A MICROSCOPIC MODEL FOR NON-FERMI-LIQUID BEHAVIOR AND CHARGE CARRIER PAIRING IN A PURELY REPULSIVE 2D ELECTRON SYSTEM

by

Mona Inesa Berciu

A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy
Graduate Department of Physics
University of Toronto

©Copyright by Mona Inesa Berciu 2000
The author has granted a non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of this thesis in microform, paper or electronic formats.

The author retains ownership of the copyright in this thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without the author's permission.

0-612-49975-8
Thesis title: A microscopic model for non-Fermi-liquid behavior and charge carrier pairing in a purely repulsive 2D electron system

Degree: Doctor of Philosophy

Year of convocation: 2000

Author: Mona Inesa Berciu

Department of Physics
University of Toronto

Abstract

This thesis examines the properties of a new microscopic model for non-Fermi-liquid behavior and d-wave pairing in a strongly correlated quasi-two-dimensional (2D) electron gas with purely repulsive interactions. The microscopic Hamiltonian for this system involves a nearest neighbor electron hopping matrix element $t$, an on-site Coulomb repulsion $U$, and a nearest neighbor Coulomb repulsion $V$. We suggest that nearest neighbor Coulomb repulsion on the energy scale of $t$ stabilizes a state in which electrons undergo a "somersault" in their internal spin-space (spin-flux). Spin-flux is a new form of spontaneous symmetry breaking in a strongly correlated electron system in which the Hamiltonian acquires a term with the symmetry of spin-orbit coupling at the mean-field level. Spin-flux modifies the single quasi-particle dispersion relations from that of a conventional antiferromagnet (AFM). When this spin-1/2 AFM insulator is doped, the charge carriers are mobile, charged, bosonic meron-vortex solitons accompanied by unoccupied states deep inside the Mott-Hubbard charge-transfer gap. This model provides a unified microscopic basis for (i) non-Fermi-liquid transport properties for low and intermediate doping, (ii) mid-infrared optical absorption, (iii) destruction of AFM long range order with doping, (iv) angled resolved spectroscopy (ARPES), (v) d-wave preformed charge carrier pairs, and (vi) a transition from the non-Fermi liquid state to a conventional Fermi-liquid metal for large doping.

The approximations used to study the 2D spin-flux Hubbard model are the unrestricted Hartree-Fock Approximation and the Configuration Interaction (CI) Method. In 1D, the
CI approximation leads to excellent agreement with the exact Bethe Ansatz solution of the Hubbard model, as well as a clear demonstration of the spin-charge separation: the charge of the doping hole is carried by charged bosonic domain-walls, while the spin of the doping hole is carried by neutral fermionic domain-walls. In 2D, the CI method suggests a precursor to the spin-charge separation: addition of a single hole leads to the appearance of a charge-carrying vortex (the meron-vortex) bound to a spin-carrying antivortex.
Acknowledgements

Most of all, I would like to thank my supervisor, Prof. Sajeev John. He gave me a very interesting problem to study and kept me pointed in the right direction all the time. He always encouraged and supported me. He helped me out of many traps and always had time to patiently listen to me. It is difficult to express in words how grateful I am for the good fortune of having been his student. Thank you.

Throughout these years I received financial support from the Ontario Graduate Scholarship Program, McLean Fellowship, Connaught Fellowship and various other scholarships from the University of Toronto. Their support is gratefully acknowledged.

I would also like to thank my family, and most especially my mother, for their support and unconditional love. I owe her all that is good in me. Mulțumesc.

Throughout my school years I was shaped by all my teachers and professors. I would like to thank all of them, and especially d-l Martin Avram, d-na Lucia Gaie, d-l Romulus Pop, d-na Viorica Florescu and d-l Gheorghe Ciobanu. Mulțumesc.

Finally, I want to thank Ovidiu for choosing me as his partner. A1.
# Contents

1 Introduction ................................................................. 1  
1.1 Motivation ............................................................... 1  
1.2 Crystal structure and model Hamiltonian ............................. 5  

2 Experimental properties .................................................. 13  
2.1 Optical and infrared spectroscopy ..................................... 13  
2.1.1 The Drude model ................................................... 13  
2.1.2 ab-plane conductivity ............................................. 14  
2.2 Transport properties .................................................... 20  
2.2.1 ab-plane resistivity ................................................. 20  
2.2.2 c-axis resistivity .................................................. 24  
2.2.3 The Hall Effect ..................................................... 27  
2.3 Magnetic properties ..................................................... 29  
2.3.1 The undoped parent compound .................................. 29  
2.3.2 Influence of hole doping on the AFM state ....................... 32  
2.3.3 Magnetic neutron scattering ...................................... 34  
2.3.4 Nuclear magnetic resonance .................................... 36  
2.4 Angle-Resolved Photoemission Spectroscopy (ARPES) ............... 37  

3 Charged bosons in a doped Mott Insulator ............................... 45  
3.1 The Static Hartree-Fock Approximation ............................... 46  
3.2 The one-dimensional Hubbard chain .................................. 49  
3.2.1 The undoped ground state ....................................... 49  
3.2.2 Solitons in the doped ground state: the spin-bag and the domain-wall  
3.2.3 Green’s functions approach ...................................... 56  
3.3 Continuum approximation: analogy between 1D and 2D soliton electronic spectra ................................. 57  
3.3.1 Electronic structure of domain walls and spin-polarons .......... 57  
3.3.2 Electronic structure of meron-vortices and skyrmions .......... 63  

4 Numerical study of multi-soliton configurations in a 2D doped antiferromagnetic Mott insulator ................................. 69  
4.1 The undoped ground state ............................................. 70  
4.2 Solitons in the doped insulator: the spin-bag and the meron-vortex  
4.2.1 The spin-bag ....................................................... 74  
4.2.2 The meron-vortex ................................................ 77  
4.2.3 The meron-antimeron pair ....................................... 82
4.3 Higher dopings: multi-soliton configurations .................................. 84
4.3.1 Charge carrier concentration of $\delta = 1/8$ ........................................ 88
4.3.2 Optical absorption ................................................................................. 89
4.3.3 The magnetic structure factor ................................................................. 91
4.4 Conclusions and critique of the method .................................................... 91

5 Quantum dynamics of charged and neutral magnetic solitons:
Spin-Charge Separation and d-wave Pairing ................................................. 95
5.1 Configuration Interaction Method ............................................................... 96
5.2 Exact solution of the 1D Hubbard Model: the Bethe Ansatz ....................... 98
5.3 Comparison between the BA, the CI and the HF results in the 1D case ........ 100
  5.3.1 The undoped ground-state: neutral domain walls ............................... 100
  5.3.2 The spin-polaron ................................................................................. 103
  5.3.3 The charged domain-wall ................................................................. 107
  5.3.4 Spin-charge separation ...................................................................... 113
5.4 CI results for the 2D system .................................................................... 116
  5.4.1 Spin-bag Dissociation: Charge-Spin Separation in 2D ......................... 116
  5.4.2 d-wave Superconductive Pairing ....................................................... 121
5.5 Conclusions ............................................................................................. 127

6 Semi-classical response of charged magnetic solitons to external fields:
The Time-Dependent Hartree-Fock Approximation ......................................... 129
6.1 The Time-Dependent Hartree-Fock Approximation .................................. 130
6.2 The one-dimensional system ................................................................... 133
  6.2.1 Motion of the charged domain wall in a static electric field ............... 133
  6.2.2 Domain-wall motion in an ac electric field ....................................... 140
  6.2.3 Motion of the charged spin-bag in a static electric field .................... 140
6.3 The Random Phase Approximation ......................................................... 140
  6.3.1 Spin waves of the undoped AFM chain ............................................ 144
  6.3.2 Spin waves of the undoped AFM plane ........................................... 145
6.4 Summary .................................................................................................. 146

7 Summary and Conclusions .......................................................................... 147

A Green’s functions method .......................................................................... 151
A.1 The half-filled antiferromagnetic background .......................................... 151
  A.1.1 The Green’s function of the undoped AFM background .................... 153
  A.1.2 Self-consistency of the antiferromagnetic background ....................... 153
A.2 Neutral domain wall solitons ................................................................... 154
  A.2.1 The neutral sharp-boundary soliton .................................................. 155
  A.2.2 The FM-core and the AFM-core neutral solitons .............................. 161
  A.2.3 Excitation energies of the neutral solitons ....................................... 164
A.3 Charged domain wall solitons ................................................................ 166
  A.3.1 The self-consistent charged solitons ................................................. 166
  A.3.2 The spin of the charged soliton ........................................................ 169
  A.3.3 Charge density of the doped solitons ............................................... 170
List of Figures

1.1 Crystal structure of the monolayer parent compound La$_2$CuO$_4$. The CuO$_2$ plane are shadowed. They are separated by a couple of insulating layers. ........................................ 6

1.2 Crystal structure of the bilayer parent compound YBa$_2$Cu$_3$O$_7$. There are two close CuO$_2$ planes per unit cell. They are separated from the other bilayers by 3 other layers. The most interesting of these is the middle layer, which is made of CuO chains. ........................................................................... 6

1.3 (a) Bonding between the 3d orbitals of a Cu$^{2+}$ atom and the 2p orbitals of two O$^{2-}$ atoms making up the unit cell of the CuO$_2$ planes. The highest anti-bonding orbital has predominantly d$_{x^2-y^2}$-$p_x$ character and contains the hole of the undoped unit cell. All the other bonding and anti-bonding orbitals obtained through hybridization are fully occupied and at much lower energies. (b) The Cu(3d$_{x^2-y^2}$) and O(2p$_{x(y)}$) orbitals which hybridize most and form the lowest bonding and highest anti-bonding states shown in Fig. 1.3(a). ........................................ 7

1.4 Phase diagram of the hole-doped system La$_{2-x}$Sr$_x$CuO$_4$ as a function of doping $x$ [17]. The undoped parent compound ($x = 0$) is an AFM insulator. With increased doping, there is a transition to an unusual metal that becomes superconducting below $T_c$. ........................................ 7

1.5 Choice of the gauge for describing the mean-field spin-flux background. Physical observables depend on the rotation matrices $T^j$ only through the plaquette matrix product $T^{12}T^{23}T^{34}T^{41}$. Shown above is the simplest (spin independent) gauge choice describing a 2$\pi$-rotation of the internal coordinate system of the electron (described by 3 Euler angles) as it encircles an elementary plaquette. This is a new form of spontaneous symmetry breaking for a strongly interacting electron system in which the mean-field Hamiltonian acquires a term with the symmetry of a spin-orbit interaction. ........ 11

2.1 Optical conductivity of LaSrCuO at 300K, for $0 \leq x \leq 0.34$ [36], and for YBaCuO at 100K, for 4 different dopings [37]. ........................................ 15

2.2 Solid lines: Optical conductivity $\sigma_1(\omega)$ of a $T_c$=92K film of YBaCuO at 20, 100, 200 and 300K. Dotted lines: Imaginary conductivity $\sigma_2(\omega)$. From [38]. 15
2.3 (a) Upper panel: Optical conductivity of a \( T_c = 89 \) K YBaCuO film above \( T_c \) with the Drude contribution subtracted. Lower panel: Total conductivity below \( T_c \). From [39]. (b) Mid-infrared contribution to the frequency-dependent conductivity of BiSrCaCuO at temperatures between 20 and 300K. The curves at and above 75K were found by subtracting a Drude-model conductivity from the total conductivity. The 20K curve is the total conductivity. From [40].

2.4 The optical conductivity of four YBaCuO crystals with, starting from the top curve, \( T_c = 90, 80, 50, \) and 30 K. The only effect of the doping on the mid-infrared band (seen in the lower panel) is an overall scaling. The onset of absorption at 150 cm\(^{-1}\) does not vary with \( T_c \). From [37].

2.5 Photoinduced absorption in three insulating parent compounds of the high temperature superconductors. Top curve is LaCuO, middle curve YBaCuO, bottom curve TiBaCaGdCuO. Under intense laser irradiation the insulating compounds develop absorption bands that resemble those of the corresponding superconducting materials [41].

2.6 Dashed line, right scale: Effective mass as a function of frequency determined from the a-axis polarized conductivity of an optimally doped YBaCuO single crystal. The temperature is 100K. Full line, left scale: The corresponding renormalized scattering rate, \( 1/\tau \). From [42].

2.7 Temperature dependence of resistivity in ceramic samples of La\(_{2-x}\)Sr\(_x\)CuO\(_4\) for different Sr content \( x \). The system undergoes an insulator to metal transition at \( x \approx 0.03 \), where superconductivity sets in. The resistivity keeps decreasing with further increase of \( x \). While the underdoped to optimally doped samples show a T-linear behavior, the overdoped samples show a \( T^2 \) behavior, reminiscent of a Fermi liquid. From [46].

2.8 Top: Comparison of the dc resistivity from Drude parameters based on far infrared transmission with transport measurements. Bottom: Temperature dependence of the quasiparticle relaxation rate. The scattering rate is linear with temperature in the non-superconducting Bi\(_2\)Sr\(_2\)CuO\(_6\), but drops rapidly below \( T_c \) in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\). From [50].

2.9 The temperature dependence of the basal plane resistivity \( \rho_{ab} \) and the c-axis resistivity \( \rho_c \), in single crystal samples of La\(_{2-x}\)Sr\(_x\)CuO\(_4\) for different doping \( x \). The anisotropy \( \rho_c/\rho_{ab} \) decreases with increased doping. In the overdoped sample, both resistivities shows the \( T^2 \) dependence, signalling the transition to a Fermi liquid. From [53].

2.10 The \( x \)-dependence of the Hall coefficient for the hole-doped La\(_{2-x}\)Sr\(_x\)CuO\(_4\) and the electron-doped Nd\(_{2-x}\)Ce\(_x\)CuO\(_4\) systems. In both cases, the Hall coefficient is inversely proportional to the doping \( x \) in the underdoped region, and increases significantly and changes sign in the overdoped regions. From [17, 57].
2.11 Temperature dependence of ab-plane resistivity (upper panel) and the reciprocal of the Hall coefficient, $1/R_H$ (lower panel) for single crystal samples of YBa$_2$Cu$_{3-x}$Zn$_x$O$_7$ with different Zn impurity content $x$. The pure sample is close to optimally doped, having a superconducting transition at $T_c = 87$K. Its Hall coefficient increases like $1/T$. As the Zn content increases, both $T_c$ and the temperature dependence of the Hall coefficient are suppressed. From [58]. ........................................ 28

2.12 Inverse correlation length $\xi^{-1}$ versus temperature in La$_2$CuO$_4$, from [69]. The solid line is the theoretical prediction of Eq. (2.4) [70]. ......................... 31

2.13 Magnetic susceptibility $\chi_m$ versus $T$ taken on ceramic samples for various oxygen contents, from the AFM to the metallic state. Large Curie terms occur at low $T$ and are partly due to spurious phases in the sample. From [71]. ........................................... 31

2.14 Temperature dependence of the $\mu sr$ frequency in La$_{2-x}$Sr$_x$CuO$_4$. The $T=0$ frequency is only slightly dependent on the Sr content, which shows that the internal magnetic field does not vary so much from the AFM to the disordered spin glass state. From [79]................................. 33

2.15 Instantaneous spin correlation length as deduced from the width of the quasielastic scattering along the two-dimensional ridge for La$_{2-x}$Sr$_x$CuO$_4$, plotted versus $x$. The solid line is the average separation between holes. From [69]............................................. 33

2.16 Left: Planar $^{63}$Cu Knight shift in optimally doped YBa$_2$Cu$_3$O$_{6.95}$ (squares) and underdoped YBa$_2$Cu$_3$O$_{6.64}$ (circles). The normal state susceptibility is temperature independent in the optimally doped compound but decreases with temperature in the underdoped compound. From [92]. Right: A compendium of Cu relaxation rates in various cuprates. Non-Korringa behavior $(1/T_1 \neq aT)$ is observed in all compounds. From [86]. .................................................. 36

2.17 Left: ARPES data showing the peak dispersion along the $(0,0)$ to $(\pi, \pi)$ direction for the insulating Sr$_2$CuO$_2$Cl$_2$ (a) and the metallic Bi$_2$Sr$_2$CaCu$_2$O$_8$ (b). The daggers beneath each spectrum are guides to the eye. The legend at the top has circles indicating the points in the 2D Brillouin zone where data were taken and is labeled with $(l,l)=(\pi, \pi)$. The dark circles in the legend are on the side of the zone where the peak is strong in the insulator and the open circles where the peak is weak. The size of the circles indicates the $k$ resolution. Right: ARPES data along the $(0,0)$ to $(\pi, 0)$ direction (a) and along the $(0,\pi)$ to $(\pi, 0)$ direction (b). The dashed line in (a) is the maximum energy for any peak in this direction. The legend is the same as in the top panel. From [90]. ............................................. 39

2.18 Fermi crossings for two Bi2212 samples of different doping. While the overdoped sample has a continuous fermi surface, the underdoped sample's Fermi surface is made of 4 disjoint arcs appearing near the $(\pi/2, \pi/2)$ point. From [91]. ............................................................ 40
2.19 Left: Destruction of the Fermi surface by the pseudogap at three doping levels (same temperature). The dotted line shows the large Fermi surface seen in the overdoped samples. As the doping is reduced, the Fermi surface (shown by a thick line) becomes gapped and only the solid arcs remain. Data show that even at low doping (leftmost panel) the minimum gap follows the original dashed Fermi surface, as shown in the second picture. From [92]. Right: Fermi surface of Bi2212 samples with different Tc's obtained by varying the doping level. For the underdoped samples for which the Fermi arcs are not continuous (the Fermi surface is gapped far from the (π/2, π/2) point), the curve shows the locus of points of minimum gap. Their shape changes little with doping. From [93].

2.20 Left: Temperature dependence of the photoemission spectra at the (π, 0) point, for an underdoped Bi 2212 sample (Tc = 79K). A sharp peak develops from the extremely broad normal state feature as the temperature is lowered. From [97]. Right: The superconducting gap as a function of the angle around the Fermi surface, for the Tc = 87K underdoped Bi2212 sample. The gap has d-wave like nodes on the zone diagonals and rises to a maximum value of about 35meV at the (π, 0) point, in agreement with the left panel picture. The open circles are the measured leading edge shifts of the raw photoemission spectra and the filled circles are the estimated gap. From [89].

2.21 Schematic phase diagram of Bi2212 as a function of doping. The filled symbols are the measured Tc's for the superconducting phase transition from magnetic susceptibility. The open symbols are the T* at which the pseudogap closes; for the Tc = 10K sample the symbol at 301K is a lower bound on T*. The region between Tc and T* is an unusual metal, with a pseudogap in the electronic excitation spectrum. Above T* the large continuous Fermi surface is regained. Below Tc, the d-wave symmetry superconductor has only four nodal points at (π/2, π/2). From [99].

2.22 Left: Momentum dependence of the gap estimated from the leading edge shift for three Bi2212 samples with Tc = 10, 83 and 87K, measured at 14K. The inset shows the Brillouin zone with a large Fermi surface enclosing the (π, π) point, with the occupied region shaded. The gaps are extremely similar in the three samples, although the Tc = 10K sample is still in the normal state and therefore its measured gap is its pseudogap, as opposed to the superconducting gap measured for the other two samples. Right: The temperature dependence of the gap for the same three samples. For the near-optimal 87K sample the gap closes at T* = 90K ≈ Tc, while for the underdoped 83K sample there is a smooth evolution of the gap through Tc. The extremely underdoped sample has a much larger gap, but its evolution is also smooth. From [99].

3.1 Magnitude S of the staggered spin of the undoped chain, as a function of U/t.

3.2 Energy per site (in units of t) of the AFM undoped background as a function of U/t, as obtained from the Hartree-Fock Approximation (full line) and from the exact Bethe Ansatz solution (dashed line).
3.3 Self-consistent charge (upper line) and spin distributions for a charged spin-bag on a 40-site chain, for $U/t = 5$. The spin-bag is a charged fermion.

3.4 Left: Self-consistent charge (upper line) and spin distributions for a domain wall centered on site (COS) on a 41-site chain, for $U/t = 5$. Right: Self-consistent charge (upper line) and spin distributions for a domain wall centered between sites (CBS) on a 41-site chain, for $U/t = 5$. The domain walls are charged bosons.

3.5 Electronic spectra for an undoped AFM chain with 40 sites (left panel), and for a 40-site chain with a charged spin-bag (right panel). $U/t = 5$.

3.6 Electronic spectra for a chain 41 sites chain with a COS domain-wall (left panel), and a CBS domain-wall (right panel). $U/t = 5$.

3.7 Excitation energy in units of $t$ of the charged spin-polaron, CBS and COS domain walls, as a function of $U/t$. The excitation energy is defined with respect to the undoped chain. Within the HFA, for $U/t < 6.5$ the charged domain-walls are the low-energy charged excitations, while for $U/t > 6.5$ the spin-polarons are the low-energy excitations. However, the HFA approximation neglects the kinetic energy gained by these charged excitation through translation along the chain. When this is taken into account within the Configuration Interaction approximation, the mobile domain-wall is found to be the low-energy charged excitation for all values of $U/t$ (see Fig. 5.9).

3.8 Top panel: Structure of an AFM-core soliton. The spins on the two sublattices rotate from one mean-field ground state to the other one, preserving the local antiferromagnetic correlations of this soliton. Bottom panel: Structure of the FM-core soliton. The spins on the two sublattices rotate in opposite directions, creating a ferromagnetic region in the core of this soliton.

3.9 Dependence of the energy of the discrete gap level on $\rho_p = \rho U S/2at$, predicted by the continuum model (full line), and by the discrete models with $U S/t = 1.2$ and 6, for an AFM-core soliton. Only the upper half $E > 0$ of the Mott-Hubbard gap is shown. The lower half is symmetrical.

3.10 The 2D analog of the neutral domain wall is a meron texture depicted as a lotus-flower configuration of the local director field $\hat{n}(\vec{r})$. As $\hat{n}(\vec{r})$ varies smoothly from one unit cell to the next, it makes a half-covering of the unit sphere $S_2$. If the meron is doped, all the components of the spin perpendicular to the plane become zero, and therefore the magnitude of the spin vanishes in the core of the charged meron-vortex.

3.11 Left: Electronic gap structure of the FM- and AFM-core 2D undoped merons as a function of the continuum parameter $\rho U S/2at$, as predicted by the continuum model; Right: Electronic gap structure of the FM- and AFM-core 1D undoped domain walls as a function of the continuum parameter $\rho U S/2at$, as predicted by the continuum model.

3.12 Left: Electronic gap structure of the FM- and AFM-core 2D skyrmion as a function of the continuum parameter $\rho U S/2at$, as predicted by the continuum model; Right: Electronic gap structure of the FM- and AFM-core 1D spin-polaron as a function of the continuum parameter $\rho U S/2at$, as predicted by the continuum model.
4.1 Left: The dispersion relation of the valence band of the undoped AFM ground state in the conventional model is plotted in the extended Brillouin zone (\( k \) is measured in units of \( \pi/a \)). The color code is indicated on the right scale. The Brillouin zone is marked by the dashed line. All the points on the Brillouin surface are at the highest possible energy, therefore they belong to the Fermi surface. Right: The dispersion relation of the valence band of the undoped AFM ground state in the spin-flux model is plotted in the extended Brillouin zone (\( k \) is measured in units of \( \pi/a \)). The color code is indicated on the right scale. The Brillouin zone is marked by the dashed line. Only the four corners of the Brillouin surface are at the highest possible energy, therefore only they belong to the Fermi surface.

4.2 A comparison between the experimentally determined \( E(\vec{k}) \) quasi-particle dispersion relation, from angle resolved photoemission studies (ARPES), for the insulating \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) (open circles with error bars) and the mean-field AFM spin-flux phase dispersion relation (full line) and the mean-field AFM conventional phase dispersion relation (dashed-dotted line). While the peak on the \((0,0)\) to \((\pi,\pi)\) is equally well described in both models, the mean-field spin-flux model gives a much better agreement for the \((\pi,0)\) to \((0,0)\) and \((\pi,0)\) to \((0,\pi)\) directions. The fitting corresponds to \( U = 2.01 \) eV, \( t = 0.29 \) eV for the spin-flux phase, and \( U = 1.98 \) eV, \( t = 0.21 \) eV in the conventional phase. The experimental results are the ARPES results of Ref. [90].

4.3 Left: Dependence of the staggered spin \( S \) of the AFM undoped compound with \( U/t \). The diamonds show the numerical results obtained in the presence of the spin-flux, while circles show numerical results for the conventional phase. The lines show the values predicted by Eqs. (4.3) and (4.6) for the two phases. The spin-flux phase has a mean-field AFM solution \( (S \neq 0) \) only for \( U/t > 3 \). As expected, \( S \rightarrow 1/2 \) in the large \( U/t \) limit, where every electron becomes localized on individual sites. Right: Dependence of the ground-state energy per site of the AFM parent compound with \( U/t \). The diamonds show the numerical results obtained in the presence of the spin-flux, while circles show numerical results for the conventional phase. The lines show the values predicted by Eqs. (4.2) and (4.5) for the two phases. The mean-field AFM spin-flux phase has a lower energy than the mean-field AFM conventional phase for all values of \( U/t \).

4.4 Left: Self-consistent spin distribution of a 10x10 lattice with a spin bag centered at \((5,5)\). The spin-bag has a small ferromagnetic core, and the magnetic order is only locally affected. Right: Self-consistent charge distribution of a 10x10 lattice with a spin bag centered at \((5,5)\). There is an average of one electron per site everywhere, except in the core of the spin-bag where the doping hole is localized.
Electronic spectrum of a spin bag on a 10x10 lattice, for $U/t = 5$ in the
spin-flux model (left) and the conventional model (right). Eigenenergies $E_{\alpha}$
are plotted as a function of $\alpha = 1, 200 (= 2N^2)$. Only the first $N^2 - 1 = 99$
states are occupied. There are two empty bound discrete levels deep into
the Mott-Hubbard gap ($\alpha = 100, 101$), one of which comes from the valence
band of the undoped AFM compound (see inset). There is also an occupied
discrete level below the valence band ($\alpha = 1$). The valence band is spin
paired, since it has an even number of levels. Thus, the total spin of the
spin-bag comes from the discrete occupied level. The spin-bag is a charged,
spin-$\frac{1}{2}$ fermion.

Excitation energy of a spin bag $E_{\text{spin-bag}}$ as a function of the lattice size
$N$. Diamonds show results for a spin-flux AFM phase, with Cyclic Boundary
Conditions (CBC, full diamonds) and free boundary conditions (FBC, empty
diamonds). Circles show results for the conventional AFM state, with CBC
(full circles) and FBC (empty circles). The Hubbard parameter is $U/t = 6$.
The bulk limit is reached for $N > 10$. In this limit, the excitation energy of
the localized spin-bag becomes independent on the size of the lattice. Right:
Excitation energy of a spin bag $E_{\text{spin-bag}}$ as a function of $U/t$, in the presence
of spin-flux (filled diamonds), and in the conventional state (circles). In the
very large $U/t$ limit, the excitation energy approaches asymptotically the
value $U/2 - 2t$. The excitation energy of a spin-bag is lower in the spin-flux
phase than in the conventional phase.

Self-consistent spin distribution of a 10x10 lattice with a meron-vortex
in the spin-flux phase. The core of the meron is localized in the center of
a plaquette, in the spin-flux phase (in the conventional phase, the core of
the meron-vortex is localized at a site). This excitation has a topological
winding number 1, since the spins on either sublattice rotate by $2\pi$ on any
curve surrounding the core. The magnitude of the staggered magnetic
moments is slightly diminished near the vortex core but is equal to that of the
undoped AFM background far from the core. Right: Self-consistent charge
distribution of a 10x10 lattice with a meron-vortex in the spin-flux phase.
Most of the doping charge is localized in the center of the meron. Far from
the core, there is an average of one electron per site.

Electronic spectrum of a meron-vortex on a 10x10 lattice, for $U/t = 5$,
in the presence of the spin-flux. Eigenenergies $E_{\alpha}$ are plotted as a function
of $\alpha = 1, 200 (= 2N^2)$. Only the first $N^2 - 1 = 99$ states are occupied
(the valence band). There are two discrete empty levels deep into the Mott-
Hubbard gap, one of which ($\alpha = 100$) comes from the valence band of the
undoped AFM parent. Merons must be created in vortex-antivortex pairs
(for topological reasons). Each pair removes two levels from the undoped
AFM valence band. Thus, the valence band remains spin paired, and the
total spin of this excitation is zero. This meron is a spinless, charged, bosonic
collective excitation of the doped antiferromagnet. Right: same as in the left
panel, for a meron-vortex in the conventional state. The only difference
is that the two bound levels drawn deep inside the Mott-Hubbard gap are
degenerate in this case.
4.9 Excitation energy (in units of $t$) of a single meron-vortex, as a function of
the meron size $N$, in the presence of the spin flux (diamonds) and without
spin-flux (circles). The lines show fits with a logarithmic dependence on
$N$, $E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}}$. The excitation energy of a meron-vortex is
always lower in the spin-flux phase than in the conventional phase. If the size
of the meron core is small enough, the excitation energy of the meron-vortex
may become smaller than the excitation energy of a spin-bag.

4.10 Left: Dependence of the coefficient $\alpha$ (in units of $t$) from the fit $E_{\text{meron}}(N) =
\alpha \ln N + \epsilon_{\text{core}}$ on $U/t$. Diamonds show results for a spin-flux phase, while
circles correspond to a conventional state. The line serves to guide the eye.
In the large $U/t$ limit $\alpha \to 0$, since in this limit all spin configurations become
degenerate and the excitation energy of the meron-vortex should equal the
excitation energy of the spin-bag. Right: Dependence of $\epsilon_{\text{core}}$ (in units of $t$)
from the fit $E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}}$ on $U/t$. Diamonds show results for
a spin-flux phase, while circles correspond to a conventional state. The line
serves to guide the eye. In the large $U/t$ limit $\epsilon_{\text{core}} \to E_{\text{spin-bag}}$, since in this
limit all spin configurations become degenerate and the excitation energy of
the meron-vortex should equal the excitation energy of the spin-bag.

4.11 Critical doping concentration, $\delta_c$, above which a charged meron-antimeron
liquid is energetically favorable compared to a gas of spin-bags. Diamonds show results for a spin-flux phase, while circles correspond to a conventional
state. The line serves to guide the eye. In the conventional phase the critical
concentrations are very large, $\delta_c > 0.3$. In the spin-flux phase, the transition
to the liquid of meron vortices takes place at dopings smaller than 0.10, for
$U/t < 8$. In the conventional phase, the critical doping is so large ($\delta_c > 0.30$)
that merons are unlikely to appear before the Mott-Hubbard gap itself closes.

4.12 Self-consistent spin distribution for a tightly bound meron-antimeron pair.
The meron (M) and the antimeron (A) are localized on neighboring plaquettes.
The total winding number of the pair is zero. The magnetic AFM order
is disturbed only on the small region where the vortices are localized. The
attraction between holes is of topological nature and on long length scale is
stronger than unscreened Coulomb repulsion between charges.

4.13 Self-consistent charge distribution for a tightly bound meron-antimeron pair.
The doping charge is mostly localized on the two plaquettes containing the
meron and antimeron cores. Due to interactions, the cores of the vortices are
somewhat distorted, with most of the charge missing from the (10,10) site
common to both cores. The two holes localized in the cores are responsible
for the fact that the meron-antimeron pair does not collapse (due to Fermi
statistics, it is impossible to have two holes at the same site).
4.14 Energy per site (in units of $t$) as a function of the electron concentration, $c = 1 - \delta$, for $U/t = 5$. Circles correspond to the lowest energies found in the random trial in the spin-flux phase (liquid of meron-vortices), while squares correspond to the best result of the random trial in the conventional phase (stripes). The dashed line shows the exact value for $U = 0$ (non-interacting case). At low doping (high electron concentration) the liquid of meron-vortices of the spin-flux phase has a lower energy than the stripes of the conventional phases. However, at higher dopings ($\delta > 0.4$) the conventional phase becomes stable.

4.15 Self-consistent spin distribution for the configuration of lowest energy found at $\delta = 0.08$ (8 holes), starting from an initial random distributions, for $U/t = 5$ in the spin-flux phase. Four meron-antimeron pairs appear. We have marked with M the plaquettes on which merons are centered, and with A the plaquettes on which antimerons are centered. A meron and an antimeron are "split" between the two opposing boundaries (we have imposed cyclic boundary conditions).

4.16 Self-consistent spin distribution for the configuration of lowest energy found at $\delta = 0.15$, starting from initial random distributions, for $U/t = 5$ in the conventional phase. A closed charged stripe appears (cyclic boundary conditions were imposed). The AFM magnetic order is switched from one phase to the other one (up $\rightarrow$ down and viceversa) as the stripe is crossed.

4.17 Left: Self-consistent spin distribution for the configuration of lowest energy found at $\delta = 1/8$, for $U/t = 5$ in the spin-flux phase. An ordered crystal of charged merons and antimerons is created. Right: Self-consistent spin distribution for the configuration of lowest energy found after adding a 5% anisotropy in the hopping integral, at $\delta = 1/8$, for $U/t = 5$ in the spin-flux phase. The merons and antimerons rearrange on horizontal lines, leading to a structure similar to that suggested by Tranquada in Ref. [110].

4.18 Optical absorption (arbitrary units) as a function of the frequency (in units of $t$) for various dopings. The Hubbard parameter is $U/t = 5$, and the corresponding self-consistent lowest-energy configurations of frozen liquids of merons and antimerons were used. The damping coefficient is $\Gamma = 0.1t$. As the doping increases, a broad band due electronic excitations from the lower Mott-Hubbard gap to the discrete, empty, meron-induced levels develops deep into the gap.

4.19 The static magnetic structure factor as a function of $(k_x, k_y)$, measured in units of $2\pi/a$. The first picture corresponds to $\delta = 0.00$ and has the large magnetic peak at $(\pi/a, \pi/a)$. As the doping increases to $\delta = 0.05$ (second picture) and $\delta = 0.08$ (third picture) this magnetic peak splits into four incommensurate satellites. The Hubbard parameter is $U/t = 5$, and the corresponding self-consistent lowest-energy configurations of frozen liquids of merons and antimerons were used.
5.1 Ground-state energy per site, in units of \( t \), of an undoped Hubbard chain of \( N \) sites and \( U/t = 5 \). The full circles show the values found directly from the Bethe Ansatz Equations (5.7, 5.8, 5.9) while the full line shows the thermodynamic limit given by Eq. (5.10). In the limit of large \( N \) the two values agree. ........................................ 100

5.2 Left: Self-consistent spin and charge distribution for a 40-site chain with two neutral domain walls, for \( U/t=5 \). The charge \( Q(i) = 1 \) everywhere. The total spin carried by each neutral domain wall is \( 1/2 \). ........................................ 101

5.3 Right: Electronic structure of the 40-site chain with the two neutral domain walls. Each domain wall has 4 discrete levels bound in its core. The spins on the two occupied bound levels are oriented in the same direction as the core spins of the domain wall. In the configuration shown in the left panel, there is a \( +1/2 \) and a \(-1/2\) domain wall, and therefore all levels are spin paired and the total spin of the chain is zero. However, for two \(+1/2\) (-\(1/2\)) domain walls, all the occupied discrete levels have \(+1/2\) (-\(1/2\)) spins, and the total spin of the chain is \(+1\) (-1). ........................................ 101

5.4 Ground-state energy (in units of \( t \)) of a chain of size \( N \), calculated with the HF (circles), CI (squares) and BA (diamonds). The left panel corresponds to \( U/t = 5 \), while the right one corresponds to \( U/t = 50 \). Although the energy scale is very different, in both cases the CI method significantly improves the agreement with the exact Bethe Ansatz solution. ........................................ 103

5.5 Dispersion band for the spin-polaron, \( E_{pol}(k) \) vs. \( k \), with \( E_{pol}(k) \) extracted from Eq. (5.15) for chains of length \( 2N = 14, 16, ..., 22 \) sites and \( U/t = 5 \). The various curves fall on top of each other, thus proving that the fit (5.15) is legitimate. Also shown is the excitation energy of the static hole-doped spin-polaron \( E_{pol}^{HF} \) (the full line), as obtained from the Unrestricted HFA. We can see that translation does indeed lower the total energy of the spin-polaron, with the most stable state corresponding to \( k = \pi/2a \). The kinetic energy gained through translation is quite small. ........................................ 106

5.6 The extra kinetic energy gained by the spin-polaron \( E_{pol}(\frac{\pi}{2a}) - E_{pol}^{HF} \) (circles) and the width of the spin-polaron band, \( E_{pol}(\frac{\pi}{2a}) - E_{pol}(0) \) (squares) as a function of \( t^2/U \). The log-log graph clearly shows the linear dependence. This is expected, since the spin-polaron must tunnel two sites to the next allowed position. This is a second order hopping process and this charged excitation is rather immobile. ........................................ 106

5.7 The effective mass \( m_{pol} \) of the spin-polaron as extracted from its dispersion band, as a function of \( U/t \). The unit of mass is \( m_e/(a^2t) \), where \( m_e \) is the free electron mass, \( a \) is the lattice constant in \( \AA \) and \( t \) is the hopping integral in \( eV \). As \( U/t \) increases the spin-polaron becomes more and more immobile. 107

5.8 The dispersion relations \( E_{dw}(k) \) vs. \( k \) for both CBS (left panel) and COS (right panel) domain walls on chains of different length \( 2N + 1 = 17, ..., 23 \), and \( U/t = 5 \). The excitation energy of the static configuration (obtained from the unrestricted HF search) is also shown as a full line. The extra kinetic energy gained through translation by the domain-wall is considerable, of the order of \( t \). ........................................ 109
5.9 Excitation energy, in units of $t$, for a charged domain wall (circles) and a charged spin-polaron (diamonds), as obtained from the CI approach. The exact excitation energy given by the Bethe-Ansatz method is shown by squares. The domain-wall CI approximation is in excellent agreement with the exact results (also see inset), while the spin-polaron CI approximation is significantly different. For comparison, we also show the excitation energies for the COS and CBS domain walls as obtained from the static HFA (up and down triangles), proving again that the extra kinetic energy gained by the moving domain wall is of order $t$ for most $U/t$ values. In contrast, the extra kinetic energy gained by the spin-polaron is of order $t^2/U + O(\ln L) \cdot \frac{L}{t}$ in the large $U/t$ limit there is almost no difference between the HF and CI results for the charged spin-polaron. We conclude that the charged domain-wall is the relevant excitation for all values of $U/t$.

5.10 The dispersion relation for a domain-wall on a chain of length $2N + 1 = 17, 19, 21$ and $U/t = 100$. In the large $U/t$ limit the dispersion relation of one single hole is given by $E_{dw}(k) = 2t \cos(ka)$ [118]. This is indeed in very good agreement with the dispersion band of the domain wall, proving again that this is the relevant charged excitation of the Hubbard chain.

5.11 The effective mass $m_{dw}$ of the domain-wall as extracted from its dispersion band, as a function of $U/t$. The unit of mass is $m_e/(a^2t)$, where $m_e$ is the free electron mass, $a$ is the lattice constant in Å and $t$ is the hopping integral in eV. As $U/t$ increases the mass of the domain-wall increases, although it is significantly smaller than the mass of the charged spin-polaron (see Fig.5.7).

5.12 Dispersion relation of the charged spin-bag $E_{ab}(\vec{k})$ (in units of $t$) plotted along lines of high symmetry in the Brillouin zone. The upper plot shows the dispersion band of the spin-bag in the conventional model, while the lower one shows the dispersion band of the spin-bag in the spin-flux model. $U/t = 5$ in both cases. Circles, squares, diamonds and triangles show the results obtained from CI analysis of 6x6, 8x8, 10x10 and 12x12 lattices. We conclude that the results are already almost converged, even for such small lattices. The full lines show the excitation energy of the spin-bag at the static HF level.

5.13 Dispersion band of the spin-bag in the conventional model (left) and the spin-flux model (right), for $U/t = 5$. We show the full 2D Brillouin zone ($k$ is measured in units of $\pi/a$), and the color code is shown at the right of each picture. The spin-bag dispersion relations have the symmetry as the dispersion relations of the underlying undoped AFM background, shown in Fig. 4.1: while the $(\pi/2a, \pi/2a)$ point corresponds to the minimum excitation energy of the spin-flux spin-bag, in the conventional model all points along the $(0, \pi)$ to $(\pi, 0)$ have almost the same energy.
5.14 Schematic representation of the self-consistent configurations used to find the lowering in energy of a charged spin-bag if it decays into a singly-charged vortex-antivortex pair which rotates about its center of mass. For the 10x10 lattice considered, the vortex and the antivortex are centered on-site, therefore the center of mass of the pair is the center of a plaquette. The hole shared by the vortex-antivortex pair is shown as full circle, centered at the center of mass. There are four possible ways to rotate the vortex-antivortex pair about its center of mass. We also add the four possible configurations with a charged spin-bag localized in each of the corners of the plaquette. The spin-bags carry both charge and spin. These four spin-bag configurations are all schematically shown in the first panel.

5.15 Dispersion band $E_{\text{pair}}(\vec{k})$ (in units of $t$) vs. $\vec{k}$ of the (un-rotated) meron-antimeron pair. The momentum units are $\pi/a$, and the color code for energy is shown at the right of the figure. For convenience, the reference energy is taken to be the static HF energy of the self-consistent configuration with the meron-antimeron pair. Thus, we see that quantum hopping lowers the overall energy of the pair by 1.29$t$. Since the meron-antimeron configuration is not rotationally invariant, the dispersion relation is also not invariant to $\pi/2$ rotations.

5.16 Left: The lowest energy dispersion band $E_{\text{pair}}(\vec{k})$ (in units of $t$) vs. $\vec{k}$ of the meron-antimeron pair. The momentum units are $\pi/a$, and the color code for energy is shown at the right of the figure. For convenience, the reference energy is taken to be the static HF energy of the self-consistent meron-antimeron pair. We see that quantum hopping and rotation lowers the overall energy of the pair by 1.76$t$. The rotational symmetry of the dispersion relation is restored (compared to Fig. 5.15). Right: The symmetry of the meron-antimeron wave-function varies through the Brillouin zone. The outside region (containing the absolute minima points $(\pi, \pi)$) has $d$-wave symmetry ($J = 2$), while the core region about the $(0, 0)$ point has $s$-wave symmetry ($J = 0$). The intermediary area is a mix of $s$+$d$ wave symmetry.

6.1 Left: Time-dependent charge distribution $Q(i, \tau)$ of a moving domain wall on a 51-sites chain; $U/t = 2.5$, $eaE/t = 5 \cdot 10^{-5}$. Time is measured in units of $\hbar/t$. Away from the trapped hole the charge is at its undoped background value of $Q(i) = 1$. Right: Snapshots of the spin configuration of the same moving domain wall. The snapshots correspond to $\tau = 100, 110, ..., 200\hbar/t$. Away from the domain wall, the staggered spin has its undoped background value $S$.

6.2 The lower panel shows the trajectory of the domain wall shown in Fig. 6.1, for a much longer period of time (up to $2000\hbar/t$). The upper panel shows the absolute error $\delta x(\tau)$ in fitting the trajectory $x(\tau)$ to a quadratic time-dependence (the non-relativistic fit) and to a relativistic fit.
6.3 The relativistic speed $c$ of the domain wall (in units of $at/\hbar$) and its rest mass $m_0$ (in units of $m_e/\bar{a}^2t$) as a function of $U/t$. The squares/circles show the values obtained from the fit of the total energy. The lines serve to guide the eye. At higher $U/t$ values where the pinning barrier is significant, one can define two sets of masses and speeds, with empty (full) circles and squares corresponding to the COS (CBS) configurations.

6.4 Left: Time-dependent charge distribution of a moving domain wall; $U/t = 2.5$, $eaE/t = 10^{-2}$. Time is measured in units of $\hbar/t$. For $\tau < 30\hbar/t$ we see the domain wall being accelerated by the electric field. As its speed increases, its size decreases (relativistic contraction). For $\tau > 30\hbar/t$ small fluctuations in the background charge appear behind the soliton. The amplitude of these collective excitations increases as the soliton goes around the chain the second and third time. The speed of the soliton remains constant from this point on. Right: Snapshots of the spin configuration of the moving domain wall for $\tau = 50.51, \ldots, 60\hbar/t$. The motion of the soliton is accompanied by fluctuations in the magnitude of all the spins, produced by the collective excitations. This is to be compared to Fig.6.1, where all the spins in the background had exactly the same magnitude as in the undoped chain.

6.5 Maximum speed of a domain wall in the presence of collective excitations, as a function of the electric field $eaE/t$. The speed is measured in units of $at/\hbar$, and the values shown correspond to $U/t = 2, 3, 4$. The large error bars are due to the fact that as the soliton emits collective excitations its center of mass oscillates as well, and therefore its motion is not just a smooth translation as in the absence of collective excitations.

6.6 Spin-wave spectra obtained from RPA for a 40-site chain with $U/t=3.4.8$ (circles, squares, diamonds). For comparison, the antiferromagnetic magnon spectra of the Heisenberg chain with $J = 11711 = 1.33, 1.0, 0.5$ are also plotted.

A.1 Left: A sharp boundary soliton created by juxtaposition of regions found in the two AFM mean-field ground-states; Right: The electronic structure of the sharp boundary soliton consists of two spin-paired bands and 4 discrete non-degenerate levels within the gap. In the large $U/t$ limit, the two strongly localized electrons occupying the gap levels correspond to the two spins bordering the sharp-boundary.

A.2 Excitation energy (in units of $t$ and measured with respect to the AFM mean-field background) of the sharp-boundary soliton, as a function of $US/t$. The dotted line shows the asymptotic value predicted by the Heisenberg model with $J = 4t^2/U$.

A.3 Top panel: Structure of an AFM-core soliton. The spins on the two sublattices rotate from one mean-field ground state to the other one, preserving the local antiferromagnetic correlations; Bottom panel: Structure of the FM-core soliton. The spins on the two sublattices rotate in opposite directions, creating a ferromagnetic region in the core of this soliton.
A.4 Left: The lower half of the electronic spectrum of an AFM-core soliton, as a function of the soliton core-radius \( \rho \). In the limit \( \rho \to 0 \), there are two discrete levels. In the limit \( \rho \to \infty \), this soliton becomes indistinguishable from the mean-field background. As the soliton core radius \( \rho \) increases, the discrete levels re-enter the bands; Right: The lower half of the electronic spectrum of a FM-core soliton, as a function of the soliton core-radius \( \rho \). In the limit \( \rho \to 0 \), there are two discrete levels. In the limit \( \rho \to \infty \), the entire chain becomes ferromagnetic and the spectrum consists of two continuum bands, the valence band corresponding to \( E \in [-US - 2t, -US + 2t] \). Here \( \gamma = (4t^2 + (US)^2)^{1/2} \) and \( \ell = (t^2 + (US)^2)^{1/2} \) ....... 163

A.5 The energy of the near midgap (\( E > 0 \)) level for the undoped FM- and AFM-core soliton, for \( US/t = 1, 3 \) and 6, as a function of the soliton core radius. For the FM-core soliton this level approaches the mid-gap, while for the AFM-core soliton it approaches the band-edge. For \( US/t < 2 \), the FM-core soliton level reaches the midgap. For \( US/t > 2 \), this level goes to \( US - 2t \), the band-edge of the FM valence band. .......... 164

A.6 Left: Excitation energies (in units of \( t \) and measured with respect to the AFM mean-field background) of the undoped FM-core soliton and AFM-core soliton, as a function of the soliton core radius \( \rho \). Here \( US/t = 5 \). In the absence of magnetic anisotropy the 1D neutral domain wall is unstable; the minimum energy occurs for \( \rho \to \infty \). ............... 165

A.7 Right: Excitation energies (in units of \( t \) and measured with respect to the AFM mean-field background) of a doped FM/AFM-core soliton, as a function of the soliton core radius \( \rho \). This estimate is obtained by adding the energy of the level occupied by the doping electron(hole) to the excitation energy of the undoped soliton. For \( US/t = 5 \), a stable, charged FM core soliton exists at \( \rho/a = 2 \). ............... 165

A.8 Left: The self-consistent spin distribution of a doped-soliton centered between sites. Here, \( US/t = 1.2 \). The magnitude of the spin is suppressed in the core of the soliton, due to the localization of the doping particle in the core. Right: Same, for doped-soliton centered at a site. ............... 167

A.9 Left: Soliton core radius of a self-consistent doped soliton centered at a site (full line) and centered between sites (dashed line), as a function of \( US/t \). ....... 168

A.10 Right: The excitation energies (in units if \( t \)) of the self-consistent doped soliton centered between sites (full line) and centered at a site (dashed line), as a function of \( US/t \). For \( US/t < 2 \), the soliton core radii are large and the two solitons become indistinguishable, giving excellent agreement with the continuum model (dotted line). For \( US/t > 2 \), the soliton radius is comparable to the lattice constant. ............... 168

A.11 Electronic spectra of the self-consistent doped solitons as a function of \( US/t \). The soliton centered at a site has a doubly-degenerate mid-gap level for all \( US/t \). For \( US/t < 2 \), the soliton centered between sites has a pair of nondegenerate levels which go towards the mid-gap as \( US/t \) decreases. For \( US/t > 2 \), a second pair of nondegenerate levels split from the bands. .... 169
A.12 Left: Electronic spectrum of a hole-doped soliton centered at a site including charge redistribution effects, as a function of $US/t$ (diamonds). All gap levels are doubly-degenerate. The lines show the approximate values found in the large $US$ limit. All levels below the mid-gap are occupied. Right: Same, for a hole-doped soliton centered between sites. All gap levels are nondegenerate. The spectra of the corresponding electron-doped solitons are obtained by inversion with respect to $E = 0$.  

A.13 Left: Excitation energies (in units of $t$) of static hole- and electron-doped solitons centered at a site, as a function of $US/t$, with no compensating positive background; Right: Excitation energies (in units of $t$) of static doped solitons centered at a site (full line) and centered between sites (dashed line), as a function of $US/t$, with a uniform, compensating positive background. The solitons centered at a site can move freely along the chain, and therefore their actual energy is lowered by an amount $2t$ relative to the static soliton.
Chapter 1

Introduction

1.1 Motivation

In 1986 Bednorz and Muller [1] discovered that the perovskite compound (BaLa)\(_2\)CuO\(_4\) exhibits high-temperature superconductivity, with a critical temperature of up to 30K. Soon after, La\(_{2-x}\)Sr\(_x\)CuO\(_4\) and YBa\(_2\)Cu\(_3\)O\(_{7-x}\) were found to have superconducting critical temperatures of 35K and 95K, respectively. Since then, many more such compounds were found, including the Tl and Hg series. The current record \(T_c\) of 135K (165K under pressure) is found in the HgBa\(_2\)Ca\(_2\)Cu\(_3\)O\(_8\) system.

Soon after these discoveries it was realized that these superconductors are not of the conventional BCS type. Superconductivity emerges through doping the insulating parent compounds, which are three-dimensional antiferromagnets (AFM). As charge carriers are introduced by doping, the long-range AFM order disappears, leading to a metallic phase with striking non-Fermi-liquid properties. Superconductivity emerges from this unconventional metal as the system is cooled. Understanding the nature of this unconventional metal appears to be the central focus of many-body theory as applied to these systems [2, 3].

The vicinity of the superconducting phase with the AFM phase as well as the non-Fermi liquid behavior of the normal state are evidence for strongly correlated electron behavior in these systems. So far, in condensed matter physics there is no systematic way to derive the non-Fermi liquid properties of this strongly correlated system. Some insight into the nature of strongly correlated electron systems comes from exactly solvable one-dimensional models, such as the 1D Heisenberg model [4], 1D XY Heisenberg model [5] and the 1D Hubbard model [6]. These models exhibit new properties, such as fermionic spin soliton states (in the Heisenberg model) and spin-charge separation (Hubbard model). Unfortunately, the Bethe Ansatz [4] which provides the foundation for the solution of these 1D problems does not provide an exact solution in higher dimensions. Instead, the concept of Luttinger-liquid in high dimensions has been proposed [7]. A microscopic derivation of such behavior
for \( d > 1 \) is still lacking. On the other hand, two alternative paradigms for non Fermi liquid in condensed matter physics have been very successful, namely the theory of charge conduction in polyacetylene [8, 9] and the Fractional Quantum Hall Effect. These theories are also based on the concepts of charge-spin separation, fermion number fractionalization and multiple soliton formation [2].

Since 1986 many proposals for theory of the high-\( T_c \) cuprates have emerged. Many of them are constructed to explain one experimental feature, but do not lend themselves naturally to explain the broad range of experimentally observed anomalies in the cuprates. Semi-phenomenological models include variants of the Fermi-liquid theory (for example, by adding by hand strong AFM correlations [10]), non-Fermi liquid models based on the presence of charged stripes theory [11, 12, 13] and the SO(5) theory of antiferromagnetism and superconductivity [14]. On the other hand, Anderson has proposed a more general framework for non-Fermi liquid based on charge-spin separation in a two-dimensional correlated electron system [7]. However, a truly microscopic picture for the decomposition of a physical electron into a charged boson and a neutral fermion has not been elucidated.

This thesis presents a microscopic model for understanding the cuprate physics. This model is consistent with Anderson's conjecture of charge-spin separation. However, the origin of this charge-spin separation is quite distinct from that of the original RVB model [7]. Our model is a direct analog of the 1D compound polyacetylene [8, 9]. In polyacetylene, the ground state dimerization of the carbon chain leads to a breaking of translational symmetry. Domain wall solitons in this bond alternation pattern tend to restore this broken symmetry. Similarly, in the cuprates, antiferromagnetic ordering of the spin-1/2 local magnetic moments leads to a breaking of translational symmetry and a two-fold degeneracy of the mean-field ground state. Magnetic solitons provide a local tunneling mechanism between the two mean-field ground states and likewise tend to restore translational symmetry while at the same time destroying long range magnetic order. Our hypothesis is that upon doping, the holes are cloaked by mobile magnetic vortex solitons. These new charged objects, which we call meron-vortices (or merons), are bosons (in a conventional quasiparticle theory, one expects the charge carriers to be fermions). In the presence of merons the electronic structure is modified, and bound levels appear deep into the Mott-Hubbard charge transfer gap. We argue that generation of merons with doping can explain (at least qualitatively) independent experimental signatures such as magnetic behavior over a large range of doping, optical data, non-Fermi liquid behavior, charge pairing, and some aspects of Angle Resolved Photoemission Spectroscopy (ARPES). Our present calculations are done at \( T = 0 \). Comparison with transport data will require a finite temperature generalization of the present work.

In Chapter 1 we introduce the model Hamiltonian used in this thesis. This model,
which we call the spin-flux model, is a generalization of the usual 2D Hubbard model which includes the most important (non-perturbational) effects of the longer range Coulomb interaction. The existence of spin-flux in a strongly correlated electron system is tantamount to the existence of a hidden law of nature which is hidden in models that neglect the long-range part of the Coulomb repulsion. It corresponds to the possibility of an electron undergoing a $2\pi$ rotation in its internal coordinate frame as it traverses a closed trajectory in external coordinate space. To our knowledge, this possibility has never before been studied in the context of correlated electron systems. Throughout the thesis we compare the predictions of this spin-flux model with those of the (widely studied) conventional Hubbard model which completely neglects long-range Coulomb interactions.

In Chapter 2, we review some of the most interesting and central experimental properties of the high-temperature cuprates, both in the normal and the superconducting state. Since the experimental field is so vast, we restrict our attention to properties which we believe are most indicative of the unusual, non-Fermi liquid and non-BCS character of the doped cuprates. Our new model provides a microscopic basis for understanding a variety of different experimental anomalies.

In Chapters 3 and 4, we treat the problem of introducing holes (charge carriers) in an AFM system using the unrestricted self-consistent Hartree-Fock method. For comparison purposes we begin by studying the 1D Hubbard model in Chapter 3. The 1D model has an exact solution, and therefore provides us with a test to gauge the accuracy of our methods. We find three types of relevant excitations in the 1D system: uncharged fermionic domain walls (which appear even in the absence of doping), fermionic charged spin-bags (or spin-polarons) and bosonic charged domain walls. A simple continuum approximation shows that the bosonic charged domain walls can be directly mapped to the bosonic charged solitons of the polyacetylene. We end Chapter 3 using this simplified continuum approximation to calculate the electronic structure of the meron-vortex, which is the 2D analog of the 1D charged domain-wall. In the continuum limit, the meron-vortex leads to the existence of a doubly degenerate mid-gap level state in the Mott-Hubbard charge-transfer gap in analogy with the midgap states induced by domain wall solitons in polyacetylene. The self-consistent lattice 2D case is studied in Chapter 4. We begin with a comparison of the undoped system treated both within the spin-flux model and the conventional model. While both models predict AFM insulating states, the spin-flux model also predicts an electronic band structure in much better agreement with the one measured experimentally through ARPES. This is very significant, since the structure of the energy levels is extremely important in describing the proper evolution of the system with doping. If just one hole is added to the planes, two types of charged excitations are identified: the fermionic charged spin-bag and the bosonic charged meron-vortex (which is a hole dressed by a magnetic spin-vortex).
Some simple energetic arguments show that vortex-antivortex pairs are the low-energy excitations of the spin-flux model in the range $3 < U/t < 8$ for dopings $\delta < 0.30\%$. This is verified by looking at higher dopings, where we show that the low-energy configurations in the spin-flux model are liquids of charged merons and antimerons, as opposed to charged stripes for the conventional model. We show that even at the static Hartree-Fock level, the liquid of merons and antimerons has properties in agreement with measured magnetic, optical and transport properties of the cuprates. The existence and stability of merons is a direct consequence of the shape of the dispersion relations of the undoped spin-flux AFM parent compound. These undoped spin-flux AFM dispersion relations are in good agreement with those measured experimentally. The dispersion relations for the electrons in the conventional Hubbard model are in disagreement with ARPES data and as a result static vortex-antivortex pairs are unstable to collapse into conventional spin-polarons in the absence of spin-flux.

The unrestricted static Hartree-Fock approximation leads to a mean-field ground state configuration which breaks symmetries of the initial Hamiltonian, namely translational and rotational invariance. These symmetries can be restored by allowing quantum hopping of the solitonic excitations along the chain. This is the essential new physics of the Configuration Interaction (CI) approximation. The results of the CI approximation are analyzed in Chapter 5. First, we analyze the 1D system. In this case, we prove that the charged bosonic domain wall excitations are the relevant excitations upon doping for all $U/t$ values. The excitation energies we obtain by including the extra kinetic energy gained through quantum hopping is in excellent agreement with the exact Bethe Ansatz solution. Also, we show that the (electron-like) spin-1/2 charged polarons decay into a charged bosonic domain wall and an uncharged fermionic domain wall, leading to spin-charge separation. The good agreement with the exact Bethe Ansatz solution suggests that the CI method is an effective method for going beyond static mean-field theory and incorporating essential tunneling effects in the 2D case. In the 2D case, we show that meron-antimeron pairs can substantially lower their energy through quantum hopping. The spin-bags, on the other hand, do not gain much energy by hopping. It is again more favorable for a spin-bag to break up into a vortex-antivortex pair which is bound by the doping charge. Such a pair is much more mobile than the spin-bag. These results further suggest that bosonic charged merons are the relevant excitations upon doping the AFM planes.

In Chapter 6 we consider the response of magnetic solitons to external electromagnetic fields. We treat the motion of the bosonic charged domain-walls of the 1D case within the Time-Dependent Hartree-Fock (TDHF) approximation. For relatively small $U/t < 5$ we prove that they have a relativistic dynamics, and find the rest mass and maximum speed. We also study the damping induced by collective excitations. However, since TDHF is a
semi-classical approximation which excludes tunneling, the method is of limited utility. We also analyze the RPA method, which is a limiting case of TDHF. We develop a new way of performing RPA, which is numerically more convenient for larger systems. We derive the spin wave spectra of the undoped parent compound, in agreement with known results. Also, the optical absorption data presented in Chapter 2 can be calculated within RPA. Although the RPA provides a basis for understanding the mid-infrared optical absorption band as well as certain features of band tailing from the upper Mott-Hubbard band, it is inadequate in treating the low frequency limit of the optical conductivity. This low frequency regime is associated with the translational motion of the charged vortex solitons in response to the electric field. For this regime, a linear response formalism based on the CI method may be required.

Finally, in Chapter 7 we summarize and discuss the main results, and suggest various avenues for further research.

1.2 Crystal structure and model Hamiltonian

The basic structure of all high-$T_c$ materials is similar, comprising alternating stacks of electronically active CuO$_2$ sheets that are usually separated by a variable number of insulating block layers [15]. In Figs. 1.1 and 1.2 we show the crystal structure of the most studied of these compounds, La$_2$Sr$_2$CuO$_4$ and YBa$_2$Cu$_3$O$_{7-x}$.

It is widely agreed that one of the central features of the cuprates is [7] that all relevant carriers of both spin and charge reside in the CuO$_2$ planes. It is these carriers that are responsible for both the magnetic and superconducting properties of the cuprates. The only role of the other planes is presumed to be that of a source of doping holes or electrons for these CuO$_2$ planes.

There is direct experimental evidence of strong electron correlations in the CuO$_2$ planes [16]. Let us consider La$_2$CuO$_4$ as an example. The valence of La is 3+, implying that La$_2$ donates a total of six electrons. Oxygen has a valence of 2- and therefore O$_4$ accommodates a total of 8 electrons. This leaves for the Cu a valence of 2+, implying a 3d$^9$ configuration. However, there is strong hybridization between the O(2p) and the Cu(3d) orbitals, as shown in Fig. 1.3(a). The hole in the Cu(3d) shell is therefore placed in the highest anti-bonding Cu-O state, which has predominantly Cu (3d$_{x^2-y^2}$) and O(2p$_z$) character (see Fig. 1.3(b)). With one hole per formula unit, one would expect La$_2$CuO$_4$ to be metallic with a half-filled conduction band. In reality, the material is an antiferromagnetic insulator with a Néel temperature of about 300K. The insulating behavior is also found above the Néel temperature, and is due to strong correlations of the electrons in the CuO$_2$ plane.

La$_2$CuO$_4$ can be doped with holes by partially replacing La$^{3+}$ by Sr$^{2+}$ or Ba$^{2+}$. The
Figure 1.1: Crystal structure of the monolayer parent compound La$_2$CuO$_4$. The CuO$_2$ plane are shaded. They are separated by a couple of insulating layers.

Figure 1.2: Crystal structure of the bilayer parent compound YBa$_2$Cu$_3$O$_7$. There are two close CuO$_2$ planes per unit cell. They are separated from the other bilayers by 3 other layers. The most interesting of these is the middle layer, which is made of CuO chains.
Figure 1.3: (a) Bonding between the 3d orbitals of a Cu$^{2+}$ atom and the 2p orbitals of two O$^{2-}$ atoms making up the unit cell of the CuO$_2$ planes. The highest anti-bonding orbital has predominantly $d_{x^2-y^2}$-$p_\pi$ character and contains the hole of the undoped unit cell. All the other bonding and anti-bonding orbitals obtained through hybridization are fully occupied and at much lower energies. (b) The Cu($3d_{x^2-y^2}$) and O($2p_{x,y}$) orbitals which hybridize most and form the lowest bonding and highest anti-bonding states shown in Fig. 1.3(a).

Figure 1.4: Phase diagram of the hole-doped system La$_{2-x}$Sr$_x$CuO$_4$ as a function of doping $x$ [17]. The undoped parent compound ($x = 0$) is an AFM insulator. With increased doping, there is a transition to an unusual metal that becomes superconducting below $T_c$. 
corresponding phase diagram is shown in Fig. 1.4. A very small doping $x \approx 0.02$ completely destroys the long-range AFM order. Simultaneously, the compound undergoes an insulator to metal transition. It is this metal that superconducts, with a critical temperature strongly dependent on the doping. The maximum $T_c$ is reached for $x \approx 0.15$. Further doping destroys the superconductor. All the other cuprate compounds have similar behavior. The undoped parent compound is an insulating antiferromagnet. Doping (either through substitution, or through removal of O atoms from other layers) leads to the appearance of the superconducting metal. The material with the maximum $T_c$ is called optimally doped, while materials less (more) doped are called underdoped (overdoped).

As discussed above, the high-temperature cuprates have a very complex chemical structure. A complete treatment of such a complicated system is clearly impossible. As usual in such situations, we will simplify the problem by using an effective Hamiltonian which includes only the most important features of the system. A first major simplification of the problem is to consider a one-band Hamiltonian describing only the hybridized $O(2p) - Cu(3d_{x^2-y^2})$ orbital, and assume that all other filled orbitals are at much lower energies, and therefore inactive.

A second major simplification is the assumption that the problem is effectively two-dimensional. This assumption clearly stems from the stacked layer structure of these compounds. If the layers between CuO$_2$ planes are inactive, as already assumed, the only 3D behavior can be driven by some direct or super-exchange coupling between neighboring CuO$_2$ planes. Such a coupling obviously affects the critical superconducting temperature, since bilayer and trilayer compounds have higher $T_c$ than monolayer compounds. However, monolayer compounds, such as LaSrCuO, which have a large separation between CuO$_2$ planes exhibit almost all of the same physics. We conjecture, therefore, that although 3D coupling is required in general for Bose condensation, superconductivity and magnetic long range order (LRO), it is rather the 2D electronic correlations that provide the central mechanism for the non-Fermi liquid behavior and charge carrier pairing. We, therefore, focus our attention on an effective Hamiltonian for electrons in 2D describing just one CuO$_2$ plane. Strictly speaking, the exact solution of such a 2D model would preclude any form of long range order except at zero temperature. However, by applying the appropriate mean-field theory for the 2D model and then considering fluctuations about this mean-field, we effectively re-introduce the role of the 3D coupling. At zero doping our model has antiferromagnetic long-range order as observed experimentally. Fluctuation corrections to the mean-field (namely charged and uncharged AFM vortices) destroy the magnetic LRO when either the temperature or the doping level is increased sufficiently.

The effective 2D Hamiltonian that can be used to describe the electrons residing in the $O(2p) - Cu(3d_{x^2-y^2})$ orbitals of the isolated CuO$_2$ plane is the generalized one-band
Hubbard model:

\[ H = - \sum_{i,j,\sigma} \left( t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + \sum_{i,j} V_{ij} n_i n_j \] (1.1)

where \( c_{i\sigma}^\dagger \) creates an electron at site \( i \) with spin \( \sigma \), \( t_{ij} \) is the hopping amplitude from site \( j \) to site \( i \) on the square lattice, \( n_i = \sum_{\sigma=1}^{2} c_{i\sigma}^\dagger c_{i\sigma} \) is the total number of electrons at site \( i \), and \( V_{ij} \) is the Coulomb interaction between electrons at sites \( i \) and \( j \). The most important terms are the nearest-neighbor hopping \( t_{ij} = t_0 \) and the on-site Coulomb repulsion \( V_{ii} = U/2 \). If only these two terms are considered, and we shift the chemical potential by \( \mu \), we obtain the well-known Hubbard model

\[ H = -t_0 \sum_{\langle i,j \rangle \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + U \sum_i n_i^{\uparrow} n_i^{\downarrow}. \] (1.2)

The notation \( \langle i, j \rangle \) means that the sites indexed by \( i \) and \( j \) are nearest neighbors. This Hubbard Hamiltonian, as well as the so-called \( t-J \) Hamiltonian that can be obtained from it through perturbation in the large \( U/t \) limit have long been considered as the simplest effective Hamiltonians that might still capture the physics of the high-temperature cuprates. However, after more than 10 years of intensive theoretical study of these Hamiltonians a comprehensive and microscopic theory of the cuprates has not emerged.

One major assumption made in writing Hamiltonian (1.2) is that we can neglect all longer range Coulomb interaction \( (V_{ij} = 0, \text{if } i \neq j) \). This is based on the Fermi-liquid theory notion of screening of the effective electron-electron interaction. However, this Fermi liquid underpinning of the Hubbard model is in contradiction with the experimental fact that the high-\( T_c \) cuprates are not Fermi-liquids. Therefore, we include in the Hamiltonian the nearest-neighbor Coulomb interaction which, as we will show, is a highly relevant perturbation. A nearest-neighbor Coulomb interaction \( V \) on the energy scale of \( t \) opens the possibility of an entirely new type of broken symmetry in the many-electron system, giving rise to qualitatively new physics.

Our starting Hamiltonian is, therefore,

\[ H = -t_0 \sum_{\langle i,j \rangle \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + U \sum_i n_i^{\uparrow} n_i^{\downarrow} + \sum_{\langle i,j \rangle} V n_i n_j \] (1.3)

It is convenient to define the bilinear combination of electron operators \( \Lambda_{ij}^\mu \equiv c_{i\sigma}^\dagger \sigma^{\mu}_{\sigma\sigma} c_{j\sigma} \), \( \mu = 0, 1, 2, 3 \), for \( i \neq j \) (summation over multiple indexes is assumed). Here \( \sigma^0 \) is the 2 \( \times \) 2 identity matrix and \( \sigma \equiv (\sigma^1, \sigma^2, \sigma^3) \) are the usual Pauli spin matrices. The quantum expectation value \( \langle \cdot \rangle \) of the \( \Lambda_{ij}^\mu \) operators are associated with charge-currents \( (\mu = 0) \) and spin-currents \( (\mu = 1, 2, 3) \). Circulating charge currents have been considered in the context of conventional flux phases [18]. Non-vanishing charge currents lead to appearance of...
electromagnetic fields, which break the time-reversal symmetry of the Hamiltonian. However, such states are not observed experimentally in the cuprate superconductors. In the following, we adopt the ansatz that there is no charge current in the ground state $\Lambda_{ij}^0 = 0$ but circulating spin-currents exist and take the form $\Lambda_{ij}^a = \frac{2e}{\hbar} i \Delta_{ij} \hat{n}_a, a = 1, 2, 3$, where $|\Delta_{ij}| = \Delta$ for all $i$ and $j$, and $\hat{n}$ is a unit vector.

Using the Pauli spin-matrix identity, $\frac{1}{2} \sigma_{\alpha\beta}^\mu (\sigma_{\alpha'\beta'}^\mu)^* = \delta_{\alpha\alpha'} \delta_{\beta\beta'}$, it is possible to rewrite the nearest-neighbor electron-electron interaction terms as $n_i n_j = 2 n_i - \frac{1}{2} \Lambda_{ij}^\mu (\Lambda_{ij}^\mu)^*$. If we neglect fluctuations in the spin-currents, we can use the mean-field factorization, $\Lambda_{ij}^\mu (\Lambda_{ij}^\mu)^* \rightarrow (\Lambda_{ij}^\mu) (\Lambda_{ij}^\mu)^* + \Lambda_{ij}^\mu (\Lambda_{ij}^\mu)^* - (\Lambda_{ij}^\mu) (\Lambda_{ij}^\mu)^*$. Thus, the quartic nearest-neighbor Coulomb interaction term is reduced to a quadratic term that is added to the hopping term leading to the effective generalized Hamiltonian

$$\mathcal{H} = - t \sum_{\langle i,j \rangle} \left( c_i^\dagger \hat{T}_{n,i,j} c_{j,i} + h.c. \right) + U \sum_i n_i^+ n_i^- . \quad (1.4)$$

Here, $T_{n,i,j}^\mu \equiv (\delta_{\alpha\alpha'} + i \Delta_{ij} \hat{n} \cdot \sigma_{\alpha\beta}) / \sqrt{1 + \Delta^2}$ are spin-dependent $SU(2)$ hopping matrix elements defined by the mean-field theory, and $t = t_n \sqrt{1 + \Delta^2}$. In deriving (1.4) we have dropped constant terms which simply change the zero of energy as well as terms proportional to $\sum n_i$, which simply change the chemical potential.

Mean-field states exhibiting spin currents have been considered earlier [19, 20]. However, the quantization of circulating spin-currents and the concept of quantized spin-flux were introduced by John and Golubentsev [21]. In particular, it was shown previously [21, 22] that the ground state energy of the Hamiltonian of Eq.(1.4) depends on the $SU(2)$ matrices $T^\mu$ only through the plaquette matrix product $T^{12} T^{23} T^{34} T^{41} \equiv \exp(i \hat{n} \cdot \vec{\sigma} \Phi)$. Here, $\Phi$ is the spin-flux which passes through each plaquette and $2\Phi$ is the angle through which the internal coordinate system of the electron rotates as it encircles the plaquette. Since the electron spinor wavefunction is two-valued, there are only two possible choices for $\Phi$. If $\Phi = 0$ we can set $T_{n,i,j}^\mu = \delta_{\alpha\alpha'}$ and the Hamiltonian (1.4) describes conventional ordered magnetic states of the Hubbard model (1.2). The other possibility is that a spin-flux $\Phi = \pi$ penetrates each plaquette, leading to $T^{12} T^{23} T^{34} T^{41} = -1$. This means that the one-electron wavefunctions are antisymmetric around each of the plaquettes, i.e. that as an electron encircles a plaquette, its wavefunction in the internal spin space of Euler angles rotates by $2\pi$ in response to strong interactions with the other electrons. In effect, the electron performs an internal "somersault" as it traverses a closed path in the CuO$_2$ plane. We call this the spin-flux phase. This uniform spin-flux phase is accompanied by a AFM local moment background (with reduced magnitude) and may be regarded as an alternative mean-field ground state of the conventional AFM phase of the Hubbard model. In the spin-flux phase, the kinetic energy term in (1.4) exhibits broken symmetry of a spin-orbit type.
This new form of spontaneous symmetry breaking occurs over and above that associated with conventional antiferromagnetism. It is also distinct from the smaller, conventional spin-orbit effects which give rise to anisotropic corrections to superexchange interactions between localized spins in the AFM [23]. We emphasize, however, that this AFM mean-field is a "false ground state" [24] at finite doping, analogous to the "false vacuum" in early models of quantum chromodynamics [25]. In the presence of charge carriers this mean-field is unstable to the proliferation of topological fluctuations (magnetic solitons) which eventually destroy AFM long range order. In this sense, the analysis which we present below goes beyond simple mean field theory. We capture the quantum dynamics of these magnetic solitons using the Configuration Interaction (CI) method. This method recaptures tunneling effects not contained in the Hartree-Fock approximation.

The major scope of this thesis is to study the consequences of the introduction of the spin-flux in the Hubbard model. For simplicity, we assume that the mean-field spin-flux parameters $T^{ij}$ are given by the simplest possible choice $T^{12}_{\alpha\beta} = -\delta_{\alpha\beta}, T^{23}_{\alpha\beta} = T^{34}_{\alpha\beta} = T^{41}_{\alpha\beta} = \delta_{\alpha\beta}$ (see Fig. 1.5). In a more general theory, they should also be treated as dynamical variables. We also investigate the corresponding results obtained for the conventional Hubbard model $T^{12}_{\alpha\beta} = T^{23}_{\alpha\beta} = T^{34}_{\alpha\beta} = T^{41}_{\alpha\beta} = \delta_{\alpha\beta}$ (see Eq. (1.2)), for two reasons. First, the conventional model has been investigated extensively, and we can compare our results with other results reported in literature to validate our approximations. More importantly, we will compare the results obtained for the conventional model with those obtained for the spin-flux model, in order to emphasize the new physical picture emerging from the spin-flux model.

Figure 1.5: Choice of the gauge for describing the mean-field spin-flux background. Physical observables depend on the rotation matrices $T^{ij}$ only through the plaquette matrix product $T^{12}T^{23}T^{34}T^{41}$. Shown above is the simplest (spin independent) gauge choice describing a $2\pi$-rotation of the internal coordinate system of the electron (described by 3 Euler angles) as it encircles an elementary plaquette. This is a new form of spontaneous symmetry breaking for a strongly interacting electron system in which the mean-field Hamiltonian acquires a term with the symmetry of a spin-orbit interaction.
We will also investigate quite extensively the 1D Hubbard model. Since the 1D chain contains no nontrivial closed loops through which spin-flux can penetrate, we set $T^\nu = 1$ in this case and thus study only the conventional 1D Hubbard model (1.2). A study of the 1D Hubbard model is extremely useful since this is one of very few Hamiltonians that have an exact solution, and this allows us to test our approximations against the exact Bethe ansatz solution. Moreover, the 1D results may be directly relevant for the 3D high $T_c$ superconductors. High $T_c$ cuprates such as $\text{YBa}_2\text{Cu}_3\text{O}_7$ and its close relatives have quasi-one-dimensional CuO chain structures. Unlike other classic one-dimensional quantum spin chains [26] which exhibit 3D AFM order at temperatures on the order of 1K, the CuO chains reveal AFM ordering at temperatures $T_N \sim 10\text{K}-80\text{K}$ [27]. Experiments measuring the dc resistivity [28], the infrared and optical conductivity [29] and the penetration depth in untwinned crystals [30] and ceramics [31] have revealed large anisotropies between the a-direction (perpendicular to chains) and the b-direction (parallel to chains). These results suggest that substantial currents are carried along the chains in both the normal and superconducting state [32]. The source of superconducting condensate on the chains has not yet been elucidated, and therefore a study of the 1D systems is interesting on its own.

Since we are studying doped systems, it is useful to note that the generalized Hubbard Hamiltonian (1.4) exhibits particle-hole symmetry provided that we add the effect of a neutralizing positive background. Consider the on-site repulsion term, which can be rewritten as:

$$U \sum_i n_{i\uparrow} n_{i\downarrow} = U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right) \left(n_{i\downarrow} - \frac{1}{2}\right) - \frac{U N}{4} + \frac{U}{2} \sum_i (n_{i\uparrow} + n_{i\downarrow}).$$

where $N$ is the total number of sites. The first term on rhs, which is the term on which the approximations are performed, has particle-hole symmetry. The second term is just a constant. The third term's contribution to the ground-state energy is $U N_e / 2$, since the total number of electrons $N_e$ is a good quantum number. Thus, if we consider as reference the half-filled system ($N_e = N$) then there is a difference of $nU$ between the energy of a configuration with $n$ doping holes ($N_e - n$ electrons), and the energy of the corresponding configuration with $n$ doping electrons ($N_e + n$ electrons). This difference which favors hole-doped configurations is an artifact of the Hamiltonian, which does not include electron-nucleus interactions. In the following chapters we will usually quote the energies of the hole-doped systems, in order to be able to compare them with other published results. However, in the physical system the relevant energy is that of the particle-hole invariant term $U(n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$. From the factorization written above, we can see that this is, in fact, the average between the energy of the hole-doped and of the electron-doped configurations. This average effectively mimics the role of a neutralizing positive background. The energy difference $nU$ is a constant dependent only on doping, not on the particular configuration at that doping, so both formulations contain the same physics.
Chapter 2

Experimental properties

Since the discovery of the high-\(T_c\) cuprate compounds [1], an enormous amount of unexplained experimental data has been collected [33]. A complete review of all the properties of the cuprates is impractical. Instead, we review some of the more striking experimental anomalies which point to the need for a rethinking of many-electron physics at the most fundamental level.

2.1 Optical and infrared spectroscopy

Before describing the optical properties of the cuprates, we will briefly review the behavior expected for a typical Fermi-liquid metal.

2.1.1 The Drude model

A metal has free charge carriers (quasiparticles) which respond to the electromagnetic fields at all frequencies. The simplest model describing their response is the Drude model [34], according to which the real part of the free charge carrier conductivity is given by

\[
\sigma_D(\omega) = \frac{\sigma_0}{1 + \omega^2 \tau^2}
\]  

where the dc conductivity is

\[
\sigma_0 = ne^2 \tau / m. 
\]

Here \(e\) and \(m\) are the charge and mass of the free charge carriers, while \(n\) is their density. The various interactions of the free carriers leading to absorption are incorporated in the scattering rate \(1/\tau\). These interactions include inter-particle scattering, scattering on phonons (or other collective excitations) and scattering on impurities.

Let us briefly analyze the dependence of the Drude conductivity on the density of charge carriers \(n\), on frequency \(\omega\) and on temperature \(T\). From Eq. (2.1) and (2.2) we see that
variations in the density $n$ of charge carriers lead to a simple scaling of the conductivity curve ($\sigma \sim n$). The Drude conductivity is also a smoothly decreasing function of $\omega$, expected to fall off like $1/\omega^2$ at high frequencies. The temperature dependence is hidden in the scattering rate $1/\tau$, and is determined by the dominant scattering mechanism. At very low frequencies ($\omega \rightarrow 0 \Rightarrow \sigma(\omega) \rightarrow \sigma_0$) the Drude conductivity is proportional to $\tau$, and thus it is straightforward to measure the temperature dependence of $\tau$ and identify the dominant scattering mechanism.

In a Fermi-liquid at high temperatures, the dominant scattering mechanism is the interaction with phonons. In this case the scattering rate increases proportionally with the temperature ($1/\tau \sim T$), because the number of scattering phonons is proportional to $T$ in this regime. At low temperatures, the phonon scattering rate varies like $T^3$ or $T^5$, and the dominant scattering mechanism becomes the inter-particle scattering, which has a $T^2$ dependence. This $T^2$ dependence is a clear signature of fermionic quasiparticles, since it shows that only quasiparticles within $k_BT$ of the Fermi surface can scatter. Finally, scattering on impurities is temperature independent.

To summarize, in a Fermi-liquid metal one expects a low-frequency conductivity that scales like $1/T^2$ at low temperatures (inter-particle scattering) and like $1/T$ at high temperatures (scattering on phonons). The conductivity is proportional to $n$ and falls off smoothly with increasing frequency $\omega$.

2.1.2 ab-plane conductivity

The typical variation of the conductivity of cuprates with doping at (constant) room temperature is shown in Fig. 2.1 [35, 36, 37]. The undoped ($x = 0$) parent compound is an insulator, and thus there is no conduction at frequencies below the charge transfer gap. The values of this gap are between 1.5-2 eV for all cuprates. At higher frequencies inter-band transitions are allowed, and an electronic band (the charge transfer band) is seen.

With doping, free charge carriers with a density $n \sim x$ are introduced on the CuO$_2$ planes. A simple inspection of the curves in Fig. 2.1 shows that the response of the free carriers is not simply Drude-like. In the lightly doped samples, one can see a broad mid-infrared absorption band with a definite maximum, yielding evidence that there are some transitions distinct from those described by the smoothly decreasing Drude absorption. A Drude-like tail is also seen at low frequencies (dc and far-infrared region). In more highly doped samples the mid-infrared band is not so clearly visible, the main reason being that the Drude tail increases rapidly with doping ($\sigma_\omega \sim n$) and covers it.

In order to decide whether the mid-infrared band is really a distinct feature from the Drude-like tail, and whether the Drude response is the one expected for a Fermi liquid, we must analyze the temperature dependence of the curves. The temperature dependence
Figure 2.1: Optical conductivity of LaSrCuO at 300K, for $0 \leq z \leq 0.34$ [36], and for YBaCuO at 100K, for 4 different dopings [37].

Figure 2.2: Solid lines: Optical conductivity $\sigma_1(\omega)$ of a $T_c=92K$ film of YBaCuO at 20, 100, 200 and 300K. Dotted lines: Imaginary conductivity $\sigma_2(\omega)$. From [38].
of the conductivity of a YBaCuO sample with fixed doping is shown in Fig. 2.2, from room temperature down to below the superconducting temperature $T_c$ [38]. This sample is in the optimally doped regime, since its superconducting temperature $T_c=92$ K is the maximum possible for this cuprate. Therefore, for $T=300$ K we see a curve similar to those corresponding to large $x$ in Fig. 2.1, in which the mid-infrared band is masked by the Drude-like tail.

As the temperature decreases towards $T_c$, we can see that the low frequency part of the graph (the Drude tail) increases strongly, roughly like $1/T$ (see the $\omega = 0$ intercepts in Fig.2.2). The rest of the curve, corresponding to $\omega > 1000$ cm$^{-1}$ (the mid-infrared region) is practically temperature independent. This very different response to temperature variations is strong evidence in favor of different origins for the mid-infrared band and the Drude-tail. Also, the $1/T$ dependence of the Drude-tail is an indication of non-Fermi liquid behavior of this metal. This latter aspect is discussed in the “Transport properties” subsection, where the dc resistivity is analyzed in detail.

Even more striking is the different behavior seen below $T_c$ (see the $T=20$K curve in Fig. 2.2), where the Drude-tail is no longer apparent, while the mid-infrared response still has the same shape as it did at 300K. The Drude tail is replaced by a $\delta(\omega)$ response due to the superconducting condensate formed from the free charge carriers. While this delta function response cannot be observed directly by optical techniques, its weight can be obtained from sum rules, and compared with the weight of the Drude-tail above $T_c$.

Such comparisons are shown in Fig. 2.3, in which the conductivity of a sample below $T_c$ is compared with the conductivity of the same sample above $T_c$, from which the low-frequency Drude-like contribution has been subtracted [39, 40]. The fact that the different curves are extremely similar demonstrates that the mid-infrared contribution is basically temperature independent (up to a broadening of the order $k_B T$), and that, indeed, the only effect of the superconducting transition is the collapse of the Drude-tail into the $\delta(\omega)$ function.

These features arise very naturally in our model, the essence of which is that holes doped into the CuO$_2$ planes are cloaked by magnetic vortices in the AFM background. Each meron-vortex has empty bound electronic levels localized near its core, and the mid-infrared band is simply associated with excitations of electrons from the valence band onto these bound levels, which lie deep inside the Mott-Hubbard gap. The fixed gap (clearly visible below $T_c$ in Fig. 2.4) is due to excitations from the top of the valence band on these bound levels, while the high-frequency tail, which falls roughly like $1/\omega$, is due to excitations of electrons from well inside the valence band.

Meron-meron interactions lead to the splitting of these discrete levels into a fairly broad band, even at very low temperatures. Since the characteristic energies of these transitions
Figure 2.3: (a) Upper panel: Optical conductivity of a \(T_c = 89\text{K} YBaCuO\) film above \(T_c\) with the Drude contribution subtracted. Lower panel: Total conductivity below \(T_c\). From [39]. (b) Mid-infrared contribution to the frequency-dependent conductivity of BiSrCaCuO at temperatures between 20 and 300K. The curves at and above 75K were found by subtracting a Drude-model conductivity from the total conductivity. The 20K curve is the total conductivity. From [40].

Figure 2.4: The optical conductivity of four YBaCuO crystals with, starting from the top curve, \(T_c = 90, 80, 50,\) and \(30\text{K}\). The only effect of the doping on the mid-infrared band (seen in the lower panel) is an overall scaling. The onset of absorption at 150 cm\(^{-1}\) does not vary with \(T_c\). From [37].
are quite large (mid-infrared region), they cannot be thermally activated and thus the only effect of the variation of temperature is a broadening of the lines, of the order of $k_B T$. Finally, the number of bound levels is proportional to the number of merons, and therefore this mid-infrared band is expected to scale with doping, but otherwise have the same shape, as seen in Fig. 2.4.

The low frequency Drude response, on the other hand, is associated with free translational motion (flow) of the charged bosonic meron-vortices along the CuO$_2$ planes. At low doping, a charged meron-vortex may be tightly bound to a neutral (fermionic) antivortex. With further doping the vortex-antivortex pairs may unbind even in the absence of external fields leading the destruction of magnetic LRO and anomalies in the spin excitation spectrum. It is plausible that an intermediate doping and temperature region exists where free neutral vortices are present but charged vortices bind into "preformed pairs" leading to anomalies in both the spin and the charge excitation spectrum (pseudo-gap region). As the temperature is lowered, the preformed pairs eventually condense into a superconducting state. This leads to the collapse of the Drude response in the superconducting $\delta(\omega)$-function response, but leaves the mid-infrared band unchanged, since the existence of the trapped electronic levels inside the merons' cores is not affected by how the merons flow (or super-flow) along the planes. The unusual temperature dependence of the Drude-tail ($1/T$ from 20K (in non-superconducting samples) up to 1000 K) can be attributed to the bosonic nature of the charged merons. A low-temperature $T^2$ variation is expected for fermionic particles, since it is a signature of the existence of the Fermi surface, but is not at all necessary for a liquid of bosons.

Another strong argument in favor of this interpretation is provided by photoinduced absorption experiments [41]. If the undoped parent compounds are illuminated with intense visible light, they develop absorption bands that resemble the mid-infrared bands of the doped compounds (see Fig. 2.5). Evidence that these bands are related to mobile carriers (and not to absorption by excitons, for example), is provided by the laser intensity dependence of the absorption bands (whose strength scales with the square root of the laser power). The effect of the laser light on the parent compound is to create electron-hole pairs, by exciting electrons over the Mott-Hubbard gap into the conduction band. However, both the electrons in the conduction band and the holes in the valence band can lower their energy if they decay into $\pm e$ charged merons (analogous to the decaying of the doping holes into merons in the doped samples). The photoinduced bands are due to electronic excitations on the discrete levels bound in the cores of these merons, exactly as in the doped compounds. The recombinations is simply due to $+e$ meron / $-e$ antimeron annihilation.

A number of other theoretical approaches for high-Tc, such as Anderson's RVB concepts [7], Varma's marginal Fermi liquid hypothesis [43] and the nested Fermi liquid theory
Figure 2.5: Photoinduced absorption in three insulating parent compounds of the high temperature superconductors. Top curve is LaCuO, middle curve YBaCuO, bottom curve TlBaCaGdCuO. Under intense laser irradiation the insulating compounds develop absorption bands that resemble those of the corresponding superconducting materials[41].

Figure 2.6: Dashed line, right scale: Effective mass as a function of frequency determined from the a-axis polarized conductivity of an optimally doped YBaCuO single crystal. The temperature is 100K. Full line, left scale: The corresponding renormalized scattering rate, 1/τ. From [42].
choose to summarize the optical properties presented above, along with the transport data, in a semi-phenomenological manner. In the optimally doped regime above $T_c$, the conductivity curve is indeed smooth (see the curves corresponding to the optimally doped crystal in Figs. 2.2, 2.4), and can be all fitted by a Drude formula, if one assumes a scattering rate of the form
\[ \frac{\hbar}{\tau} = \max(k_B T, \hbar \omega). \] (2.3)
and allows for some (roughly logarithmic) variation of the effective mass with frequency (see Fig. 2.6). Eq. (2.3) emphasizes in fact the two distinct regimes in the conductivity curve, a low-frequency part which is strongly temperature dependent (in a $1/T$ fashion) and a higher frequency (mid-infrared) part which is basically temperature independent, and where the conductivity tail falls like $1/\omega$.

2.2 Transport properties

2.2.1 ab-plane resistivity

The typical variation of the dc resistivity of a cuprate as a function of doping and temperature is presented in Fig. 2.7 [45, 46]. Several regimes can be identified. At very low dopings, the system is an insulator with a very large resistivity. The resistivity decreases dramatically upon doping, and at a doping around $x = 0.03$ there is an insulator-to-metal transition. For all cuprates, this insulator-to-metal transition seems to be accompanied by the occurrence of superconductivity ($\rho \to 0$ for $T < T_c$). In other words, at $T = 0$ as a function of doping the system jumps from an insulating ground state to a superconducting ground state, and there appears to be no normal metallic ground state in between. As the doping is further increased, the critical temperature $T_c$ first increases (underdoped to optimally doped region), then decreases to zero (overdoped region) and afterwards the system remains metallic down to $T = 0$ (extremely overdoped region).

In the insulating regime (extremely low doping) the $T$-dependence of the resistivity can be fitted reasonably well to the Mott formula for variable range hopping conductivity [47, 48]
\[ \rho(T) \sim \exp \left( \left( \frac{T_o}{T} \right)^{D-1} \right) \]
where $D = 2$ is the dimensionality of the system. Thus, the low-temperature conduction in the insulating phase seems to occur by variable range hopping of localized holes.

In the underdoped regime, the temperature dependence is linear in $T$ for temperatures $T > T^*$. The linear $T$ dependence disappears below $T^*$, signalling the opening of a pseudogap. We discuss the significance of the pseudogap in the underdoped samples in the
Figure 2.7: Temperature dependence of resistivity in ceramic samples of La_{2-x}Sr_xCuO_4 for different Sr content x. The system undergoes an insulator to metal transition at x ≈ 0.03, where superconductivity sets in. The resistivity keeps decreasing with further increase of x. While the underdoped to optimally doped samples show a T-linear behavior, the overdoped samples show a T^2 behavior, reminiscent of a Fermi liquid. From [46].

ARPES section. As the doping increases the pseudogap temperature $T^* \rightarrow T_c$, and in the optimally doped region all cuprates have a resistivity $\rho(T) \sim T$ from $T_c$ up to as much as 700K [49]. Another universal feature of optimally doped cuprates is that they have no residual resistivity ($\rho(T)$ extrapolates to 0 for $T \rightarrow 0$). Thus, in the optimally doped region

$$\rho(T) = BT \quad \text{for } T > T_c,$$

where $B = 10 \pm 5 \Omega/K/layer$ for all optimally doped cuprates. Finally, in the overdoped region there is a gradual transition from the T-linear to a T^2 dependence in the dc resistivity. The T-linear resistivity has attracted much attention as a possible indication for non-Fermi liquid behavior of these metals. As discussed in the "Optical and infrared spectroscopy"
subsection, the \( \omega \to 0 \) region of the conductivity curve is reasonably well fitted by a Drude formula (see Eqs. (2.1,2.2) ). Then, the dc resistivity is given by

\[
\rho(T, \omega = 0) = \frac{m}{ne^2\tau}
\]

where \( m \) and \( e \) are the mass and charge of the free charge carriers, \( n \) is their density and \( \frac{1}{\tau} \) is their characteristic scattering rate. All the temperature dependence of \( \rho \) can be attributed to the scattering rate \( 1/\tau \).

In an ordinary Fermi liquid the electron-electron scattering gives a \( T^2 \) dependence of the relaxation rate. This \( T^2 \) behavior is related to the quadratic energy dependence of the quasiparticle lifetime \( \frac{1}{\tau} \sim |\epsilon - \epsilon_F|^2 \), and is a hallmark of a Fermi liquid [34].

There have been attempts to attribute the \( 1/\tau \sim T \) scattering rate to scattering on phonons, which is known to have this characteristic behavior in the large \( T \) limit (the number of phonons increases linearly with \( T \) in this regime). Contradictions arise, however, when the data are examined in detail. First, the low-\( T \) resistivity is linear down to 20K in some compounds, and in this regime one expects a \( T^3 \) or \( T^5 \) behavior of the electron-phonon scattering rate. Second, the cuprates have a large number of Einstein-like optical phonon branches at energies between 150 - 1000K, and they should contribute to \( 1/\tau \) once they are thermally activated. In contrast to this expectation, the resistivity remains linear up to 1000K, with absolutely no variations seen at the characteristic temperatures of the optical phonons, implying that the scattering of the free carriers is completely unaffected by these optical branches. Third, the scattering rate is quickly suppressed below \( T_c \) (see Fig. 2.8). The upper panel of Fig. 2.8 compares the dc resistivity obtained from the Drude parameters based on a Drude-model fit of the far-infrared conductivity data (open circles) with the dc resistivity obtained from transport measurements (the line), for two compounds: the extremely underdoped \((T_c \to 0)\) Bi\(_2\)Sr\(_2\)CuO\(_6\) (2201) and optimally doped Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\) (2212) [50]. The agreement between the two types of measurements is very good. The lower panel of Fig. 2.8 shows the scattering rate inferred from the Drude analysis of the far-infrared data. For \( T > T_c \) we see the \( T \)-linear behavior of the optimally doped sample, quite similar to that of the underdoped sample. Below \( T_c \), however, there is a very rapid drop in the scattering rate of the superconducting sample. This suppression is very unlike phonon scattering of normal superconductors. In conventional BCS superconductors nothing happens (to first order) to the phonons as the material becomes superconductor, and therefore the scattering rate does not change dramatically at \( T_c \). In strong-coupling BCS superconductors, such as lead, the scattering rate actually increases for a range of temperatures just below \( T_c \). The rapid suppression of \( 1/\tau \) at \( T_c \) is a unique property of high-\( T_c \) superconductors. All these arguments point against scattering on phonons as the dominant scattering process, and also against a BCS-like theory of superconductivity, based
on phonon mediated pairs.

The rapid decay of the scattering rate below $T_c$ seen in Fig. 2.8 is also confirmed in measurements of microwave conductivity [51] and heat conductivity [52], which show a dramatic increase below $T_c$. This is associated with the increase of the quasiparticle lifetime (due to a collapse of the scattering rate). This collapse suggests the opening of a gap in the spectrum of excitations responsible for the large normal resistivity above $T_c$. Such a gap is opened for the charge carriers themselves, since they condense in a superfluid at $T_c$. Thus, we must conclude that the most likely excitations responsible for the linear $T$ resistivity above $T_c$ are the charge carriers themselves, or at least that the scattering mechanism is electronic in nature [7, 35].

This conclusion reopens the question of the non-Fermi liquid behavior: if the scattering mechanism is electronic, a $T^2$ dependence must be observed at low temperatures in any canonical Fermi liquid. The only possible conclusion is that the normal state of the underdoped and optimally doped compounds is a non-Fermi liquid metal. A transition towards
a Fermi-liquid takes place in the overdoped region, and is signalled by the transition to an $\rho(T) \sim T^2$ behavior.

As mentioned before, the non-Fermi nature of the underdoped and optimally doped metal is a straightforward consequence of our model, in which the metallic state is a liquid of charged merons. These merons are bosons, and therefore characteristics related to a liquid of fermions do not apply. Above $T_c$, the charged merons respond to a dc electric field by flowing along the CuO$_2$ planes. We have not investigated the temperature dependence in detail yet, but the scattering of charged merons from thermally and doping induced vortices as well as thermally excited spin waves should lead to highly non-Fermi-liquid transport in the ab plane. The transition to a Fermi-liquid at large dopings is also predicted in our theory, since at large dopings the spin-flux state which stabilizes the merons becomes unstable to the conventional state. Indeed the entire Mott-Hubbard charge-transfer gap collapses in the overdoped regime.

Another feature that is plausible in our model is the fact that the insulator-to-metal transition takes place at virtually the same concentration where the long-range antiferromagnetic order (LR AFM) is destroyed ($x = 0.03$ for La$_2$CuO$_4$). By insulator-to-metal transition we mean the transition with increased doping from an (insulating) state with divergent resistivity as $T \to 0$ to a (metallic, superconducting) state with vanishing resistivity below $T_c$ (see Fig. 2.7). One key feature of the merons is that they are topological excitations (the magnetic vortex has a $+/ -1$ winding number, depending on whether spins rotate by $+/-2\pi$ on any loop surrounding the core of the vortex). As such, they may be created only in meron-antimeron pairs, of total topological number $+1 + (-1) = 0$. At extremely low dopings the number of tightly bound meron-antimeron pairs is small, and although each pair disturbs the local AFM order, most of the spins are still outside any pair and therefore oriented according to the LR AFM order. However, for a concentration around $x = 0.02 - 0.05$ the areas occupied by different pairs start to overlap. This leads to a complete destruction of the LR AFM order while at the same time allowing the charged merons to coalesce into a quantum liquid. It is this liquid of charged merons that we associate with the metallic state.

2.2.2 c-axis resistivity

Given the stacked-planes structure of the cuprates, considerable anisotropy between the ab-plane and c-axis properties is expected. This is indeed observed for resistivity measurements, although the magnitude of the anisotropy as well as its temperature dependence show quite a large diversity among the high-$T_c$ compounds. However, there seems to be no correlation between the behavior of the c-axis resistivity, $\rho_c$, and $T_c$ [53]. This poses a serious question to those theoretical models in which the interlayer coupling strength
Figure 2.9: The temperature dependence of the basal plane resistivity $\rho_{ab}$ and the c-axis resistivity $\rho_c$, in single crystal samples of La$_{2-x}$Sr$_x$CuO$_4$ for different doping $x$. The anisotropy $\rho_c/\rho_{ab}$ decreases with increased doping. In the overdoped sample, both resistivities show the $T^2$ dependence, signalling the transition to a Fermi liquid. From [53].

plays a crucial role. A fairly typical behavior is shown in Fig. 2.9, where the evolution of c-axis resistivity with doping is shown for a LaSrCuO sample. In the underdoped to optimally doped samples the c-axis resistivity is insulator like, and is generally well fitted by an $1/T^2$ temperature dependence [54, 55]. In the extremely overdoped (non-superconducting) regime $\rho_c(T)$ becomes metallic, and $\rho_c/\rho_{ab}$ becomes nearly temperature independent, signalling the transition to a Fermi-liquid behavior (see lowest panel of Fig. 2.9). The anisotropy ratio $\rho_c/\rho_{ab}$ decreases with increasing doping. Roughly the same type of behavior is seen in other compounds as well. For example, the optimally doped YBaCuO is already metallic, although the underdoped samples are insulator like [53].

The metallic behavior of the overdoped samples is in good agreement with the Fermi-liquid metal picture that seems to be appropriate for these samples. The anisotropy $\rho_c/\rho_{ab}$ ~
100 (for overdoped LaCuO) is in fairly good agreement with anisotropies between the in-plane vs. c-axis hopping integrals as measured from the exchange integrals \( J \sim t^2/U \), and more importantly, from superconducting penetration depths. The same temperature dependence for both in-plane and c-axis resistivities in this regime also reinforces the Fermi-liquid picture: transport is due to the same processes in both directions, the anisotropy being due to different hopping integrals (or effective masses) of the charge carriers.

The sharp increase in the anisotropy of the underdoped samples, its strong temperature behavior as well as the insulating character of c-axis resistivity are, on the other hand, strong arguments against a Fermi-liquid behavior of these underdoped samples. First of all insulating behavior alone is inconsistent with a Fermi liquid. The strong temperature dependence of \( \rho_c/\rho_{ab} \) as well as its increase with decreasing doping \( x \) suggests that the mechanism of conduction in the c-direction becomes very different in character from that of the ab-planes, for the underdoped samples.

This kind of highly anisotropic conductivity is not unknown, and is usually due to the fact that the charge carrier is not the tunneling entity (the electron), but some form of soliton, as in polyacetylene [8]. In Anderson’s theory [7], each electron decomposes into a charge carrying (bosonic) holon, and a neutral (fermionic) spinon. The holons are responsible for in-plane charge conduction. However, for c-axis conduction a holon must recombine with a spinon, since only a “whole” electron can be transferred between planes.

Qualitatively the same type of picture holds in our model as well. The charge carriers responsible for the in-plane conductivity are the merons, i.e. doping holes dressed by magnetic vortices. Hopping of a single hole between planes means either leaving behind the undoped magnetic vortex (which is energetically expensive and unstable), or the disintegration of the magnetic vortex as well. However, since vortices can only be created in pairs with winding numbers \( \pm 1 \), disintegration of the undoped vortex also implies disintegration of its doped counterpart, and this is again an expensive process, since it leaves an undressed hole on the plane. Finally, the hopping hole encounters the same kind of problem on the new plane: in order to be stable, it should be dressed by a magnetic vortex, but creation of one isolated vortex is forbidden. As the doping (and hence the number of merons) increases, the subgap electronic states which they induce tend to be less localized. At some point, the very cores of the merons (defined as the region where the hole is localized) start to overlap, and from this point on we can no longer really distinguish the vortices (there are not enough undoped sites (or spins) left to dress each hole). For higher dopings a transition towards a Fermi-like metal takes place, the holes being now the charge carriers. This picture agrees with the transition from a non-Fermi liquid metal to a Fermi-liquid behavior at high dopings.
The Hall Effect

The Hall effect is a very useful transport probe, because it provides information on both the carrier density $n$ as well as the charge $q$ of the carriers. In a typical metal, the Hall coefficient is given by $R_H \sim 1/nq$.

The variation of the in-plane Hall coefficient with doping, for the hole-doped La$_{2-x}$Sr$_x$CuO$_4$ and the electron-doped Nd$_{2-x}$Ce$_x$CuO$_4$ compounds are shown in Fig. 2.10 [45, 56]. In the following, we will concentrate on hole-doped compounds characteristics. In the underdoped region, the sign of $R_H$ and the $1/R_H \sim x$ behavior clearly show that it is the doping holes that respond to the magnetic field, and not the electrons themselves. This correlates with the resistivity measurements, which also show that the Drude peak scales like the hole density $x$, not like the $1-x$ electron density. The fact that the mobile charge carriers are positively charged is an argument against Fermi-liquid behavior in the underdoped compounds, since the Fermi-liquid theory predicts that the electron-like quasiparticles should respond to electric fields. The positive Hall coefficient is observed in all hole-doped compounds, in the underdoped regime. However, in the overdoped regime some hole-doped compounds show a negative Hall coefficient, signalling the transition towards a Fermi-liquid behavior.

The most unusual feature of the Hall coefficient, however, is its temperature dependence in the underdoped and optimally doped regime (the overdoped samples have an almost $T$-independent Hall coefficient, again in agreement with Fermi-liquid behavior in this regime). For all the superconducting cuprates the Hall coefficient increases monotonically with de-
Increasing temperature [56]. Moreover, whenever the superconducting transition temperature $T_c$ is intentionally suppressed, the $T$ dependence of $R_H$ is also suppressed (see Fig. 2.11). The strongest temperature dependence is observed in the optimally doped YBaCuO compound, for which $R_H \sim 1/T$ up to 300K. The underdoped YBaCuO has a weaker temperature dependence, $R_H \sim 1/(T - T_c)$. Similar behavior is observed in the trilayer Bi 2223. The bilayer and monolayer Bi 2212 and Bi 2201 as well as the Tl compounds show a weaker $1/(T - T_c)$ temperature dependence for all dopings. The LaSrCuO compound has a more unusual behavior, having a Hall coefficient temperature-independent in the very underdoped regime. However, as the optimally doped regime is approached, a quite strong temperature dependence is regained [56].

It has been pointed out [59] that the overall temperature dependence of $R_H$ in YBaCuO is reminiscent of that of the magnetic susceptibility $\chi$. This similar temperature behavior of both $R_H$ and $\chi$ is consistent with our theory, since an applied magnetic field in the
c-direction will produce a weak ferromagnetic polarization of the ab-plane antiferromagnet. This canting of the spins in the c-direction leads to gyrotropic dynamics for magnetic vortices. In other words, a Hall like response is expected for charged merons arising purely from magnetic exchange interactions rather than from the conventional Hall response that is mediated by the Lorentz force \( \vec{F} = q\vec{v}/c \times \vec{B} \) [62]. Since the spin tilt is proportional to the susceptibility, the direct link between susceptibility and the Hall coefficient (leading to the anomalous temperature dependence of the later) is plausible.

Temperature dependent Hall coefficients are not unusual for systems with multiple charge carriers with different masses and mobilities (holes and electrons, for instance). However, in all the cuprates it is generally observed that the shape of \( R_H(T) \) is very little affected by pressure [45, 56]. This makes the two-carrier interpretation of the temperature-dependent Hall effect very unlikely. If the observed \( R_H \) is an outcome of a delicate balance between contributions from different carrier types, it is natural to expect that the balance could be easily tipped by pressure to yield a significant change in the T-dependence of \( R_H \).

In contrast to the in-plane Hall coefficient (magnetic field perpendicular to CuO\(_2\) planes), the Hall coefficient measured with the magnetic field parallel to the CuO\(_2\) planes is very small, negative and temperature independent [63, 64, 65], suggesting that the charge carrier responsible for it are the electrons. This clearly shows, again, that motion in the c-direction is only possible through tunneling of electrons between planes, in agreement with the c-axis resistivity data.

### 2.3 Magnetic properties

#### 2.3.1 The undoped parent compound

The undoped parent compounds of all superconducting cuprates exhibit long range antiferromagnetic order within the CuO\(_2\) planes [66]. Given their planar structure, the superexchange interactions between the Cu magnetic moments are expected to be much larger in the CuO\(_2\) planes than between planes. The large Néel temperatures (\( T_N = 340 \text{K} \) for LaCuO, \( T_N = 410 \text{K} \) for YBaCuO [67]) indicate that these exchange interactions must be strong.

At \( T=0 \), the intensity of the magnetic Bragg peaks gives the saturated magnetic moment \( m_o = (0.61 \pm 0.05)\mu_B \) [66]. The maximum value for the magnetic moment of a Cu\(^{2+}\) in the 3d\(_{2z^2-\gamma^2}\) state in an octahedral symmetry is \( m_o = g\mu_B S = 1.05\mu_B \). The observed spin reduction is assigned partly to a large zero point motion for the quantum spins \( S = 1/2 \), but also to covalency with the oxygen 2p orbitals, which reduces the magnitude of the moment localized on the 3d Cu orbital (see Fig. 1.3).

The magnetic properties of the undoped system can be well described with a spin Hamil-
tonian of the general form

\[ \mathcal{H} = \sum_{ij} \left[ J^{(ab)}_{ij} (S^x_i S^x_j + S^y_i S^y_j) + J^{(c)} S^z_i S^z_j \right] + \sum_{\alpha\beta} J_{\alpha\beta} \vec{S}_\alpha \cdot \vec{S}_\beta. \]

The first term describes in-plane interactions. Since it is known that in the ground state the spins are lying in the plane, a weak anisotropy of the in-plane coupling must be introduced, so that \( J^{(ab)} = J, \ J^{(c)} = J - \Delta J \), with \( \Delta J \ll J \). The second term of the Hamiltonian describes coupling between different layers. If the cuprate has bilayers, the intra-bilayer coupling \( J_b \) is expected to be stronger than the inter-bilayer coupling \( J_L \), although both should be much weaker than \( J \). Other corrections may be added, such as an in-plane Dzyaloshinski-Moriya interaction \([68]\) \( J_{\alpha\beta} (S^z_i S^z_j - S^z_i S^z_j) \) for cuprates with tilted CuO octahedra (LaCuO), leading to a slight ferromagnetic component at low \( T \) in the \( c \)-direction.

The various exchange parameters can be obtained by mapping the spin-wave spectrum of the undoped cuprates, and comparing it with the theoretical prediction of the spin Hamiltonian. The exchange coupling \( J \) is approximately equal to 1500K in LaCuO \([72]\), 1700K in YBaCuO \([73]\). These values indicate that \( T_N \) is much weaker than the mean-field value \( 4JS(S+1)/3 \), and therefore that low-dimensional effects as well as smaller spin values must dominate the magnetic ordering. As expected, the other exchange parameters are very small. For YBaCuO, for instance, \( \Delta J = 10^{-4}J \) and \( J_L = 10^{-5}J \) \([73]\). The large in-plane \( J \) value is responsible for very strong two-dimensional spin correlations well above \( T_N \), in the paramagnetic state. The characteristic correlation length is shown in Fig. 2.12, and is found to be well described by \([70]\)

\[ \xi = a \left( 1 + \frac{k_B T}{J} \right)^{-1} \exp \left( \frac{J}{k_B T} \right). \]

This formula was obtained by Chakravarty from renormalized calculations within a simple Heisenberg model, taking in consideration the quantum nature of the 2D correlations. This model also explains the variation of the susceptibility with temperature. As seen in Fig. 2.13, the susceptibility of the undoped parent is also affected by the strong 2D spin correlations, since it is quite far from a Curie-like temperature dependence \( 1/(T + T_N) \). The susceptibility decreases with \( T \) for \( T > T_N \) but goes through a flat maximum around 800K.

The origin of the 3D magnetic ordering at \( T_N \) is very revealing of the nature of magnetic fluctuations in the system. It is well known that for a single CuO\(_2\) layer, the long range order (LRO) may only occur at \( T = 0 \). Thus, it is expected that the 3D ordering is driven
Figure 2.12: Inverse correlation length $\xi^{-1}$ versus temperature in La$_2$CuO$_4$, from [69]. The solid line is the theoretical prediction of Eq. (2.4) [70].

Figure 2.13: Magnetic susceptibility $\chi_m$ versus $T$ taken on ceramic samples for various oxygen contents, from the AFM to the metallic state. Large Curie terms occur at low $T$ and are partly due to spurious phases in the sample. From [71].
by the weak interplane exchange $J_\perp = 10^{-5}J$, at a temperature of the order

$$k_B T_N = J_\perp \left( \frac{\xi}{a} \right)^2 \quad (2.5)$$

where $a$ is the lattice constant. The right hand side of Eq. (2.5) is the energy gained through coherent coupling between all the spins in a correlation disk of radius $\xi$ in one layer with the spins in a similar disk in the next layer. Below $T_N$ the thermal fluctuations are not strong enough to destroy this coherent coupling, and therefore 3D ordering is established. Eq. (2.5) suggests that $T_N$ should be very sensitive to variations of $J_\perp$. Contrary to such expectations, it was found that in YBaCuO substitution of up to 30% of the intermediary Cu(1) by Ga only induces a 2% change in $T_N$ [74]. Even if the interlayer spacing is changed (by inserting two layers of PbO between the CuO$_2$ bilayers of the YBaCuO, obtaining the YSr$_2$Pb$_2$Cu$_3$O$_{10}$ compound), $T_N$ remains unchanged at 410K [75]. This implies that $T_N$ is driven by a purely two-dimensional phenomenon, which was identified as a Kosterlitz-Thouless transition [76]. In the presence of even a small anisotropy $\Delta J$, a two-dimensional antiferromagnet should undergo a Kosterlitz-Thouless transition at a finite temperature $T_{KT}$, at which the two-dimensional correlation length $\xi$ diverges. If $\xi \to \infty$ as $T \to T_{KT}$, even an infinitesimal $J_\perp$ between planes will then drive the 3D ordering at a temperature $T_N$ only slightly larger than $T_{KT}$ (see Eq.(2.5)). In such a case, the absence of variations of $T_N$ with changes in $J_\perp$ becomes quite natural. Eq.(2.5) also implies that the long range magnetic order is strongly affected if the 2D correlation length $\xi$ is diminished. This is possible if perturbations are introduced directly in the planes, either by substitution of the Cu sites, or by hole-doping.

2.3.2 Influence of hole doping on the AFM state

It is well known that if one dilutes an AFM through substitution of some magnetic sites by non-magnetic impurities, its Néel temperature decreases and eventually, for large enough disorder, the 3D LRO disappears. The limit $T_N = 0$ is reached when the concentration of impurities approaches the percolation limit $x_c \sim 0.6$ [77]. Similar effects are expected in the cuprates, if one dopes the AFM planes with holes. However, it has been a surprise to find out that hole doping is much more detrimental to the 3D LRO than substitution of the Cu$^{2+}$ by Zn$^{2+}$, a non-magnetic ion. In fact, hole doping drives $T_N$ to zero for a very low doping $x \sim 2 - 5\%$ in LaCuO [78, 79, 80]. Similar behavior is observed in all the cuprates, in which the 3D LRO is quickly destroyed for very small concentrations of holes localized on the CuO$_2$ planes.

The variation of $T_N$ is accompanied by a reduction of the staggered magnetization given by the magnitude of the magnetic Bragg peaks. This may correspond to a reduction of
Figure 2.14: Temperature dependence of the $\mu$SR frequency in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The $T=0$ frequency is only slightly dependent on the Sr content, which shows that the internal magnetic field does not vary so much from the AFM to the disordered spin glass state. From [79].

Figure 2.15: Instantaneous spin correlation length as deduced from the width of the quasielastic scattering along the two-dimensional ridge for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, plotted versus $x$. The solid line is the average separation between holes. From [69].
the local magnetic moments with doping, or introduction of some disorder in the magnetic structure induced by the doping holes. Techniques such as μsr and nmr, which measure the local field on the Cu site, indicate that the local moment is quite independent of doping [79]. As seen from Fig. 2.14, while the Néel temperature falls from over 300K to less than 10K as doping increases to \( x = 0.05 \), the average magnetic moment (proportional to the \( T=0 \) μsr frequency) only decreases by about 25%. Such measurements lead to the conclusion that the reduction of the staggered magnetization is due to a large modification of the magnetic properties of the Cu sites near the doped hole. It is estimated that up to 100 Cu sites may be affected by the presence of a single hole [66]. Another interesting fact is provided from measurements of the variation of the 2D spin correlation length \( \xi \) with doping and temperature [69]. As shown in Fig. 2.15, the correlation length coincides quantitatively with the average distance between holes (shown as a full line in Fig. 2.15), and is also found to be basically temperature independent, from 5 to 300K. This indicates that while hole doping severely restricts the correlation length, the dynamics of holes apparently does not play a major role in the determination of \( \xi \).

The features described above are very natural consequences of our model. In our model holes doped into the planes are dressed by magnetic vortices, creating the so-called merons. For topological reasons, the creation of a vortex of winding number +1 must be accompanied by the creation of an antivortex, of winding number −1. Thus, at low dopings the holes are expected to be localized on tightly bound meron-antimerons pairs. Such a pair distorts the orientation of up to 100 neighbor Cu spins. For very low dopings, these pairs are far from each other, and there are many spins on the plane whose orientations are not affected by any pair. Thus, most of the spins maintain the LR AFM order. However, as the doping increase to about 2−5% the areas occupied by each meron-antimeron pairs start to overlap with those occupied by the neighboring pairs. At this moment the orientation of all the spins on the CuO₂ planes is affected by at least one pair of vortices, and therefore the LRO is completely lost. The local order, however, is still AFM. This picture explains the extremely low doping necessary for the disappearance of LR AFM order, as well as the fact that the spin correlation length is basically equal to the average distance between holes (vortices) and it does not depend strongly on the temperature-dependent dynamics of the hole. Each hole carries its vortex with it, and therefore the correlation length \( \xi \) is roughly the same.

2.3.3 Magnetic neutron scattering

Neutron scattering experiments are very useful in the study of magnetic order and excitations of ordered magnetic systems. This is due to the fact that the neutron has a magnetic moment which interacts with the electronic moments. Furthermore, the wavelength and
energy of thermal neutrons are such that large areas of the Brillouin zone can be investigated.

Elastic neutron scattering is useful in the AFM ordered state, where the magnetic Bragg peaks arise. The position of these peaks allow identification of the magnetic order structure, while their intensity is related to the local staggered magnetization.

Inelastic neutron scattering can be used to map the imaginary part of the magnetic susceptibility function $\chi(q, \omega)$. In the low-$T$ regime of the ordered AFM insulator, this provides information about the dispersion relations $\omega(q)$ of spin waves. In the metallic regime, this provides information about excitation of an electron across the Fermi surface with an energy boost $\hbar \omega$, momentum boost $\hbar q$, and with spin flip. The main drawback of this technique is that it requires large crystals. For this reason, only the LaCuO and the YBaCuO cuprates have been investigated in detail so far.

As discussed before, the undoped parent compounds have LR AFM order, with the main magnetic Bragg peak at $(\pi, \pi)$. With doping, this peak splits into four incommensurate peaks symmetrically placed at $(\pi + \delta, \pi + \delta)$, where the shift $\delta$ increases proportionally with doping $x$ up to around $x = 0.12$, where it seems to saturate [81]. This behavior was initially observed in the LaSrCuO compound, but has very recently been observed in YBaCuO as well [82], and therefore we can assume that it may be a common feature of all cuprates.

An early interpretation of these incommensurate peaks was based on the assumption of a large nested Fermi surface [83]. The nesting vectors vary continuously with increased doping, and therefore the four corresponding incommensurate peaks vary accordingly with doping. However, this explanation is contradicted by ARPES measurements, according to which there exists no large Fermi surface in the underdoped state (see the “ARPES” section). Another interpretation is linked to the generation of spiral spin-density waves states with doping [84]. The pitch of the spiral states is linearly dependent on doping concentration, leading to the appearance of the four incommensurate peaks.

The magnetic structure factor calculated for our static doped spin configurations also shows the incommensurate peaks, with a shift increasing with doping, in good agreement with the observed behavior in LaCuO. In this case, the appearance of the incommensurate peaks is directly related to the form factor of the single meron-vortex. The position of the peaks is determined by either the size of the vortex, or the core size, whichever is larger. Thus, at low doping the dominant length is the average vortex size, which is strongly dependent on doping. However, as the doping increases over a certain limit, the vortex size becomes comparable with the core size, and the position of the peaks is no longer dependent on doping. In LaSrCuO, such a saturation of the peaks positions with doping is indeed observed for $\delta \geq 0.12$. This phenomenology is analogous to appearance of incommensurate peaks in one-dimensional compounds, due to generation of domain-walls [85]. We have not
attempted simulation of bilayers yet, and therefore agreement with the YBaCuO results has not been studied. However, it is likely that the fairly weak interactions between the two layers will not destroy the appearance of the incommensurate peaks.

2.3.4 Nuclear magnetic resonance

NMR is a versatile tool which allows one to probe the electronic state at different nuclear sites in the lattice as well as different parts of $\vec{q}$ space. The measurable quantities are the Knight shift $K_\perp$, the spin-relaxation rate $1/T_1$ and the spin-spin relaxation rate $1/T_2c$.

The Knight shift is proportional to the real part of the susceptibility $\chi(\vec{q} = 0, \omega)$, measuring the polarization of electrons by the applied magnetic field. The spin-lattice relaxation rate is related to the imaginary part of the susceptibility through $1/T_1 \sim T \sum_{\vec{q}} F(\vec{q})^2 \chi''(\vec{q}, \omega)/\omega$ (for a one-band model). Here $F(\vec{q})$ is the atomic structure factor.
Each planar Cu nucleus is strongly interacting with the electrons of its four nearest neighbor Cu nuclei. All these neighbors belong to the same magnetic sublattice, and therefore $1/T_1$ predominantly probes the $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$ part of the susceptibility. From the electronic point of view, $1/T_1$ is proportional to the phase space available to the scattered electron. In a Fermi liquid, this is of order $k_B T$, while in a conventional superconductor it varies like $\exp\left(-\Delta/k_B T\right)$. Also, in a Fermi liquid the electrons exhibit a temperature-independent Pauli spin susceptibility. Thus, one expects to measure a temperature independent Knight shift and a $T$–linear spin-lattice relaxation rate $1/T_1$ (the Korringa law). Instead, measurements of these quantities in the high-$T_c$ cuprates indicate an anomalous temperature dependence of the susceptibility.

The Knight shift appears to be temperature independent above $T_c$ in the optimally doped case, see Fig. 2.16, left. However, in the underdoped compounds it decreases with temperature [87]. This is sometimes interpreted as a pseudogap effect. The spin-lattice relaxation rate has non-Korringa behavior for all cuprates [88]. Fig. 2.16, right, shows a compendium of non-Korringa Cu relaxation rates. Not only the temperature dependence is unusual, but also the magnitude is an order of magnitude larger than expected. The planar O atoms, as well as other nuclei exhibit Korringa relaxation, with the expected order of magnitude. The explanation for this dissimilar behavior is thought to be due to the fact that O atoms are equally coupled to both sublattices of the Cu lattice, and therefore the effect of any anomalous antiferromagnetic correlations cancels out.

### 2.4 Angle-Resolved Photoemission Spectroscopy (ARPES)

Angle-resolved photoemission spectroscopy (ARPES) is a spectroscopy in which photons of certain energy are absorbed by the material and electrons are ejected out. By measuring the energy and the emergence angle of the electron, the momentum and the energy of the filled electronic states (states below the Fermi surface) can be inferred. For the cuprates, this technique is especially useful due to the 2D character of the CuO$_2$ planes, which allows for a full determination of the 2D momentum of the occupied electronic states in the CuO$_2$ planes. By varying the angle between the sample normal and the direction of the detected photoelectron, it is possible to map out the $\mathbf{k}$ dependence of the filled states below the Fermi energy. The measured ARPES intensity is given by [89]

$$ I(\mathbf{k}, \omega) = I_o(\mathbf{k}) f(\omega) A(\mathbf{k}, \omega) $$

where $\mathbf{k}$, the in-plane momentum, gives the location in the 2D Brillouin zone and $\omega$ is the energy of the initial state measured relative to the chemical potential (Fermi level). $I_o(\mathbf{k})$ includes kinematic factors and the (squared) dipole matrix element of the Fermi Golden
Rule. It depends, in addition to \( \tilde{k} \), on the incident photon energy and polarization. The energy \( \omega \) and temperature \( T \) dependence of the ARPES intensity are entirely controlled by the \( f(\omega)A(\tilde{k}, \omega) \) factor in the range of interest. Here \( A(\tilde{k}, \omega) = -1/\pi ImG(\tilde{k}, \omega + i0^+) \) is the initial state spectral function, while the Fermi distribution \( f(\omega) = (\exp(\omega/T) + 1)^{-1} \) ensures that we are only looking at the occupied part of the spectral function.

Using Dyson's equation and the definition of the irreducible self-energy, the Green's function for the interacting system is given by \( G(\tilde{k}, \omega) = 1/(\omega - \varepsilon(\tilde{k}) - \Sigma(\tilde{k}, \omega)) \), where \( \varepsilon_0(\tilde{k}) \) is the energy of the independent quasiparticle relative to the Fermi energy and \( \Sigma(\tilde{k}, \omega) \) is the self-energy gained through interactions with the other quasiparticles. When there are quasiparticles in the interacting system, near the Fermi surface \( (\omega = 0) \) there is a single solution to the equation \( \varepsilon(\tilde{k}) = \varepsilon_0(\tilde{k}) + \Sigma'(\tilde{k}, \varepsilon(\tilde{k})) \). In addition, in a Fermi liquid \( \Sigma \) is analytic around this solution so that \( \partial \Sigma'/\partial \omega \) is a constant. Kramers-Kröning relation then implies \( \Sigma'' \sim -\omega^2 \). As a result, the quasiparticle contribution to the Green's function may then be approximated by

\[
G(\tilde{k}, \omega) = \frac{1}{1 - \frac{\partial \Sigma'}{\partial \omega}(\omega - \varepsilon(\tilde{k})) - i\omega^2} = \frac{Z}{\omega - \varepsilon(\tilde{k}) - i\omega^2}
\] (2.7)

There is an incoherent contribution to the Green's function as well, as required by normalization. From Eq.(2.7) we see that the spectral function \( A(\tilde{k}, \omega) \) is expected to be a Lorentzian centered at the quasiparticle energy \( \varepsilon(\tilde{k}) \) and with a width characterized by the quasiparticle life-time \( 1/\tau \sim \omega^2 = |\varepsilon(\tilde{k})|^2 \). As its energy moves towards the Fermi level, the quasiparticle life-time is expected to increase and the Lorentzian looks more like a \( \delta \)-function. Thus, in a typical metal one expects to see a clear quasiparticle Lorentzian peak for states below the Fermi energy and the dispersion energy \( \varepsilon(\tilde{k}) \) can be mapped. As the Fermi energy is approached, the Fermi distribution \( f(\omega) \) cuts off the quasiparticle peak, allowing a measurement of the Fermi momentum, and a mapping of the Fermi surface.

In cuprates, it is expected that the dispersion relation and the Fermi surface are strongly dependent on doping and temperature. We analyze the doping dependence first. The ARPES intensities along three directions in the Brillouin zone for the \( \text{Sr}_2\text{CuO}_2\text{Cl}_2 \) parent compound are shown in Fig.2.17 [90]. In the left panel of Fig.2.17 the dispersion relation along the \((0, 0)\) to \((\pi, \pi)\) line is shown. A very broad peak can be seen well below the Fermi energy \( (\omega = 0) \), and its dispersion relation can be easily tracked. The highest energy is reached at \((\pi/2, \pi/2)\), at about -0.8eV. The fact that there is no crossing of the \( \omega = 0 \) energy (i.e. no Fermi surface) is in agreement with the insulating character of the parent compound. For comparison, ARPES data along the same direction is shown for the optimally doped (metallic) \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \). For the metal, the dispersion relation of the broad peak can be followed as \( \tilde{k} \) varies from \((0, 0)\) to \((\pi/2, \pi/2)\), where the crossing of the Fermi line takes
Figure 2.17: Left: ARPES data showing the peak dispersion along the (0,0) to (π,π) direction for the insulating Sr$_2$CuO$_2$Cl$_2$ (a) and the metallic Bi$_2$Sr$_2$CaCu$_2$O$_8$ (b). The daggers beneath each spectrum are guides to the eye. The legend at the top has circles indicating the points in the 2D Brillouin zone where data were taken and is labeled with (1,1)=(π,π). The dark circles in the legend are on the side of the zone where the peak is strong in the insulator and the open circles where the peak is weak. The size of the circles indicates the k resolution. Right: ARPES data along the (0,0) to (π,0) direction (a) and along the (0,π) to (π,0) direction (b). The dashed line in (a) is the maximum energy for any peak in this direction. The legend is the same as in the top panel. From [90].

As the doping increases, the cuprates become metallic and a Fermi surface is observed. The ARPES data for the insulating parent compound on the (0,0) to (π,0) and the (0,π) to (π,0) directions is shown in right panel of Fig.2.17(a) and (b). The dispersion on the (0,π) to (π,0) line is very similar to the one observed on the (0,0) to (π,π) line, the point of highest energy being again (π/2,π/2). On the other line, however, there is no peak and basically no dispersion is observed. Thus, we conclude that the top of the valence band in the insulating parent compound is at (π/2,π/2), and that the dispersion relation is isotropic around it. As shown later, this is in excellent agreement with the dispersion relations obtained in our spin-flux Hubbard model, even at the mean-field level.
of the Brillouin zone, where no Fermi surface exists, the position of the points of minimum gap basically follows the same geometry as the large optimally doped Fermi surface [93] (see right panel of Fig. 2.19). This evolution of the Fermi surface with doping is now interpreted as the opening of a pseudogap in the underdoped samples (see Fig. 2.19). The pseudogap pushes more and more levels away from the Fermi level, leaving a smaller Fermi surface as the doping decreases. No evidence for a pseudogap exists in the overdoped regions, and the large Fermi surface seems to be typical for all investigated overdoped cuprates.

The large Fermi surface of the optimally doped samples was initially thought to support the Fermi liquid theory. The extreme broadness of the ARPES peaks contradicts this picture. It is widely agreed now that the ARPES data indicates that conventional quasiparticles do not exist in the normal state. In fact, it was argued [94] that the shape of the ARPES peak as well as its evolution with temperature provides clear evidence for spin-charge separation. As shown in Fig. 2.20, as the temperature is lowered the extremely broad peak seen at high temperatures splits into a well-defined quasiparticle-like peak, followed by a second much broader feature [95, 96]. Laughlin interprets this double-peaked photoemission line as evidence for a bound state (the sharp peak) plus an unbound continuum (the second much broader peak), which merge into a continuum of unbound states at high temperatures [94]. In our picture, the high-temperature metallic state corresponds to a liquid of unbound merons and antimerons. As the temperature is lowered, more and more merons and antimerons bind into pairs leading eventually to the superconducting condensate. Thus, it is tempting to associate the well-defined peak seen at low temperatures with extraction of an electron from a bound meron-antimeron pair, while the broad feature in ARPES is associated with extracting the electron from a free (unbound) meron.

Figure 2.18: Fermi crossings for two Bi2212 samples of different doping. While the overdoped sample has a continuous Fermi surface, the underdoped sample's Fermi surface is made of 4 disjoint arcs appearing near the ($\pi/2, \pi/2$) point. From [91].
Figure 2.19: Left: Destruction of the Fermi surface by the pseudogap at three doping levels (same temperature). The dotted line shows the large Fermi surface seen in the overdoped samples. As the doping is reduced, the Fermi surface (shown by a thick line) becomes gapped and only the solid arcs remain. Data show that even at low doping (leftmost panel) the minimum gap follows the original dashed Fermi surface, as shown in the second picture. From [92]. Right: Fermi surface of Bi2212 samples with different Tc's obtained by varying the doping level. For the underdoped samples for which the Fermi arcs are not continuous (the Fermi surface is gapped far from the (π/2, π/2) point), the curve shows the locus of points of minimum gap. Their shape changes little with doping. From [93].

Figure 2.20: Left: Temperature dependence of the photoemission spectra at the (π, 0) point, for an underdoped Bi 2212 sample (Tc = 79K). A sharp peak develops from the extremely broad normal state feature as the temperature is lowered. From [97]. Right: The superconducting gap as a function of the angle around the Fermi surface, for the Tc = 87K underdoped Bi2212 sample. The gap has d-wave like nodes on the zone diagonals and rises to a maximum value of about 35meV at the (π, 0) point, in agreement with the left panel picture. The open circles are the measured leading edge shifts of the raw photoemission spectra and the filled circles are the estimated gap. From [89].
or antimeron. In this respect, it is interesting to remark that the separation of the bound and continuum peaks does not appear at the superconducting transition $T_c$, but rather at the pseudogap temperature $T^*$. For instance, in Fig.2.20 the two features can still be easily observed at 85-90K, although the slightly underdoped sample becomes superconducting at 79K.

In the superconducting state, ARPES allows a direct measurement of the superconducting gap and its variation with $\mathbf{k}$ along the Fermi surface. The superconducting gap has nodes at the $(\pi/2, \pi/2)$ points, in agreement with the d-wave symmetry (see Fig.2.20, right). The d-wave symmetry of the superconducting gap is observed for all dopings [98, 99]. This is also consistent with our model of pairing of charged merons with charged antimerons. In Chapter 5, we show using the CI method that the lowest energy configuration of the "Cooper pair" of our model exhibits a wavefunction with d-wave symmetry.

The temperature evolution of the Fermi surface in the underdoped cuprates is summarized in the left panel of Fig.2.19 as well. The d-wave node below $T_c$ (left panel) becomes a gapless arc above $T_c$ (middle panel) and expands with increasing $T$ to form a full Fermi surface above $T^*$ (right panel), the pseudogap temperature. This pseudogap temperature and the critical temperature for a Bi2212 sample are shown in Fig.2.21 [99]. The evolution of the Fermi surface can easily be summarized as follows: below $T_c$, there are four nodal $\omega = 0$ points at $(\pi/2, \pi/2)$. These same four points are the top of the valence band in the insulating state. As the doping or the temperature increase the Fermi arcs develop,
Figure 2.22: Left: Momentum dependence of the gap estimated from the leading edge shift for three Bi2212 samples with $T_c = 10.83$ and 87K, measured at 14K. The inset shows the Brillouin zone with a large Fermi surface enclosing the $(\pi, \pi)$ point, with the occupied region shaded. The gaps are extremely similar in the three samples, although the $T_c = 10K$ sample is still in the normal state and therefore its measured gap is its pseudogap, as opposed to the superconducting gap measured for the other two samples. Right: The temperature dependence of the gap for the same three samples. For the near-optimal 87K sample the gap closes at $T^* = 90K \approx T_c$, while for the underdoped 83K sample there is a smooth evolution of the gap through $T_c$. The extremely underdoped sample has a much larger gap, but its evolution is also smooth. From [99].

until the pseudogap line $T^*$ is crossed. For $T > T^*$ a full continuous large Fermi surface is observed.

This smooth evolution of the superconducting gap into a pseudogap as $T$ increases suggests that the two are closely related and determined by the same kind of physics. In fact, in the ARPES data there is no difference between the superconducting gap and the pseudogap, except that the linewidths are very broad above $T_c$, while for $T << T_c$ they become resolution limited [99]. This close relationship between the two is also seen in Fig.2.22, in which the minimum gap along the Fermi surface line is measured at $T=14K$ for three Bi2212 samples, with $T_c = 10K, 83K$ and 87K. At this temperature, the two slightly underdoped samples $T_c = 83K, 87K$ are superconducting, while the underdoped $T_c = 10K$ sample is still in the normal state. However, the gaps shown in Fig.2.22 are extremely similar for all three samples, with the much larger error bars on the normal sample points due to much broader peaks. Their maximum gap $|\Delta|$ is also very similar as $T \rightarrow 0$ (see right panel of Fig.2.22). The gap of the extremely underdoped 10K sample is just slightly larger, while its superconducting temperature is almost an order of magnitude smaller than that of the 83K and 87K samples. This behavior is incompatible with BCS theory, which predicts proportionality between the gap and the superconducting temperature ($\Delta(T = 0) = 3.5k_BT_c$ for weak coupling).

The presence of the pseudogap is also observed in many other types of measurements, such as c-axis conduction, ab-plane resistivity, tunneling spectroscopy, specific heat, Raman
scattering, nuclear magnetic resonance (relaxation times) etc [92]. While there are variations in the pseudogap temperature $T^*$ obtained from different probes, its behavior with doping and order of magnitude is the same. These differences may be attributed to the fact that various experiments probe different parts of the Fermi surface (or averaged sums over the whole Fermi surface). Since the pseudogap at different points closes at different temperatures, as schematically shown in Fig.2.19, such variations are to be expected [99].

One of the proposals offered to explain this unusual gap evolution is that pre-formed pairs exist at all temperatures $T<T^*$, but coherence between pairs occurs only below $T_c$, where the material superconducts [100]. This is in qualitative agreement with our picture. In our model there is a strong pair coupling between merons and antimerons, of topological nature, at low temperatures. Each vortex must be in the vicinity of an antivortex in order to minimize the superexchange energetic cost, and since each vortex carries one hole, this interaction is an effective pair interaction. For a sufficiently large number of pairs and low enough temperature, the flow of the different pairs becomes coherent. In other words, superconductivity is related to superfluidity (dynamics) of the bosonic pairs, rather than discontinuous changes in electronic structure at $T_c$.
Chapter 3

Charged bosons in a doped Mott Insulator

In this chapter we treat the problem of introducing holes (charge carriers) in an AFM system using the static unrestricted self-consistent Hartree-Fock Approximation (HFA). The HFA is introduced in the first section. We begin this chapter with a study of the 1D Hubbard model. Using the HFA, we find two types of relevant charged excitations in the 1D system: fermionic charged spin-bags (or polarons) and bosonic charged domain walls. These are collective mode excitations which dominate the low-energy charge excitation spectrum of the 1D doped Mott insulator. Their relevance as the charge excitations of the 1D chain is clearly demonstrated in Chapter 5, where a detailed comparison with the exact Bethe Ansatz solution of the 1D Hubbard model is performed.

We then introduce a simple continuum approximation. The continuum model is constructed in such a way that the local antiferromagnetic correlation between nearest neighbor sites is treated exactly, but fluctuations from one unit cell to another have slow spatial variations. We demonstrate that some of the properties of the domain walls described by the lattice model can be accurately recaptured in the continuum approximation. Also, we prove that the bosonic charged domain walls can be directly mapped to the bosonic charged solitons of the polyacetylene. This substantiates our claim that our model is a direct analog of the polyacetylene model.

We then use the same continuum approximation to investigate the properties of skyrmion and meron excitations of the 2D AFM Mott insulator (the exact self-consistent HFA lattice treatment of this problem is addressed in Chapter 4). This simple continuum treatment clearly points out the direct analogy between the 1D charged excitations and the 2D charged excitations of the Mott AFM insulator. We demonstrate that the FM-core meron induces a degenerate pair of localized electronic midgap states within the Mott-Hubbard charge gap, which are independent of the meron core radius. On the other hand, the AFM-core meron
exhibits a pair of non-degenerate sub-gap electronic states which approach the midgap as the core radius of the meron approaches zero. Merons may be regarded as half-skyrmions. They are the two-dimensional analogues of magnetic domain wall solitons in the one-dimensional antiferromagnet and they exhibit electronic properties analogous to domain walls in the polyacetylene [8]. The skyrmion texture is analogous to the one-dimensional spin-polaron. It induces nondegenerate localized electronic states which traverse the Mott-Hubbard charge gap from valence to conduction band (and vice versa) as the skyrmion core radius varies from small to large values. This simple continuum approximation enables us to gain some valuable insight in the structure of charged collective excitations of the 2D AFM. These 2D results are confirmed in Chapter 4, where we characterize these charged solitonic structures within the self-consistent HFA.

3.1 The Static Hartree-Fock Approximation

One of the best known approximations for the many-electron problem is the Static Hartree-Fock Approximation (HFA). In this approximation the many-body problem is reduced to one-electron problems in which each electron moves in a self-consistent manner depending on the mean-field potential of the other electrons in the system. While this method is insufficient by itself to capture all of the physics of low dimensional electronic systems with strong correlations, it provides a valuable starting point from which essential fluctuation corrections can be included. In particular, we use the Hartree-Fock method to establish the electronic structure and the static energies of various magnetic soliton structures. Later we improve on this static approximation using a more general variational method (the Configuration Interaction method) which recaptures essential dynamic effects beyond this simple HF mean-field theory.

Since the many-body problem is decomposed into effective one-electron problems at the HF level, the many-body wavefunction $|\Psi\rangle$ must be a Slater determinant of one-electron orbitals. The one-electron orbitals are found from the condition that the total energy of the system is minimized

$$\delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0 \tag{3.1}$$

In the following, we will specialize the discussion for the generalized Hubbard Hamiltonian (see Section 1.2)

$$H = -t \sum_{\langle i,j \rangle} (c^\dagger_{i\alpha} T_{\alpha\beta} c_{j\beta} + h.c.) + U \sum_{i} c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \tag{3.2}$$
A Slater determinant trial-wavefunction is of the form

$$|\Psi\rangle = \prod_{p=1}^{N_e} a_p^\dagger |0\rangle,$$

where $|0\rangle$ is the vacuum state, $N_e$ is the total number of electrons in the system and the one-electron states are given by

$$a_p^\dagger = \sum_{i,\sigma} \phi_n(i, \sigma) c_{i\sigma}^\dagger$$

The one-particle wave-functions $\phi_n(i, \sigma)$ must form a complete and orthonormal system, if the transformation $(c_{i\sigma}^\dagger, c_{i\sigma}) \rightarrow (a_p^\dagger, a_p)$ is to be unitary.

Using the wavefunction (3.3) in equation (3.1), and minimizing with respect to the one-particle wavefunctions $\phi_n(i, \sigma)$, we obtain the Hartree-Fock eigen-equations:

$$E_n\phi_n(i, \alpha) = -t \sum_{j \in V_i} T_{\alpha\beta}^n \phi_n(j, \beta) + U \sum_{\beta} \left( \frac{1}{2} \delta_{\alpha\beta} Q(i) - \bar{\sigma}_{\alpha\beta} \tilde{S}(i) \right) \phi_n(i, \beta)$$

where $(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices and

$$Q(i) = \langle \Psi | c_{i\alpha}^\dagger c_{i\alpha} | \Psi \rangle = \sum_{p=1}^{N_e} \sum_{\alpha} |\phi_p(i, \alpha)|^2$$

and

$$\tilde{S}(i) = \langle \Psi | \frac{1}{2} c_{i\alpha}^\dagger \bar{\sigma}_{\alpha\beta} c_{i\beta} | \Psi \rangle = \frac{1}{2} \sum_{p=1}^{N_e} \sum_{\alpha, \beta} \phi_p^*(i, \alpha) \bar{\sigma}_{\alpha\beta} \phi_p(i, \beta)$$

represent the expectation value of the charge and spin at the site $i$, and must be computed self-consistently. The notation $j \in V_i$ appearing in (3.5) means that the sum is performed over the sites $j$ which are nearest-neighbors of the site $i$. Strictly speaking, the self-consistent Hartree-Fock equations (3.5, 3.6, 3.7) must be satisfied only by the occupied orbitals $p = 1 \ldots N_e$, but can be used to compute the empty (hole) orbitals as well.

The ground-state energy of the system in the HFA is given by

$$E_{GS} = \langle \Psi | H | \Psi \rangle = \sum_{p=1}^{N_e} E_p - U \sum_i \left( \frac{1}{4} Q(i)^2 - \tilde{S}(i)^2 \right)$$

The approximation scheme described so far is the Unrestricted Hartree-Fock Approximation. This is so because we did not impose any other constraints on the HF ground-state wavefunction $|\Psi\rangle$. Strictly speaking, the ground-state wavefunction must fulfill symmetry requirements which restrict its form. For example, in addition to being a solution of Eqns. (3.5, 3.6, 3.7), the ground-state wavefunction should also be an eigenfunction of differ-
ent symmetry operations with which the Hamiltonian commutes. If these symmetries are enforced, the method is called Restricted Hartree-Fock Approximation.

In this section we report results obtained with the Unrestricted HFA. The reason for this is that the Unrestricted HF wavefunction leads to lower energies than the Restricted HF wavefunctions, since breaking rotational and translational symmetries in this case implies that electronic correlations are partially taken into account\[16\]. As we report in the following, the HF wavefunction of the doped systems breaks the translational invariance, since the hole is localized somewhere on the lattice. In Chapter 5, we will improve the approximation by restoring the translational invariance of the ground-state wavefunction.

In the undoped (half-filled) case, the self-consistent Hartree-Fock equations can be solved analytically for the infinite system, the one-particle wave-functions being simple plane-waves. However, doping the system leads to the appearance of inhomogeneous solutions (because of the Unrestricted HF search). Infinite systems can no longer be treated, and therefore we restrict ourselves to finite chains (lattices) in 1D (2D), and solve the unrestricted self-consistent Hartree-Fock equations numerically. The numerical procedure is straightforward: we start with an initial spin and charge distribution $\tilde{S}(i)$ and $Q(i)$, numerically solve the eigenproblem (3.5) and find the HF eigenenergies and wavefunctions $E_n$ and $\varphi_n(i, \alpha)$. These are used in Eqs. (3.6) and (3.7) to calculate the new spin and charge distribution, and the procedure is repeated until self-consistency is reached.

Numerically, we define self-consistency by the condition that the largest variation of any of the charge or spin components on any of the sites of the lattice is less that $10^{-6}$ between successive iterations.

Before ending this section, let us mention the fact that the HF solution is the exact solution of the factorized Hamiltonian

$$\mathcal{H}_{HF} = -t \sum_{\alpha,\beta} \left(c^\dagger_{\alpha i} T_{\alpha \beta} c_{\beta i} + h.c. \right) + U \sum_{\alpha, \beta} C^\dagger_{\alpha i} \left(\frac{\delta_{\alpha \beta}}{2} Q(i) - \tilde{S}(i) \tilde{\sigma}_{\alpha i} \right) c_{\beta i} + U \sum_i \left(\tilde{S}^2(i) - \frac{1}{4} Q^2(i) \right)$$

(3.9)

with $Q(i)$ and $\tilde{S}(i)$ given by Eqs. (3.6, 3.7).

For convenience, in some of the following sections we will modify this by adding the quantity

$$-U \sum_{\alpha, \beta} \frac{1}{2} \delta_{\alpha \beta} c^\dagger_{\alpha i} c_{\beta i} + U \sum_i \frac{1}{2} Q(i)$$

(3.10)

Obviously, the effect of this term is only to shift the HF energies by $U/2$, but the total energy (and self-consistent distributions) will remain unaffected. The reason for which this extra manipulation is convenient is that it transforms $Q(i) \rightarrow Q(i) - 1$ in the interaction term, and therefore there is contribution only from doped sites ($Q(i) \neq 1$).
3.2 The one-dimensional Hubbard chain

3.2.1 The undoped ground state

For the undoped system we can solve the self-consistent HF equations for an infinite system. The HF ground state is found to have long range antiferromagnetic order. The Mermin-Wagner theorem states that the true ground-state of any one dimensional isolated system cannot have long range order (LRO) and that LRO is absent in 2D systems for non-zero temperatures. However, the physical systems we are modeling, namely CuO chains and CuO$_2$ planes of high-$T_c$ compounds, are embedded in a 3D crystal and exhibit LRO even at moderate temperatures. As such the Hartree-Fock ground state may be a more useful representation of the physical system than wavefunctions based on the exact solution of a strictly 1D or 2D system.

Using the spin and charge distributions $Q(i) = 1$ (one electron per site) and $\tilde{S}(i) = (-1)^i S \tilde{\varepsilon}_z$ (AFM order in the arbitrary direction $\tilde{\varepsilon}_z$), we solve (3.5) and find two electronic bands characterized by the dispersion relations

$$E_{\sigma}^{\uparrow/\downarrow} = \pm \sqrt{\varepsilon_k^2 + (US)^2} \quad k \in (-\pi/2a, \pi/2a]$$

where $\varepsilon_k = -2t \cos (ka)$ is the dispersion relation of non-interacting electrons and $a$ is the lattice constant. Each of these levels is doubly-degenerate ($\sigma = \pm 1$). If the wavefunction corresponding to spin 'up' is concentrated mainly at the odd sites, then the wavefunction corresponding to spin 'down' is concentrated mainly at the even sites, and vice versa (see Eqs. (A.5), (A.6) of Appendix A).

Given the symmetry of the spectrum and the fact that only half the states are occupied, one can easily see that in the ground state all the states in the valence band ($E_k^\uparrow < 0$) are occupied, while all the states in the conduction band ($E_k^\downarrow > 0$) are empty. The two bands are separated by the usual Mott-Hubbard gap opened at the Fermi surface ($k = \pm \pi/2a$), of magnitude $2US$.

Using the valence band wavefunctions (Eq. (A.6)) in Eqs. (3.6) and (3.7), we obtain

$$Q(i) = 1 \quad \tilde{S}(i) = (-1)^i S \tilde{\varepsilon}_z \frac{US}{2N} \sum_k \frac{1}{|E_k^\uparrow|}$$

In other words, the solution is self-consistent provided that

$$S = \frac{US}{N} \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + (US)^2}}$$

where $N$ is the number of sites and the sum is performed over the Brillouin zone $k \in (-\pi/2a, \pi/2a]$. This equation has three solutions. One is trivial ($S = 0$). Since for $S \neq 0$
the equation depends only on $S^2$, we can see that the ground state is doubly-degenerate: both $+S$ and $-S$ satisfy it and give rise to self-consistent ground-states which differ from each other only through the fact that all the spins are flipped from one ground-state to the other one.

Strictly speaking, the HF solution gives an infinite number of degenerate ground states, because the direction $\vec{\varepsilon}$ is arbitrary (this is a direct consequence of the fact that the Hubbard model is rotationally invariant). However, since a real chain is embedded in a 3D crystal, crystal field interactions will lift the rotational degeneracy, and fix one particular direction of orientation for the spins (for instance, along the chains). Consequently one particular direction $\vec{\varepsilon}$ is favored, and the mean-field ground state is doubly degenerate.

The dependence of $S$ on $U/t$ is shown in Fig. 3.1. In the weak interaction limit $U/t \ll 1$, $S \to 0$. The electrons have the same probability of spin up or down at any site, the gap is closed and the electronic band is very broad ($4t$), showing that the electrons move freely (are delocalized) along the chain. In the strong interaction limit $U/t \gg 1$, $S \to \frac{1}{2}$. The bands become very thin ($\sqrt{(US)^2 + 4t^2} - US \to 2t^2/US$), showing that the electrons are strongly localized each at one site, each having its $\frac{1}{2}$-spin in the $\vec{\varepsilon}$ direction. The AFM structure is energetically favorable because it allows a lowering of the energy by virtual hopping of electrons on their neighboring sites. Since all the states of the valence band are occupied, the energy of the HF ground state is simply given by:

$$E_{GS} = 2 \sum_k E_k'' + NU \left( S^2 + \frac{1}{4} \right)$$  \hspace{1cm} (3.14)

where $S$ is given by the self-consistency condition (3.13). The magnitude of the ground
state energy per site, in units of $t$, is plotted in Fig. (3.2) as a function of $U/t$ (the full line). The following features can be observed: in the $U/t \to 0$ limit (noninteracting electrons), the energy of the ground state has, indeed, the expected value $E_{GS} \to -4Nt/\pi$. In the strong interaction limit $U/t \to \infty$, the energy of the ground state goes to zero as expected (since in this limit every site is single occupied and there is virtually no hopping). For comparison, the exact ground-state energy obtained from the Bethe Ansatz (see Section 5.2) is also shown (dotted line). The asymptotic value of the HF energy is found to be given by $E_{CS} \to -2Nt^2/U$. It is well known that in this limit, the Hubbard model is equivalent to an AFM Heisenberg model, with a coupling constant $J = 4t^2/U$ [101], and that its true ground state energy per site is $E_{GS} \to -NJ\ln 2 = -2.77Nt^2/U$. This suggests that the Hartree-Fock method is a good starting point, from which to incorporate fluctuation corrections which lower the energy.

3.2.2 Solitons in the doped ground state: the spin-bag and the domain-wall

We have shown that the undoped mean-field ground state of the quasi 1D Hubbard model is an insulator, with the valence band completely filled and the conduction band completely empty. Normally, we would expect that if we dope such a system, the doping holes will occupy the states at the top of the valence band. Thus, this band would be partially filled and the system would be a metal.

However, this cannot be true in this case, as suggested by an argument attributed to Sawatzky [102]. Let us consider a chain with $N$ sites in the limit as the hopping integral $t \to 0$. At half filling, there are $N$ electrons in the system, one at each site. It is straightforward to see that in this case there are two electronic bands, one of energy $U$ and one of zero energy. Each of these bands has exactly $N$ states, because one can place an extra electron at any of the $N$ sites, and the energy of the system would increase by $U$ (therefore there are $N$ states in the conduction band). Similarly, there are $N$ states in the valence band (of zero energy), because one can take an electron from any of the $N$ sites without paying any energy. So, indeed, the undoped ground state is an insulator.

What happens if there are only $N - 1$ electrons in the system? In this case, there are only $N - 1$ states in the conduction band of energy $U$ (because only if we place an extra electron at one of the $N - 1$ occupied states does the energy of the system increase by $U$). Similarly, there are only $N - 1$ states in the valence band (obtained by removing any of the initial $N - 1$ electrons from the system). The two missing states are associated with adding the electron on the site initially empty. In the limit of infinitesimal hopping ($t \to 0$), these two states simply correspond to adding either an up-spin electron or a down-spin electron to the unoccupied site. Clearly, these two states have the same energy as $t \to 0$. In fact, as $t \to 0$, the energy of these states must approach the mid-gap energy. This is due to the
charge invariance symmetry of the system. If we assume, for instance, that the 2 states are above the midgap, and repeat the same reasoning for a system with \( N + 1 \) electrons initially, it results that the 2 states must be below the midgap, which is a contradiction. Moreover, these two states are obviously localized states (they are centered on the site that was initially empty). All the states in the bands are delocalized, so the two localized states can only exist somewhere deep in the electronic gap.

The effect of turning on the hopping \( t \neq 0 \) is to broaden the valence and conduction band, but the rest of the conclusions remain the same. Thus, based on this simple argument, we expect to see a radical modification of the electronic spectrum with doping. As discussed in the following section, the Hartree-Fock Approximation gives indeed solutions that roughly fit the above description.

If we solve numerically the HF equations (3.5,3.6,3.7) for a \( N \)-site chain with \( N - 1 \) electrons, we find three types of charged self-consistent solutions: the spin-bag (or spin-polaron) (Fig.3.3), the domain wall centered on site (COS domain wall) (Fig.3.4, left) and the domain-wall centered between sites (CBS domain wall) (Fig.3.4, right). The spin-polaron is created by trapping the hole in a small ferromagnetic core, which only affects the LR AFM order locally. The domain walls are topological excitations, since the AFM order is rotated by \( \pi \) as one goes through the domain wall. Therefore, in order to impose cyclic boundary conditions, we must consider an odd-number chain (or we may take an even-number chain and add two holes, leading to the appearance of a pair of domain and anti-domain walls). The localization length of the hole depends on \( U/t \), increasing as \( U/t \) decreases for all three excitations. The spin and charge at sites far from the distortion equal the undoped ground state values.

The electronic spectra corresponding to the configurations shown in Figs. 3.3 and 3.4 are shown in Figs. 3.5 and 3.6. First panel in Fig. 3.5 corresponds to the undoped ground state of a \( N = 40 \) sites chain. As discussed before, the electronic spectrum consists of two bands of \( N = 40 \) states each. The valence band is completely filled, the conduction band is completely empty, and there is a large gap between them. Adding one hole on the same \( N = 40 \) sites chain, and keeping the cyclic boundary conditions, leads to the appearance of the spin-bag shown in 3.3. Its electronic structure is shown in the right panel of Fig. 3.5. There is a localized level \( (n = 1) \) well below the valence band, the valence band is left with 38 states, there are 3 localized levels deep inside the Mott-Hubbard gap, and finally the conduction band also has 38 levels. Since there are \( N - 1 = 39 \) electrons in the system, only the localized level below the valence band and the valence band states are occupied. Since the valence band is spin paired (having an even number of states), this means that the total spin of this excitation is \( 1/2 \), associated with the spin of the electron on the localized level. The fact that the spin-bag carries a \( 1/2 \)-spin is also easy to deduce from Fig. 3.3, because
Figure 3.3: Self-consistent charge (upper line) and spin distributions for a charged spin-bag on a 40-site chain, for $U/t = 5$. The spin-bag is a charged fermion.

Figure 3.4: Left: Self-consistent charge (upper line) and spin distributions for a domain wall centered on site (COS) on a 41-site chain, for $U/t = 5$. Right: Self-consistent charge (upper line) and spin distributions for a domain wall centered between sites (CBS) on a 41-site chain, for $U/t = 5$. The domain walls are charged bosons.
Figure 3.5: Electronic spectra for an undoped AFM chain with 40 sites (left panel), and for a 40-site chain with a charged spin-bag (right panel). $U'/t = 5$.

Figure 3.6: Electronic spectra for a chain 41 sites chain with a COS domain-wall (left panel), and a CBS domain-wall (right panel). $U'/t = 5$. 
of the small ferromagnetic core. Thus, we conclude that the spin-bag is a charged fermion.

The domain wall electronic structures are shown in Fig. 3.6, that of the CBS domain wall in the right panel, and the COS domain wall in the left panel. In this case, we study a chain with \( N - 1 = 40 \) electrons and \( N = 41 \) sites, so that we can impose cyclic boundary conditions again. We can see that in both cases there are 4 localized levels inside the Mott-Hubbard gap, \( N - 1 = 40 \) occupied states in the valence band, and 38 states in the conduction band. The localized levels of the COS domain wall are degenerate. The degeneracy is lifted for the CBS domain wall, and the upper discrete level is pushed quite close to the lower edge of the conduction band. However, it is still a localized level (this is easily checked by plotting its wavefunction). Thus, in both cases we have a full spin-paired valence band, and therefore the total spin of these excitations is zero. They also carry the charge of the hole, therefore the domain walls are charged bosons, exactly like the charged solitons of the polyacetylene.

In order to establish which of these excitations is the low-energy excitation upon doping, we must compare their excitation energies (defined with respect to the undoped (half-filled) ground state). The excitation energies of the hole-charged excitations as a function of \( U/t \) are plotted in Fig. (3.7). As we can see, the domain walls are the low-energy excitations for \( U/t < 6.5 \), while the spin-polarons become the low-energy excitations for \( U/t > 6.5 \). As \( U/t \to 0 \), the core size of the domain-walls diverges roughly like \( t/U \). As a result, in this limit the COS and the CBS domain-walls are very extended objects and therefore degenerate. However, as \( U/t \) increases the core becomes more and more localized, and the degeneracy between the COS and the CBS domain-walls is lifted. The CBS domain-wall is energetically less expensive in this limit.

However, this static HFA does not take into account the lowering of energy of these excitations due to translations along the chain. From the simple inspection of the spin distributions of the spin-bag and of the domain wall, we can easily deduce that while a domain wall can move freely along the chain, the spin-bag is rather immobile. This is so because moving the center of the domain wall by one site (by interchanging the hole with the spin at the right or at the left) only necessitates some rearrangement of the magnitude of the core spins, while their orientation is automatically correct. Thus, we expect that a domain wall may lower its energy by an amount of the order \( t \) through hopping along the chain. However, if a spin-bag moves only by one site, the moved spin must be flipped (which means, in fact, that the total spin of the spin-bag changes from \( +1/2 \) to \( -1/2 \), or viceversa). This is obviously a costly (and unlikely) process. The spin-bag can tunnel to the second nearest neighbor directly, in which case the spin-flip is not necessary. However, this is a second order process, and therefore we expect that a spin-bag can only lower its energy by an amount of the order \( t^2/U \). As we demonstrate in Chapter 5, these qualitative
arguments are actually true, and it is the charged bosonic domain wall that proves to be the relevant charged excitation of the Hubbard model for all values of $U/t$.

3.2.3 Green’s functions approach

The numerical approach described above for solving the Hartree-Fock equations has the advantage that it can easily be used to treat any doping, the method is fast and therefore a "good" initial guess is not essential. In fact, by starting with random initial distributions for the spin and charge distributions $\tilde{S}(i)$ and $Q(i)$, and making many searches, we can make sure that we really found the lowest energy self-consistent distributions corresponding to a certain doping. The obvious disadvantage of this approach is that it only works for finite (not too long) chains.

We can study the problem of one doping hole (electron) on an infinite chain by using Green’s functions. In particular, we studied in detail domain walls with this method, although it can very easily be used for the study of spin-bags as well. This Green’s function approach has the advantage of allowing direct calculation of quantities such as local and total density of states, which are not obtainable from finite chain analysis. However, it is restricted to the study of just one hole (at most, a tightly-bound pair of holes) configu-
rations, and it depends essentially on the ability to calculate the Green's function of the undoped Hartree-Fock AFM ground state analytically. This is possible in 1D, but not in 2D.

A full overview of the method and the results obtained are given in Appendix A. Besides the self-consistent charged domain-walls we already described, a number of un-self-consistent configurations, such as FM and AFM-core domain-walls, are also considered.

3.3 Continuum approximation: analogy between 1D and 2D soliton electronic spectra

The properties of lattice solitons, which we have described so far, can be elegantly recaptured by means of a continuum model. The appropriate continuum model is constructed in such a way that the local antiferromagnetic correlation between nearest neighbor sites is treated exactly, but fluctuations from one unit cell (consisting of two spins) to another have slow spatial variations. This also provides a foundation for constructing the appropriate continuum model for the two-dimensional antiferromagnet (described in Section V) where the lattice model is very cumbersome.

One of the difficulties of a discrete model is that the HF one-electron equations \( H\phi(n) = E\phi(n) \) are recurrence relations. In the continuum model, these recurrence relations are replaced by differential equations, which in turn have analytical solutions.

3.3.1 Electronic structure of domain walls and spin-polarons

The simplest continuum approximation consists of expanding the dispersion relations near the Brillouin zone edge \( k_0 = \pm \pi/2a \). If we expand the free-electron dispersion relations \( \epsilon_k = 2t \cos (ka) \) near this point, we get the approximate value \( \epsilon_k = -2ta(k - k_0) \). Changing the reference point from \( k = 0 \) to \( k = k_0 \) in the reciprocal space, we can write:

\[
\epsilon_k - 2ta(k - k_0) \rightarrow 2ta\frac{d}{dx}.
\]

The hopping Hamiltonian can then be approximated by (see Eqs. A.1, A.2 in Appendix A):

\[
\mathcal{H}_{k.e.} = -\sum_k \Phi_k^\dagger \begin{pmatrix} 0 & -2ta \\ -2ta & 0 \end{pmatrix} \Phi_k = \int dx \Phi^\dagger(x) \begin{pmatrix} 0 \\ -2ta\tau_x \frac{d}{dx} \end{pmatrix} \Phi(x).
\]

In what follows, the Pauli matrices \( \sigma_{x,y,z} \) are associated to the spin-space, while the Pauli matrices \( \tau_{x,y,z} \) are associated to the site-space. Here \( \Phi(x) \) is a 4-component spinor describing the two components of electron spin on each of the two lattice sites constituting a unit cell.
Figure 3.8: Top panel: Structure of an AFM-core soliton. The spins on the two sublattices rotate from one mean-field ground state to the other one, preserving the local antiferromagnetic correlations of this soliton. Bottom panel: Structure of the FM-core soliton. The spins on the two sublattices rotate in opposite directions, creating a ferromagnetic region in the core of this soliton.

Similarly, the interaction part of the Hamiltonian becomes:

\[ H_{\text{int}} = \int dx \Phi(x) \left[ -U \cdot \begin{pmatrix} \bar{S}_1(x) \cdot \sigma & 0 \\ 0 & \bar{S}_2(x) \cdot \sigma \end{pmatrix} - \frac{U}{2} (1 - Q(x)) \right] \Phi(x) \]

where \( \bar{S}_{1,2}(x) \) is the expectation value of the spin at the site \( 1(2) \) of the unit cell located at \( x \), and \( Q(x) \) is the charge at a site.

In the undoped case, we study two types of undoped domain-walls, namely the FM-core and the AFM-core domain-walls. \( Q(x) = 1 \) for both the AFM-core and the FM-core solitons (see Fig. 3.8). However,

\[
\begin{align*}
\bar{S}_1(x) &= S \left( \cos(\theta(x)) \hat{e}_x + \sin(\theta(x)) \hat{e}_y \right) \\
\bar{S}_2(x) &= S \left( (-1)^b \cos(\theta(x)) \hat{e}_x - \sin(\theta(x)) \hat{e}_y \right).
\end{align*}
\]

For an AFM-core soliton, we choose \( b = 1 \), whereas for the FM-core soliton we choose \( b = 0 \). Here \( \theta(x) \) describes the direction of the local spin with respect to the chain axis. The continuum Hamiltonian for the AFM/FM-core soliton is given by:

\[ H = \int dx \Phi(x)^\dagger \left\{ -2t a \tau_x \frac{d}{dx} - U S A \tau_z (\sin \theta A \sigma_z + \cos \theta \sigma_x) \right\} \Phi(x) \]

where \( A = 1 \) for the AFM-core soliton and \( A = \tau_z \) for the FM-core soliton.

The electronic structure of the mean-field, AFM background states (\( \theta(x) = \pm \frac{\pi}{2} \)) of this Hamiltonian is made up of two bands with dispersion relations \( E^\pm_k = \pm \sqrt{(U S)^2 + 4a^2 t^2 k^2} \), separated by a Mott-Hubbard gap of magnitude \( 2 U S \). In the presence of a soliton, the angle \( \theta(x) \) describes the rotation between the two ground states, and is characterized by a soliton core radius \( \rho \). For a domain-wall we choose \( \theta(x) = \frac{\pi}{2} \tanh(\frac{x}{\rho}) \). Introducing the dimensionless variables

\[
\zeta = \frac{x U S}{2a t}, \quad e = \frac{E}{U S}, \quad \text{and} \quad \rho_c = \frac{\rho}{2a t},
\]

The spin on the two sublattices rotate from one mean-field ground state to the other one, preserving the local antiferromagnetic correlations of this soliton. Bottom panel: Structure of the FM-core soliton. The spins on the two sublattices rotate in opposite directions, creating a ferromagnetic region in the core of this soliton.
the domain-wall spectrum is obtained by solving the eigenvalue problem:

\[ \begin{align*}
-d & - \tau_z (\sin \theta(\zeta) \sigma_z + A \cos \theta(\zeta) \sigma_x) \\
\end{align*} \]

where \( \theta(\zeta) = \frac{\pi}{2} \tanh \frac{\zeta}{\mu_c} \). Unlike the lattice model, in which there are two independent parameters \( U S/t \) and \( \rho/a \), here we have just one parameter \( \rho_c \).

The AFM-core soliton

Since the AFM-core soliton Hamiltonian commutes with the operator \( P = \tau_x \sigma_y \), the eigenfunctions \( \phi(\zeta) \) can be chosen to be eigenfunctions of \( P \) as well. Since \( P^2 = 1 \) and \( P \) is hermitian, its eigenvalues are \( \pm 1 \). We perform a unitary transformation with \( U = \exp(-i \frac{\pi}{4} \tau_y \sigma_y) \) such that \( P \) becomes diagonal, i.e. \( U^{-1} P U = \tau_z \). Labelling the eigenvalues of \( \tau_z \) by \( s = \pm 1 \), we obtain the differential equation for the new two-component function \( \eta(\zeta) = U \phi(\zeta) \):

\[ \begin{align*}
- \sigma_y d & - (\cos \theta(\zeta) \sigma_x + \sin \theta(\zeta) \sigma_z) \\
\end{align*} \]

This shows that if there is a level with the quantum numbers \( (e, s) \) there is another level with the quantum numbers \( (-e, -s) \), as expected for charge-conjugation invariance. Clearly, the discrete levels on either side of the mid-gap have different parities. We can see from the structure this equation that the levels are non-degenerate, since there is no matrix which anticommutes with all three Pauli matrices.

Using the method presented in Reference [21], we numerically evaluate the gap structure. There are only two levels in the gap, with energies varying from 0 to the band-edges, as \( \rho_c \) varies from zero to infinity. In Fig. 3.9 we present a comparison between the results of
the continuum model with that of the discrete AFM-core soliton model for various values of $US/t$. In the large $\rho_c$ limit the agreement is very good for many choices of $US/t$. For small $\rho_c$ values, the agreement is best when $US/t$ is small as expected, since for a given $\rho_c$, smaller $US/t$ values correspond to bigger $\rho/a$ values.

The excitation energy of the continuum AFM-soliton is similar to that of the lattice AFM soliton. The band contribution to the total soliton energy varies slowly with $\rho_c$, leaving the main contribution to the discrete levels. For the undoped soliton, only the discrete level with $E < 0$ is occupied, and the energy of this level decreases as $\rho_c$ increases. As the soliton expands, its excitation energy diminishes, until it becomes indistinguishable from the AFM mean-field background.

**The FM-core soliton**

Since FM-core soliton Hamiltonian commutes with the operator $P = \tau_z \sigma_z$ (with eigenvalues $\pm 1$), the eigenfunctions $\varphi(\zeta)$ can be chosen such that they are eigenfunctions of $P$ as well. We perform a unitary transformation with $U = \exp(-i\frac{\zeta}{4}\tau_z \sigma_z)$ such that $U^{-1}PU = \tau_z$. Once again, labelling the eigenvalues of $\tau_z$ by $s = \pm 1$, we obtain the differential equation for the new two-component function $\eta(\zeta) = U\varphi(\zeta)$:

$$-i\sigma_z \frac{d}{d\zeta} (-\cos \theta(\zeta)\sigma_z + s \sin \theta(\zeta)\sigma_z) \eta(\zeta) = e\eta(\zeta)$$

For the FM-core soliton (unlike the AFM-core soliton), the matrix $\sigma_y$ anticommutes with the Hamiltonian. Therefore, if there is a state $\varphi$ with the quantum numbers $(e, s)$, then there is another state $\sigma_y \varphi$ with the quantum numbers $(-e, s)$ as expected by charge-conjugation invariance. Another difference is that for the FM-core soliton, levels with energies in the different halves of the gap have the same parity (instead of opposite parity for AFM-soliton). Using the same argument as before, there are no degenerate discrete levels, except at $e = 0$. This is verified by numerical calculations. Numerically, we find only a doubly-degenerate level at $e = 0$, and the corresponding wavefunction is given by:

$$\eta_s(\zeta) = C \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-\int_0^\zeta \sin \theta(\zeta') + i s \cos \theta(\zeta')} = \pm 1$$

Here, $C$ is a normalization constant.

**Self-consistent theory of the doped domain-wall in the continuum model**

In the case of doped domain-wall soliton, a self-consistent solution for the spin degrees of freedom is possible if we take $Q(x) = 1$. The self-consistent solution of the discrete case suggests a parameterization of the form $\vec{s}_1(x) = -\vec{s}_2(x) = S \tanh (\frac{\zeta}{\rho}) \vec{\sigma}$. It turns out that
with this parameterization, the continuum model has a simple analytical solution. In fact, it maps onto the continuum polyacetylene model [8, 103]. The total "electronic" Hamiltonian is given by:

$$\mathcal{H}_{el} = \int dx \Phi^\dagger(x) \left\{ -2t a i \tau_z \frac{d}{dx} - U S \tau_z \sigma_z \tanh \frac{x}{\rho} \right\} \Phi(x)$$

Using the dimensionless variables defined earlier, the eigenvalue problem reduces to:

$$\left\{ -i \tau_z \frac{d}{d\zeta} - \tanh \left( \frac{\zeta}{\rho_c} \right) \tau_z \sigma_z \right\} \phi(\zeta) = e \phi(\zeta)$$

Using the fact that the Hamiltonian commutes with $\sigma_z$, and introducing the quantum number $s$ (defined by $\sigma_z \phi_s(\zeta) = s \phi_s(\zeta)$), the eigen-equation reduces to a pair of two-component equations:

$$\left\{ -i \tau_z \frac{d}{d\zeta} - s \tanh \left( \frac{\zeta}{\rho_c} \right) \tau_z \right\} \phi_s(\zeta) = e \phi_s(\zeta), \ s = \pm 1$$

This equation can be written in a more familiar form if we perform a rotation by $\frac{\pi}{2}$ about the $O_\gamma$ axis in the site-space. This rotation is implemented by the matrix $U = \exp(-i \frac{\pi}{4} \tau_y)$. The rotated Hamiltonian $U^\dagger \mathcal{H}_{HF} U$ and the rotated wavefunction $\psi_s(\zeta) = U \phi_s(\zeta)$ satisfy the equation:

$$\left\{ -i \tau_z \frac{d}{d\zeta} + s \tanh \left( \frac{\zeta}{\rho_c} \right) \tau_z \right\} \psi_s(\zeta) = e \psi_s(\zeta) \quad (3.15)$$

For $s = 1$ this equation is identical to the corresponding equation for charged solitons in polyacetylene (Eq.(7) from [103]). From Eq. (3.15) we can see that $\psi_{-1}(\zeta) = \tau_z \psi_{+1}(\zeta)$. Therefore, for $s = -1$ we obtain the same spectrum. This shows that the spectrum of this doped soliton is identical to the spectrum of the polyacetylene soliton. In the polyacetylene case, the spin is a trivial degree of freedom and each level is doubly-degenerate as a result. The soliton structure induces phase-shifts in the band wave-functions and therefore the calculation of the excitation energy of the doped domain wall follows exactly the steps described in [103]. This yields the result that the doped soliton is stable when $\rho_c = 1$ or $\rho/a = 2t/US$. In this particular case, the spectrum of the soliton is made up of a doubly-degenerate level at the midgap plus the two bands. The soliton excitation energy is given by $US/\sqrt{2}$. The results of the continuum model are in good agreement with the results of the discrete model in the small $U/t$ (large $\rho$) limit.

It is straightforward to verify that this calculation is self-consistent with respect to the expectation value of the spin. The band wavefunctions are given by:

$$\psi_{+1,k}(\zeta) = \begin{pmatrix} u_k(\zeta) \\ v_k(\zeta) \end{pmatrix} \quad \text{and} \quad \psi_{-1,k}(\zeta) = \begin{pmatrix} u_k(\zeta) \\ -v_k(\zeta) \end{pmatrix}$$
where the detailed expressions for \( u_k(\zeta) \) and \( v_k(\zeta) \) in the case \( \rho_c = 1 \) are given in Reference ([103]). Explicitly, we have even solutions:

\[
\begin{align*}
\left\{ \begin{array}{l}
u_k(\zeta) + i v_k(\zeta) = \sqrt{\frac{2}{L}} \frac{i}{1+i k} [k \cos k \zeta - \tanh \zeta \sin k \zeta] \\
u_k(\zeta) - i v_k(\zeta) = \sqrt{\frac{2}{L}} \frac{i}{1+i k} \sin k \zeta
\end{array} \right.
\end{align*}
\]

and odd solutions:

\[
\begin{align*}
\left\{ \begin{array}{l}
u_k(\zeta) + i v_k(\zeta) = \sqrt{\frac{2}{L}} \frac{i}{1+i k} [k \sin k \zeta + \tanh \zeta \cos k \zeta] \\
u_k(\zeta) - i v_k(\zeta) = \sqrt{\frac{2}{L}} (-i) \sqrt{\frac{1-i k}{1+i k}} \cos k \zeta
\end{array} \right.
\end{align*}
\]

Here, the dimensionless wave-vector \( k \geq 0 \) is measured in units of \( US/2at \). Rotating these wavefunctions back to the initial representation, we obtain the band wavefunction:

\[
\begin{align*}
\phi^+_1(\xi,k) &= \frac{1}{\sqrt{2}} \left( u_k(\zeta) - v_k(\zeta), 0, u_k(\zeta) + v_k(\zeta), 0 \right) \\
\phi^-_1(\xi,k) &= \frac{1}{\sqrt{2}} \left( 0, u_k(\zeta) + v_k(\zeta), 0, u_k(\zeta) - v_k(\zeta) \right)
\end{align*}
\] (3.16)

The wavefunctions of the two midgap levels are given by:

\[
\begin{align*}
\phi^+_1(B)(x) &= \frac{1}{2\sqrt{\cosh} (\frac{L}{a})} \left( -1, 0, -i, 0 \right) \\
\phi^-_1(B)(x) &= \frac{1}{2\sqrt{\cosh} (\frac{L}{a})} \left( 0, i, 0, 1 \right)
\end{align*}
\] (3.17)

In the doped domain-wall, all the levels in the valence band are occupied, and the midgap levels are either empty or doubly occupied. Therefore, the only contribution to the expectation value of the spins comes from the band. Using these wavefunctions, the expectation value of the spin in the \( z \)-direction is given by:

\[
S_z(\zeta) = \frac{1}{4} < \tau_z \sigma_z >_{\text{band}} = \frac{1}{4} \sum_{\zeta,k} \phi^*_\sigma(\zeta) \tau_z \sigma_z \phi_\sigma(\zeta) = - \sum_k \text{Re} \left( u_k^*(\zeta) v_k(\zeta) \right) = S \tanh(\zeta)
\]

where \( S = \frac{1}{2L} \sum_k \frac{US}{\sqrt{(US)^2 + 4a^2 \tau_k^2}} \) and \( L = Na \) is the length of the chain. This demonstrates the self-consistency, since we have shown previously that the magnitude \( S \) satisfies this condition (see Eq. (3.13)). The expectation values for the spin in the \( x \) and \( y \) directions are zero.

It is straightforward to verify that this doped soliton has no spin, but carries the charge of the doping electron (hole). For each energy level in the band, there are an equal number of eigenfunctions with up ( \( s = +1 \) ) and down ( \( s = -1 \) ) spin \( \sigma_z \). Since all the levels in the band are occupied, the total spin is zero. On the other hand, the doped soliton has a charge \( \pm e \), which is localized in the core region with a probability density given by that of the midgap level. For a hole-doped soliton only the valence band is occupied and the
The expectation value of the probability (charge) density is given by:

\[ \rho(x) = \sum_{k,n} \phi_{k, n}^* \phi_{k, n} = 2 \sum_k (|u_k|^2 + |v_k|^2) = \frac{1}{a} \left[ 1 - \frac{1}{2 \cosh^2 \left( \frac{z}{\rho} \right)} \cdot \tan^{-1} \frac{t}{U S} \right] \]

The total charge (in units of the electron charge) at one site is given by \( Q(x) = a \rho(x) \). The total number of electrons in the chain is given by:

\[ \int_{-L/2}^{L/2} \rho(x) dx = N - \frac{2}{\pi} \tan^{-1} \left( \frac{t}{U S} \right) \]

where \( L = Na \) is the length of the chain and \( N \) is the number of sites. In the limit \( US/t \to 0 \) (weak-coupling), this goes indeed to \( N - 1 \), as expected for one extra hole.

### 3.3.2 Electronic structure of meron-vortices and skyrmions

In this section we demonstrate the analogy between 1D domain walls and spin-polarons, and 2D merons and skyrmions, respectively, in the continuum approximation. In order to keep this section self-contained, we review the main points in the derivation of the 2D continuum Hamiltonian.

As discussed in Section 1.2, we assume that the 2D lattice Hamiltonian of the spin-flux model is given by equation 1.4. The mean-field background consists of antiferromagnetically aligned local magnetic moments whose Hartree-Fock energy has been lowered by the inclusion of uniform spin-flux. This is expressed formally by setting the product of the electron hopping matrices \( T^{12} T^{23} T^{34} T^{41} = -1 \) around any elementary plaquette. We choose the simplest spin-independent gauge in which \( T^{12} = -1 \) for one link of each plaquette, but \( T^{ij} = 1 \) for the remaining three links (see Fig. 1.5). The spectrum is independent of the choice of the gauge. For undoped solitons we choose \( Q_i = 1 \) and, since we are interested only in the electronic spectra, we drop the constant terms.

We introduce an eight-component annihilation operator \( \phi(\vec{r}) \) for up and down spin electrons at the four sites of the square unit cell located at \( \vec{r} \), and the corresponding eight-component Bloch operator \( \phi_{\vec{k}} = N^{-1/2} \sum_{\vec{r}} e^{-i \vec{k} \cdot \vec{r}} \phi(\vec{r}) \). Here \( N \) is the number of unit cells and the sum is performed over all the unit cells. \( \vec{k} \) is restricted to the first Brillouin zone, which in this case is defined by \( k_x \in \left[ \frac{-\pi}{2a}, \frac{\pi}{2a} \right], k_y \in \left[ \frac{-\pi}{2a}, \frac{\pi}{2a} \right] \). In terms of the Bloch operators, the Hamiltonian can be rewritten as:

\[ \mathcal{H} = \sum_{\vec{k}} \phi_{\vec{k}}^\dagger [\epsilon_{\vec{k}} \alpha_x + \epsilon_{\vec{k}} \alpha_y + U \beta] \phi_{\vec{k}} \]

where \( \epsilon_{\vec{k}} = -2t \cos ka \), \( a \) is the lattice constant, and \( \alpha_x, \alpha_y \) and \( \beta \) are \( 8 \times 8 \) matrices whose structure is dependent on our choice for the mean-field parameters \( T^{ij} \) and \( S_i \). Explicitly
Here \( I \) is the 2 \( \times \) 2 identity matrix in the spin space, and \( \vec{\tau} \) and \( \vec{T} \) are two sets of 2 \( \times \) 2 Pauli matrices describing hopping in the \( x- \) and \( y- \)directions respectively. We will use the \( \vec{\sigma} \) Pauli matrices to describe the internal spin-space of the electron. These matrices appear in the interaction term,

\[
\beta = \begin{pmatrix}
\vec{S}_1 \vec{\sigma} & 0 & 0 & 0 \\
0 & \vec{S}_2 \vec{\sigma} & 0 & 0 \\
0 & 0 & \vec{S}_3 \vec{\sigma} & 0 \\
0 & 0 & 0 & \vec{S}_4 \vec{\sigma}
\end{pmatrix},
\]

where \( \vec{S}_i \) describes the expectation value of the spin at the \( i = 1 \ldots 4 \) site of the unit cell.

In the undoped AFM state we have \( \beta = S \tau_z \sigma_z \) (assuming that the spins are oriented in the \( z- \)direction), and the dispersion relations are given by \( E_k = \pm \sqrt{(\epsilon_k^x + \epsilon_k^y) + (US)^2} \).

Due to the relativistic form of the dispersion relations, the Fermi surface at half-filling (\( E_F = 0 \)) collapses to the four corner points of the Brillouin zone, \( \vec{k}^0 = (\pm \pi/2a, \pm \pi/2d) \).

The continuum approximation consists, as in the 1D case, in linearizing the electron-dispersion relations about one of these isolated Fermi points. By replacing \( \cos(k;\alpha) \) with \( (k_i - k_i')a \rightarrow -ia\partial_i, \ i=x,y \). Using the dimensionless variables \( x \rightarrow x \frac{U_x}{2a}, y \rightarrow y \frac{U_y}{2a} \) and \( E \rightarrow E \frac{U_d}{2S} \), the Schrödinger equation becomes:

\[
[i\alpha_x \partial_x + i\alpha_y \partial_y + \frac{1}{S} \beta] \psi(\vec{r}) = E \psi(\vec{r})
\]

As in the case of the domain walls in one-dimension, there are two distinct types of undoped meron-vortex configurations in two-dimensions. For a meron with an AFM core we may parameterize the interaction matrix \( \beta \) by the relations

\[
\vec{S}_1 = -\vec{S}_2 = \vec{S}_3 = -\vec{S}_4 = S\hat{n}.
\]

Here, \( \hat{n} = (\sin(\theta(r)) \cos(\mu \phi), \sin(\theta(r)) \sin(\mu \phi), \cos(\theta(r)) \) plays the role of a plaquette director field, around which there are 4 antiferromagnetically correlated local moments. For the FM-core meron, the required parameterization is given by

\[
\vec{S}_1 = \vec{S}_3 = S\hat{n}, \vec{S}_2 = \vec{S}_4 = -S(\hat{n} - 2\hat{n}_z).
\]

Here, \( \mu \) is the vortex winding number and we choose the angle \( \theta(r) = 2 \tan^{-1}(r/\rho) \) for \( r < \rho \) and \( \theta(r) = \frac{\pi}{2} \) for \( r > \rho \). The angle of the plaquette director field with respect to the \( z- \)axis
varies from 0, in the core of the meron, to \( \pi/2 \), in the asymptotic region, as shown in Fig. 3.10.

It is straightforward to see that the two undoped merons have the same asymptotic structure, but their cores are very different: while for the AFM-core soliton the spins are antiferromagnetically aligned on each unit cell and rotate slowly in the same direction as the plaquette vector, for the FM-core soliton spins on the two sublattices rotate in opposite directions, such that they become parallel (ferromagnetic) in the core of the soliton. With these parameterizations we have:

\[
\mathcal{J} = \mathcal{S} \tau_z \sin \theta(r) (\cos(\mu \phi) \sigma_x + \sin(\mu \phi) \sigma_y) + \mathcal{S} \mathcal{A} \tau_z \cos \theta(r) \sigma_z = \mathcal{S} \mathcal{A} \tau_z U^\dagger(r) \sigma_z U(r)
\]

where \( U(r) = e^{\mu \phi(r)A \sigma_z/2} e^{i \mu \omega_r \phi(r)/2} \). Here, \( \mathcal{A} = 1 \) for an AFM-core meron, while \( \mathcal{A} = \tau_z \) for a FM-core meron. In polar coordinates, the kinetic energy terms reduce to:

\[
\begin{align*}
&i \alpha_x \partial_x + i \alpha_y \partial_y = e^{-i \gamma_z} \left[ i \alpha_x \left( \partial_r + \frac{1}{2r} \right) + i \alpha_y \frac{\partial \phi}{r} \right] e^{i \gamma_z} \\
\end{align*}
\]

where \( \alpha_z = -\gamma_z \). With this choice, the three \( \alpha \)-matrices satisfy the cyclic algebra \([\alpha_i, \alpha_j] = i \epsilon_{ijk} \alpha_k\). We introduce a radial wavefunction \( \eta(r) \) defined by \( \phi(r) = e^{i(\alpha_x + \mu \sigma_z + 2\mu_\phi/r)} \eta(r)/\sqrt{r} \), to obtain the radial Schrödinger equation,

\[
\left[ i \alpha_x \partial_r + \frac{\alpha_y}{r} \left( \frac{\mu}{2} \sigma_z + \ell \right) + \mathcal{A} \tau_z \sigma(r) \right] \eta(r) = e\eta(r)
\]

Figure 3.10: The 2D analog of the neutral domain wall is a meron texture depicted as a lotus-flower configuration of the local director field \( \hat{n}(\theta) \). As \( \hat{n}(\theta) \) varies smoothly from one unit cell to the next, it makes a half-covering of the unit sphere \( S^2 \). If the meron is doped, all the components of the spin perpendicular to the plane become zero, and therefore the magnitude of the spin vanishes in the core of the charged meron-vortex.
Here, $\sigma(r) \equiv e^{-iA_\gamma y/2} \sigma_z e^{iA_\gamma y/2}$ and $\ell$ is an angular momentum quantum number. Since we are using the dimensionless variables $r \to r \frac{US}{2a}$ and $E \to e = \frac{E}{US}$, the only independent parameter is $\rho \frac{US}{2a}$, as in the 1D case. Since the meron does not carry additional spin-flux, only integer values of $\ell$ are allowed. The solution of this equation can be simplified by noting that the plaquette parity operator $P \equiv \tau_z \gamma_y$ commutes with $H_r$. It follows that the eigenfunctions of $H_r$ can be labelled according to the eigenvalues of $P$, which we denote as $s_1 = \pm 1$. Introducing the unitary matrix $U_1 = e^{i \frac{\pi}{2} \tau_x \gamma_z}$, and noting the $U_1^+ P U_1 = \gamma_z$, the transformed radial equation becomes

$$\left\{ -is_1 \tau_x \partial_r + \frac{\tau_y}{r} \left( \frac{\mu}{2} \sigma_z + \ell \right) + A \tau_z (\sigma_z \cos \theta + \sigma_x \sin \theta) \right\} \eta = E \eta$$

For either the FM-core or AFM-core solitons, if $\eta$ is an eigenfunction with quantum numbers $(E, s_1, \ell)$, it follows that $\sigma_y \eta$ is another eigenfunction with quantum numbers $(-E, -s_1, -\ell)$. Therefore the spectrum is always symmetric about $E = 0$. For the AFM-core undoped meron ($A = I$), it follows that $\tau_x \eta$ is another eigenfunction with quantum numbers $(-E, -s_1, \ell)$. As a consequence, the $\ell \neq 0$ levels of the AFM-core solitons are doubly degenerate whereas the $\ell = 0$ levels are non-degenerate. For the FM core soliton ($A = \tau_z$), the state $\tau_x \sigma_z \eta$ is another eigenfunction with quantum numbers $(E, -s_1, \ell)$. As a consequence, all of the levels of the FM-core undoped meron are doubly degenerate. We can see that for $\ell = 0$ the structure of the levels and the quantum numbers associated with them are analogous to the 1D undoped domain-wall case. For the AFM-core undoped meron, for every state labelled by quantum numbers $(E, s_1)$ there is another state $(-E, -s_1)$. In the FM-structure, for every state $(E, s_1)$ there is another state $(-E, s_1)$.

Numerical calculations also give a very similar gap structure, as shown in Fig.3.11. The AFM-core meron has two nondegenerate gap levels with opposite parity, which go towards the mid-gap as $\rho \frac{US}{2at} \to 0$ and towards the band-edges in the limit $\rho \frac{US}{2at} \to \infty$. The FM-core
meron has a doubly-degenerate level at the midgap. This close similarity between the 1D and 2D structures can be seen for other magnetic textures as well. In particular, the 2D skyrmion structure is analogous to the 1D spin-polaron. The 1D spin-polaron may be regarded as a bound pair of domain wall solitons and the 2D skyrmion is topologically equivalent to a bound pair of merons (see Fig.3.12). For the skyrmion we choose \( \theta(r) = 2 \tan^{-1}(r/\rho) \) and for the spin-polaron we choose \( \theta(x) = 2 \tan^{-1}(x/\rho) \). In this case, a truly FM-core does not exist, since at \( r = 0 (x = 0) \) the arrangements of the spins of a unit cell is the same as that of a unit cell in the asymptotic region, except that all spins are flipped. In the asymptotic region we have an AFM-arrangement. This means that in the core we have an AFM-arrangement as well. Consequently we can set \( A = 1 \). All the symmetries of the Hamiltonian remain as for the meron (domain wall), and in the large \( \rho \frac{U S}{2 \alpha} \) limit the band structure is basically the same. It consists of two non-degenerate levels which go towards the band edges. In the small \( \rho \frac{U S}{2 \alpha} \) limit, the levels crossover and go towards the opposite band-edge, instead of going towards the midgap (see Fig.3.12).

Finally, we discuss the nature of the charged meron, obtained by doping the 2D antiferromagnet with a hole. In analogy with the charged domain wall soliton in 1D we expect that the local magnetic moment amplitude in the core of the meron will be suppressed. The undoped meron has a “lotus-flower” structure (see Fig.3.10). It resembles a planar vortex in the plaquette director field in the asymptotic region. In the core region, the plaquette vector points in a direction perpendicular to the 2D plane. In analogy with the doped 1D soliton, we assume that the effect of doping the 2D meron is simply to remove the components of spin perpendicular to the plane, and the “lotus-flower” is reduced to a planar vortex in which the local moment amplitude vanishes in the core region. Remarkably, for this charged meron-vortex configuration, it is possible to obtain an analytic solution for the mid-gap electronic structure. We set \( \cos \theta \equiv 0 \) and we take the same “doped” parame-
It is straightforward to show that the meron radial equation has a doubly-degenerate mid-gap level, whose wavefunctions are given, up to a normalization constant, by:

$$\eta_{1=1}^*(r) = \frac{\sqrt{r}}{\cosh (r/\rho_c)} \begin{pmatrix} 1 & 0 & -1 & 0 \end{pmatrix} \quad \text{and} \quad \eta_{1=-1}^*(r) = \frac{\sqrt{r}}{\cosh (r/\rho_c)} \begin{pmatrix} 0 & 1 & 0 & -1 \end{pmatrix}$$

The midgap levels $\phi(r) \sim \frac{n(r)}{\sqrt{r}}$ have exactly the same form as the midgap levels of the doped 1D domain-wall soliton. For the doped meron-vortex, the gap states are empty and the valence band continuum states are fully occupied. It is straightforward to verify that these occupied states are spin-paired, as was the case for the charged domain wall in the one-dimension. As a result, the charged vortex soliton carries no net spin, and behaves as a bosonic excitation in the 2D antiferromagnet.

This concludes our study of the analogy of charged and neutral excitations of the 1D and 2D antiferromagnets in this simplified continuum model. In the following chapter we study the charged meron-vortices and spin-bags (which can be thought of as extremely localized charged skyrmions) in the static Hartree-Fock Approximation, and show that many of the properties deduced from the continuum model hold true. We also study multi-soliton configurations induced by doping as well as some magnetic and optical properties of such configurations. The conclusions about the general validity of the HFA in dealing with such systems appear at the end of the Chapter 4.
Chapter 4

Numerical study of multi-soliton configurations in a 2D doped antiferromagnetic Mott insulator

One of the long standing questions regarding the high-temperature compounds is the type of excitations that appear on the CuO$_2$ planes, as holes are introduced into the AFM parent compound. In the following, we use the Static Hartree-Fock Approximation (described in Section 3.1) to analyze the charged excitations of the spin-flux and conventional Hubbard models (see Sec. 1.2). This chapter is organized as follows: in the first section, we compare the half-filled AFM mean-field ground states of the conventional model and the spin-flux model. The direct comparison between the two Hamiltonians is justified by an alternative interpretation of the spin-flux model as being the Hubbard Hamiltonian projected in an extended Hilbert space which includes antiperiodic wave functions $[21]$. In this context, the spin-flux and conventional Hubbard model are projections of the same Hamiltonian in different Hilbert subspaces, and therefore their ground-state energies may be compared using the usual variational trial wavefunction principle. We show that the spin-flux model mean-field ground state always has a lower energy, and that it has a single quasiparticle dispersion relation which is consistent with angle-resolved photo-emission studies (ARPES). This suggests that the spin-flux model is a suitable starting point for studying the behavior of the parent compounds upon doping. Then we consider the problem of adding just one hole to the AFM background. We study in detail two possible soliton excitations, the fermionic charged spin bag and the bosonic charged meron-vortex, for both the conventional and the spin-flux model. Using a simple energetical argument, we propose a phase diagram for each of these excitations showing which is the relevant excitation for various $U/t$ values and various dopings. In the conventional phase we find that the spin bag is the relevant excitation at all dopings and all values of $U/t$. In the spin-flux phase, we find that for
intermediate $U/t$ values and low dopings, the meron-vortices are the relevant excitations. Since the spin-flux phase has the lower energy, this means that a liquid of meron-vortices appears on the lattice upon doping. This suggests a plausible explanation for various unusual (non-Fermi-liquid) properties of the underdoped and slightly overdoped cuprate compounds. We then study multi-soliton configurations, by doping more holes into the lattice. The results obtained are in good agreement with those predicted from the simple phase diagrams inferred. We also show that at higher doping (overdoped samples) the conventional phase has a lower energy than the spin-flux phase, and therefore a transition to a conventional Fermi-liquid takes place in this regime. Finally, we calculate the optical and static magnetic response of underdoped cuprate containing a frozen liquid of meron vortices, and show that it is consistent with the experimental measurements.

4.1 The undoped ground state

It is experimentally observed that the ground-state of the undoped Mott insulator has long-range AFM order. Accordingly, we choose a spin distribution at the site $i = \vec{e}_x i_x a + \vec{e}_y i_y a$ of the form $\vec{S}(i) = (-1)^{x+y} S \vec{e}$, where $\vec{e}$ is the unit vector of some arbitrary direction, while the charge distribution is $Q(i) = 1$. The results for the conventional AFM are well known. In this case, we choose the Brillouin zone to be a rotated square defined by 

$$-\frac{\pi}{a} \leq k_x + k_y, k_x - k_y \leq \frac{\pi}{a}$$

(see Fig. 4.1, left panel). The dispersion relations are given by

$$E^\pm(k) = \pm E(k) = \pm \sqrt{\epsilon^2(k) + (US)^2}$$

(4.1)

where each level is two-fold degenerate and $\epsilon(k) = -2t (\cos(k_x a) + \cos(k_y a))$ is the one-electron dispersion relation of the non-interacting conventional state. The HF ground-state energy is given by (see Eqn. (3.14))

$$E_{GS} = -2 \sum_k E(k) + N^2 U \left( S^2 + \frac{1}{4} \right).$$

(4.2)

where the self-consistent value for the staggered spin $S$ satisfies the energy minimization condition

$$S = \frac{1}{N^2} \sum_k \frac{US}{E(k)}.$$

(4.3)

In the spin-flux phase, it is more convenient to choose a square unit cell, in order to simplify the description of the $T^j$ phase-factors. We make the simplest gauge choice compatible with the spin-flux condition for the $T$-matrices, namely that $T^{12} = T^{23} = T^{34} = -T^{41} = 1$ (see Fig. (1.5)). This leads to the reduced square Brillouin zone $-\pi/2a \leq k_x, k_y \leq \pi/2a$ shown in Fig. 4.1, right panel. The dispersion relations for the AFM configuration are
given by:

\[ E_{sf}^\pm(\vec{k}) = \pm E_{sf}(\vec{k}) = \pm \sqrt{\epsilon_{sf}^2(\vec{k}) + (US)^2} \]  

(4.4)

where each level is four-fold degenerate and \( \epsilon_{sf}(\vec{k}) = -2t\sqrt{\cos (k_xa)^2 + \cos (k_ya)^2} \) are the noninteracting electron dispersion relations in the presence of spin-flux. The HF ground-state energy is given by

\[ E_{GS}^{sf} = -4 \sum_{\vec{k}} E_{sf}(\vec{k}) + N^2U \left( S^2 + \frac{1}{4} \right) \]  

(4.5)

where the AFM local moment amplitude is determined by the condition

\[ S = \frac{2}{N^2} \sum_{\vec{k}} \frac{US}{E_{sf}(\vec{k})}. \]  

(4.6)

In both cases, at half-filling the valence band is completely filled and the conduction band is completely empty. Therefore, in both the conventional and spin-flux phases, a Mott-Hubbard gap of magnitude \( 2US \) opens between the valence and the conduction bands. However, the Fermi surfaces are very different. In the conventional phase, all the points of the Brillouin surface belong to the nested Fermi surface, while in the spin-flux phase the Fermi surface collapses to four points \((\pm \pi/2a, \pm \pi/2a)\). This means that the introduction
of the spin-flux leads to a lowering of the energies of all the other points of the conventional nested Fermi surface, and thus for a strongly interacting electron system the energy of the entire system is lower in the spin-flux phase.

It is interesting to note that the quasi-particle dispersion relation obtained in the presence of the spin-flux closely resembles the dispersion as measured through angle-resolved photoemission studies (ARPES) in a compound such as Sr$_2$CuO$_2$Cl$_2$ [90] (see Fig. 4.2). Namely, there is a a peak centered at $(\pi/2, \pi/2)$ with an isotropic dispersion relation around it, observed on both the $(0,0)$ to $(\pi,\pi)$ and $(0,\pi)$ to $(\pi,0)$ lines. The spin-flux model in HFA exhibits another smaller peak at $(0,\pi/2)$ which is not resolvable in existing experimental data. This minor discrepancy may be due to next nearest neighbor hopping or other aspects of the electron-electron interaction which we have not yet included in our model [104]. The quasi-particle dispersion relation of the conventional phase has a large peak at $(\pi/2, \pi/2)$ on the $(0,0)$ to $(\pi,\pi)$ line (see Fig. 4.2), but it is perfectly flat on the $(0,\pi)$ to $(\pi,0)$ line. Also, it has a large crossing from the upper to the lower band-edge on the $(0,0)$ to $(0,\pi)$ line. This dispersion relation is very similar to that of the $t-J$ model (see Ref. [90]).
While both the conventional and spin-flux model predict AFM insulators at half-filling (at least at the HF level), the fact that the spin-flux also provides a much better agreement with the dispersion relations, as measured by ARPES, is extremely important. As we have already seen in the 1D case, one of the expected effects of doping is the appearance of discrete levels deep inside the Mott-Hubbard gap. Naturally, these levels are drawn into the gap from the top (bottom) of the undoped valence (conduction) bands, so the types of excitations created by doping will strongly depend on the topology of the Fermi surface. The ARPES spectroscopy measures, in fact, the dispersion relations of the photoinduced charged excitations. In Chapter 5 we prove that these charged excitations (spin-bags and meron-vortices) have dispersion relations which closely mimic the dispersion relations of the undoped system, but also lead to significant broadening of the ARPES lines. Due to this similarity, starting with the correct dispersion relations near the Fermi surface is of paramount importance, and gives a strong argument in favor of the spin-flux model.

The self-consistent solutions of Eqs. (4.2), (4.3), (4.5) and (4.6) are shown in Fig. 4.3 (continuous lines). The left panel of Fig. 4.3 shows the magnitude of the staggered spin as a function of \( U/t \). In the large \( U/t \) limit \( S \) goes to \( 1/2 \), as expected. In the small \( U/t \) limit there is a solution with \( S \to 0 \) only for the conventional phase. The spin-flux phase admits an AFM \( (S \neq 0) \) mean-field solution solution only for \( U/t > 3 \). The ground-state

![Graph showing the dependence of staggered spin S on \( U/t \).]
energies per site are shown in right panel of Fig. 4.3, as a function of $U/t$. The energy of the spin-flux phase is lower than the energy of the conventional phase, suggesting that spin-flux provides a better mean-field starting point from which to describe fluctuation effects on the system. As mentioned previously, this lowering of the total energy is due to the collapse of the Fermi surface.

In the large $U/t$ limit, the Hubbard model at half-filling is equivalent with the Heisenberg model [101]. This equivalence remains true in the presence of spin-flux since the Heisenberg exchange coupling involves only the product of phase factors $T^i_jT^{ij} = 1$:

$$\mathcal{H} = \frac{4t^2}{U} \sum_{\langle i,j \rangle} |T^i_j|^2 \left( \bar{s}_i \bar{s}_j - \frac{1}{4} \right).$$

This equivalence between the conventional and spin-flux phases is indeed observed in all our numerical simulations when the electron concentration is at, or extremely near, half-filling. The small differences are due to higher order virtual hopping corrections to the Heisenberg model. The most significant differences between the spin-flux AFM and the conventional AFM occur at intermediate $U/t$ values.

The analytical results described above provide a useful check for our self-consistent numerical scheme. The circles and diamonds of Fig. 4.3 show the numerical results obtained for a $N \times N$ sites lattice in the “bulk” limit. There is perfect agreement with the analytic results. If we use cyclic boundary conditions, which require an even value for $N$, the “bulk” limit is reached for $N \geq 10$.

4.2 Solitons in the doped insulator: the spin-bag and the meron-vortex

4.2.1 The spin-bag

If we introduce just one hole in the plane, the self-consistent solution we get is a conventional spin-polaron or “spin-bag” (see Fig. 4.4). This type of excitation is the 2D analog of the 1D spin-polaron. The doping hole is localized around a particular site, leading to the appearance of a small ferromagnetic core around that site. The spin and charge distribution at the other sites are only slightly affected. In fact, the localization length of the charge depends on $U/t$, and becomes very large as $US \to 0$, since in this limit the Mott-Hubbard gap closes. For intermediate and large $U/t$, the doping hole is almost completely localized on the five sites of the ferromagnetic core. The static spin-configuration surrounding the hole makes charge transport very difficult since motion of the hole outside the ferromagnetic core will create a string of antiferromagnetic bond defects. The hole may circumvent this self-trapped configuration by further twisting the AFM background. However, the subgap
The electronic level induced by the spin-bag ensures that it has a lower Hartree-Fock energy than a hole in the valence band of a spiral (twisted) magnetic background state.

The spin-bag is a charged fermion, as can be seen by direct inspection of its charge and spin distributions (see Fig. 4.4). The electronic spectrum in the presence of the hole-doped spin-bag (see Fig. 4.5) reveals that two levels are drawn deep into the Mott-Hubbard gap. These are the first empty levels, suggesting that one of the discrete gap levels emerged from the upper edge of the valence band, while the other one emerged from the lower edge of the conduction band. There are also an odd number of occupied discrete levels which split from the lower edge of the valence band (one in the spin-flux case, three in the conventional phase). This means that the valence band continues to have an even (spin-paired) number of levels, and therefore its contribution to the total spin is zero. However, the excitation carries the spin localized on the occupied discrete levels. Since there is an odd number of such levels, the spin of the excitation is a half-integer spin.

We define the excitation energy of a spin-bag as the difference between the energy of a self-consistent configuration with a spin-bag and the energy of the undoped AFM background. In the left panel of Fig. 4.6 we show the variation of this excitation energy with the size $N$ of the lattice, for $U/t = 6$, for both cyclic and free boundary conditions. As expected, the excitation energy of the spin-bag does not depend on the size of the lattice, for $N \geq 10$. The variation of the excitation energy of the spin-bag with $U/t$ is shown in the right panel of Fig. 4.6.

In the very large $U/t$ limit, this energy goes asymptotically from above to $U/2 - 2t$. 

Figure 4.4: Left: Self-consistent spin distribution of a 10x10 lattice with a spin bag centered at (5.5). The spin-bag has a small ferromagnetic core, and the magnetic order is only locally affected. Right: Self-consistent charge distribution of a 10x10 lattice with a spin bag centered at (5.5). There is an average of one electron per site everywhere, except in the core of the spin-bag where the doping hole is localized.
Figure 4.5: Electronic spectrum of a spin bag on a 10x10 lattice, for $U/t = 5$ in the spin-flux model (left) and the conventional model (right). Eigenenergies $E_\alpha$ are plotted as a function of $\alpha = 1.200 (= 2N^2)$. Only the first $N^2 - 1 = 99$ states are occupied. There are two empty bound discrete levels deep into the Mott-Hubbard gap ($\alpha = 100.101$), one of which comes from the valence band of the undoped AFM compound (see inset). There is also an occupied discrete level below the valence band ($\alpha = 1$). The valence band is spin paired, since it has an even number of levels. Thus, the total spin of the spin-bag comes from the discrete occupied level. The spin-bag is a charged, spin-$\frac{1}{2}$ fermion.

Figure 4.6: Left: Excitation energy of a spin bag $E_{\text{spin-bag}}$ as a function of the lattice size $N$. Diamonds show results for a spin-flux AFM phase, with Cyclic Boundary Conditions (CBC, full diamonds) and free boundary conditions (FBC, empty diamonds). Circles show results for the conventional AFM state, with CBC (full circles) and FBC (empty circles). The Hubbard parameter is $U/t = 6$. The bulk limit is reached for $N > 10$. In this limit, the excitation energy of the localized spin-bag becomes independent on the size of the lattice. Right: Excitation energy of a spin bag $E_{\text{spin-bag}}$ as a function of $U/t$, in the presence of spin-flux (filled diamonds), and in the conventional state (circles). In the very large $U/t$ limit, the excitation energy approaches asymptotically the value $U/2 - 2t$. The excitation energy of a spin-bag is lower in the spin-flux phase than in the conventional phase.
This can be understood from the fact that in this limit, a hole-doped spin-bag should cost no Coulomb energy, since we simply remove an electron from a site. An electron-doped spin-bag, on the other hand, costs $U$, since we have a doubly occupied site. In both cases, the doping charge can move within the ferromagnetic core, lowering its energy by $2t$. The average energy, therefore, is $U/2 - 2t$ as obtained numerically.

4.2.2 The meron-vortex

In the previous discussion it was suggested that the charged spin-bag is relatively immobile in the AFM background whereas a twisted magnetic background would facilitate electrical conductivity. In this section we present another self-consistent charged soliton, the meron-vortex (see Fig.4.7). It is the direct analog of the 1D charged domain wall. This excitation has a topological (winding) number 1 (i.e. the spins on each sublattice rotate by $2\pi$ on any closed contour surrounding the center of the meron). As such, this excitation cannot appear alone in an infinitely extended AFM plane by the introduction of a single hole into the plane. From a topological point of view, this is so because the AFM background has a winding number 0, and the winding number must be conserved, unless topological excitations migrate over the boundary into the considered region. Also, the excitation energy of the meron-vortex diverges logarithmically with the size of the lattice. This means that an isolated hole introduced in the AFM plane is initially dressed into a spin-bag excitation. Nevertheless, we study the characteristics of the isolated meron-vortex, since this provides a foundation for understanding multiple meron-antimeron configurations at higher dopings, which are no longer topologically or energetically forbidden.

In order to get a self-consistent meron solution, we start with a spin configuration with a winding number of unity. Successive iterations conserve this winding number, but adjust the magnitude of the spins and distribution of charges until self-consistency is reached. In this case, it is useful to use free boundary conditions, since cyclic boundary conditions would distort the spins near the edges of the sample such that they orient in the same direction with the spins on the opposite edge, affecting the excitation energy.

From Fig. 4.7 we can see that the meron-vortex is a charged boson, since the total spin of such a configuration is zero, while it carries the doping charge. Its electronic spectrum is shown in Fig. 4.8. In the presence of the hole-doped meron-vortex we see a pair of levels drawn deep into the gap. In the conventional AFM state these two levels are degenerate, whereas in the spin-flux phase the degeneracy is lifted. This is a direct consequence of the fact that the self-consistent meron-vortex of the spin-flux phase is localized at the center of a plaquette (as shown in Fig. 4.7) while a self-consistent meron-vortex in the conventional state is localized at a site. If the charge dependent terms are removed from the meron-vortex Hamiltonian, this pair of levels is exactly at the mid-gap of the Mott-Hubbard gap for any
Figure 4.7: Left: Self-consistent spin distribution of a 10x10 lattice with a meron-vortex in the spin-flux phase. The core of the meron is localized in the center of a plaquette, in the spin-flux phase (in the conventional phase, the core of the meron-vortex is localized at a site). This excitation has a topological winding number 1, since the spins on either sublattice rotate by $2\pi$ on any curve surrounding the core. The magnitude of the staggered magnetic moments is slightly diminished near the vortex core but is equal to that of the undoped AFM background far from the core. Right: Self-consistent charge distribution of a 10x10 lattice with a meron-vortex in the spin-flux phase. Most of the doping charge is localized in the center of the meron. Far from the core, there is an average of one electron per site.

Figure 4.8: Left: Electronic spectrum of a meron-vortex on a 10x10 lattice, for $U/t = 5$, in the presence of the spin-flux. Eigenenergies $E_\alpha$ are plotted as a function of $\alpha = 1.200 (= 2N^2)$. Only the first $N^2 - 1 = 99$ states are occupied (the valence band). There are two discrete empty levels deep into the Mott-Hubbard gap, one of which ($\alpha = 100$) comes from the valence band of the undoped AFM parent. Merons must be created in vortex-antivortex pairs (for topological reasons). Each pair removes two levels from the undoped AFM valence band. Thus, the valence band remains spin paired, and the total spin of this excitation is zero. This meron is a spinless, charged, bosonic collective excitation of the doped antiferromagnet. Right: same as in the left panel, for a meron-vortex in the conventional state. The only difference is that the two bound levels drawn deep inside the Mott-Hubbard gap are degenerate in this case.
value of \( U/t \), as predicted in Reference [105, 106]. These two levels are the first unoccupied levels, suggesting that one of them emerges from the valence band, while the other one emerges from the conduction band. Moreover, they split from the \((\pi/2, \pi/2)\) peaks of the electron dispersion relation (the Fermi points of the spin-flux phase) [105, 106]. This process is consistent with the opening of the hole pockets near \((\pi/2, \pi/2)\) in the underdoped cuprates.

The bosonic nature of the meron-vortex can be inferred from its electronic spectrum as well. In this case (see Fig. 4.8) only the extended states of the valence band are occupied, and therefore they are the only ones contributing to the total spin. Since only one state is drawn from the valence band into the gap, becoming a discrete bound level, it appears that an odd (unpaired) number of states was left in the valence band. However, one must remember that for topological reasons, merons must appear in vortex-antivortex pairs. Thus, the valence band has an even number of (paired) levels, and the total spin is zero. This argument of the bosonic character of the meron-vortex is identical to that for the charged domain wall in polyacetylene [106, 8, 9].

The excitation energy of the meron as a function of the lattice size is shown in Fig. 4.9, for a fixed \( U/t \). This excitation energy was obtained by subtracting the energy of an AFM undoped background (with free boundary conditions) from the energy of the meron-configuration. As in the case of the spin-bag excitation, it is energetically more expensive to excite a meron in the conventional phase than in a spin-flux phase, for all possible values of \( U/t \). The dependence of the excitation energy on \( N \) may be fitted to the expected form \( E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}} \). The dependence of \( \alpha \) and \( \epsilon_{\text{core}} \) on \( U/t \) are shown in Fig. 4.10. Both vanish as \( S \to 0 \) (corresponding to \( U \to 3t \) for the spin-flux phase and \( U \to 0 \) for the conventional phase). In the very large \( U \) limit, \( \alpha \to 0 \) and \( \epsilon_{\text{core}} \to U/2 \) as expected. In the intermediate \( U/t \) region, the core energy of the meron-vortex in the spin-flux phase is energetically less expensive than that of the meron vortex of the conventional phase due to the spreading of its charged core over the four sites of a plaquette.

Comparing the energy of a meron in a finite size sample with that of a spin-bag, we can obtain a crude estimate of the critical doping concentration at which a transition from the spin-bags to a liquid of charged meron-vortices may take place. Comparing Fig. 4.10 with Fig. 4.6, we see that \( \epsilon_{\text{core}} < E_{\text{spin-bag}} \) for small and intermediate \( U/t \). This means that the excitation energy of a meron-vortex is smaller than that of a spin-bag, provided that the effective size \( N_{\text{eff}} \) of the meron is smaller than \( N_o \) defined by \( E_{\text{meron}}(N_o) = \alpha \ln(N_o) + \epsilon_{\text{core}} = E_{\text{spin-bag}} \). The effective size is given by the sample size \( N \) or the distance to the core of the nearest anti-meron, whichever is smaller. This suggests that for an infinite lattice and finite doping, meron-vortex excitations have lower energies than spin-bag excitations, provided that each hole is dressed by a meron or antimeron-vortex and that the average separation
Figure 4.9: Excitation energy (in units of $t$) of a single meron-vortex, as a function of the meron size $N$, in the presence of the spin flux (diamonds) and without spin-flux (circles). The lines show fits with a logarithmic dependence on $N$, $E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}}$. The excitation energy of a meron-vortex is always lower in the spin-flux phase than in the conventional phase. If the size of the meron core is small enough, the excitation energy of the meron-vortex may become smaller than the excitation energy of a spin-bag.

Figure 4.10: Left: Dependence of the coefficient $\alpha$ (in units of $t$) from the fit $E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}}$ on $U/t$. Diamonds show results for a spin-flux phase, while circles correspond to a conventional state. The line serves to guide the eye. In the large $U/t$ limit $\alpha \to 0$, since in this limit all spin configurations become degenerate and the excitation energy of the meron-vortex should equal the excitation energy of the spin-bag. Right: Dependence of $\epsilon_{\text{core}}$ (in units of $t$) from the fit $E_{\text{meron}}(N) = \alpha \ln N + \epsilon_{\text{core}}$ on $U/t$. Diamonds show results for a spin-flux phase, while circles correspond to a conventional state. The line serves to guide the eye. In the large $U/t$ limit $\epsilon_{\text{core}} \to E_{\text{spin-bag}}$, since in this limit all spin configurations become degenerate and the excitation energy of the meron-vortex should equal the excitation energy of the spin-bag.
between the vortex and the antivortex is less than \(N_o\). Clearly, this may occur if the doping concentration \(\delta\) is larger than the critical value \(\delta_c \equiv 1/N_o^2\). We plot this critical concentration as a function of \(U/t\) in Fig. 4.11, for both conventional and spin-flux phases.

In the conventional phase we see that the purported critical concentration for the dissociation of spin-bags into charged meron-antimeron pairs is larger than 0.30. At such large doping concentrations the average size of the excitation is \(N_e < 2\), and the distinction between merons and spin-bags is blurred. We conclude, therefore, that there is no clear transition from a state with spin-bag excitations to a state with meron excitations as the doping increases. In other words, the only relevant excitations for the conventional AFM phase are spin-bags, within the Hartree-Fock approximation. In the spin-flux phase, the situation is very different. For a broad range of intermediate values of \(U/t\) the critical concentration \(\delta_c\) is small and the distinction between spin-bags and merons remains clear. This suggests that for these values of \(U/t\) there are two distinct types of Hartree-Fock ground-states, as a function of doping. At very low dopings, the spin-bag excitations are energetically more favorable. Since spin-bags affect the magnetic order only locally, the long range AFM order is still preserved in their presence. However, if the concentration increases beyond \(\delta_c\), it is energetically favorable for each hole to be dressed into a meron or antimeron-vortex. In this case, the long range AFM order can be destroyed, leaving behind
either power-law decaying magnetic correlations or short range AFM on the length scale of the average distance between vortices.

4.2.3 The meron-antimeron pair

In the above estimate of the critical concentration $\delta_c$, we assumed that the merons and antimerons are uniformly distributed. However, the actual critical concentration $\delta_c$ may be lowered when the tendency of merons and antimerons to form tightly bound pairs (of total winding number 0) is considered. In Figs. 4.12 and 4.13 we show the self-consistent spin and charge distributions for the lowest energy configuration found when we put 2 holes on the AFM lattice, in the spin-flux model. This configuration consists of a meron and an antimeron centered on neighboring plaquettes. As a result of the interaction, the cores of the vortices are somewhat distorted, and most of the charge is missing from the (10,10) site which is common to both cores. If the vortices were uncharged, a total collapse of the vortex-antivortex pair would be plausible. However, for charged vortices, the fermionic nature of the underlying electrons prevents two holes from being localized at the same site, in spite of the bosonic character of the collective excitation.

A very interesting feature of this tightly bound meron-antimeron solution is that the attraction between the charged vortices is of purely topological nature, and appears even though the electronic Hubbard Hamiltonian (see Eq.(1.4)) contains only repulsive electron interactions. Vortex-antivortex attraction varies as the logarithm of the distance between the cores, and therefore the pair of vortices should remain bound even if full Coulomb repulsion exists between the charged cores. Thus, the process of nucleation of meron-antimeron pairs upon doping provides a very natural scenario for the existence of pre-formed pairs in the underdoped regime.

There is another possible self-consistent state for the system with two holes, consisting of two spin-bags far from each other (such that their localized wave functions do not overlap). The excitation energy of such a pair of spin-bags is simply twice the excitation energy of a single spin-bag. When this excitation energy is compared to the excitation energy of the tightly bound meron-antimeron pair, we find that it is higher by 0.15$t$ (for $U/t = 5$). This would suggest that spin-bags are always unstable to the creation of charged meron-antimeron pairs within the spin-flux phase, and that the critical doping concentration, $\delta_c$, should be set equal to zero. A more realistic determination of the critical hole concentration for the nucleation of meron-antimeron pairs requires the incorporation of the long range Coulomb repulsion between charge carriers in the doped Mott insulator.

The situation in the high-$T_c$ copper-oxide materials is probably more complex, and depends on the nature of the doping process. If the charge carrier concentration is low and uniformly distributed, the average distance between holes is large. At low temperatures,
Figure 4.12: Self-consistent spin distribution for a tightly bound meron-antimeron pair. The meron (M) and the antimeron (A) are localized on neighboring plaquettes. The total winding number of the pair is zero. The magnetic AFM order is disturbed only on the small region where the vortices are localized. The attraction between holes is of topological nature and on long length scale is stronger than unscreened Coulomb repulsion between charges.

Figure 4.13: Self-consistent charge distribution for a tightly bound meron-antimeron pair. The doping charge is mostly localized on the two plaquettes containing the meron and antimeron cores. Due to interactions, the cores of the vortices are somewhat distorted, with most of the charge missing from the (10,10) site common to both cores. The two holes localized in the cores are responsible for the fact that the meron-antimeron pair does not collapse (due to Fermi statistics, it is impossible to have two holes at the same site).
it is possible that these holes are trapped somewhere in the vicinity of their donors in the form of spin-bags. If two spin-bags encounter each other, they should indeed decay into a tightly bound meron-antimeron pair. Since such a pair distorts the AFM background only in a very small region, magnetic LRO is preserved. At low temperatures and low dopings, these meron-antimeron pairs may remain pinned to the donor atoms or other forms of disorder, giving rise to the appearance of a spin-glass type phase of the magnetic background. At higher dopings the pinning potential of the donor atoms is screened and the soliton-soliton interactions are stronger than pinning energies. For concentrations greater than some critical concentration, it is possible that charged meron-antimeron pairs are no longer tightly bound and AFM long range order is completely destroyed.

If this scenario is applicable to the high-$T_c$ copper oxide materials, it is tempting to associate the charge carriers in the doping regime relevant to superconductivity with meron-vortices. Besides the magnetic order, another extremely important issue is the dynamics of solitons. For instance, in the intermediate $U/t$ regime, a spin-bag as depicted in this model (see Fig. 4.4) is basically immobile, since moving would mean leaving behind a string of ferromagnetically aligned spins. It is plausible [107] that the kinetic energy of localization of the hole could be lowered if the spin-bag (spin-polaron) has a ferromagnetically aligned core, within which the hole is free to move. Another possibility [108] is that a spiral twist in the AFM background accompanies the hole as it moves. The meron-vortex may be regarded as a self-consistent realization of the twist-accompanied hole which is topologically stable even when the charge carrier is stationary. The vortex in the AFM background surrounding the hole facilitates mobility of charge since hopping of the vortex core to a neighboring plaquette leads to a less severe distortion of the AFM exchange coupling between neighboring spins. Since meron-vortices have a bosonic nature, the non-Fermi liquid nature of the metal from which superconductivity emerges is also quite natural.

### 4.3 Higher dopings: multi-soliton configurations

For higher carrier concentrations, there is some arbitrariness in choosing the initial spin and charge configurations from which to begin the iterative self-consistency scheme. Since a variety of different self-consistent states may be realized starting from different initial configurations, we adopt a probabilistic approach. We give random numbers as the initial components of the spin distribution, and also choose randomly the sites where the holes are initially localized. This iterative process is repeated many times, and the self-consistent configuration of lowest energy is finally selected. As we mentioned before, the relation between the energy per site of the hole-doped configuration and that of the equivalent electron-doped configuration is given by $e_{\text{hole}}(\delta) = e_{\text{electron}}(\delta) - U\delta$ where $\delta$ is the average
number of charge carriers per site. For convenience, we plot the energy of the hole-doped configurations as a function of doping. The results obtained in the random searches are summarized in Fig. 4.14, where the energy per site (in units of $t$) of the self-consistent hole-doped configurations is plotted as a function of the electron concentration. They correspond to $U/t = 5$, and a $10 \times 10$ lattice with cyclic boundary conditions. For $\delta = 0.01$ and 0.02 (corresponding to one and two holes, respectively) we recapture the results presented in the previous section. In the spin-flux phase, a single isolated hole forms a spin-bag, whereas the lowest energy configuration found for two holes is the tightly bound meron-antimeron pair shown in Figs. 4.12,4.13. For 2 holes we also find a number of self-consistent metastable states, containing widely separated spin-bags.

For a doping up to about 0.30, (which corresponds to an electron density $c = 0.70$ to 1), the lowest energy configurations always correspond to various arrangements of meron-antimeron pairs in the spin-flux phase. As an example, we show the spin configuration of lowest energy found for 8 holes, $c = 0.08$ (see Fig.4.15). We can see 4 meron-antimeron pairs arranged such that each meron is surrounded by antimerons and viceversa. This state appears to be a crystal of meron-antimeron pairs, in the sense that the lattice obtained through translations of the $10 \times 10$ lattice shown in Fig.4.15 has an ordered distribution of meron-antimeron pairs. This crystallization is very likely an artifact of the zero tempera-

![Figure 4.14: Energy per site (in units of $t$) as a function of the electron concentration. $c = 1 - \delta$, for $U/t = 5$. Circles correspond to the lowest energies found in the random trial in the spin-flux phase (liquid of meron-vortices), while squares correspond to the best result of the random trial in the conventional phase (stripes). The dashed line shows the exact value for $U = 0$ (non-interacting case). At low doping (high electron concentration) the liquid of meron-vortices of the spin-flux phase has a lower energy than the stripes of the conventional phases. However, at higher dopings ($\delta > 0.4$) the conventional phase becomes stable.](image-url)
ture, semiclassical, static Hartree-Fock approach. Incorporation of dynamics and fluctuations in the model may lead to the melting of this crystal into a quantum liquid of mobile meron-antimeron pairs. However, as discussed in the next section, ordered arrays of merons and antimerons may play an important role at some special dopings.

As the doping becomes larger than 0.20, the density of vortices is so large that we obtain configurations which have a meron or antimeron vortex localized on almost each plaquette, leading to a state where long range AFM correlations are completely lost. As a consequence, the doping charge is quite uniformly distributed over the whole lattice, and the magnitude of the staggered spin decreases considerably. The apparent overlap of the charge carrier wavefunctions, here, suggests that quantum corrections to the Hartree-Fock approximation may be substantial in this doping range and that the charge carriers here form a novel type of quantum liquid. Finally, at very large doping ($\delta > 0.4$), the entire spin-flux phase is energetically unstable to the formation of a conventional electron gas. This is expected, since (see Eqs. (3.1) and (3.4)) the bottom of the valence band in the spin-flux phase is higher than that of the valence band in the conventional phase. At very low electron concentrations, the energy per site approaches that of the non-interacting ($U = 0$) electron model (see Fig.4.15), as expected.
In contrast to the above picture of a meron-liquid in the spin-flux phase, the lowest energy configurations at low dopings in the conventional AFM phase always consists of charged stripes [11, 12]. For example, in Fig.4.16 we show the selfconsistent spin configuration found for $c = 0.15$, where all the spin-bags assemble in a closed stripe (the stripe must close due to the cyclic boundary conditions). We have also calculated the energies of ordered horizontal and diagonal stripes. This necessitates bigger lattices, so that the cyclic boundary conditions are satisfied. For $U/t = 5$ we find basically no difference between the energies of such stripes and that of the closed stripes obtained from the random initial conditions. The instability of the spin-bags to stripe formation has also been proven in the three-band Hubbard model and the t-J model [13]. However, as seen from Fig.4.14, such states have higher energies than the liquid of meron-antimeron pairs of the spin-flux phase. We have also tried to obtain horizontal and diagonal stripes in the spin-flux phase, by starting with an initial configuration containing such a stripe. However, they converge to the liquid of meron-antimeron pairs rather than self-consistent stripe configurations.

At large dopings, the conventional phase becomes energetically more favorable and more and more discrete levels are drawn into the Mott-Hubbard gap. Due to overlap of the charge carrier wavefunctions, these levels spread into a broad impurity-like band. Also, the staggered magnetization $S$ at each site is strongly suppressed, leading to shifts of the

![Figure 4.16: Self-consistent spin distribution for the configuration of lowest energy found at $\delta = 0.15$, starting from initial random distributions, for $U/t = 5$ in the conventional phase. A closed charged stripe appears (cyclic boundary conditions were imposed). The AFM magnetic order is switched from one phase to the other one (up $\rightarrow$ down and viceversa) as the stripe is crossed.](image)
band edge energies (roughly given by $\pm US$). These two effects conspire to close the Mott-Hubbard gap, and lead to the formation of a conventional, Fermi-liquid with a partially-filled band for dopings $\delta > 0.3$.

In summary, the static HF analysis suggests a picture of three distinct regimes. At very low dopings, we have a collection of tightly bound meron-antimeron pairs and/or spin-bags, which preserve the long range AFM order. When the doping exceeds some critical value $\delta_c$, a transition to a quantum liquid of meron-antimeron pairs occurs, and is accompanied by the destruction of the AFM long range order. Since these charged merons are spinless bosons this metallic state will invariably exhibit non-Fermi-liquid properties. As the doping further increases, the spin-flux state itself is unstable, the Mott-Hubbard gap closes and the system reverts to a conventional Fermi-liquid. Although our static Hartree-Fock analysis points to the above picture, it does not describe soliton dynamics and quantum fluctuation effects pertinent to the quantum liquid phase of merons. In addition, a more careful treatment of the long range part of the Coulomb repulsion between charge carriers may be needed in the non-Fermi-liquid phase where the conventional arguments of screening are inapplicable [109]. Finally, a more realistic model must include the interactions of the doping charges with the impurity charges located in nearby planes, and the influence of structural distortions of the CuO$_2$ planes. The last issue is pertinent to the meron crystal phase at the special doping $\delta = 1/8$, which we discuss below.

4.3.1 Charge carrier concentration of $\delta = 1/8$

The $\delta = 1/8$ doping is very special, because in some compounds [111] superconductivity is completely suppressed at this doping. A very simple and natural explanation of this suppression is that the charge carriers become immobile. Within our picture of a charged meron liquid, at a doping of 1/8, we find a self-consistent structure consisting of a crystal of merons and antimerons (see Fig. 4.17, left). Neutron scattering reveals that for $\delta = 1/8$, the $\frac{\pi}{a}(1,1)$ AFM magnetic peak splits into four peaks situated at $\frac{\pi}{a}(1,1 \pm \frac{1}{8})$ and $\frac{\pi}{a}(1 \pm \frac{1}{8},1)$ [112, 110]. For the calculated meron crystal shown in the left panel of Fig. 4.17, the magnetic structure factor exhibits four peaks with the correct distances between the peaks. However, they are rotated by $45^\circ$ (they appear along the diagonals, not along the horizontals) relative to the observed neutron scattering peaks. This picture can be brought into agreement with experiments by introducing a small anisotropy in the electron hopping within the copper-oxide plane. The addition of such a perturbation to our model is justified by the experimentally observed distortion of the lattice from the usual low-temperature orthorhombic (LTO) structure to the low-temperature tetragonal (LTT) structure at this doping [113]. In the LTT structure the atomic displacements form a horizontal (or vertical) structure, and very likely favor the pinning of horizontal (vertical) stripes. The easiest
way to mimic this structural distortion is to add a small anisotropy in the magnitude of the hopping integral, with the same periodicity. For a 3% anisotropy, the half-filled stripe structure predicted by Tranquada [110] becomes stable (see right panel of Fig.4.17). The self-consistent stripe configuration obtained in the presence of the small anisotropy is made up of merons and antimerons packed along horizontal lines. This example illustrates that a more realistic model including the effects of such structural distortions and possibly the interaction with the impurity charges is required for a quantitative comparison with experiments.

4.3.2 Optical absorption

As we mentioned before, in the presence of each meron or antimeron-vortex, two electronic levels, one from the valence band and one from the conduction band, are drawn deep into the gap. In the presence of multi-soliton interactions these levels spread into a broad impurity band within the larger Mott-Hubbard gap. Since these localized states are empty (for the hole-doped system), electrons can be optically excited to them from the valence band. Consequently, a broad optical absorption band appears inside the Mott-Hubbard gap. In Fig.4.18 we show the evolution of the optical absorption with doping. The absorption was calculated through straightforward perturbation theory, after a term coupling the doping charge to an external vector potential field [114] was added to the mean-field Hamiltonian.
This leads to the following formula for the electric conductivity tensor

\[
\sigma_{ij}(\omega) = \frac{1}{i\omega} \sum_{\alpha=1}^{N_e} \sum_{\beta=\alpha+1}^{N_e} \left[ \frac{\eta_{\beta\alpha}^1 \eta_{\beta\alpha}^2}{\hbar \omega - (E_{\alpha} - E_{\beta}) + i\Gamma} \right. \\
\left. - \frac{\eta_{\beta\alpha}^1 \eta_{\beta\alpha}^2}{\hbar \omega + (E_{\alpha} - E_{\beta}) + i\Gamma} \right]
\]

where

\[
\eta_{\alpha,\beta} = \frac{i\epsilon t}{\hbar} \sum_{\langle i,j \rangle} \left[ (\vec{r}_j - \vec{r}_i) \phi^*_{\alpha}(i) T^{ij} \phi_{\beta}(j) - (\vec{r}_i - \vec{r}_j) \phi^*_{\alpha}(j) T^{ji} \phi_{\beta}(i) \right]
\]

is the matrix element between an occupied state \( \alpha \) and an empty state \( \beta \) of the density of current operator \( \vec{j} \). Here, \( N_e \) is the number of occupied states, \( N^2 \) is the total number of states and \( \Gamma \) is a phenomenological damping coefficient. The calculation is approximate, in the sense that we did not include the variation of the spin and charge distribution due to the modification of the wave-function in the external field. A more detailed calculation involving a time-dependent generalization of the Hartree-Fock method (the random phase approximation) will be presented elsewhere. In order to mimic the interaction with spin-waves and other damping effects on the excited electronic states we assumed that the
subgap levels are homogeneously broadened with a spectral width of $\Gamma = 0.1t$. This leads to a smooth optical absorption even for a $10 \times 10$ lattice. As the doping increases, two effects are apparent. The first is the appearance of a broad absorption band deep into the gap. This is due to the soliton gap states, and significant weight is transferred into it from the conduction band. The second effect is that the overall charge-transfer gap itself decreases since doping decreases the average self-consistent value of $S$, leading to a shift in the mean-field position of the valence and conduction band edges. This second effect is less apparent in Fig.4.18, because of the fairly large damping we chose. It is well known that the optical absorption of the doped compounds contains a broad mid-infrared band and a Drude-like tail starting from very low frequencies [35]. It is reasonable to associate the broad mid-infrared band with electronic transitions from the valence band to the vortex mediated impurity band (see Fig.4.18). On the other hand, the Drude tail component is associated with the translational motion of the bosonic meron-vortices. This may be described in a time-dependent Hartree-Fock (TDHF) approximation.

4.3.3 The magnetic structure factor

We can characterize the evolution of the magnetic long range order with the doping by looking at the magnetic structure factor. We have calculated the static magnetic structure factor,

$$S(\tilde{Q}) = \frac{1}{N^2} \sum_{i,j} e^{i\tilde{Q}\cdot(\vec{r}_i - \vec{r}_j)} \bar{S}(i) \bar{S}(j),$$

assuming that the spins are frozen in the self-consistent configuration. The results are shown in Fig.4.19. The AFM parent compound has a large peak at $(\pi/2, \pi/2)$, as expected. As the doping increases, this peak splits into four incommensurate peaks, whose positions shift with the doping. This is in agreement with the observed behavior of some cuprate compounds [112, 110].

4.4 Conclusions and critique of the method

In the last two chapters we presented a numerical study of the Hartree-Fock approximation of the one-band generalized Hubbard model. We started with the 1D case in Chapter 3. Doping of the AFM background leads to two types of static self-consistent solutions, namely the charged fermionic spin-bag and the charged bosonic domain-wall. Although at the level of the Hartree-Fock approximation the spin-bag is the low-energy excitation, we argued that this is just an artifact of neglecting the motion of these excitations along the chains. The domain-wall is much more mobile, and therefore expected to lower its energy considerably more than the immobile spin-bags. Thus, we expect that the charge carriers are the charged
domain walls, which are bosons. This is clearly demonstrated in the next chapter, where we use the Configuration Interaction Method to allow quantum dynamics of solitons along the chain. The conduction mechanism based on charged bosonic domain-walls is very similar to that of the polyacetylene. In fact, in Section 3.3.1 we prove that in a continuous approximation, the charged domain wall of the 1D Hubbard model exactly maps over the charged bosonic soliton of the polyacetylene. Using the same simple continuum model we also demonstrate the analogy between solitonic structures in 1D antiferromagnets, such as the domain-wall and the spin-polaron, and solitonic structure of 2D antiferromagnets, such as the meron-vortex and the spin-bag (which is analogous to a small-core skyrmion). This analogy is a direct consequence of the introduction of the spin-flux in the 2D Hubbard model (see Section 1.2). The spin-flux leads to the collapse of the large nested Fermi surface of the AFM background to four points, as observed experimentally (see Fig. 4.2).
Since the spin-flux dispersion relations are isotropic around these four 2D Fermi points, the Schrödinger equation describing the 2D solitonic excitations in the continuum model is reduced to effectively 1D (radial) equations. The structure of these radial equations is very similar to that of the equations of 1D corresponding solitons, leading to a direct analogy between their gap structures.

In the 2D case, we have shown that at low dopings, the spin-flux phase provides a better starting point than the conventional phase, having both a lower overall energy and better agreement with experimentally measured dispersion relations. Two types of self-consistent charged excitations are again identified: the spin-bag (direct analog of 1D spinbag) and the meron-vortex (direct analog of the 1D domain wall). As their 1D counterparts, the spin-bag is a rather immobile charged fermion and the meron-vortex in a mobile charged boson. Simple energetical arguments as well as numerical simulations show that for $U/t$ in the intermediate range, the lowest energy configurations found in the doping regime relevant to superconductivity, consists of a liquid of meron and antimeron-vortices. These meron-vortices accommodate each of the doping holes in an impurity band that occurs within the Mott-Hubbard charge transfer gap. The key ingredient that distinguishes our model from previous studies of the Hubbard model is the concept of spin-flux. In its absence, our analysis reproduces the conventional AFM, in which there is a tendency for stripe formation at low doping, as predicted by many other authors [11, 12, 13]. However, introduction of spin-flux into the AFM leads to a lower mean-field energy state, in which the doping holes find it energetically favorable to be cloaked by vortices of the magnetic background. This cloaking stabilizes the magnetic vortex, and also facilitates the mobility of holes in the AFM background. At extremely low doping the holes are either paired in tightly bound meron-antimeron pairs, or become spin-bags (which may be thought of as a collapsed charged meron-neutral antimeron pair). Increasing doping creates a liquid of meron-antimeron pairs, completely destroying AFM order. This picture is consistent with angle-resolved photo-emission studies of the quasi-particle dispersion relation, the appearance of a broad mid-infrared optical absorption band with doping and various aspects of the neutron scattering data. It also offers a microscopic mechanism for the non-Fermi liquid characteristic of the metallic state from which superconductivity emerges.

One of the great challenges in the understanding of charge carrier pairing is that an attractive force must emerge from a purely repulsive many-electron Hamiltonian. This problem is exacerbated by the fact that the standard arguments of screening of the Coulomb repulsion are based on Fermi-liquid theory and may be inapplicable to a doped Mott insulator. Our model, based on charged vortex solitons, provides a very natural strong attractive force between charge carriers which is of topological origin and which can lead to binding of charge carriers even in the absence of screening. Moreover, the presence of vortices in
the AFM background will lead to a large renormalization of the spin-wave spectrum. This may in turn be related to the observed pseudo-gap phenomenon in the high $T_c$ cuprates [92]. As the doping increases further, the spin-flux phase is unstable to the formation of a conventional Fermi liquid, in which the Mott-Hubbard gap is closed.

All of our results, so far, are based on a static Hartree-Fock mean-field theory. In spite of the simplicity of our approximation, the calculated properties of our model are consistent with a variety of independent experimental signatures of the cuprate superconductors. We believe that it is reasonable to proceed beyond this mean-field theory to understand in greater detail the quantum and dynamical properties of the meron-liquid. One of the most important steps is to turn on the quantum dynamics of the charged solitons. This is expected to lower the energy of the meron-antimeron pairs even more, thus making the liquids of merons more stable. Also, a more proper way of calculating the response functions of the systems, by including soliton translations, is necessary. The long range part of the Coulomb repulsion between doping charges may play a more important role in the properties of this novel quantum liquid than it does in a conventional Fermi liquid where standard screening arguments apply. Also, additional interactions such as crystal field effects and conventional spin-orbit interaction [23], which help to stabilize uncharged meron-vortices, may need to be added in the starting Hamiltonian. These considerations may, in turn, shed light on the microscopic mechanism of high-temperature superconductivity and the detailed characteristics of the non-Fermi-liquid state from which it arises.
Chapter 5

Quantum dynamics of charged and neutral magnetic solitons: Spin-Charge Separation and d-wave Pairing

The 1D Hubbard model is exactly solvable. The solution, based on the Bethe Ansatz, is unique to one-dimension, and cannot be extended to higher dimensions. As such, it becomes very important to find an approximation which gives very good agreement with the exact Bethe Ansatz solution and which can also be generalized to 2D systems. The Configuration Interaction (CI) method is such an approximation. The CI method provides a systematic way to improve and go beyond the Hartree-Fock Approximation, by allowing quantum dynamics of the solitons.

We start this chapter with a detailed description of the CI method, followed by a very brief description of the exact Bethe Ansatz solution for the 1D Hubbard chain. A detailed comparison between the exact Bethe Ansatz results and the approximate CI and HF results for the 1D Hubbard chain is given. The main results are that the charged bosonic domain-wall soliton is identified as the charged excitation of the 1D Hubbard chain for all values of $U/t$, and its excitation energy and dispersion band as predicted by the CI method are in excellent agreement with the Bethe Ansatz results. We also show that in the CI treatment a charged fermionic spin-bag dissociates into a charged bosonic domain-wall (which carries charge but no spin) and a neutral fermionic domain-wall (which carries spin but no charge). This is a very clear demonstration of the spin-charge separation. Again, good agreement with the exact Bethe-Ansatz results is found. We then use the CI method to analyze the effect of turning on the quantum dynamics of the charged solitons of the 2D plane. We find that the charged fermionic 2D spin-bag is also unstable to dissociation into a magnetic
vortex-antivortex pair which shares the doping charge. This is suggestive of spin-charge separation in 2D. The meron-antimeron pair is also analyzed carefully. We show that this pair is very mobile, thus substantiating the claim that a liquid of such pairs is a metal. More importantly, we show that the meron-antimeron pair has two stable configurations. The most stable one has d-wave pairing, while a second less stable configuration has s-wave pairing.

5.1 Configuration Interaction Method

Consider a system with \(N_o\) electrons. The basic idea of the CI method is that the ground-state wavefunction is not just a \(N_o \times N_o\) Slater determinant (as in the HFA), but a judiciously chosen linear combination of such Slater determinants \([115, 116]\). Of course the set of all possible Slater determinants with all possible occupation numbers generated from a complete set of one-electron orbitals constitute a complete set of the \(N\)-particle Hilbert space. Our aim is to pick out a subset of these Slater determinants which captures the essential physics of the quantum “spin liquid”. Let us assume there are \(N\) such \(N_o \times N_o\) Slater determinants, \(|\Psi_1\rangle, ..., |\Psi_N\rangle\). Then, the CI ground-state wavefunction is given by

\[
|\Psi\rangle = \sum_{i=1}^{N} \alpha_i |\Psi_i\rangle
\]  

(5.1)

where the coefficients \(\alpha_i\) are chosen such that the minimization principle is fulfilled

\[
\frac{\delta}{\delta \alpha_i} \left( \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right) = 0 \quad \text{for } i = 1, N
\]  

(5.2)

Eq. (5.2) leads to the system of CI equations

\[
\sum_{j=1}^{N} \mathcal{H}_{ij} \alpha_j = E \sum_{j=1}^{N} \mathcal{O}_{ij} \alpha_j \quad \text{for } i = 1, N
\]  

(5.3)

where \(E = \langle \Psi | \mathcal{H} | \Psi \rangle / \langle \Psi | \Psi \rangle\) is the energy of the system in the \(|\Psi\rangle\) state, \(\mathcal{H}_{ij} = \langle \Psi_i | \mathcal{H} | \Psi_j \rangle\) are the matrix elements of the Hamiltonian in the basis of Slater determinants \(|\Psi_i\rangle, i = 1, N\}, and \(\mathcal{O}_{ij} = \langle \Psi_i | \Psi_j \rangle\) are the overlap matrix elements of the Slater determinants (which are not necessarily orthogonal). Since such linear systems of equations are easily solved, the CI solution can be easily found once the basis of Slater determinants \(|\Psi_i\rangle, i = 1, N\} is chosen. If we denote by \(\phi_p^{(n)}(i, \sigma)\) the \(p = 1, N_o\) one-electron occupied orbitals of the Slater
determinant \(|\Psi_n\rangle\), these matrix elements are given by

\[
\mathcal{O}_{nm} = \text{Det} \left( \begin{array}{ccc}
\beta_{1,1}^{nm} & \cdots & \beta_{1,N_o}^{nm} \\
\vdots & \ddots & \vdots \\
\beta_{N_o,1}^{nm} & \cdots & \beta_{N_o,N_o}^{nm}
\end{array} \right)
\] (5.4)

and

\[
\mathcal{H}_{nm} = \mathcal{T}_{nm} + \mathcal{V}_{nm}
\] (5.5)

The expectation values of the hopping and on-site interaction parts of the generalized Hubbard Hamiltonians (1.4) are:

\[
\mathcal{T}_{nm} = \sum_{p=1}^{N} \text{Det} \left( \begin{array}{ccc}
\beta_{1,1}^{nm} & \cdots & \beta_{1,N_o}^{nm} \\
\vdots & \ddots & \vdots \\
\beta_{N_o,1}^{nm} & \cdots & \beta_{N_o,N_o}^{nm}
\end{array} \right)
\]

and

\[
\mathcal{V}_{nm} = U \sum_{i \neq j} \sum_{p_1 \neq p_2} \text{Det} \left( \begin{array}{ccc}
\beta_{1,1}^{nm} & \cdots & \beta_{1,N_o}^{nm} \\
\vdots & \ddots & \vdots \\
\beta_{N_o,1}^{nm} & \cdots & \beta_{N_o,N_o}^{nm}
\end{array} \right)
\]

where

\[
\beta_{ph}^{nm} = \sum_{i,\sigma} \phi_h^{(n)*}(i, \sigma) \phi_p^{(m)}(i, \sigma)
\]

\[
t_{p_1 p_2}^{nm} = -t \sum_{(r,j)} (\phi_{p_1}^{(n)*}(i, \alpha) T_{nj}^{pi} \phi_{p_2}^{(m)}(j, \beta) + h.c.)
\]

\[
u_{p_1 p_2}^{nm}(i) = \phi_{p_2}^{(n)*}(i \uparrow) \phi_{p_1}^{(m)}(i \uparrow)
\]

\[
d_{p_1 p_2}^{nm}(i) = \phi_{p_2}^{(n)*}(i \downarrow) \phi_{p_1}^{(m)}(i \downarrow)
\]

We now consider the specific choice of the Slater determinant basis \(|\Psi_i\rangle, i = 1, N\}. Strictly speaking, one may choose the proper basis of Slater determinants from the general principle of minimization of energy, by requiring that they satisfy the condition

\[
\frac{\delta}{\delta \phi_p^{(n)}(i, \sigma)} \left( \frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right) = 0 \quad n = 1, N; p = 1, N_o
\] (5.6)

However, implementation of this full trial-function minimization scheme (also known as a multi-reference self-consistent mean-field approach) is very difficult, and it becomes unmanageable numerically even for medium-sized systems. Instead, we will select the Slater determinant basis \(|\Psi_i\rangle, i = 1, N\} so as to restore any symmetries of the starting Hamiltonian that were broken by the mean-field HF theory. An obvious member of this set is the
Unrestricted HF wave-function studied in the previous chapter, since it is a Slater determinant, and most specifically the one that satisfies (5.6) by itself (in other words, if the \( \alpha \) coefficients corresponding to the other Slater determinants in Eq.(5.1) are set to zero).

Since this Unrestricted HF wavefunction is not translationally invariant (the doping hole is always localized somewhere along the chain), we can restore the translational invariance of the CI ground-state wavefunction by also including in the basis of Slater determinants all the possible lattice translations of this Unrestricted HF wavefunction. In 2D, we must also include all the possible non-trivial rotations.

Obviously, all the translated HF Slater determinants lead to the same HF ground-state energy \( \langle \Psi_n | \mathcal{H} | \Psi_n \rangle = E_{GS} \) as defined by Eq. (3.8). Thus, we can see that the physical interpretation of the CI method is that it is the most straightforward way of lifting the degeneracy between states with the hole-induced configuration localized at different sites, thus restoring the translational invariance lost through the unrestricted HF search. We may identify the lowering in the total energy due to the lifting of this degeneracy as the extra kinetic energy the doping-induced configuration saves through hopping along the chain. In addition, quantum fluctuations in the internal structure of a magnetic soliton can be incorporated by including the lowest order excited state configurations of the static Hartree-Fock energy spectrum. This addition can also recapture changes in the “shape” of the soliton as it undergoes quantum mechanical motion through the crystal.

In this chapter, we only report results for hole-doped configurations. As mentioned in Sect. 1.2, the energies of the corresponding electron-doped configuration are obtained by adding \( nU \) to the energy of the hole-doped configuration, where \( n \) is the number of doping charges. However, in this chapter we calculate kinetic energies of various spin-polarons and domain walls, which are at most of the order \( t \). While these kinetic energies are the same for both hole-doped and electron-doped configurations, it is obviously more convenient to avoid the large \( nU \) extra contribution to the energy of the electron-doped configurations.

### 5.2 Exact solution of the 1D Hubbard Model: the Bethe Ansatz

Before reporting the results obtained in the CI approximation for the 1D Hubbard model, we briefly describe the exact Bethe Ansatz solution of this problem [6], for comparison purposes.

Consider a chain with \( N \) sites, \( N_o \) electrons of which \( M \) have spin-down. Here, \( N_o \leq N \) and \( M \leq N_o/2 \). Any wavefunction satisfying the many-body Schrödinger equation \( \mathcal{H} | \Psi \rangle = E | \Psi \rangle \) is characterized by \( N_o \) quasi-momenta \(-\frac{\pi}{a} < k_j \leq \frac{\pi}{a}\) describing the motion of the \( N_o \) charges (\( a \) is the lattice constant), and \( M \) rapidities, \( \Lambda_n \), describing the spin ordering. Using the Bethe Ansatz (BA) and imposing periodic boundary conditions, it can be shown
that the quasi-momenta and the rapidities satisfy the so-called Bethe Ansatz equation (see, for instance, Reference [117])

\[
\exp (ik_j Na) = \prod_{\alpha=1}^{M} \frac{\sin (k_j a) - \Lambda_\alpha + \frac{U}{4} i}{\sin (k_j a) - \Lambda_\alpha - \frac{U}{4} i}
\]

(5.7)

\[
\prod_{j=1}^{N_a} \frac{\Lambda_\alpha - \sin (k_j a) + \frac{U}{4} i}{\Lambda_\alpha - \sin (k_j a) - \frac{U}{4} i} = \prod_{\alpha=1}^{M} \frac{\Lambda_\alpha - \Lambda_{\alpha+1} + \frac{U}{4} i}{\Lambda_\alpha - \Lambda_{\alpha+1} - \frac{U}{4} i}
\]

(5.8)

The total energy and the total crystal momentum are then given by

\[
E = -2 \sum_{j=1}^{N_a} \cos (k_j a) \quad P = \sum_{j=1}^{N_a} k_j
\]

(5.9)

The ground state is always given by real \(k\)'s and \(\Lambda\)'s. Excited states are usually described by complex rapidities in so-called "string" structure.

We have solved the Bethe Ansatz equations iteratively, starting with a guess for the set of real rapidities \(\Lambda_\alpha\) (related to the solution of the 1D Heisenberg chain, as described in [117]). Then, we solve Eq. (5.7) and find the quasi-momenta \(k_j\), which we use in Eq.(5.8) to find the new set of real rapidities. The procedure is repeated until self-consistency is reached.

We can check our numerical procedure for a few particular cases. First, the ground-state energy of a half-filled \(N = N_o\) chain in the thermodynamic limit is known to be given by [16]

\[
E = -4 |t| N \int_0^{\infty} \frac{dx J_0(x) J_1(x)}{x(1 + \exp (xU/(2|t|)))}
\]

(5.10)

where the \(J_\nu(x)\) are cylindrical Bessel functions. In Fig. 5.1 we plot the ground-state energy per site, in units of \(t\), obtained for a half-filled chain of various lengths \(N\), for \(U/t = 5\). While for very low values of \(N\) there are large variations between the energies of chains with even and odd number of unit cells, as \(N\) increases the energies obtained converge towards the thermodynamic value of Eq. (5.10) (shown as the full line). We consider chains with an even number of sites (integer number of unit cells), since we know that the ground-state has AFM correlations. Similar curves were obtained for various other values of \(U/t\).

The other well known limit which we use as a check on our numerical procedure refers to the energy of a chain with just one hole, in the \(U/t \to \infty\) limit. In this limit, double occupancy is forbidden by the large on-site interaction, and therefore the only possible motion is that of the hole. The total energy of the chain equals the energy of the hole, since the single occupied sites give little contribution to energy. In this limit the contributions from the AFM correlations of the electron spins are of the order of \(t^2/U\). They are negligible for finite chains. It is straightforward to show [118] that the hole's dispersion relation
in 1D is exactly that of a free particle, and therefore the total energy of the chain is $E(k) = -2t \cos(ka)$. Then, the total ground-state energy of the system with one hole, in the $U/t \to \infty$ limit, must be $E = -2t$. In the following section, we show that this is indeed the limit we obtain numerically from the BA equations as well.

5.3 Comparison between the BA, the CI and the HF results in the 1D case

5.3.1 The undoped ground-state: neutral domain walls

In Chapter 3, we showed (Fig. 3.2) a comparison between the exact ground-state energy of a half-filled chain, as given by the BA treatment (Eq. (5.10)) and that obtained from the HFA, in the thermodynamic limit. As expected, the HFA is exact for $U = 0$ (no interactions), and provides a reasonable upper bound for the ground-state energy for $U > 0$.

The HF Slater determinant of the undoped AFM ground state is already invariant to translations by $2a$ (AFM order must be preserved). As a result, we must find some other self-consistent undoped excited states that can be combined with the HF ground state to create the CI basis of Slater determinants. The lowest energy self-consistent excited state is the undoped (neutral) domain-wall, shown in Fig.5.2. Since the AFM order rotates by $\pi$ when crossing the domain wall, we consider either one domain wall on an odd-site
Figure 5.2: Left: Self-consistent spin and charge distribution for a 40-site chain with two neutral domain walls, for $U/t=5$. The charge $Q(i)=1$ everywhere. The total spin carried by each neutral domain wall is $1/2$.

Figure 5.3: Right: Electronic structure of the 40-site chain with the two neutral domain walls. Each domain wall has 4 discrete levels bound in its core. The spins on the two occupied bound levels are oriented in the same direction as the core spins of the domain wall. In the configuration shown in the left panel, there is a $+1/2$ and a $-1/2$ domain wall, and therefore all levels are spin paired and the total spin of the chain is zero. However, for two $+1/2$ ($-1/2$) domain walls, all the occupied discrete levels have $+1/2$ ($-1/2$) spins, and the total spin of the chain is $+1$ ($-1$).
chain, or a pair of domain walls on an even-site chain, in order to be able to impose cyclic boundary conditions. We are interested in even-site chains, so we show a typical self-consistent configuration containing two neutral domain walls. An analysis similar to the one performed for the charged domain-walls (see Section 3.2.2) suggests that each neutral domain wall carries a spin $1/2$ (with a projection in the same direction as its core spins), and no charge. Thus, this excitation is a neutral fermion. This is confirmed from the electronic structure shown in Fig.5.3.

We can find self-consistent configurations having the two neutral domain-walls at all possible distances from each other, either having opposite orientations (i.e. total chain spin 0) or same orientations (total chain spin ±1). Since the AFM ground state has total spin 0, and states with different total spin do not mix, we need only include in the set of CI Slater determinants $|\Psi_i\rangle$ states of total spin zero, i.e. those having the neutral domain walls “paired” (with opposite orientations). Since all the possible configurations with two neutral domain-walls have very similar energies, they must all be included along with the AFM undoped ground state in making up the variational trial wavefunction. Indeed, we must include both AFM undoped states in the CI set, as well as the excited states each containing a pair of opposite spin neutral domain walls. This can be easily seen from Fig.5.2, where half of the chain is in one AFM ground state, and the other half is in the other (flipped) ground state. Therefore, this state will have equal overlap with both AFM ground states, although the AFM ground-states themselves are orthogonal to each other. For an $N$-site chain, the CI set contains a total of $2 + N(N-2)/2$ Slater determinants, two being the undoped AFM ground states, and the rest being the $N-2$ possible states with paired domain-walls at different distances from each other, each of which can be translated $N/2$ times along the chain.

The total ground-state energy found with the HF (circles), CI (squares) and BA (diamonds) methods for chains of different lengths $N$ for $U/t = 5$ and $U/t = 50$ are shown in Fig. 5.4. For all three methods the total energy of the chain is proportional to the length of the chain. The addition of the configurations with a pair of neutral domain walls in the CI method improves the ground-state energy considerably. It is obvious, however, that as the length of the chain increases configurations with two, three, four and more pairs of neutral domain walls should be included in the CI set in order to arrive at a perfect agreement with the exact Bethe Ansatz solution. In Section 5.3.3 we will define a charged domain wall energy and show that this agrees almost perfectly with the Bethe Ansatz solution. It is interesting to remark that even if only the configurations with one pair of neutral domain walls are included, the CI ground state is such that $\langle S_z(i)\rangle = 0$ for any site $i$ of the chain, although the antiferromagnetic correlations remain very strong. This is a consequence of the fact that CI set of Slater determinants contains an equal number of states with the spin
at the site i up and down, so in average each spin expectation value is vanishing.

5.3.2 The spin-polaron

We now move to the discussion of charge carriers in the doped quantum antiferromagnet. Consider a spin-polaron on a chain with $2N$ sites (the number of sites must be an even number so that we can impose cyclic boundary conditions). This type of excitation was discussed in Sect. 3.2.2, and a self-consistent charged spin-polaron on a chain with 40 sites is shown in Fig. 3.3. Using the CI method we evaluate the kinetic energy saved by the charged spin-bag if it can quantum mechanically tunnel along the chain. For this, we include in the CI set of Slater determinants the HF states with the spin-polaron centered on all possible sites of the lattice, obtained from the initial configuration through translation. In this case we only need to include in the set of Slater determinants $|\Psi_i\rangle$ configurations translated by an even number of sites from the initial HF configuration. The reason for this is that the spin-polarons are spin-$1/2$ excitations. Let $|\Psi_{\text{even}}\rangle, |\Psi_{\text{odd}}\rangle$ be the HF determinants for the spin-polaron centered at an even and odd site, respectively, and let $S_z = \sum_i S_z(i) = \frac{1}{2} \sum_{i,\sigma} \sigma c_\sigma^\dagger c_\sigma$ be the total spin operator in the $z$-direction. Then, $S_z|\Psi_{\text{even}}\rangle = \frac{1}{2}|\Psi_{\text{even}}\rangle$ while
$S_z |\Psi_{odd}\rangle = -\frac{1}{2} |\Psi_{odd}\rangle$ (or vice versa), and therefore $\langle \Psi_{odd}|\Psi_{even}\rangle = 0$. Since the Hubbard Hamiltonian commutes with $S_z$, it follows that $\langle \Psi_{odd}|H|\Psi_{even}\rangle = 0$. From the CI equation (5.3) we conclude that there is no mixing between states with the spin-polaron on one sublattice and states with the polaron on the other sublattice. This is simply an expression of the fact that states with different total spins are in different Hilbert subspaces and do not mix. Thus, for a chain with $2N$ sites we only need to mix $N$ Slater determinants in order to obtain the spin-polaron ground-state within the CI method.

If the initial self-consistent HF spin-polaron configuration $|\Psi_1\rangle$ is composed of the one-particle occupied orbitals $\phi_p^{(1)}(i, \sigma)$, the one-particle orbitals of the state $|\Psi_n\rangle$ translated by $2na$ will simply be chosen as $\phi_p^{(n+1)}(i, \sigma) = \phi_p^{(1)}(i - 2n, \sigma)$ (cyclic boundary conditions are assumed). The overlap matrices $O_{nm}$ and $H_{nn}$ may be calculated and the CI matrix equation (5.3) solved. Numerically, the largest amount of time is spent computing the $H_{nn}$ matrix elements. Due to various symmetries, there are only $N/2$ distinct matrix elements in this case.

Given the structure of the CI equation (5.3), we can readily see that its solutions must be of the form

$$|\Psi_k\rangle = \sum_{n=1}^{N} e^{i kn 2\pi a} |\Psi_n\rangle$$

where $a$ is the lattice constant and there are $N$ distinct $k$ values. These values satisfy the periodicity condition

$$e^{ikN 2\pi a} = 1$$

since translating any spin-polaron configuration by the total chain length $2Na$ leaves the configuration unchanged. Therefore, the distinct $k$ values are

$$k = m \frac{\pi}{Na} , m = 0, 1, ..., N - 1,$$

i.e. are restricted to the $[0, \pi/a)$ region (or, symmetrically, the $(-\pi/2a, \pi/2a)$ interval). This restricted Brillouin zone for the polaron is due to its motion on only one sublattice, and corresponds to states with spin-up (for instance). Then, the band corresponding to the spin-polaron on the other sublattice will have the same structure, but will correspond to spin-down states. In other words, we obtain the typical spin-degenerate band expected for fermions.

Having the general form of the wavefunction, it is straightforward to find the dispersion relation of the spin-polaron

$$E(k) = \frac{\langle \Psi_k|H|\Psi_k\rangle}{\langle \Psi_k|\Psi_k\rangle} = \frac{\sum_{n=1}^{N} \exp (2ika(n-1)) H_{1n}}{\sum_{n=1}^{N} \exp (2ika(n-1)) O_{1n}}$$

In deriving the last equation, we used the symmetry properties of the matrices $H_{nm}$ and
\[ \mathcal{O}_{nm}, \text{ namely that the } (nm) \text{ matrix element only depends on } n - m. \] Strictly speaking, the energy \( E(k) \) is the energy of the whole chain plus the polaron, and will strongly depend on the length of the chain. We extract the dispersion relation of the spin-polaron from a fit of the form

\[ E(k) = 2N e_{GS} + E_{pol}(k) \tag{5.15} \]

where \( e_{GS} \) is interpreted as the undoped ground-state energy per site (since for a very long chain, most of the sites are unaffected by the presence of the single spin-polaron), and we define \( E_{pol}(k) \) as the dispersion relation of the spin-polaron. In other words, the energy of the spin-polaron is just the difference between the energy of the chain with the spin-polaron, and that of an undoped chain. We have verified numerically that the solutions of the CI equation (5.3) are indeed of the form \( \alpha_{\ell}(k) = \exp(ik2na) \), with \( k \) given by Eq. (5.13), and that the total energies \( E(k) \) given by Eq. (5.14) are identical to those obtained numerically from Eq. (5.3). Also, the value \( e_{GS} \) obtained from the fit in Eq. (5.15) is virtually identical to that obtained for the undoped chain in the HF treatment.

We plot \( E_{pol}(k) \) versus \( k \) in Fig. 5.5, for \( U/t = 5 \) and chains of various lengths. The various curves fall on top of each other, thus proving that the fit (5.15) is legitimate. Also shown is the excitation energy of the static hole-doped spin-polaron \( E_{pol}^{HF} \) (the full line), as obtained from the Unrestricted HFA (this excitation energy was also defined with respect to the energy of the undoped chain). Clearly, translation lowers the total energy of the spin-polaron, with the most stable state corresponding to \( k = \pi/2a \). The total kinetic energy gained is, however, only of the order of \( t^2/U \). This is shown in Fig. 5.6, where we plot both the kinetic energy gained \( E_{pol}(\pi/2a) - E_{pol}^{HF} \) (circles) and the width of the spin-polaron band, \( E_{pol}(\pi/2a) - E_{pol}(0) \) (squares), as a function of \( t^2/U \). The log-log graph clearly shows the linear dependence. This fact is not surprising, since the spin-polaron must tunnel two sites to the next spin-allowed position, and this is a second order hopping process. Clearly, this charged fermionic excitation is relatively immobile.

We estimate an effective mass for the spin-polaron near the bottom of its dispersion band using the parabolic fit

\[ E_{pol}(\frac{\pi}{2a} + k) = E_{pol}(\frac{\pi}{2a}) + \frac{\hbar^2 k^2}{2m_{pol}}. \tag{5.16} \]

The effective mass \( m_{pol} \) is expected to become very large in the \( U/t \to \infty \) region, where the spin-polaron is immobile (its band is very flat). This is indeed seen in Fig.5.7, where we plot this effective mass as a function of \( U/t \). The unit of mass is \( m_e/(a^2t) \), where \( m_e \) is the free electron mass, \( a \) is the lattice constant in Å and \( t \) is the hopping integral in eV.

In the next section we compare the CI spin-polaron energy with the exact energy of the doping hole obtained from Bethe Ansatz. As it turns out the Bethe Ansatz solution
Figure 5.5: Dispersion band for the spin-polaron, $E_{pol}(k)$ vs. $k$, with $E_{pol}(k)$ extracted from Eq. (5.15) for chains of length $2N = 14, 16, \ldots, 22$ sites and $U/t = 5$. The various curves fall on top of each other, thus proving that the fit (5.15) is legitimate. Also shown is the excitation energy of the static hole-doped spin-polaron $E_{pol}^{HF}$ (the full line), as obtained from the Unrestricted HFA. We can see that translation does indeed lower the total energy of the spin-polaron, with the most stable state corresponding to $k = \pi/2a$. The kinetic energy gained through translation is quite small.

Figure 5.6: The extra kinetic energy gained by the spin-polaron $E_{pol}(\frac{\pi}{2a}) - E_{pol}^{HF}$ (circles) and the width of the spin-polaron band, $E_{pol}(\frac{\pi}{2a}) - E_{pol}(0)$ (squares) as a function of $t^2/U$. The log-log graph clearly shows the linear dependence. This is expected, since the spin-polaron must tunnel two sites to the next allowed position. This is a second order hopping process and this charged excitation is rather immobile.
suggests that the true charge carrier is a domain wall soliton rather than a spin-polaron.

5.3.3 The charged domain-wall

To investigate an isolated charged domain wall, we consider chains with an odd number \((2N+1)\) of sites. As discussed in Sect. (3.2.2), there are two types of self-consistent charged domain-walls, namely the COS (centered on site) domain wall and the CBS (centered between sites) domain wall. Typical self-consistent configurations with such domain walls are shown in Fig. 3.4. Since the domain walls are bosons \((S_v|\Psi\rangle = 0)\), there is no apriori reason why we should only keep configurations with the domain-wall localized on one sublattice (moreover, this is inconsistent for the CBS domain wall). Indeed, even for the COS domain wall, it turns out that there is non-vanishing overlap between states with the domain-wall centered on different sublattices, and therefore we must include all possible translations in the CI Slater determinant set \(|\Psi_i\rangle\). We generate the translations with an even number \(2n\) of lattice sites in the same way as for the spin-polaron, \(\phi_p^{(2n+1)}(i, \sigma) = \phi^{(1)}(i - 2n, \sigma)\). However, for translations with an odd number \(2n-1\) of sites we must also rotate all the spins by \(\pi\), so that the AFM order on the two sides of the domain-wall remains the same \(\phi_p^{(2n)}(i, \uparrow) = \phi^{(1)}(i - (2n - 1), \downarrow), \phi_p^{(2n)}(i, \downarrow) = \phi^{(1)}(i - (2n - 1), \uparrow)\). For a \(2N+1\)-site chain, there are \(2(2N+1)\) distinct COS domain wall configurations, and \(2(2N+1)\) distinct CBS domain wall configurations. The reason for the factor 2 is that translation of a domain
wall by $2N + 1$ sites takes it into a domain wall centered at the same site as in the initial configuration, but with all spins flipped, due to the $\pi$-difference in the AFM ordering of the spins on the two sides of the domain wall. A second translation around the whole chain is necessary in order to regain the initial configuration. As a result, there is a four-fold increase in the number of possible configurations for a domain wall, as compared to a spin-polaron on a chain of almost the same length.

Let us first consider only including one type of domain wall (either COS, or CBS), in the CI wavefunction. In this case, we can again conclude that the solutions of Eq. (5.3) must be of the form

$$|\Psi_k\rangle = \sum_{n=1}^{2(2N+1)} e^{i k n a} |\Psi_n\rangle$$

(5.17)

where $|\Psi_n\rangle$ is the configuration translated by $n - 1$ sites from the initial HF configuration $|\Psi_1\rangle$. The periodicity condition is now

$$e^{i k 2(2N+1)a} = 1$$

(5.18)

and therefore the acceptable values of $k$ are given by

$$k = m \frac{\pi}{(2N + 1)a}, \quad m = 0, 1, ..., 2(2N) - 1$$

(5.19)

Thus, the domain-wall dispersion band is extended over the full Brillouin zone $[0, 2\pi]$ (or the symmetric version $(-\pi, \pi]$). The dispersion relation is given by

$$E(k) = \frac{\langle \Psi_k | \mathcal{H} | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle} = \frac{\sum_{n=1}^{2(2N+1)} \exp(i k (n - 1)a) \mathcal{H}_{nn}}{\sum_{n=1}^{2(2N+1)} \exp(i k (n - 1)a) \mathcal{O}_{nn}}$$

(5.20)

As in the case of the spin-polaron, we extract the dispersion relation of the domain-wall from $E(k)$ by substracting the energy of the undoped chain

$$E_{dU}(k) = E(k) - (2N + 1)e_{GS}$$

(5.21)

In Fig. 5.8 we show the dispersion relations $E_{dU}(k)$ vs. $k$ for both CBS (left panel) and COS (right panel) domain walls on chains of different length $2N + 1$, and $U/t = 5$. The excitation energy of the static configuration (obtained from the unrestricted HF search) is also shown. Again, various dispersion curves fall on top of each other, validating the fit of Eq. (5.21). Comparing Fig. 5.8 with Fig. 5.5, it is immediately apparent that the dispersion band of the domain walls is much wider. In fact, the band of the COS domain wall extends up to $4t$ (not shown). Comparing the bottom of the dispersion band to the static HF excitation energy of domain wall (shown as a full line), we see that translational motion lowers the energy of the domain wall by about $t$ (as opposed to only $0.3t$ for a spin-polaron). While the
Figure 5.8: The dispersion relations $E_{dw}(k)$ vs. $k$ for both CBS (left panel) and COS (right panel) domain walls on chains of different length $2N + 1 = 17, ... , 23$, and $U/t = 5$. The excitation energy of the static configuration (obtained from the unrestricted HF search) is also shown as a full line. The extra kinetic energy gained through translation by the domain-wall is considerable, of the order of $t$.

bottom of the dispersion band is basically identical for both types of domain walls, the top is very different. However, excited states with energy $E(k) > 0$ require the incorporation of the excited state configurations of the single Slater determinant (from static Hartree-Fock). Clearly these excited state static configurations have energies comparable to the moving domain wall at high energy parts of the dispersion curve. The most likely candidates are those configurations in which electrons from the top of the valence band are excited into the bound discrete levels. If only one such excitation takes place, the energy of the static configuration is raised by $\approx U/2$ (the difference between the energy of the level at the top of the valence band, and that of the first empty localized level), and therefore such configurations should influence the band structure for $E(k) > 0$. We have checked that this is indeed true, by mixing such configurations in the CI Slater determinant set. This modifies the upper part of the dispersion relation, but leaves the bottom unchanged. We are most interested in the kinetic energy gained by the domain wall through translation ($E(k) < 0$ region), and therefore in the following we will neglect these higher-energy processes.

A technical issue that emerges is what happens if we mix both the COS and the CBS domain wall configurations when calculating the CI wavefunction. One might expect that since either set of configurations by itself predicts similar energies at the bottom of the dispersion band, there might be some supplementary lifting of degeneracies lowering the
overall energy further if both sets are superposed. However, this is not the case. The reason is that each set of configurations by itself generates basically the same CI wavefunctions \( |\Psi_k\rangle \) at the bottom of the dispersion band rather than different ones. Hence, there is no degeneracy to begin with. This can easily be seen numerically if we analyze the eigenvalues of the overlap matrix \( O_{nm} \). Suppose that \( \lambda \) is an eigenvalue of this matrix, and that \( (\alpha_i)_{i=1,N} \) is the corresponding normalized eigenvector (for simplicity, we use \( N \) as the dimension of the overlap matrix, as we did in Sect. 5.1). Defining \( |\Psi\rangle = \sum_{i=1}^{N} \alpha_i |\Psi_i\rangle \) it is straightforward to show that \( \langle \Psi | \Psi \rangle = \lambda \). When we mix both sets of configurations together, we find many vanishing eigenvalues \( \lambda = 0 \), which imply \( |\Psi\rangle = 0 \) (numerically, we use the Singular Value Decomposition technique as a diagnostic for vanishing eigenvalues). This proves that we started with a set of Slater determinants \( |\Psi_i\rangle \) which contains redundant linearly dependent combinations. We remove these linearly dependent states to find the CI ground-state. In particular, by mixing COS and CBS domain wall configurations, the resulting low-energy spectrum is the same as that found by using only the CBS domain wall configurations. This is not surprising, since at higher values of \( U/t \) there is a significant difference between the HF energies of the COS and CBS domain walls, and the CBS configurations are the lower energy configurations.

The previous analysis gives us the lowest energy of a single charge carrier in the chain with a domain wall that can be obtained within the CI approximation. It is interesting to compare this energy to the one obtained from the Bethe Ansatz. However, it is not appropriate to directly compare the total chain energies. The reason, as already proved, is that there is a large contribution to these energies proportional to the number of sites in the chain, the proportionality constant being the undoped ground-state energy per site (see Eq. (5.21)). We already know that the HFA gives a higher undoped energy per site than the exact BA energy (see Fig. 3.2), and the CI approach does not improve it unless we also add states with pairs of uncharged domain-walls. Our aim is to isolate the energy of the doping hole. Therefore, we compare \( E_{dw}(\frac{M}{2}) \) (the lowest CI energy of the domain wall itself) with the corresponding doping hole energy extracted from the Bethe Ansatz. This comparison is shown in Fig. 5.9. In order to find the doping hole energy from the Bethe Ansatz, we evaluate the exact ground-state energy of chain with \( 2N + 1 \) sites and \( 2N \) electrons ( half \( M = N \) of which have spin-down), for various values of \( N \). This set of energies is seen to be well fitted by an expression of the form \( E(N) = (2N + 1)e_{GS} + E_0 \), where \( e_{GS} \) is in excellent agreement with the BA ground-state value predicted by (5.10). As in the CI approach, we identify \( E_0 \) with the energy of the doping hole. These BA energies \( E_0 \) are shown as squares in Fig. 5.9, and they indeed go to \(-2t\) in the \( U/t \to \infty \) limit, as expected. In the \( U/t \to 0 \) limit, the energy of the doping hole is expected to go to zero, since in this \( U = 0 \) limit the system is a metal.
The CBS domain-wall energies $E_{dw} = E_{ci}(\frac{\pi}{a})$ are shown as full circles in Figure 5.9. The agreement with the Bethe Ansatz energy is striking. For $U/t \geq 5$, the fit (5.21) is excellent and the error bars on the domain wall energies are extremely small. However, as $U/t \to 0$, the size of the domain wall increases significantly (it is around 20 sites for $U/t = 2$) and therefore extremely long chains need to be considered for a good fit. The longest chain we considered had 41 sites, and this is the reason why the error bars are increasing. The two upper lines correspond to the static HF energies obtained for a self-consistent CBS domain wall (triangle down) and a COS domain wall (triangle up). The diamonds show the CI results for the spin-polaron. We can indeed see that the translational motion of the domain wall included in the CI approach drastically lowers its overall energy, the kinetic energy saved being of the order $t$ over most of the $U/t$ parameter range.

The agreement between the domain-wall energy as calculated in the CI approach and the exact doping-hole energy as given by the Bethe Ansatz is quite remarkable, over the whole range of $U/t$ parameters. The only disagreement appears for $U/t \leq 2$, where, as explained, the domain-walls become extremely delocalized and the numerical calculations are very difficult. The CI solution is not exact, because the HF description of the AFM background
Figure 5.10: The dispersion relation for a domain-wall on a chain of length $2N + 1 = 17, 19, 21$ and $U/t = 100$. In the large $U/t$ limit the dispersion relation of one single hole is given by $E_{dw}(k) = 2t \cos(ka)$ [118]. This is indeed in very good agreement with the dispersion band of the domain wall, proving again that this is the relevant charged excitation of the Hubbard chain.

Figure 5.11: The effective mass $m_{dw}$ of the domain-wall as extracted from its dispersion band, as a function of $U/t$. The unit of mass is $m_e/(a^2t)$, where $m_e$ is the free electron mass, $a$ is the lattice constant in $\AA$ and $t$ is the hopping integral in $eV$. As $U/t$ increases the mass of the domain-wall increases, although it is significantly smaller than the mass of the charged spin-polaron (see Fig.5.7).
is not exact. As explained before, the description of the AFM background can be greatly improved by adding pairs of neutral domain-walls in the configurations. Such an enterprise would make the CI method extremely cumbersome, due to the extreme increase in the number of possible configurations. However, when the contribution of this background is removed, we see that the CI picture of a single charged domain wall moving around the chain agrees very well with the exact solution. This further suggests that the interaction between the charged domain wall and the neutral domain wall pair is relatively weak. The agreement with the Bethe Ansatz is not limited to the bottom of the charged domain wall dispersion curve. In the large $U/t$ limit, the domain-wall dispersion band is indeed given by $E_{dw}(k) = 2t\cos(ka)$, as required [118]. For example, the dispersion relation for domain-wall corresponding to $U/t = 100$ is shown in Fig. 5.10. At such high $U/t$ values, the typical energy of the configurations containing electrons excited on the mid-gap levels is of order $U/2$. They do not influence the lowest domain wall band. As $U/t$ is decreased, these excited configurations simply modify the high energy part of the domain-wall dispersion relation.

We compute an effective mass for the domain-wall from its dispersion relation near $\pi/a$,

$$E_{dw}(k + \frac{\pi}{a}) = E_{dw}(\frac{\pi}{a}) + \frac{\hbar^2 k^2}{2m_{dw}}$$

This effective mass is shown in Fig. 5.11. The values obtained are indeed small compared to the spin-polaron effective masses (see Fig. 5.6).

In conclusion, the mobile charged bosonic domain wall excitation is the relevant charged excitation of the 1D chain described by the Hubbard model for all values $U/t$. In the static HFA, the charged spin-polaron appeared to be the lower energy excitation for $U/t > 6.5$. However, HFA neglects the kinetic energy due to motion along the chain. When this is taken into consideration in the CI method, the much higher mobility of the charged domain-wall enables it to gain enough kinetic energy to become the lowest excitation.

5.3.4 Spin-charge separation

The comparison shown in Fig.5.9 raises question of what happens if one adds a hole to an even-site chain. The charged spin-polaron is too immobile and does not gain enough energy from translations. In fact, for $U/t > 10$ the difference between the CI energy of the charged spin-polaron and the BA energy of the doping hole is about $0.5t$ (see Fig.5.9). A configuration with a single charged domain-wall is also impossible, both because of the cyclic boundary conditions, and because a $2N$ site chain with $2N - 1$ electrons has a total spin $1/2$ (the spin of the unpaired electron), while the charged domain wall is a boson. An even-site chain with a bosonic charged domain-wall is possible, however, provided that a neutral spin-1/2 domain wall is also created. Thus, it is possible that the charged spin-bag
dissociates into a charged bosonic domain-wall and a neutral fermionic domain wall, both of which are much more mobile.

We demonstrate this spin-charge separation effect using the set of all the possible configurations with a pair of a charged and a neutral domain walls in the CI method. Again, since states with different spins do not mix, we need only keep configurations in which the uncharged domain wall has the same spin, either $+1/2$, or $-1/2$. As in the undoped case, configurations with a pair of domain walls connect the two possible AFM ground states, so we expect that in this case, the CI energy fit will give a better description of the AFM background as well.

We perform the CI analysis for chains with lengths of 12 to 22 sites, and $U/t = 50$. We choose this rather high $U/t$ value for illustrative purposes. In this regime we see a dramatic lowering of the CI energy in agreement with the BA solution. For 2D systems containing charged and neutral vortex solitons, we consider the more physically interesting parameter regime $U/t = 5$ (see Sections 5.4.1 and 5.4.2). The large $U/t$ regime of the 1D model, nevertheless, makes the physical picture most transparent. The CI energy of the $N$-site chain with one charged domain wall and one neutral domain wall is found to be $E_{CI}^{\text{pair}}(N)/t = -1.798 - 0.048N$, while the fit to the exact Bethe Ansatz ground state energy of a chain with $N$ (even) sites and $N - 1$ electrons is $E_{BA}(N)/t = -1.8257 - 0.0552N$ (the number of significant digits indicates the accuracy). For comparison, the CI energy of the chain with a spin-polaron is $E_{CI}^{\text{pol}}(N)/t = -1.358123 - 0.039984N$ (all these fits are for the lowest energy found, i.e. the bottom of the dispersion relation in the CI method). Clearly, the excitation energy $E_{\text{par}} = -1.798t$ of the doped-undoped pair of domain-walls is in very good agreement with the excitation energy of the doping hole as predicted by the Bethe Ansatz solution $E_{\text{hole}} = -1.8257t$ (relative error is 1.5%). The spin-polaron excitation energy $E_{\text{pol}} = -1.358123t$ has a relative error of 26%. As expected, we also see an improvement in the background energy per site in the presence of this pair of domain-walls. The HF prediction in the thermodynamic limit is (for $U/t = 50$) $e_{\text{HF}}^{\text{FS}} = -0.039936t$, in agreement with the fit from the CI method for the spin-polaron. The BA ground-state energy per site is, at the thermodynamic limit, $e_{\text{BA}}^{\text{FS}} = -0.05536t$, in agreement with the BA fit. The ground-state energy per site obtained from the CI fit for the domain-walls pair is $e_{\text{CI}}^{\text{FS}} = -0.048t$, showing the expected significant improvement over the HF value. As discussed previously, an even better agreement can be achieved if more pairs of uncharged domain-walls are included. This result provides a very clear illustration of the spin-charge separation phenomenon known to exist in the 1D Hubbard model. Upon doping, the relevant charge excitation is not the spin-polaron, which is a quasiparticle-like excitation which carries both the spin and the charge of the doping hole. Instead, we find two different excitations, a charged bosonic domain-wall (carries charge but no spin) and a
neutral fermionic domain-wall (carries spin but no charge).

Another interesting result of this analysis is that the excitation energy needed to add a hole to an even-site chain is different from that needed to add a hole to an odd-site chain. For instance, for $U/t = 50$ the fit of the exact Bethe Ansatz ground state energy of a chain with $N$ odd sites and $N - 1$ electrons is $E_{BA}(N)/t = -1.9526 - 0.0551N$ (this was the value used in the comparison with the single charged domain-wall shown in Fig. 5.9). For $N$ even we find $E_{BA}(N)/t = -1.8257 - 0.0552N$. The range of values for $N$ used are similar (12-22 vs. 11-23). Also, the undoped ground-state energy per site in both even and odd chains agree well with the value predicted in the thermodynamic limit. We conclude that this $\Delta E = 0.127t$ excitation energy difference between the even and the odd chain really exists for the doped system, and it persists even in the thermodynamic limit $N \to \infty$. Such a difference would be irreconcilable if the excitation was a local quasiparticle, in which case different boundary conditions are expected to introduce variations of the order $O(1/N)$. However, in the case of the charge-spin separation, there is a simple interpretation. A doped chain with an odd $N$ number of sites has an even $N - 1$ number of electrons. Its ground state has zero spin (all electrons are paired). This is well described by a single charged domain-wall. On the other hand, the doped chain with an even $N$ number of sites has an odd $N - 1$ number of electrons, and therefore its total spin is $1/2$ (the spin of the unpaired electron). As a result, we need both a charged domain wall and a neutral spin-1/2 domain wall in order to describe this chain. We associate the difference $\Delta E$ in excitation energies with the energy necessary to create the neutral spin-1/2 domain-wall plus some interaction energy between the charged and the uncharged domain-walls. As already argued, we expect this interaction energy between domain-walls to be very small, otherwise the pairs of neutral domain-walls which we know must exist in a proper description of the whole chain would modify the energy of the charged domain-wall significantly and the agreement between CI and BA excitation energies would not exist. This result may be verified independently by finding the excitation energy of a single undoped spin-1/2 domain wall. This is straightforward to do by considering undoped chains with an odd number of sites. At the HF level, cyclic boundary conditions impose the existence of an undoped domain-wall in this case. The BA analysis also suggests that an undoped spin-1/2 carrier must exist in this case, since at half-filling the odd-site chain has an odd number of electrons, and therefore one is (spin) unpaired. The fit of the exact BA ground-state energy of the odd-site chain with $N = 9 - 21$ sites and $U/t = 50$ is $E_{BA}(N)/t = 0.1195 - 0.0552N$, i.e. the excitation energy of the spin-1/2 neutral domain wall is $0.1195t$, very close to $\Delta E = 0.127t$. This confirms both our interpretation and the fact that interactions between domain-walls are small. The confirmation of this interpretation within the CI method is somewhat more difficult. The reason is that including only the configurations with a single
same-spin neutral domain-wall is not enough, since the spin-1/2 domain wall must tunnel two lattice sites to the next allowed configuration. As in the case of the charged spin-bag, this process is of second order and therefore the extra kinetic energy saved within CI is only of order $t^2/U$. Thus, we should include at least three neutral domain-walls in the CI configurations. The number of possible configurations is greatly increased in this case, making the numerical simulations much more difficult. Work is in progress to investigate this matter, as well as perform the same analysis for a broader range of $U/t$ values.

These results clearly confirm the validity and accuracy of the CI method. The quantum motion of the solitons along the chain allowed within CI, provides the key for close agreement with the exact Bethe-Ansatz results. The CI results clearly distinguish the charge and the spin carriers of the Hubbard chain, namely the bosonic charged domain-wall and the spin-1/2 neutral domain wall.

5.4 CI results for the 2D system

The generalization of the CI method to 2D systems is straightforward. In 2D, translations should be allowed in both $x$ and $y$ directions. Furthermore, if the self-consistent configuration is not rotationally-invariant (e.g. a meron-antimeron pair), all possible rotations must be performed as well. By rotation we mean changing the relative position of the meron and antimeron while keeping their center of mass fixed. The main difference is a purely technical one, namely the computation time. The computation time for one matrix element $H_{nm}$ scales roughly like $N^9$, where $N$ is the number of sites and the number of configurations included in the CI set scales as $N!/N_s!((N - N_s)!$ when $N_s$ solitons are present. For both an $N$-site chain and an $N \times N$ lattice, the HF “bulk” limit is reached for $N \geq 10$. In the 1D case we used chains with $N = 10 - 25$, and numerical calculations can be easily performed. However, in 2D the smallest acceptable system has 100 sites, leading to an enormous increase in the computation time. Nevertheless, our small sample of results in 2D are very suggestive of a simple and clear physical picture. We describe this picture below.

5.4.1 Spin-bag Dissociation: Charge-Spin Separation in 2D

The charged spin-bag carries a spin 1/2. Since configurations with different total spin do not mix, it is enough to include in the CI set only configurations with the spin bag localized on the same magnetic sublattice. This is in direct analogy with the 1D charged spin-bag behavior. Let us denote by $|\Psi_{(0,0)}\rangle$ the initial static Hartree-Fock configuration, and by $|\Psi_{(n,m)}\rangle$ the configuration obtained through its translation by $n$ sites in the $x$-direction and $m$ sites in the $y$-direction. The condition that only configurations on the same sublattice are included means that $n + m$ must be an even number, and the cyclic boundary conditions
mean that $0 \leq n \leq N - 1, 0 \leq m \leq N - 1$, for a $N \times N$ lattice. As explained in detail in the 1D analysis, mixing configurations with the charged spin-bag localized at different sites and then subtracting out the contribution of the undoped AFM background allows us to calculate the dispersion band of the spin-bag

$$E_{ab}(\vec{k}) = E(\vec{k}, N) - N^2 e_{GS}$$

(5.22)

where the total lattice energy

$$E(\vec{k}, N) = \frac{\langle \Psi_{\vec{k}} | \mathcal{H} | \Psi_{\vec{k}} \rangle}{\langle \Psi_{\vec{k}} | \Psi_{\vec{k}} \rangle}$$

and the CI wave-function

$$|\Psi_{\vec{k}}\rangle = \sum_{(n,m)} \exp(i(k_x n + k_y m)a)\Psi_{(n,m)}$$

are the solutions of the CI equation (5.3).

An analysis of the dependence of the spin-bag dispersion relation $E_{ab}(\vec{k})$ on the size $N \times N$ of the lattice is shown in Fig.5.12, for the conventional model (upper panel) and spin-flux model (lower panel), and $U/t = 5$. We used 6x6, 8x8, 10x10 and (only for the spin-flux model) 12x12 lattices. The dispersion relation is plotted along lines of high symmetry of the full Brillouin zone. For comparison, we also show the excitation energy obtained in the static HFA as a full line. For both models, we see that the spin-bag dispersion band is almost converged, even though we used quite small lattices. The convergence is somewhat slower in the spin-flux case, as seen most clearly at the $(0,0)$ point. Although the values obtained from the four lattices all differ at $(0,0)$, the extremum values correspond to the 6x6 and the 8x8 lattices, while the values for the 10x10 and 12x12 lattices are indistinguishable. We conclude that the fit (5.22) is legitimate. From Fig.5.12 we also see that the dispersion relations for the spin-bag in the two different models have very different shapes. The dispersion relations over the full 2D Brillouin zone are shown in Fig. 5.13, and they are seen to mimic the electronic dispersion relation of the underlying undoped AFM background, shown in Fig. 4.1. This is in agreement with the quasi-particle behavior of this charged spin-1/2 spin-bag. In the conventional model, the undoped AFM background has a Fermi surface along the $(0, \pi)$ to $(\pi, 0)$ line, and it is exactly along this line that the spin-bag dispersion band has a minimum. Similarly, the lowest energy of the spin-bag of the spin-flux model is at $(\pi/2, \pi/2)$, corresponding to the Fermi points of the underlying undoped spin-flux AFM background.

The extra kinetic energy saved by the spin-bag through quantum hopping is $0.37t$ in the conventional model and $0.56t$ in the spin-flux model (for $U/t = 5$). Since the spin-bag
Figure 5.12: Dispersion relation of the charged spin-bag $E_{ab}(k)$ (in units of $t$) plotted along lines of high symmetry in the Brillouin zone. The upper plot shows the dispersion band of the spin-bag in the conventional model, while the lower one shows the dispersion band of the spin-bag in the spin-flux model. $U/t = 5$ in both cases. Circles, squares, diamonds and triangles show the results obtained from CI analysis of 6x6, 8x8, 10x10 and 12x12 lattices. We conclude that the results are already almost converged, even for such small lattices. The full lines show the excitation energy of the spin-bag at the static HF level.
Figure 5.13: Dispersion band of the spin-bag in the conventional model (left) and the spin-flux model (right), for $U/t = 5$. We show the full 2D Brillouin zone ($k$ is measured in units of $\pi/a$), and the color code is shown at the right of each picture. The spin-bag dispersion relations have the symmetry as the dispersion relations of the underlying undoped AFM background, shown in Fig. 4.1: while the $(\pi/2a, \pi/2a)$ point corresponds to the minimum excitation energy of the spin-flux spin-bag, in the conventional model all points along the $(0, \pi)$ to $(\pi, 0)$ have almost the same energy.

Figure 5.14: Schematic representation of the self-consistent configurations used to find the lowering in energy of a charged spin-bag if it decays into a singly-charged vortex-antivortex pair which rotates about its center of mass. For the 10x10 lattice considered, the vortex and the antivortex are centered on-site, therefore the center of mass of the pair is the center of a plaquette. The hole shared by the vortex-antivortex pair is shown as full circle, centered at the center of mass. There are four possible ways to rotate the vortex-antivortex pair about its center of mass. We also add the four possible configurations with a charged spin-bag localized in each of the corners of the plaquette. The spin-bags carry both charge and spin. These four spin-bag configurations are all schematically shown in the first panel.
is only allowed to stay on one magnetic sublattice, it must tunnel two lattice constants to the next allowed site. Consequently, we expect that the energy gained through hopping (of order $t^2/U$) is small. This is confirmed, for the spin-bag of the conventional Hubbard model in [115]. As in the 1D case, we conclude that the spin-bag is a rather immobile quasiparticle-like excitation.

In the 1D model we saw that it is energetically favorable for a spin-bag to decay into a charged bosonic domain wall and a neutral fermionic domain wall, resulting in spin-charge separation. The analog of the 1D charged bosonic domain wall is the 2D charged bosonic meron-vortex of the spin-flux model. If the spin-bag decays into a charged meron-vortex, a magnetic antivortex must also be created for topological reasons. Unlike the pair of domain walls in the 1D case, the vortex-antivortex pair is tightly bound by a topological binding potential that increases as the logarithm of the vortex-antivortex separation. Therefore, we expect that the doping charge is shared between the two magnetic vortices. One technical problem for testing this hypothesis is that such a configuration (a vortex-antivortex pair sharing one doping hole) is not self-consistent at the static Hartree-Fock level. In the static approximation we required two doping holes to stabilize two vortex cores and create a meron-antimeron pair. Since the doubly-charged meron-antimeron pair is stable and self-consistent, we choose the two states obtained by adding one electron in either of the two lower energy localized gap electronic states of a self-consistent meron-antimeron pair, as the basis Slater determinants for the CI calculation. These wavefunction are not invariant to rotations, because the meron-antimeron pair is not (see Figs. 4.12, 4.13). Therefore, we must also include the the configurations obtained through $\pi/2$ rotations about their fixed center of mass. One interesting question is how much rotational energy is gained as a result of the decay of the spin-bag into a singly-charged vortex-antivortex pair. To answer this, we use a CI set of 12 Slater determinants, 8 of which are the configurations of the vortex-antivortex pair, and 4 of which are spin-bag configurations rotated about the center of mass. These configurations are shown schematically in Fig. 5.14. The vortex and antivortex are centered on-site, and share a doping hole (shown as a full circle). There are four possible arrangements of the pair around its center of mass, and each arrangement has two different Slater determinants (determined by which vortex carries the charge) associated with it. We also add the four possible spin-bags shown on the first plaquette, so that the center of mass of the total configurations is fixed. Since the spin-bags belong to different sublattices, they have different spins, as indicated.

The lowest energy CI state found has an energy of $-1.19t$ (with respect to the undoped AFM background). This means that dissociation of the spin-bag into a singly-charged vortex-antivortex pair which rotates about its center of mass lowers the energy of the spin bag by $0.37t$ (the HF energy of the charged spin-bag is $-0.82t$). Thus, a remarkable amount
of energy is saved through this dissociation and rotation process (hopping over the whole lattice of the charged spin-bag only saves $0.56t$ of translational kinetic energy). Another very interesting point is that the CI wavefunction describing this process mixes states with the charged spin-bag on different sublattices (i.e., states with different total spin). This is now possible because the state describing a vortex-antivortex pair is not an eigenstate of any of the total spin operators. There are non-zero spin expectation values in both in-plane directions when vortices are created. As a result, such a wavefunction has non-zero overlap with both a $+1/2$ and a $-1/2$ spin-bag state. This also shows that the question of what carries the spin $1/2$ of the spin-bag in the vortex-antivortex configuration is problematic. This is in marked contrast to the 1D case, where all the domain-wall configurations have spins oriented in the same direction, and therefore the spin is a good quantum number for all states.

So far we have considered only rotational degrees of freedom of the singly-charged meron-antimeron pair. A further energy reduction occurs if the singly-charged vortex-antivortex pair is also allowed to translate over the whole lattice, as well as rotate. Since a vortex-antivortex is much more mobile than the charged spin-bag, it is very likely that the kinetic energy saved through quantum hopping will be large (of the order of $t$). We conclude that it is energetically advantageous for a spin-bag to decay into a much more mobile singly-charged vortex-antivortex pair.

This scenario opens a new avenue for research into how the system evolves with doping. If each hole is dressed into a singly-charged vortex-antivortex pair, when two such pairs overlap it is possible that both doping charges move to the same pair, creating a doubly-charged meron-antimeron pair. These pre-formed charge pairs may condense into a superconducting state at low temperatures. The other uncharged vortex-antivortex pair may either collapse and disappear (this is likely to happen at low-temperatures) or remain as a magnetic excitation of the system (at higher temperatures), mediating the destruction of the long-range AFM order, the renormalization of the spin-wave spectrum and the opening of the spin pseudogap.

5.4.2 d-wave Superconductive Pairing

From the static HF analysis we found that the most stable static self-consistent configuration with two doping holes added to the AFM background of the spin-flux model is the meron-antimeron pair, for $3 < U/t < 8$. At larger $U/t$, two charged spin-bags become more stable, in the static HF approximation. This is in close analogy to the prediction that the spin-bag is energetically more favorable than the doped static domain-wall for $U/t > 6.5$, in the HFA of the 1D Hubbard model. However, in the 1D case the charged domain-wall is considerably more mobile than the charged spin bag, gaining a kinetic energy of the order
of $t$ as opposed to $t^2/U$ energy gained by the spin-bag. As a result, when this kinetic energy is taken into account within the CI method, the charged domain-wall is found to be the relevant charged excitation for all values of $U/t$. A similar picture emerges in the 2D case, because the meron-vortices are much more mobile than the spin-bags.

For the 2D system, we have shown that the charged spin-bag has very similar behavior to the 1D charged spin-bag. The analog of the 1D charged bosonic domain-wall is the 2D charged bosonic meron-vortex. We now consider the properties of the doubly-charged meron-antimeron pair. All the numerical results quoted in the rest of this section refer to a meron-antimeron pair on a 10x10 lattice, in the spin-flux model with $U/t = 5$. We have not yet been able to perform an analysis of scaling of the pair energy with different lattice sizes due to computational constraints. The 6x6 and 8x8 lattices are too small to accommodate a meron-antimeron pair. Even on the 10x10 lattice the pair is somewhat squeezed, as seen by the fact that the meron and the antimeron move from being centered on neighboring plaquettes (as for the 20x20 lattice) to the opposite corners of the same plaquette. However, this is a small effect.

As already discussed, the meron-antimeron pair is not rotationally invariant. We can find the rotational kinetic energy saved by the pair as it rotates about its center of mass, in direct analogy with the study performed for the singly-charged vortex-antivortex pair. In the present case, only 4 configurations need to be included, corresponding to the four possible self-consistent arrangements of the meron and antimeron about their fixed center of mass (see Fig. 5.14). Simple rotation by $\pi/2$ of the one-particle orbitals about the center of mass is not, however, sufficient to generate the rotated configurations. First of all, the $\pi/2$ rotation also changes the spin-flux parameterization. If the spin-flux of the initial configuration is $T^{12} = -1, T^{23} = T^{34} = T^{41} = 1$, a $\pi/2$ rotation leads to a state corresponding to the rotated spin-flux $T^{12} = 1, T^{23} = -1, T^{34} = T^{41} = 1$. Thus, following the $\pi/2$ rotation, a canonical transformation must be performed in order to restore the initial spin-flux parameterization. For the case cited above, this simply implies the change in the one-particle orbitals $\phi_p(i_x, i_y, \sigma) \rightarrow -\phi_p(i_x, i_y, \sigma)$ for all sites $(i_x, i_y)$ which are a type '2' site of the unit cell, in other words sites with even $i_x$ and odd $i_y$ (also, see Fig. 1.5). The second observation is that the rotation by $\pi/2$ also changes (flips) all the spins of the AFM background surrounding the pair. Thus, an extra $\pi$ rotation about an axis perpendicular to the lattice plane is necessary to restore the alignment of the AFM background. Following these transformations it is straightforward to generate the Slater determinants $|\Psi_2\rangle, |\Psi_3\rangle$ and $|\Psi_4\rangle$ corresponding to the meron-antimeron pairs rotated by $\pi/2, \pi$ and $3\pi/2$ from the initial self-consistent HF meron-antimeron pair described by $|\Psi_1\rangle$. The CI method can be used to find the rotational energy saved by superposing these rotated meron-antimeron configurations. The lowest CI energy found is 0.46$t$ below the energy of
the static pair, and corresponds to d-wave symmetry. By this we mean that the coefficients \( a_i \), multiplying the 4 rotated states in the CI wave-function \( |\Psi\rangle = \sum_{i=1}^{4} \alpha_i |\Psi_i\rangle \) satisfy the condition \( \alpha_1 = -\alpha_2 = \alpha_3 = -\alpha_4 \).

Translation of a pair over the whole lattice can also be investigated. Since the pair does not carry any spin, all possible translations must be included (there is no restriction to same magnetic sublattice configurations). This leads to a total of \( N^2 \) possible configurations for a \( N \times N \) lattice. Again, when various configurations are generated from the initial self-consistent HF meron-antimeron state \( |\Psi_1\rangle \), care must be taken to preserve the same spin-flux parameterization and the same AFM background orientation. This can be achieved performing transformations similar to the ones described above. As a result of performing the CI method on the set of translated states, we find the dispersion relation of the (un-rotated) meron-antimeron pair. This is shown in Fig. 5.15. For convenience, we choose the reference point to be the HF energy of the self-consistent meron-antimeron configurations. Thus, it is immediately apparent that quantum hopping of the meron-antimeron pair lowers its total energy by an extra \( 1.29t \). Two other interesting features are observed in Fig. 5.15. The first one is that the dispersion relation is not invariant to rotations by \( \pi/2 \). This is due to the fact that the translated meron-antimeron is not rotationally invariant. More important is the fact that the minima of the dispersion relation are about the \((n, r)\) points. This is a consequence of the fact that we are investigating the dependence of the energy on the total momentum \( \vec{k} \) of the pair. Since the mass of the pair is twice the mass of either meron or antimeron, the momentum of the pair is also twice the momentum of either the meron or the antimeron. This suggests that the most stable state corresponds, indeed, to both the meron and the antimeron having momenta of \((\pi/2, \pi/2)\), as expected for the spin-flux model. The doubling of the size of the Brillouin zone is also a direct consequence of this doubling of total momentum (for comparison with undoped dispersion relation, see Fig. 4.1).

However, to obtain the true energy of the charged pair, we must really mix all rotated and all translated meron-antimeron configurations. All have the same static HF energy and are equally important in the CI method. Therefore, we consider a total of \( 4N^2 \) configurations. Let us denote by \( |\Psi_0(0, 0)\rangle \) the initial self-consistent static Hartree-Fock meron-antimeron configuration, and by \( |\Psi_{\theta}(n, m)\rangle \) the configuration obtained through its translation by \( n \) sites in the x-direction and \( m \) sites in the y-direction, as well as a rotation by an angle of \( \theta \pi/2 \) of the pair about its center of mass, where \( 0 \leq \theta \leq 3 \). The cyclic boundary conditions imply that \( 0 \leq n \leq N - 1, 0 \leq m \leq N - 1 \). The CI wavefunctions are then given by:

\[
|\Psi_{\vec{k}}\rangle = \sum_{(n, m)} e^{i(k_x n + k_y m)\alpha} \left( \sum_{\theta=0}^{3} \alpha_\theta |\Psi_{\theta}(n, m)\rangle \right)
\]

(5.23)
Figure 5.15: Dispersion band \( E_{\text{pair}}(k) \) (in units of \( t \)) vs. \( \vec{k} \) of the (un-rotated) meron-antimeron pair. The momentum units are \( \pi/a \), and the color code for energy is shown at the right of the figure. For convenience, the reference energy is taken to be the static HF energy of the self-consistent configuration with the meron-antimeron pair. Thus, we see that quantum hopping lowers the overall energy of the pair by \( 1.29t \). Since the meron-antimeron configuration is not rotationally invariant, the dispersion relation is also not invariant to \( \pi/2 \) rotations.

Figure 5.16: Left: The lowest energy dispersion band \( E_{\text{pair}}(k) \) (in units of \( t \)) vs. \( \vec{k} \) of the meron-antimeron pair. The momentum units are \( \pi/a \), and the color code for energy is shown at the right of the figure. For convenience, the reference energy is taken to be the static HF energy of the self-consistent meron-antimeron pair. We see that quantum hopping and rotation lowers the overall energy of the pair by \( 1.76t \). The rotational symmetry of the dispersion relation is restored (compared to Fig. 5.15). Right: The symmetry of the meron-antimeron wave-function varies through the Brillouin zone. The outside region (containing the absolute minima points \( (\pi, \pi) \)) has d-wave symmetry \( (J = 2) \), while the core region about the \( (0, 0) \) point has s-wave symmetry \( (J = 0) \). The intermediary area is a mix of s+d wave symmetry.
The dispersion relation $E_{\text{pair}}(\mathbf{k}) = \langle \Psi_k | \mathcal{H} | \Psi_k \rangle / \langle \Psi_k | \Psi_k \rangle - E_{\text{pair}}^{HF}$ obtained from this complete set is shown in the left panel of Fig. 5.16. The reference point is again the HF energy of the self-consistent meron-antimeron pair $E_{\text{pair}}^{HF}$. Thus, we see that the total kinetic energy saved by the freely moving meron-antimeron pair is $1.76t$. This, indeed, equals the sum $0.46t + 1.29t$ of rotational and translational kinetic energies found before (the number of significant figures indicates the estimated accuracy of the computational method). The rotational invariance of the dispersion band is also restored.

The rotational symmetry of the meron-antimeron pair wavefunction, defined by the coefficients $(\alpha_\theta)$, varies through the Brillouin zone, as shown in the right panel of Fig. 5.16. The absolute minima points $(\pi, \pi)$ and the area around them correspond to pairs with d-wave symmetry. By this, we mean that the coefficients $\alpha_\theta$ have the form

$$\alpha_\theta = \exp \left( iJ \frac{\pi}{2} \right) \alpha$$

(5.24)

with $J = 2$, i.e. $\alpha_0 = -\alpha_1 = \alpha_2 = -\alpha_3$. The core area, about the local minimum (0,0) point, corresponds to s-wave symmetry. In this region the coefficients $(\alpha_\theta)$ again satisfy Eq. (5.24), but for $J = 0$, i.e. $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3$. The intermediary area appears to be a mixture of different $J$ values. A simple decomposition of the form (5.24) is no longer possible, although a sum of such terms corresponding to different $J$ values is. Since we only have rotations by $\pi/2$, a unique identification of the composite symmetry is not possible. However, the energy of the states in this intermediary area is at the top of the dispersion band. As argued in previous cases, in order to find the correct CI states for energies well above the static HF value (i.e. larger than zero, in this case) we must add to the CI set the first set of excited states. For a meron-antimeron pair, excitation of an electron from the valence band onto the empty localized levels inside the Mott-Hubbard gap costs about $1.5t$ of energy, for $U/t = 5$, so such states should contribute significantly in the CI states with positive energies. For this same reason, we do not show the upper three high-energy bands obtained besides the low-energy one shown in Fig. 5.16, since adding the excited states should modify their dispersions quite drastically. Consequently, both the energy and the symmetry of the states in the intermediary area may be somewhat different than the ones shown in Fig. 5.16. However, the minimum areas around the $(\pi, \pi)$ and the (0,0) points are at energies well below zero, and therefore their energies and rotational symmetry are unaffected by additions of higher energy configurations to the CI set.

The fact that we obtain two distinct minima is not very surprising. As argued before, we expect that individual merons and antimerons are created with momenta of $(\pm \pi/2, \pm \pi/2)$. As a result, two different couplings are possible. A $(\pi/2, \pi/2)$ meron can pair with a $(\pi/2, \pi/2)$ antimeron, creating a pair of total momentum $(\pi, \pi)$. This is the most stable coupling, leading to the lowest possible energy of $-1.76t$ below the static HF energy. This
pair has d-wave symmetry. The second possible coupling is between a \((\pi/2, \pi/2)\) meron and a \((-\pi/2, -\pi/2)\) antimeron. This pair has a total momentum of \((0,0)\), and s-wave symmetry. However, this coupling is less strong. For the \(U/t = 5\) case considered, the energy of the s-wave (0, 0) pair is 1.28\(t\) above the energy of the d-wave \((\pi, \pi)\) pair. The existence of both d-wave and s-wave pairing, and the dominance of the d-wave pairing, have been established experimentally for the high-Tc cuprates [119]. We are not aware of any other microscopic theory that predicts the two types of pairing to appear in different regions of the Brillouin zone, as is the case in our theory.

The total kinetic energy saved by the meron-antimeron pair through quantum hopping and rotation is 1.76\(t\). This is indeed of the order of \(t\), as expected since the pair is not restricted to one magnetic sublattice, and therefore tunneling is not required for motion. As a result, we expect that the energy saved by the meron-antimeron pair for larger values of \(U/t\) is comparably large. On the other hand, we have shown that a spin-bag only saves 0.56\(t\) for \(U/t = 5\), in the spin-flux model, and this energy scales like \(t^2/U\). In fact, we argued that it is likely that a spin-bag may dissociate into a singly-charged mobile vortex-antivortex pair. However, even if the dissociation does not occur, we see that the kinetic energy saved by a pair of spin-bags is significantly smaller than the kinetic energy saved by the meron-antimeron pair. Moreover, even at the static HF level, the meron-antimeron pair costs less energy than the pair of spin-bags if \(3 < U/t < 8\). This shows that for \(U/t = 5\) the meron-antimeron pair is even more favorable energetically than the HFA predicts. This strongly suggests that the \(U/t\) range where meron-antimeron pair formation occurs may extend well beyond the \(U/t = 8\) limit found within the HFA. In the 1D case, we showed that the range of stability of the charged domain wall versus the charged spin-bag is extended (from the HF prediction of \(U/t = 6.5\)) all the way to \(U/t \to \infty\). A numerical analysis must be performed in order to ascertain if the limit is extended to infinity in the 2D case as well. This meron-antimeron picture may provide an alternative to earlier pictures based on Nagaoka's theorem \(^1\) [107] and the spiral magnetic state [120].

\(^1\)Nagaoka proved that for \(U/t = \infty\) and a bipartite 3D crystal, addition of one doping hole to the AFM half-filled background forces all the spins to become ferromagnetic. For a large finite \(U/t\) value, he showed that the transition to the ferromagnetic state is expected provided that enough holes are added to the AFM background. A simple physical argument for this behavior is that at half-filling and large \(U/t\), the superexchange energy saved through AFM ordering is of the order of \(NJ\), where \(N\) is the number of sites and \(J = 4t^2/U\) is the exchange integral. If a hole is added to the AFM background, it is expected to be very immobile, since motion leaves behind strings of parallel spins (or the hole must tunnel among allowed positions). However, if the whole background becomes ferromagnetic, the hole can move freely and is expected to lower its energy by an energy \(\alpha t\), where \(\alpha\) depends on the dimensionality of the system. Thus, for a total of \(n\) holes added, the transition from the AFM with immobile holes to the ferromagnet with mobile holes takes place when \(n > N J\), leading to a critical doping concentration of \(\delta = n/N > \beta t/U\), with \(\beta\) of the order of unity. Thus, for infinite \(U/t\) the transition takes place for even one hole added to an infinite lattice, while for a finite \(U/t\) a finite doping is necessary to accomplish this.

In 1D it can be shown analytically that the ferromagnetic transition is rigorously excluded [118]. For the 2D Hubbard model such a proof does not exist, and the problem is of obvious interest for the cuprates. There have been attempts to solve the problem numerically, but there is no consensus in the results obtained by various authors using various approximations. In this context, generation of mobile meron-vortices with doping may be energetically more favorable than a ferromagnetic transition even as \(U/t \to \infty\), since the charged merons do gain an energy of the order of \(t\) while also preserving the AFM correlations.
5.5 Conclusions

The Configuration Interaction Approximation allows us to consider the effects of the quantum translational and rotational motion of the solitons, which are absent at the Static Hartree-Fock level.

In 1D, we showed that a charged bosonic domain wall can lower its kinetic energy by about \( t \) for all \( U/t \) values, while the immobile charged spin-polaron can only lower its kinetic energy by the order of \( t^2/U \). As a result, the charged bosonic domain wall is the low energy excitation of the Hubbard chain for all values of \( U/t \), and its excitation energy and dispersion band are in good agreement with the predictions of the exact Bethe-Ansatz solution. We also showed that it is energetically favorable for the quasiparticle-like charged (spin-1/2) spin-bag to dissociate into a charged bosonic domain wall (which carries the charge but no spin) and a neutral spin-1/2 domain wall (which carries the spin but no charge). Clearly the CI method recaptures the physics of spin-charge separation known to exist in the 1D Hubbard model. The results obtained in the 1D case clearly illustrate the importance of adding quantum hopping to the treatment of the doped system. The CI method provides us with a simple understanding of the behavior of the charged excitations of the Hubbard chain, as well as a straightforward demonstration of the spin-charge separation. It may be fruitful to perform a more detailed study of the interaction between various types of domain walls, as well as various correlation functions and response functions for detailed comparison with exact results. The results obtained so far using the CI approximation are in very good agreement with the exact Bethe Ansatz solution. We believe that the CI method is likewise a very powerful tool for describing effects beyond mean-field theory in 2D.

For 2D systems, numerical calculations are much more time consuming. However, our preliminary results are quite suggestive. Combined with the expertise gained in the 1D case, they lead us to a simple physical picture. In direct analogy with the 1D results, we find that the bosonic charged meron-vortices are much more mobile than the fermionic charged spin-bags. The extra kinetic energy gained by the meron-vortices is very likely to extend their region of stability beyond the \( U/t = 8 \) limit suggested in the HFA. There are also strong indications that a charged spin-bag may also decay into a singly-charged vortex-antivortex pair, analogous to the spin-charge separation in the 1D case. Nucleation of such pairs of vortices with doping is expected to further influence the magnetic behavior of the cuprates.

The symmetry of the meron-antimeron pairs emerges very clearly from this treatment. We find two regions of stability of the meron-antimeron pair. Pairs with total momentum of \( (\pi, \pi) \) have d-wave symmetry, and are the most stable. Pairs with total momentum \( (0,0) \) have s-wave symmetry and have a smaller gap. Thus, we find that different pairing appears
in different regions of the Brillouin zone. These results agree with numerous experiments, which show that a strong d-wave component and a smaller s-wave component mix in the superconducting state of the cuprates. However, a derivation of the explicit consequences of this picture must be pursued and a comprehensive comparison with the experiments remains to be done.
Chapter 6

Semi-classical response of charged magnetic solitons to external fields: The Time-Dependent Hartree-Fock Approximation

The Time-Dependent Hartree-Fock Approximation (TDHF) goes beyond the Static HFA by allowing calculation of dynamical properties, such as response to external fields. Although TDHF does not recapture certain tunneling effects described by the CI method, it does provide a valuable semi-classical description of linear and non-linear response to external fields. For example, TDHF enables us to describe the acceleration of charged magnetic solitons by an electric field as well as the damping of this soliton motion by the creation of electron-hole pairs across the Mott-Hubbard charge transfer gap. In addition, collective excitations, such as spin-waves, are described within the Random-Phase Approximation (RPA), which is a limiting case of the TDHF.

In this chapter we analyze the dynamics of a charged 1D domain-wall in the presence of an external electric field. The electric field interacts with the charge trapped in the core of the domain-wall, creating a force which moves the domain-wall along the chain. The isolated charged domain-wall has relativistic dynamics, with the highest possible speed being the Fermi velocity of free (non-interacting) electrons. However, if enough energy is absorbed by the soliton from the external electric field, particle-hole excitations across the Mott-Hubbard gap are created, leading to damping of the the motion of the domain-wall. We study this damping and show that it has a non-linear dependence on the external electric field. We also analyze the spin-wave collective excitations using RPA.
6.1 The Time-Dependent Hartree-Fock Approximation

The properties of a many-body quantum system described by a Hamiltonian $\mathcal{H}$, are completely determined by the solution of the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial \tau} |\Psi(\tau)\rangle = \mathcal{H}|\Psi(\tau)\rangle. \tag{6.1}$$

This equation can in turn be rewritten as the solution of the variational problem

$$\delta \int d\tau \langle \Psi(\tau)|i\hbar \frac{\partial}{\partial \tau} - \mathcal{H}|\Psi(\tau)\rangle = 0. \tag{6.2}$$

An approximate solution of the Schrödinger equation (6.1) can be obtained using a restricted trial wavefunction in (6.2). The Time-Dependent Hartree-Fock Approximation (TDHF) consists in restricting the trial wavefunction to a single Slater determinant [121]. In other words, we again treat the system in the independent-electron approximation, but we allow the self-consistent potentials experienced by each electron to be time-dependent. As in previous chapters, we restrict the discussion to the generalized Hubbard Hamiltonian (see Sec. 1.2).

A Slater determinant trial-wavefunction for a system with $N_e$ electrons is of the form

$$|\Psi(\tau)\rangle = \prod_{\rho=1}^{N_e} a_\rho^+(\tau)|0\rangle, \tag{6.3}$$

where $|0\rangle$ is the vacuum state and the one-particle states are given by

$$a_n^+(\tau) = \sum_{i,\sigma} \phi_n(i, \sigma, \tau) c_{i\sigma}^+. \tag{6.4}$$

The one-particle wave-functions $\phi_n(i, \sigma, \tau)$ are chosen to form a complete orthonormal system, so that the transformation $(c_{i\sigma}^+, c_{i\sigma}) \rightarrow (a_n^+, a_n)$ is unitary.

Using the wavefunction (6.3) in equation (6.2), and minimizing with respect to the one-particle wavefunctions $\phi_n(i, \sigma, \tau)$, we obtain the TDHF equations:

$$i\hbar \frac{\partial}{\partial \tau} \phi_n(i, \alpha, \tau) = -t \sum_{\beta, \sigma} T^{ij}_{\alpha\beta} \phi_n(j, \beta, \tau) + U \sum_{\beta} \left( \frac{1}{2} \delta_{\alpha\beta} Q(i, \tau) - \sigma_{\alpha\beta} S(i, \tau) \right) \phi_n(i, \beta, \tau) \tag{6.5}$$

where $(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices and

$$Q(i, \tau) = \sum_{\rho=1}^{N_e} \sum_{\alpha} |\phi_\rho(i, \alpha, \tau)|^2 \tag{6.6}$$
and

\[ \vec{S}(i, \tau) = \frac{1}{2} \sum_{p=1}^{N_o} \sum_{\alpha, \beta} \phi_p(i, \alpha, \tau) \vec{\sigma}_{\alpha\beta} \phi_p(i, \beta, \tau) \]  

(6.7)

represent the expectation value of the charge and spin at the site \( i \). The notation \( j \in V_i \) appearing in (6.5) means that the sum is performed over the sites \( j \) which are nearest-neighbors of the site \( i \). Strictly speaking, equation (6.5) must be satisfied only by the occupied orbitals \( p = 1, N_o \), but can be used to compute the empty orbitals as well.

The (static) Hartree-Fock Approximation is regained easily from the TDHF, if we assume that

\[ \phi_n(i, \alpha, \tau) = \exp \left( -\frac{i}{\hbar} E_n \tau \right) \phi_n(i, \alpha) \]  

(6.8)

Eqs. (3.5,3.6,3.7) follow immediately from Eqs. (6.5,6.6,6.7).

In Chapters 3 and 4 we showed that doping 1D or 2D systems leads to the appearance of localized spin distortions which trap the hole. Since the resulting charged objects (domain wall and spin-polarons in 1D, merons and spin-bags in 2D) are responsible for the transport properties of the system, it is interesting to elucidate their dynamics and their effective masses. Accordingly, we use the TDHF equations (6.5,6.6,6.7) to compute the time evolution of the Slater determinant describing the system. Since the static self-consistent configurations found within HFA satisfy the TDHF equations, we must either deform the initial self-consistent configurations, or add an external field in order to obtain nontrivial dynamics. We choose the latter, since the introduction of an electric field induces translational motion of our charged magnetic solitons. For simplicity, we choose the gauge in which the electric potential \( \phi = 0 \) and the electric field \( E(\tau) = -\partial / \partial \tau \vec{A}(\tau) \). We choose to denote times by \( \tau \) in order to avoid confusion with the hopping integral \( t \). The addition of a vector potential to the hopping Hamiltonian follows the standard prescription, \( t_{ij} \rightarrow t_{ij} \exp \left( -\frac{i e}{\hbar} \int_{\vec{r}_i}^{\vec{r}_j} \vec{A} d\vec{r} \right) \). In the absence of magnetic fields, \( \vec{A} \) is spatially uniform. Therefore, \( \int_{\vec{r}_i}^{\vec{r}_j} \vec{A} d\vec{r} = \vec{A}(\tau)(\vec{r}_j - \vec{r}_i) \), and the introduction of the external field is equivalent to the replacement

\[ T^{\nu\mu}_{\alpha\beta} \rightarrow T^{\nu\mu}_{\alpha\beta} \exp \left( -\frac{i e}{\hbar} \vec{A}(\tau)(\vec{r}_j - \vec{r}_i) \right) \]

in the TDHF equations [122].

In principle, one can integrate the TDHF equations (6.5,6.6,6.7) directly, using a Runge-Kutta method. However, this is time consuming, since each one-electron wave-function has phase factors which oscillate very quickly in time (these are the equivalents of the \( \exp - \frac{i E_n \tau}{\hbar} \) part in Eq. (6.8)). Such overall phase factors do not contribute to \( Q(i, \tau) \) or \( \vec{S}(i, \tau) \) (see Eqs. (6.6,6.7)). It is preferable to avoid the computational work necessary to trace all these quick variations in time. This is possible if we write the time-evolution equations for expectation values of two electron operators rather than the one-particle
wavefunctions [123].

We define

\[ \lambda_\alpha(l, i, \tau) = \langle \Phi(\tau) | \left( \begin{array}{c} c_{i\uparrow}^+ \\ c_{i\downarrow}^+ \end{array} \right) \cdot \sigma_\alpha \cdot \left( \begin{array}{c} c_{i\uparrow} \\ c_{i\downarrow} \end{array} \right) | \Phi(\tau) \rangle = \sum_{n=1}^{N_c} \phi_n^*(l, \tau) \sigma_\alpha \phi_n(i, \tau) \]  

(6.9)

where \( \sigma_0 \) is the 2 x 2 unit matrix, \( \sigma_x, \sigma_y \) and \( \sigma_z \) are the Pauli spin matrices, and

\[ \phi_n(i, \tau) = \left( \begin{array}{c} \phi_n(i, \uparrow, \tau) \\ \phi_n(i, \downarrow, \tau) \end{array} \right). \]

With these definitions \( Q(i, \tau) = \lambda_\alpha(i, i, \tau), \tilde{S}(i, \tau) = \frac{1}{2} \tilde{\chi}(i, i, \tau) \).

Using the TDHF equations (6.5,6.6,6.7) and the definition (6.9), we obtain the equations of evolution for the two-operator expectation values

\[ i\hbar \frac{\partial}{\partial \tau} \lambda_\alpha(l, i, \tau) = -t \sum_{j \in V_l} T^{lj} \lambda_\alpha(l, j, \tau) + t \sum_{j \in V_l} T^{jl} \lambda_\alpha(j, l, \tau) \]

\[ + \frac{U}{2} [\lambda_\alpha(i, i, \tau) - \lambda_\alpha(l, l, \tau)] \lambda_\alpha(l, i, \tau) - \frac{U}{2} \left[ \tilde{\chi}(i, i, \tau) - \tilde{\chi}(l, l, \tau) \right] \cdot \tilde{\chi}(l, i, \tau) \]  

(6.10)

and

\[ i\hbar \frac{\partial}{\partial \tau} \tilde{\chi}(l, i, \tau) = -t \sum_{j \in V_l} T^{lj} \tilde{\chi}(l, j, \tau) + t \sum_{j \in V_l} T^{jl} \tilde{\chi}(j, l, \tau) \]

\[ + \frac{U}{2} [\lambda_\alpha(i, i, \tau) - \lambda_\alpha(l, l, \tau)] \tilde{\chi}(l, i, \tau) - \frac{U}{2} \left[ \tilde{\chi}(i, i, \tau) - \tilde{\chi}(l, l, \tau) \right] \lambda_\alpha(l, i, \tau) \]

\[ -i \frac{U}{2} \left[ \tilde{\chi}(i, i, \tau) + \tilde{\chi}(l, l, \tau) \right] \times \tilde{\chi}(l, i, \tau). \]  

(6.11)

It is straightforward to show that the time-dependent equations (6.5) or (6.10, 6.11) conserve the total charge and total spin (more generally, the expectation value of any operator which commutes with the Hamiltonian). In the absence of external fields, the total energy is also conserved.

The system of Eqs. (6.10, 6.11) can also be obtained from the Heisenberg equations of motion describing the time-evolution of the various quadratic operators. Due to the interaction term, these equations contain quartic operator terms on the rhs. The approximation done in obtaining (6.10, 6.11) is the typical Hartree-Fock factorization \( \langle a_i^+ a_2 a_3^+ a_4 \rangle = \langle a_i^+ a_2 \rangle \langle a_3^+ a_4 \rangle - \langle a_i^+ a_4 \rangle \langle a_3^+ a_2 \rangle \). We numerically integrate these equations, choosing as initial values the corresponding expectation values in the static self-consistent configuration considered.

In the following, we use the lattice constant \( a \) as the unit of distance; the hopping matrix element \( t \) as the unit of energy, and \( \hbar/t \) as the unit of time. The electric field is given as
the dimensionless quantity $eaE/t$. We are interested in the regime $eaE/t < 1$.

### 6.2 The one-dimensional system

#### 6.2.1 Motion of the charged domain wall in a static electric field

For a static electric field $E$ along the chain, the vector potential is $A = -\tau E$. Fig. 6.1 shows the typical evolution of the domain wall along the chain, for very small electric fields. We can see that as the domain wall accelerates, it moves along the chain and passes successively through the COS and CBS configurations.

As already discussed, for $U/t < 3$, there is basically no difference between the COS and CBS domain wall excitation energies. However, as $U/t$ increases and the domain wall becomes more localized, the two configurations have different excitation energies. This difference acts as a Peierls potential. This means that if the domain wall is initially in the lower, CBS configuration, it can only start moving (in the absence of tunneling) if the electric field is such that $eaE/2$ overcomes the washboard potential barrier (in other words, the domain wall must gain enough energy as it moves half a lattice constant between the two configurations to overcome the difference in energies). We have checked numerically that this is true. Indeed, if the electric field is too small, the domain wall slowly oscillates about the lower energy CBS position, but cannot tunnel to the next low-energy CBS configuration. The absence of tunneling in the semi-classical TDHF is well known. This means that this method is not suitable to describe charged soliton dynamics in the large $U/t$ limit.

From Fig. 6.1 we can clearly define the trajectory of the domain wall as the position of its center in time, $x(\tau)$. The trajectory (for a much longer evolution time) is shown in Fig. 6.2, in the lower panel (cyclic boundary conditions were imposed for the odd-number site chain with the domain wall). Here, we follow the domain wall going around the chain many times, as it is accelerated by the weak electric field. As usual, distances are measured in units of $a$ and times in units of $\hbar/t$. The upper panel shows the absolute error $\Delta x(\tau) = x_{fit}(\tau) - x(\tau)$ for a classical (non-relativistic) motion fit of the form $x_{fit}(\tau) = x_o + a\tau^2/2$ (the dash-dotted line) and for a fit containing the first relativistic correction $x_{fit}(\tau) = x_o + a\tau^2/2 - a^3\tau^4/8c^2$ (the full line). Here $a = eE/m_o$ is the expected acceleration of the domain wall, $m_o$ is its rest mass, and $c$ is the maximum speed the domain wall could have if its motion is relativistic.

Before continuing this analysis, we emphasize that we have fixed the tolerances in the numerical integration program such that the trajectory is unchanged if we further lower them. This means that the absolute error in the trajectory is smaller than the thickness of the line.

The fits shown in the upper panel of Fig. 6.2 strongly suggest that the motion of the domain wall is relativistic. The coefficients in the fit allow us to calculate the rest mass $m_o$.
Figure 6.1: Left: Time-dependent charge distribution $Q(i, \tau)$ of a moving domain wall on a 51-sites chain: $U/t = 2.5$, $e\alpha E/t = 5 \cdot 10^{-5}$. Time is measured in units of $\hbar/t$. Away from the trapped hole the charge is at its undoped background value of $Q(i) = 1$. Right: Snapshots of the spin configuration of the same moving domain wall. The snapshots correspond to $\tau = 100, 110, \ldots, 200\hbar/t$. Away from the domain wall, the staggered spin has its undoped background value $S$.

of the soliton as well as its maximum allowed speed $c$. Another indication of relativistic dynamics is that $m_0c^2$ equals the excitation energy of the static domain wall, as computed in the static HFA (the relative error is always less than 1%). This is quite remarkable, since the two compared quantities are computed with very different methods. Here we define the excitation energy of the static domain wall by the average between the excitation energy of the hole-doped and the electron-doped domain wall (or the excitation energy of a domain wall if we started with the particle-hole invariant Hubbard model, as discussed at the end of Section 1.2.) Relativistic Lorentz contraction is also observed. As the speed of the domain wall increases, its core size decreases.

We can also prove that the motion of the soliton is relativistic from the dependence of its energy on its speed. We have checked numerically that the energy of the domain wall (defined as the energy of the chain containing the moving domain wall minus the energy of an undoped, AFM background) varies in time as $E(\tau) = E_0 + \epsilon E(x(\tau) - x_0)$, where its rest energy, $E_0$, is the excitation energy of the static domain wall. This is the expected result from conservation of energy, since the system absorbs energy from the electric field as the
charged domain wall accelerates. The speed of the soliton is simply \( v(\tau) = \frac{dx(\tau)}{d\tau} \). We can fit the total energy of the soliton either as \( E(\tau) = E_0 + m_v u^2(\tau)/2 \) (classical kinetic energy), or as \( E(\tau) = m_v c^2 / \sqrt{1 - u^2(\tau)/c^2} \) (relativistic energy). Again, the relativistic fit is better for a broad range of velocities. In the following, we use the relativistic energy vs. velocity \( u^2 = c^2 - m_v^2 c^2 / E^2 \) to compute \( c \) and \( m_v \). In the trajectory fit \( x(\tau) \) we are forced to consider higher and higher relativistic corrections as the speed increases, and the process is more cumbersome.

The dependence of the rest mass \( m_v \) and the relativistic speed \( c \) on \( U/t \) are shown in Fig. 6.3. The rest mass is measured in units of \( m_e / \tilde{a}^2 \tilde{t} \) (\( m_e \) is the electron mass, \( \tilde{a} \) is the lattice constant measured in Å, and \( \tilde{t} \) is the hopping integral measured in eV). The relativistic speed \( c \) is measured in units of \( a \hbar / t \). The relativistic speed \( c \) is a constant, given roughly \( 2at/\hbar \), the Fermi speed of the free electrons in the half-filled non-interacting chain. Clearly the domain-wall is a collective electronic excitation and therefore it cannot move faster than the fastest electronic speed, since its motion necessitates readjustments of all electron wavefunctions. The domain-wall mass increases significantly as \( U/t \) increases. The natural unit of mass for the domain wall is the electron mass \( m_e \), which is obtained from an expression involving the parameters \( a, t \) and the constant \( \hbar \).

As \( U/t \) increases, the pinning potential (the difference in energy between COS and CBS
domain-wall configurations) becomes significant (see Fig.3.7). This pinning potential appears as a periodic, washboard type potential for the domain wall. Thus, the acceleration of the domain-wall under the influence of the electric field involves oscillations as the soliton moves between the (lower energy) CBS configuration, and the (higher energy) COS configuration. This superimposed oscillatory motion is due to the inability of the semi-classical TDHF to describe direct tunneling between the low-energy CBS configurations. A direct consequence of this is that the effective soliton mass varies between two limits, depending on the fit. The lower limit is obtained if only the CBS configuration are included in the fit, while the upper limit corresponds to only COS configurations. Any other fit interpolates between the two. We choose to interpret this as if rest mass of the soliton varies in going from the COS to the CBS configuration and back. Thus, we can define two rest masses, corresponding to the COS and CBS soliton, shown as empty and full circles in Fig.6.3. Since quantum tunneling is forbidden in this treatment, we expect that these masses are larger than the values obtained by the CI method.

The relativistic dynamics of the domain wall solitons is related to the fact that the equations of evolution for a classical AFM Heisenberg model are Lorentz-invariant [124]. Therefore, any static solution of those equations can be boosted into relativistic motion.
The relativistic limiting speed $c$, in this case, is the spin-wave velocity, since in a Heisenberg system, all the information between spins at different sites is exchanged through spin-waves. However, in order to obtain stable finite-size soliton solutions of the classical AFM Heisenberg equations, one needs to add anisotropies and/or magnetic fields. As a result, the effective rest masses of the solitons are proportional to these anisotropies. Lorentz invariance carries over to the Hubbard model at half-filling in the $U/t \rightarrow \infty$ limit since it is equivalent to a quantum AFM Heisenberg model, with $J = 4t^2/U$. However, we are in a regime of $U/t$ where this equivalence is not precise and more importantly we are studying a charged system which is distinct from a Heisenberg magnet. As discussed above, the relativistic speed for the charged soliton is an electronic speed, and the effective mass is of the order of the electronic mass. Nevertheless, the relativistic motion has its underpinnings in the antiferromagnetic correlations of the background spins.

So far, we have described soliton motion resulting from weak electric fields applied for fairly short periods of time. At higher fields and/or longer times, the system gains enough energy from the external electric field to excite collective excitations that damp the motion of the domain wall. A typical picture showing the motion of a domain wall in a higher electric field is shown in Fig.6.4. We identify two regimes. In the initial period $0 < \tau < 30$, the soliton is the only excitation on the chain, and is being accelerated by the electric field (this is the relativistic regime studied above). However, when the speed exceeds a certain limit we observe excitations created behind the soliton. These excitations are small fluctuations in the charge background $Q(i)$ and the staggered spin $S_z(i)$. The nature of these excitation is evident from their frequencies, which are comparable with the Mott-Hubbard charge-transfer gap. These excitations occur when there is enough energy in the system to excite electrons on the formerly unoccupied levels, either those localized in the core of the soliton or those in the valence band. These excitations damp the motion of the soliton. As a result, the soliton continues its motion with a constant speed, the energy gained from the electric field going into the excitation of more such electronic excitations (we can see their amplitude increasing continuously behind the soliton). In addition to electron-hole pair excitations, we expect Cerenkov radiation when the soliton velocity exceeds the spin-wave velocity. This, however, requires the incorporation of magnetic anisotropy in the system and a linearization of the spin-excitation spectrum about the direction of anisotropy. In the mean-field theory described above we do not consider rotations of the spin degrees of freedom.

We study the dependence of the viscous drag coefficient of the domain wall (due to the generation of quasiparticles) on $U/t$, the intensity of the field, the length of the chain and the number of domain walls on the chain. The only significant dependences found are on $U/t$ and $eaE/t$. These are shown in Fig.6.5. We observe that as the magnitude
of the electric field increases, so does the maximum speed of the domain wall as expected for classical damped motion. However, since the isolated domain wall is a relativistic object, its maximum speed cannot be larger than c. Accordingly, we observe a saturation of the maximum speed for large electric fields. This non-linear $E$ vs. $v$ behavior may be measurable experimentally, since the dc conductivity is defined as $env/E$, where $n$ the concentration of domain-walls.

Another type of low-energy collective excitation is the spin-wave. Spin waves (transversal oscillations $S_x(i), S_y(i)$ of the spin) are not excited if we start from the static self-consistent configuration polarized purely in the $z$-direction. However, if we add minute spin components in the $xy$ plane in the initial state, the spin waves are excited as the soliton accelerates. In the absence of any anisotropy, spin waves cause the direction of the staggered spin to rotate through the whole 3D spin-space. The domain wall, however, remains well defined.
in spin space, since the $\pi$ jump in the antiferromagnetic order is preserved. This rotation of the staggered spin through all possible 3D orientations is expected, since the effect of this Goldstone mode is to restore the broken symmetry of the system (in this case, the broken symmetry is that $\vec{z}$ is chosen as the direction of the staggered spin). In a real system, where the 1D chain is embedded in a larger 3D structure, there are small anisotropy effects (such as crystal fields) to break the symmetry. In this case, rotation of the staggered spin is confined to small angles relative to the direction of anisotropy.

We have also investigated the additional effect of spin waves on damping the motion of a domain wall. While there is a decrease in the maximum speed reached by the domain wall, the effect is relatively small and within the error bars shown in Fig.6.5. We believe that this may be a consequence of the small $U/t$ values considered. On the other hand, the behavior of the system is expected to be dominated by the magnetic degrees of freedom in the large $U/t$ limit. In the small $U/t$ limit, the charge degrees of freedom dictate the behavior of the system. However, due to the fact that the semi-classical TDHF does not describe tunneling, the study of the motion of charged domain walls for larger $U/t$ values and the influence of spin-waves requires a more general variational formulation such as that of the CI method.

Figure 6.5: Maximum speed of a domain wall in the presence of collective excitations, as a function of the electric field $e\vec{E}/t$. The speed is measured in units of $a\vec{t}/\hbar$, and the values shown correspond to $U/t = 2, 3, 4$. The large error bars are due to the fact that as the soliton emits collective excitations its center of mass oscillates as well, and therefore its motion is not just a smooth translation as in the absence of collective excitations.
6.2.2 Domain-wall motion in an ac electric field

As in the case of static electric fields, one can distinguish two different regimes in the response of the domain-wall to an ac electric field. If the intensity of the fields is fairly small and its frequency fairly large, we observe the motion of the domain wall to be that of a charged relativistic particle in an ac electric field with no damping.

More interesting is the other regime, where damping takes place. In this case, we observe absorption of energy from the domain wall to the excitations of the charge and spin background. In addition to damping from excitations created by the domain-wall itself, in a real system collective excitations are thermally activated.

6.2.3 Motion of the charged spin-bag in a static electric field

This problem cannot be studied realistically within TDHF, since this semi-classical approximation does not describe tunneling. The charged spin-bag has a spin $1/2$, as discussed in Section 3.2. As a result, a spin bag must remain on the same AFM sublattice. Moving to the other sublattice involves a spin-flip, a process which is forbidden in the absence of external magnetic fields. Thus, a spin-bag must tunnel a total of two lattice constants to the next allowed position. The TDHF can only describe how the system climbs over the potential barrier, which in this case is very high. Numerically, this is seen from the fact that the electric field must be extremely large $(eaE/t \sim 1)$ before the spin-bag moves at all. At such large fields the energy gained from even a very small translation is large enough to excite the doping hole into the valence band (field ionization of the spin-bag).

The results from Configuration Interaction method (which allows quantum tunneling) suggest that the actual propagation mechanism for the charged spin-bag is to dissociate into a charged bosonic domain-wall and a neutral spin-$1/2$ domain wall (see Section 5.3.4). The wavefunction describing such a process is much more complicated than the Slater determinant allowed for by the TDHF.

In conclusion, TDHF is of limited value in describing the nonlinear dynamics of the charged excitations. Its utility is limited to domain-walls in the small $U/t$ limit. However, as we show below, TDHF is well suited for characterizing linear collective excitations, such as spin-waves and plasmons.

6.3 The Random Phase Approximation

The Random-Phase Approximation (RPA) is a limiting case of the TDHF Approximation, in which one assumes that a weak time-dependent external field induces small oscillations of the system about its static self-consistent Hartree-Fock ground-state. This method allows
the identification of the normal modes (collective modes) of the system, as well as calculation of response functions (susceptibilities) in the linear approximation.

Since the reference state is the self-consistent static HF solution $|\Psi_o\rangle$, it is convenient to work directly with the one-particle operators which diagonalize this state (see Eqs. (3.3), (3.4), (6.3), (6.4))

$$a_n^\dagger = \sum_{i,\sigma} \phi_n(i, \sigma) c_{i\sigma}^\dagger \quad \text{and} \quad |\Psi_o\rangle = \prod_{p=1}^{N_o} a_p^\dagger |0\rangle$$

with $\phi_n(i, \sigma)$ the one-particle wavefunctions of the self-consistent HF Slater determinant. In terms of these operators, a general linear coupling to an external time-dependent field is described by interaction

$$\mathcal{H}_{ext} = \lambda \sum_{n,m} f_{nm}(t) a_n^\dagger a_m.$$  \hspace{1cm} (6.12)

Here, $\lambda$ characterizes the strength of the weak external field ($\lambda \ll 1$) and is introduced as a device to keep track of the order of perturbation. Some examples are the coupling to external electric fields $\hat{\rho} \rho(t)$ or $\vec{j} \cdot A(t)$ or magnetic fields $\vec{S} \cdot \vec{B}(t)$. The density of charge $\rho$, the density of current $\vec{j}$ and the spin $\vec{S}$ operators are all quadratic combinations of electron creation and annihilation operators.

Using perturbation theory, the wave-function of the system in the presence of $\mathcal{H}_{ext}$ has the general form $|\Psi(t)\rangle = |\Psi_o(t)\rangle + \lambda |\Psi_1(t)\rangle + \ldots$, where $|\Psi_o(t)\rangle = \exp(-\frac{i}{\hbar} E_{GSM}(t)|\Psi_o\rangle$ is the ground-state wavefunction. The first order perturbation in the wave-function induces small (first-order) deviations of the self-consistent Hartree-Fock fields from their ground-state self-consistent values as follows:

$$Q(i, t) = \langle \Psi(t) | \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} | \Psi(t) \rangle = Q(i) + \lambda q(i, t) + O(\lambda^2)$$  \hspace{1cm} (6.13)

$$\vec{S}(i, t) = \langle \Psi(t) | \frac{1}{2} \sum_{\alpha,\beta} c_{i\alpha}^\dagger \vec{S}_{\alpha\beta} c_{i\beta} | \Psi(t) \rangle = \vec{S}(i) + \lambda \vec{s}(i, t) + O(\lambda^2)$$  \hspace{1cm} (6.14)

where $Q(i) = \langle \Psi_o | \sum_{\alpha} c_{i\alpha}^\dagger c_{i\alpha} | \Psi_o \rangle$ and $\vec{S}(i) = \langle \Psi_o | \frac{1}{2} \sum_{\alpha,\beta} c_{i\alpha}^\dagger \vec{S}_{\alpha\beta} c_{i\beta} | \Psi_o \rangle$. Thus, to first order in perturbation theory, the effective perturbation of the mean-field Hamiltonian (see Eq. (6.5)) is given by

$$\mathcal{H}_{eff} = \mathcal{H}_{ext} + \lambda U \sum_{i,\alpha,\beta} c_{i\alpha}^\dagger \left( \frac{1}{2} \delta_{\alpha\beta} q(i, t) - \vec{s}_{\alpha\beta} \vec{s}(i, t) \right) c_{i\beta} = \lambda \sum_{n,m} V_{nm}(t) a_n^\dagger a_m,$$  \hspace{1cm} (6.15)

where

$$V_{nm}(t) = f_{nm}(t) + U \sum_{i,\alpha,\beta} \phi_n^\ast(i\alpha) \left( \frac{1}{2} \delta_{\alpha\beta} q(i, t) - \vec{s}_{\alpha\beta} \vec{s}(i, t) \right) \phi_m(i\beta).$$  \hspace{1cm} (6.16)

To leading order in perturbation theory, the perturbed wave-function (up to an arbitrary
phase factor) is given by:

\[ |\Psi(t)\rangle = e^{-\frac{i}{\hbar} E_{\text{ext}} t} \left( |\Psi_0\rangle + \lambda \sum_{p=1}^{N_e} \sum_{h=N_v+1}^{N} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{V_{hp}(\omega) \exp(-i\omega t)}{\hbar \omega - (E_h - E_p) + i\eta} a_h^{\dagger} a_p |\Psi_0\rangle + O(\lambda^2) \right) \]  

(6.17)

Here \( V_{hp}(\omega) \) is the Fourier transform of \( V_{hp}(t) \) (see Eq. 6.16), and \( E_h, E_p \) are the one-particle energies of the unperturbed hole and particle orbitals \( \phi_n, \phi_p \). This result shows that the external perturbation adds particle-hole excitations to the ground-state wavefunction, as expected. Although the wavefunction (6.16) does not appear as a single Slater determinant, it can be reexpressed as a single TDHF Slater determinant if all orders in perturbation theory are retained.

The wavefunction \( |\Psi(t)\rangle \) must satisfy the self-consistency conditions (6.13), (6.14), up to the first order in the perturbation parameter \( \lambda \). These conditions lead to a closed system of equations for the parameters \( q(i,t) \) and \( s'(i,t) \). Once this system is solved for these parameters, the matrix elements \( V_{nm}(t) \) of (6.16) can be evaluated, and the perturbed wave-function (6.17) is determined. This, in turn, yields the response of the system to the external field.

We define the coefficients

\[ D_{\alpha\beta}(i,t) = \bar{s}_{\alpha\beta} s(i,t) - \frac{1}{2} \delta_{\alpha\beta} q(i,t). \]  

(6.18)

Using the wavefunction (6.17) the self-consistency equations (6.13), (6.14) become

\[ D_{\alpha\beta}(i,\omega) = \sum_{\alpha_1, \beta_1, \alpha_2, \beta_2} \sum_{\alpha_1, \beta_1, \alpha_2, \beta_2} \Gamma^{\alpha_1, \beta_1}_{\alpha_2, \beta_2} \left( \frac{\phi_{\alpha_1}(i, \alpha_1) \phi_{\beta_1}(i, \beta_1) V_{hp}(\omega)}{\hbar \omega - (E_h - E_p) + i\eta} - \frac{\phi_{\alpha_2}(i, \alpha_2) \phi_{\beta_2}(i, \beta_2) V_{ph}(\omega)}{\hbar \omega - (E_h - E_p) + i\eta} \right) \]  

(6.19)

where \( \Gamma^{\alpha_1, \beta_1}_{\alpha_2, \beta_2} = \delta_{\alpha_1, \alpha_2} \delta_{\beta_1, \beta_2} - \delta_{\alpha_1, \beta_2} \delta_{\alpha_2, \beta_1} \) and

\[ V_{nm}(\omega) = f_{nm}(\omega) - U \sum_{\alpha_2} \phi_{\alpha}^{\dagger}(i, \alpha) D_{\alpha\beta}(i,\omega) \phi_{\alpha}(i, \beta). \]  

(6.20)

We consider a system with \( N \) states (corresponding to \( N/2 \) sites times two spins per site) and \( N_e \) electrons. For each frequency, \( \omega \), we have \( 2N \) unknown \( D_{\alpha\beta}(i,\omega) \) elements, and \( 2N_e(N - N_e) \) unknown matrix elements \( V_{hp}(\omega) \) and \( V_{ph}(\omega) \).

It is straightforward to verify that this system of equations (6.19), (6.20) is indeed equivalent to the conventional RPA matrix equation [125]. For this, we define

\[ X_{hp} = \frac{V_{hp}(\omega)}{\hbar \omega - (E_h - E_p) + i\eta}, \quad Y_{hp} = \frac{V_{ph}(\omega)}{\hbar \omega - (E_h - E_p) + i\eta} \]

and eliminate the \( D_{\alpha\beta}(i,\omega) \) elements from the system. This leads immediately to the RPA.
The RPA matrix for the Hubbard model is given by:

\[ A_{hp,h'p'} = \delta_{pp'} \delta_{hh'} (\epsilon_h - \epsilon_p) + a_{hp',ph'} \]

\[ B_{hp,h'p'} = a_{hh',pp'} \]

with

\[ a_{hp,h'p'} = U \sum_i \left( \phi_h^n(i \uparrow) \phi_p^n(i \downarrow) - \phi_p^n(i \uparrow) \phi_h^n(i \downarrow) \right) \left( \phi_{h'}(i \uparrow) \phi_{p'}(i \downarrow) - \phi_{p'}(i \uparrow) \phi_{h'}(i \downarrow) \right) \]

Once the ground-state self-consistent Hartree-Fock eigenenergies and eigenfunctions \( E_n, \phi_n(i\alpha) \) are known, it is straightforward to set up the RPA matrix equation (6.21) and compute the response of the system to the weak external field \( f \). The non-trivial solutions of the RPA equation in the absence of external fields \( (f_{nm}(t) = 0) \) are the normal (collective) modes of the system. Modes for which \( s_x(i,t) \neq 0, s_y(i,t) \neq 0 \) and \( s_z(i,t) = q(i,t) = 0 \), are spin-waves, whereas modes for which \( q(i,t) \neq 0, s_x(i,t) \neq 0 \) and \( s_z(i,t) = s_y(i,t) = 0 \) are charge excitations (plasmons). In the doped systems more general charge-spin collective modes exist, with all four perturbation fields simultaneously different from zero (e.g. spin-waves bound to the core of a doped soliton).

However, the conventional RPA equation (6.21) is cumbersome since the dimension of the RPA matrix, \( 2N(N - N_e) \), is extremely large, and numerical calculations can be performed only for very small systems (in 2D, up to \( 4 \times 4 \) lattices). This is circumvented in our formulation of the RPA by solving the system (6.19),(6.20) for the \( 2N \) variables \( D_{\alpha\beta}(i,\omega) \) first. Eliminating \( V_{hp} \) and \( V_{ph} \), we obtain another matrix equation

\[ \sum_{j\alpha'\beta'} M_{\alpha\beta,\alpha'\beta'}(i,j,\omega) D_{\alpha'\beta'}(j,\omega) = d_{\alpha\beta}(i,\omega) \]  

(6.22)

where

\[ M_{\alpha\beta,\alpha'\beta'}(i,j,\omega) = \delta_{\alpha\alpha'} \delta_{\beta\beta'} \delta_{ij} + U \sum_{p=1}^{N_e} \sum_{h=N_e+1}^{N} \sum_{\sigma\sigma'} T_{\alpha\beta}^{\sigma\sigma'} \]

\[ \left( \frac{\phi_p^n(i\sigma)\phi_h(\sigma')\phi_p^n(j\alpha')\phi_p^n(j\beta')}{\hbar \omega - (E_h - E_p) + i\eta} - \frac{\phi_h^n(i\sigma)\phi_p^n(i\sigma')\phi_p^n(j\alpha')\phi_h^n(j\beta')}{\hbar \omega + (E_h - E_p) + i\eta} \right) \]

(6.23)
and

\[ d_{\alpha\beta}(i\omega) = \sum_{\mu=1}^{N_{c}} \sum_{\delta=N+1}^{N} \sum_{\alpha^\prime} \mathcal{R}_{\alpha\alpha^\prime
}(\phi_p^{\ast}(i\sigma)\phi_h(i\sigma')[f_{hp}(\omega) - \frac{\phi_h^{\ast}(i\sigma)\phi_p(i\sigma')f_{ph}(\omega)}{\hbar\omega - \left(E_h - E_p \right) + i\eta} - \frac{\phi_h^{\ast}(i\sigma)\phi_p(i\sigma')f_{ph}(\omega)}{\hbar\omega - \left(E_h - E_p \right) + i\eta}] \]  
(6.24)

In the absence of the external field \(d_{\alpha\beta} = 0\), the collective modes of the system are given by the non-trivial solutions of \(\det |M_{\alpha^\prime\alpha'}(i,j,\omega)| = 0\) (see Eq. (6.22)).

The advantage of this new formulation is the small dimension of the matrix \(M\), as compared to the RPA matrix. For example, if we consider a system near half-filling \(N_c \sim N/2\), then the dimension of the RPA matrix is \(N^2/2\), while the dimension of the \(M\) matrix is \(2N\). This simplification allows us to solve the problem in the \(M\) formulation for systems for which the RPA matrix is unmanageable numerically. The drawback of the \(M\)-matrix formulation is that one must solve the system (6.22) for each frequency \(\omega\) of interest.

Physically, this dimension difference can be understood in the following way. The matrix RPA approach (6.21) calculates the one-particle Green's functions \(X_{hp}, Y_{hp}\) for all possible particle-hole excitation and annihilation processes. Since any perturbative evolution can be decomposed as a sum of such elementary processes, once these Green's functions are known the problem is solved. The \(M\)-matrix approach, on the other hand, first calculates the self-consistent Hamiltonian in the presence of the perturbation, and then finds the corresponding wave-function and response of the system. In order to have the self-consistent Hamiltonian, the perturbations in the Hartree-Fock fields \(q(i,t) = Q(i,t) - Q(i)\) and \(s(i,t) = S(i,t) - S(i)\) are needed, and these are provided by the solutions \(D_{\alpha\beta}(i,\omega)\) of Eq. (6.22).

### 6.3.1 Spin waves of the undoped AFM chain

The undoped AFM chain exhibits a branch of gapless spin-waves (Goldstone modes). From the analogy with the Heisenberg model (which is valid for large \(U/t\)), these spin-waves have a spectrum of the form \(E_{\text{sw}}(k) = J\sin(ka)\). The results obtained from the \(M\)-matrix approach for a chain of 40 sites and \(U/t = 3, 4, 8\) (circles, squares, diamonds) are shown in Fig.6.6. The eigenergies are the values \(\omega\) for which \(\det |M_{\alpha^\prime\alpha'}(i,j,\omega)| = 0\). For each eigenergy we find the corresponding solution \(D_{\alpha\beta}(i,\omega)\) from Eq.(6.14). This solution is of the form \(s_z(i,\omega) \neq 0, s_y(i,\omega) \neq 0, s_z(i,\omega) = q(i,\omega) = 0\), i.e. it is a spin-wave. Straightforward Fourier transformation of \(s_z(i,\omega), s_y(i,\omega)\) gives the momentum \(k\) of the spin-wave. Since the chain is finite, only spin-waves with certain momenta \(k\) within the Brillouin zone are excited. For comparison, full lines are the spin-wave spectra predicted by the Heisenberg model, for \(J = 4t^2/U = 1.33, 1, 0.5\). The agreement is excellent for \(U/t = 8\), and reasonable for \(U/t = 3\). The Heisenberg model is a second-order perturbation approximation to the Hubbard model. The deviations in spin-wave spectra between the two models is of the order \(t^4/U^3\) and thus very small.
The M-matrix also has non-trivial solutions for energies $\omega \geq 2US$. These solutions all have $q(i, \omega) \neq 0$, and are associated with charge excitations across the Mott-Hubbard gap.

The characterization of the collective excitations of the doped chains is more complex. As a result of the inhomogeneity introduced by the localized charge, the momentum $k$ is no longer a good quantum number. Also, various mixed excitations appear, such as spin-waves bound to the charged core, and low-energy charge excitations related to the deformation of the charged core.

6.3.2 Spin waves of the undoped AFM plane

For the 2D planes, we can again identify the spin-wave spectra exactly as in the 1D case, and compare them to the Heisenberg spin-wave spectrum. The comparison is very similar to that of the 1D case. One difficulty in this case is that there are much fewer $k$-points due to the much smaller linear size of the 2D sample (e.g. for a $10 \times 10$ lattice there are 5 $k$-points on the symmetry lines in the Brillouin zone). For the doped sample, the coupled charge-spin excitation spectrum is complex.
6.4 Summary

Due to the semi-classical nature of the TDHF method, it can only be used to characterize the dynamics of domain-walls for rather small values of the Hubbard parameter $U/t < 5$. For this case, we find a relativistic dynamics, with the maximum relativistic speed given by the Fermi velocity of non-interacting electrons, and the rest mass of the domain wall of the order of the electron mass.

TDHF also describes the interactions of charged domain-walls with plasmon and spin-wave collective excitations. For small $U/t$, plasmons damp the soliton motion. The spin-waves act to restore the broken symmetry of the mean-field background.

The RPA method is a limiting case of the TDHF. It leads to the identification of the collective modes and evaluation of response functions. We have identified an alternative way of performing RPA suitable for medium and large systems for which the conventional RPA matrix approach is numerically impractical. However, the RPA time evolution of the system is simply linearized dynamics in the neighborhood of the static Hartree-Fock state. A clear way to improve both TDHF and RPA is to start from a Configuration Interaction state. This would mean a homogeneous ground state even for the doped system (simplifying characterization of collective excitations) and also would allow tunneling (translational) motion of the charged solitons and therefore a calculation of the entire response function of the system.
Chapter 7

Summary and Conclusions

This thesis presents a study of the strongly correlated, purely repulsive 1D electron systems as described by the generalized spin-flux Hubbard model. This model is believed to have direct relevance for understanding the high-temperature superconductivity as well as a host of unusual magnetic, optical, transport, ARPES, etc. properties of the cuprates.

The key ingredient that distinguishes our model from previous studies of the Hubbard model is the concept of quantized spin-flux [21]. The spin-flux is a direct non-trivial consequence of adding longer range Coulomb repulsion in the generalized Hubbard model. Inclusion of the spin-flux, even at the mean-field level, leads to a renormalization of the electronic spectrum of the half-filled AFM system which is in good agreement with dispersion relations measured experimentally through Angle Resolved Photoemission Spectroscopy.

We first studied the consequences of doping the 2D AFM using the static self-consistent unconstrained Hartree-Fock Approximation. As a result of the modified dispersion relations in the presence of the spin-flux, a new type of charged collective excitation is stabilized. This is the meron-vortex, which is a doping-hole trapped in the core of an antiferromagnetic vortex. This excitation carries charge but no spin, and it is a direct analog of the 1D charged bosonic domain wall of the Hubbard model, as well as of the charged bosonic domain wall of the polyacetylene. In analogy to these 1D excitations, the meron-vortex is also a topological object, characterized by a topological number \( \nu = \pm 1 \). This topological number is the winding number of the spins on any closed loop in real space surrounding the core of the vortex. In contrast to the 1D case, in 2D the non-trivial topological number of the vortex leads to a strong topological attraction between a vortex \((\nu = 1)\) and an antivortex \((\nu = -1)\). The attraction potential increases logarithmically with the distance between the vortex cores, and as a result it is stronger than even fully unscreened Coulomb repulsion between the doping charges trapped in the cores of the vortices. Thus, we automatically obtain an extremely strong pairing attraction between a meron and an antimeron. At low doping \((\delta < 0.4)\), a liquid of such meron-antimeron pairs is found to describe the ground-
state of the system, at the static Hartree-Fock level, for $3 < U/t < 8$. Since the charge carriers are collective meron excitations conventional charged quasiparticles of Fermi-liquid theory are absent. At higher dopings ($\delta > 0.4$) the spin-flux phase becomes unstable to the conventional model, leading to a homogeneous, Fermi-like liquid. In the absence of the spin-flux, the meron-antimeron pairs are not stable, and the ground-state of the doped system is a collection of charged stripes.

Even in this simplest static HFA (Chapters 3 and 4) the appearance of a liquid of meron-vortices with doping can explain some of the unusual experimental features of the cuprate compounds. However, quantum hopping of the charged solitons is extremely important for a proper description of interactions with electric fields, as well as a characterization of all dynamic properties. This quantum hopping is excluded in the static HFA, but can be described within the Configuration Interaction (CI) Approximation.

As a diagnostic of the CI method, we first studied the 1D Hubbard model. This enabled us to gauge its accuracy against the exact solution of the 1D model, given by the Bethe Ansatz. In addition to quite remarkable agreement between the energy of the mobile charged bosonic domain-wall excitation (as given by the CI method) and the exact energy of the doping hole (as given by Bethe Ansatz solution), we also obtained a clear demonstration of the spin-charge separation in 1D. The quasiparticle-like charged fermionic spin-polaron was shown to decay into a charged bosonic domain wall (which carries the charge but no spin) and a neutral fermionic domain wall (which carries the spin but no charge). These results clearly confirm the validity and accuracy of the CI method. They also suggest that the essence of the Bethe solution is recaptured by allowing the quantum hopping of the charged excitations.

In 2D, the CI method clearly shows that the meron-antimeron pair is mobile, thus substantiating the claim that a liquid of such pairs should have metallic properties. The CI method also allows us to identify the rotational symmetry of the meron-antimeron pair. The most stable pairs have d-wave symmetry, and a total momentum of $(\pi, \pi)$. A second region of stability, at much higher energies, has pairs with s-wave symmetry and total momentum $(0, 0)$. The appearance of both d-wave and s-wave symmetry, with a dominant (more stable) d-wave component is consistent with numerous experiments. There are also strong indications of the possibility of spin-charge separation in 2D, through the decay of the quasiparticle-like charged fermionic spin-bag into a singly-charged vortex-antivortex pair.

Addition of the spin-flux to the Hubbard model thus leads to a microscopic model which recaptures some of the more puzzling aspects of the cuprate physics. We find strong attractive pairing in a purely repulsive electron system, which suggests the existence of preformed meron-antimeron pairs with d-wave symmetry up to quite high temperatures. With
the incorporation of three-dimensional couplings, such a liquid of bosons is expected to Bose condense at low temperatures, leading to d-wave superconductivity. Nucleation of meron-antimeron pairs with doping also explains the rapid loss of long range antiferromagnetic order. At the same time, antiferromagnetic correlations with a coherence length equal to the average hole separation survive to much higher dopings. A liquid of bosonic charge carriers naturally exhibits non-Fermi-liquid properties. Another argument for this is that the meron-vortices are collective charged excitations created through the decay of quasiparticle-like charged fermionic spin-bags. Thus, there are no quasiparticles left in the system. The existence of well-defined quasiparticles is the cornerstone of Fermi-liquid theory. The sub-gap electronic structure of levels bound in the meron-cores explain the appearance of the mid-infrared gap that develops with doping. These are present both above and below the superconducting transition temperature $T_c$. Finally, in the overdoped region a transition to a conventional Fermi-liquid is predicted.

We believe that this microscopic picture warrants further development. One of the more obvious directions is the study of the response functions of the quantum liquid of meron-antimeron pairs. A simple Random-Phase Approximation treatment is not enough, since the essential quantum motion of the charged solitons is absent in these approximations. A generalization of the CI method for time-dependent Hamiltonians describing interactions of the system with external fields is warranted. This should also allow calculation of the spectrum of the low-energy excitations, such as spin-waves and other collective modes in the quantum liquid phase at non-vanishing temperatures. The long range part of the Coulomb repulsion between doping charges may also play a more important role in the properties of this novel quantum liquid than it does in a conventional Fermi liquid where standard screening arguments apply. Additional interactions such as crystal field effects and conventional spin-orbit interaction, which help to stabilize uncharged meron-vortices, may need to be added in the starting Hamiltonian before quantitative comparison with the experimental data can be made.

Other avenues of study are the investigation of the superconducting state itself, as well as that of the pseudogap region. As argued in Chapter 2, a possible interpretation of these phenomena, in qualitative agreement with our picture, is that pre-formed pairs exist for temperatures $T < T^*$, but coherence between pairs occurs only below $T_c$, where the system becomes superconducting (the bosonic charged meron-antimeron pairs Bose condense). We believe that nucleation of singly-charged vortex-antivortex pairs, as well as doubly-charged meron-antimeron pairs with doping may provide a basis for the rich phase diagram of the cuprates. A quantitative description of the superconductivity must also include 3D interactions between CuO$_2$ planes.
Appendix A

Green's functions method

In this Appendix we provide a full description of the Green's function method for treatment of magnetic solitons on the 1D Hubbard chain. This method allows the study of one doping hole (electron) on an infinite chain by using Green's functions. In particular, we studied in detail domain walls with this method, although it can very easily be used for the study of spin-bags as well. This Green's function approach has the advantage of allowing direct calculation of quantities such as local and total density of states, which are not obtainable from finite chain Hartree-Fock analysis. However, it is restricted to the study of just one hole (at most, a tightly-bound pair of holes) configurations, and it depends essentially on the ability to calculate the Green's function of the undoped Hartree-Fock AFM ground state analytically. This is straightforward in 1D, but not in 2D.

A.1 The half-filled antiferromagnetic background

We first consider the electronic structure of the undoped 1D antiferromagnet with long range order (LRO). This LRO is induced by the magnetic interaction of electrons in the chain with other electrons in the 3D crystal in which the chain is embedded.

We start with the mean-field factorized 1D Hamiltonian (see (3.9))

$$\mathcal{H} = -t \sum_{\iota,\sigma} \left( c_{\iota+1,\sigma}^{\dagger} c_{\iota,\sigma} + c_{\iota+1,\sigma}^{\dagger} c_{\iota,\sigma} \right) - U \sum_{\iota,\alpha,\beta} c_{\iota,\alpha}^{\dagger} \left( \vec{S}(i) \cdot \vec{\sigma}_{\alpha,\beta} \right) c_{\iota,\beta} + U \sum_{\iota} \left( \vec{S}^2(i) + 1/4 \right) \quad (A.1)$$

where $\vec{S}(i) = (-1)^{i+1} \vec{e}_z$ ($\vec{e}_z$ is a unit vector of some arbitrary direction) and $Q(i) = 1$ are the mean-field choice for the total spin and charge at each site $i$ of an undoped AFM. The value of $S$ is determined self-consistently.

It is useful to introduce the spinor fields $\chi_i^+ = \left( c_{i,\uparrow}^{\dagger} \quad c_{i,\downarrow}^{\dagger} \right)$ and the Bloch operators $\chi_k^{(i)} = N^{-1/2} \sum_x \exp(-ikx) \chi_x^{(i)}$. Here $x_i = 2na + (i-1)a$ is the position of the site $i = 1, 2$ of the $n^{th}$ unit cell. The sum is performed over all the $N$ unit cells. Using the four-component
operators $\Phi_k^\dagger = \left( \chi_k^{(1)^\dagger} \chi_k^{(2)^\dagger} \right)$, the electronic part of the mean-field Hamiltonian (A.1) can be expressed as:

$$\mathcal{H}_{el} = \sum_k \Phi_k^\dagger \begin{pmatrix} U \sigma_z & \epsilon_k \\ \epsilon_k & -U \sigma_z \end{pmatrix} \Phi_k$$

(A.2)

The sum is performed over the first Brillouin zone $-\pi/2a < k \leq \pi/2a$ and $\epsilon_k = -2t \cos(ka)$.

We introduce the conduction- and valence-band operators $\left( \chi_k^+, \chi_k^- \right) = \Phi_k^\dagger U$, where:

$$U = \begin{pmatrix} 0 & -\alpha_k^{(-)} & \alpha_k^{(+)} \\ \alpha_k^{(+)} & 0 & -\alpha_k^{(-)} \\ -\alpha_k^{(-)} & 0 & \alpha_k^{(+)} \end{pmatrix}$$

(A.3)

$$\alpha_k^{(\pm)} = \sqrt{\frac{1}{3} \left( 1 \mp \frac{U_S}{E_k} \right)}$$

and $E_k = \sqrt{\epsilon_k^2 + (US)^2}$. The Hamiltonian can be expressed as:

$$\mathcal{H}_{el} = \sum_k E_k \left( \chi_k^+ \chi_k^- - \chi_k^{+\dagger} \chi_k^- \right)$$

(A.4)

Thus, the electronic part of the undoped AFM mean-field Hamiltonian (A.1) consists of two electronic bands characterized by the dispersion relations:

$$E_k^{c/v} = \pm \sqrt{\epsilon_k^2 + (US)^2} \quad k \in (-\pi/2a, \pi/2a]$$

where $\epsilon_k = -2t \cos(ka)$ and $a$ is the lattice constant. The conduction band has doubly-degenerate levels described by the dispersion relation $E_k^c = E_k$ while the valence band has doubly-degenerate levels described by $E_k^v = -E_k$. The bands are separated by the Mott-Hubbard gap of magnitude $2US$ opened at the Fermi points $(k_o = \pm \pi/2a)$. The one-electron band wavefunctions are given by:

$$\mathcal{C}_{k\sigma}(m, \sigma) = \langle m \sigma | c_{k\sigma}^\dagger | 0 \rangle = \frac{\delta_{\sigma,\sigma'} e^{ikma}}{\sqrt{N}} \left( \alpha_k^{(\sigma \sigma')} e_m + \alpha_k^{(\sigma' \sigma)} o_m \right)$$

(A.5)

$$\mathcal{V}_{k\sigma}(m, \sigma) = \langle m \sigma | v_{k\sigma}^\dagger | 0 \rangle = \frac{\delta_{\sigma,\sigma'} e^{ikma}}{\sqrt{N}} \left( \alpha_k^{(-\sigma \sigma')} e_m - \alpha_k^{(-\sigma' \sigma)} o_m \right)$$

(A.6)

Here $e_m = 1$ if $m$ is an even number and 0 if $m$ is an odd number, and $o_m = 1 - e_m$. Each of these levels is doubly-degenerate, corresponding to spin 'up' and spin 'down' degrees of freedom: if the wavefunction corresponding to spin 'up' is concentrated mainly at the odd sites, then the degenerate wavefunction corresponding to spin 'down' is concentrated mainly at the even sites, and vice versa. At half-filling, all the states in the valence band ($E_k^v < 0$) are occupied, while all the states in the conduction band ($E_k^c > 0$) are empty.
A.1.1 The Green's function of the undoped AFM background

The matrix elements of the Green's function $\hat{G}^u(E) = 1/(E - \mathcal{H}_{el})$ in the site-spin basis space are given by:

$$G^u_{\sigma\sigma'}(m, n; E) = \langle m\sigma|\hat{G}^u(E)|n\sigma'\rangle = \delta_{\sigma,\sigma'} \sum_k \left[ \frac{C_{k\sigma}(m, \sigma)C_{k\sigma}^*(n, \sigma)}{E - E_k - i\eta} + \frac{V_{k\sigma}(m, \sigma)V_{k\sigma}^*(n, \sigma)}{E + E_k - i\eta} \right].$$

Substituting the band wavefunctions and performing the sum over the Brillouin zone, we obtain the following expressions for the Green's functions of the chain in the ground state:

a) If $m$ and $n$ are both even or both odd, then:

$$G^u_{\sigma\sigma}(m, n; E) = (E + (-1)^m\sigma U S) \left\{ \begin{array}{ll}
-i|m-n|e^{-|m-n|\phi}(2t^2 \sinh 2\phi)^{-1} & \text{if } |E| \leq U S \\
l e^{-|m-n|\phi}(2t^2 \sin 2\phi)^{-1} & \text{if } U S \leq |E| \leq \gamma \\
e^{-|m-n|\phi}(2t^2 \sinh 2\phi)^{-1} & \text{if } \gamma \leq |E| 
\end{array} \right.$$

b) If $m$ and $n$ have different parities, then:

$$G^u_{\sigma\sigma}(m, n; E) = \left\{ \begin{array}{ll}
i e^{-|m-n|\phi}(2t \cosh \phi)^{-1} & \text{if } |E| \leq U S \\
i e^{-|m-n|\phi}(2t \sin \phi)^{-1} & \text{if } U S \leq |E| \leq \gamma \\
e^{-|m-n|\phi}(2t \sinh \phi)^{-1} & \text{if } \gamma \leq |E| 
\end{array} \right.$$

The angle $\phi > 0$ is defined by:

$$\phi = \left\{ \begin{array}{ll}
sinh^{-1}(\sqrt{(US)^2 - E^2}/2t) & \text{if } |E| \leq U S \\
\sin^{-1}(\sqrt{\gamma^2 - E^2}/2t) & \text{if } U S \leq |E| \leq \gamma \\
\sinh^{-1}(\sqrt{E^2 - \gamma^2}/2t) & \text{if } \gamma \leq |E| 
\end{array} \right.$$

and $\gamma = \sqrt{4t^2 + (US)^2}$.

A.1.2 Self-consistency of the antiferromagnetic background

The LDOS (local density of states) projected onto site $n$ and spin direction $\sigma$, is defined in terms of the one-electron Green's function:

$$\rho^u_{n\sigma}(E) = \text{sgn}(E) \frac{1}{\pi} \Im G^u_{\sigma\sigma}(n, n; E).$$

Using the Green's function of the undoped AFM background, we obtain the Local Density of States of the undoped chain to be given by

$$\rho^u_{n\sigma}(E) = \frac{\text{sgn}(E)(E + (-1)^m\sigma U S)}{\pi \sqrt{[E^2 - (US)^2][[(US)^2 + 4t^2 - E^2]]}}.$$
for $US \leq |E| \leq \sqrt{(US)^2 + 4t^2}$ and 0 otherwise.

The total number of states per site per spin-direction in each one of the bands can be calculated by integrating the LDOS over the corresponding ranges of energies. The results are shown in Table A.1.

<table>
<thead>
<tr>
<th># states</th>
<th>$n=$even</th>
<th>$n=$odd</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma = \uparrow$</td>
<td>$\sigma = \downarrow$</td>
<td>$\sigma = \uparrow$</td>
</tr>
<tr>
<td>$\int_{\text{f.band}} dE \rho_{\text{f.band}}^\sigma(E) = \frac{1}{2} + S_0$</td>
<td>$\frac{1}{2} - S_0$</td>
<td>$\frac{1}{2} - S_0$</td>
</tr>
<tr>
<td>$\int_{\text{v.band}} dE \rho_{\text{f.band}}^\sigma(E) = \frac{1}{2} - S_0$</td>
<td>$\frac{1}{2} + S_0$</td>
<td>$\frac{1}{2} + S_0$</td>
</tr>
</tbody>
</table>

Table A.1: Number of states per site, per spin direction, in the valence and conduction bands.

Here,

$$S_0 = \frac{US}{2N} \sum_k \frac{1}{E_k}$$  \hspace{1cm} (A.7)

In the ground state, at half-filling, there is one electron per site:

$$Q(i) = \int_{\text{v.band}} dE \left( \rho_{\text{f.band}}^\sigma(E) + \rho_{\text{n.b}}^\sigma(E) \right) = 1.$$  

Also, the spin at each site is given by:

$$S^z(i) = \frac{1}{2} \int_{\text{v.band}} dE \left( \rho_{\text{f.band}}^\sigma(E) - \rho_{\text{n.b}}^\sigma(E) \right) = (-1)^{l_{i-1}} S_0$$  

$$S^y(i) = 0; \quad S^x(i) = 0.$$  

This mean-field solution is made self-consistent by requiring that the resulting spin, $S_0$, in equation (A.7) is equal to the assumed spin amplitude $S$. This condition of self-consistency is identical to the one obtained using the HF method (see Eq. (3.12)). The self-consistent staggered spin $S$ as a function of $U/t$ is plotted in Fig. 3.1.

Since all the states of the valence band are occupied, the energy of the AFM mean-field ground-state is simply given by:

$$E_{\text{GS}} = 2 \sum_k E_k'' + 2NU \left( S^2 + \frac{1}{4} \right)$$  

where $S = S_0$ in Eq. (A.7). This mean-field ground-state energy is also identical to that obtain through straightforward HF method, as given by Eq.(3.14). The dependence of the ground-state AFM background energy as a function of $U/t$ is shown in Fig. 3.2.

### A.2 Neutral domain wall solitons

A sharp-boundary soliton is a domain wall consisting of a simple juxtaposition of two halves of chain found in the two mean-field ground states (see Fig.A.1). We treat this case in some detail, since it serves as "reference case" for more general extended solitons. Also, analytic
calculations are possible and one can gain insight into the charge, spin and statistics of such solitons.

A.2.1 The neutral sharp-boundary soliton

The Green's functions for the Hamiltonian of the sharp-boundary soliton can be calculated analytically. We summarize our results below. In order to obtain a sharp-boundary soliton we must cut the chain, flip all the spins of one of the halves and then paste the two halves back together. We calculate, below, the Green's functions at each stage.

The Green's functions for a semi-infinite chain

Let $\mathcal{H}_{cl}$ be the hamiltonian for the mean-field AFM background state, and $G^{0}_{\alpha\beta}(n, m; E)$ the corresponding Green's function. In order to find the hamiltonian for half of this chain, we cut this chain between sites $-1$ and $0$. Assuming that the two halves of the chain do not interact, the Hamiltonian for the chain with the cut is $[126, 127] \mathcal{H}_{cl}^{h} = \mathcal{H}_{cl} + V_h$, where the potential $V_h$ describing the cut is chosen such that:

$$\langle n\sigma|\mathcal{H}_{cl}^{h}|n'\sigma' \rangle = 0$$

if $n$, $n'$ are on different sides of the cut, and

$$\langle n\sigma|\mathcal{H}_{cl}^{h}|n'\sigma' \rangle = \langle n\sigma|\mathcal{H}_{cl}|n'\sigma' \rangle$$
if \( n, n' \) are on the same side of the cut. The required \( V_h \) is given by \( \langle n\sigma|V_h|n'\sigma' \rangle = -\langle n\sigma|H_{el}|n'\sigma' \rangle \) if \( n, n' \) are on different sides of the cut and vanishes otherwise.

Since \( H_{el} \) is diagonal in the spin-space, all the other operators are diagonal in the spin-space. Therefore, Dyson’s equation for the chain with the cut is:

\[
G_{\sigma\sigma}^h(n, m; E) = G_{\sigma\sigma}^u(n, m; E) + \sum_{n', m'} G_{\sigma\sigma}^u(n, n'; E) < n'\sigma|V_h|m'\sigma > G_{\sigma\sigma}^h(m', m; E)
\]

Suppose that we first calculate the Green’s function for the right-hand side of the chain, \( n, m, m' \geq 0 \). In this case, the only nonvanishing term in the sum corresponds to \( n' = -1, m' = 0 \) and \( < -1\sigma|V_h|0\sigma > = t \). Then, Dyson’s equation can be solved and we find the Green’s function for the right-hand side of the chain:

\[
G_{\sigma\sigma}^{hR}(n, m; E) = G_{\sigma\sigma}^u(n, m; E) + \frac{G_{\sigma\sigma}^u(n, -1; E)G_{\sigma\sigma}^u(0, m; E)}{1 - tG_{\sigma\sigma}^u(0, -1; E)}
\]

where \( n \geq 0, m \geq 0 \).

The Green’s function for the left-hand side of the chain is calculated in the same way. We also flip the spins of this half, which means changing \( US \rightarrow -US \) in all expressions. We will denote by \( \tilde{G}_{\sigma\sigma}^u(n, m; E) \) the Green’s function obtained as a result of this substitution. Then, the Green’s function for the left-hand side of the chain is given by:

\[
G_{\sigma\sigma}^{hL}(n, m; E) = \tilde{G}_{\sigma\sigma}^u(n, m; E) + \frac{\tilde{G}_{\sigma\sigma}^u(n, 0; E)\tilde{G}_{\sigma\sigma}^u(-1, m; E)}{1 - t\tilde{G}_{\sigma\sigma}^u(-1, 0; E)}
\]

where \( n < 0, m < 0 \).

Thus, we can define the Green’s function for the two disconnected halves of the chain:

\[
G_{\sigma\sigma}^h(n, m; E) = \begin{cases} 
G_{\sigma\sigma}^{hR}(n, m; E) & \text{if } n \geq 0, m \geq 0 \\
G_{\sigma\sigma}^{hL}(n, m; E) & \text{if } n < 0, m < 0 \\
0 & \text{otherwise}
\end{cases}
\]

**Green’s function for the sharp-boundary chain**

In order to obtain the Green’s function for the sharp-boundary chain, we have to reconnect the two halves of the chain by subtracting the potential \( V_h \) added previously. Dyson’s equation for the Green’s function of the sharp-boundary soliton is:

\[
G_{\sigma\sigma}^s(n, m; E) = G_{\sigma\sigma}^h(n, m; E) - tG_{\sigma\sigma}^h(n, 0; E)G_{\sigma\sigma}^s(-1, m; E) - tG_{\sigma\sigma}^h(n, -1; E)G_{\sigma\sigma}^s(0, m; E)
\]

This equation can be solved exactly and one obtains the following results:
a) if \( n, m \geq 0 \), then:

\[
G_{\sigma\sigma}^*(n, m; E) = G_{\sigma\sigma}^{hR}(n, m; E) + t^2 \frac{G_{\sigma\sigma}^{hR}(n, 0; E)G_{\sigma\sigma}^{hL}(-1, 1; E)G_{\sigma\sigma}^{hR}(0, m; E)}{F_{\sigma}(E)}
\]

b) if \( n \geq 0, m < 0 \), then:

\[
G_{\sigma\sigma}^*(n, m; E) = -t \frac{G_{\sigma\sigma}^{hR}(n, 0; E)G_{\sigma\sigma}^{hL}(-1, m; E)}{F_{\sigma}(E)}
\]

c) if \( n < 0, m \geq 0 \), then:

\[
G_{\sigma\sigma}^*(n, m; E) = -t \frac{G_{\sigma\sigma}^{hL}(n, -1; E)G_{\sigma\sigma}^{hR}(0, m; E)}{F_{\sigma}(E)}
\]

d) if \( n, m < 0 \), then:

\[
G_{\sigma\sigma}^*(n, m; E) = G_{\sigma\sigma}^{hL}(n, m; E) + t^2 \frac{G_{\sigma\sigma}^{hL}(n, -1; E)G_{\sigma\sigma}^{hR}(0, 0; E)G_{\sigma\sigma}^{hL}(-1, m; E)}{F_{\sigma}(E)}
\]

Here,

\[
F_{\sigma}(E) = 1 - t^2 \frac{G_{\sigma\sigma}^{hR}(0, 0; E)G_{\sigma\sigma}^{hL}(-1, -1; E).}
\]

**Densities of states in the gaps:** \( |E| \leq US \) and \( |E| \geq ((US)^2 + 4t^2)^{1/2} \)

The appearance of discrete states in the gap is related to the existence of poles in the Green's functions. From the expression of Green's functions for the sharp-boundary soliton, one can see that such poles appear at the energies \( E \) satisfying the condition \( F_{\sigma}(E) = 0 \). Since this condition is spin dependent, it is apparent that the direction of the spin is well defined (and unique) on each one of these levels.

The LDOS can be calculated using the identities:

\[
\frac{1}{F_{\sigma}(E)} = \lim_{\eta \to 0} \frac{1}{F_{\sigma}(E - i\eta)} = P \frac{1}{F_{\sigma}(E)} + i\pi \sum_{\text{roots}} \frac{\delta(E - E_0)}{|dF_{\sigma}(E)|_{E_0}}
\]

where \( E_0 \) are the simple roots of the equation \( F_{\sigma}(E) = 0 \), i.e. the energies of the discrete levels.

The LDOS is proportional to the imaginary part of the Green's function. This yields the following expressions for the LDOS. In the internal gap \( |E| \leq US \),

\[
\rho_{\sigma\sigma}^*(E) = \frac{1}{2\sqrt{1 + \lambda^{-2}}} \left[ \sqrt{\lambda^2 + 1 - \lambda} \right]^{N(n)} (\delta_{\sigma \uparrow} \delta(E - E_{\uparrow}^+) + \delta_{\sigma \downarrow} \delta(E - E_{\downarrow}^-))
\]

(A.8)
In the external gaps $|E| \geq \sqrt{(US)^2 + 4t^2}$,

$$
\rho_{n\sigma}^\ast (E) = \frac{1}{2\sqrt{1 + \lambda^{-2}}} \left[ \sqrt{\lambda^2 + 1 - \lambda} \right]^{N(n)} \left( \delta_{\sigma,\uparrow} \delta(E - \tilde{E}^\uparrow_\downarrow(E - \tilde{E}^\downarrow_\downarrow) \right) \tag{A.9}
$$

Here, $\lambda \equiv US/t$ and

$$
N(n) = N(-n - 1) = \begin{cases} 
n & \text{if } n \geq 0 \text{ is even} \\
n + 1 & \text{if } n \geq 0 \text{ is odd} 
\end{cases} \tag{A.10}
$$

Thus, 4 discrete levels are found to appear in the gaps. Two of the discrete levels appear inside the Mott-Hubbard gap ($|E| < US$),

$$
E^{\uparrow}_\downarrow = -t + \sqrt{(US)^2 + t^2} > 0,
\quad E^{\downarrow}_\downarrow = t - \sqrt{(US)^2 + t^2} < 0
$$

and the other two appear in the two external gaps ($|E| > \sqrt{4t^2 + (US)^2}$):

$$
\tilde{E}^{\uparrow}_\downarrow = t + \sqrt{(US)^2 + t^2} > 0,
\quad \tilde{E}^{\downarrow}_\downarrow = t - \sqrt{(US)^2 + t^2} < 0.
$$

The spin projections for these nondegenerate levels are indicated in Fig. A.1. This soliton preserves charge-conjugation symmetry: for each level of energy $E$ and spin $\sigma$ there is another level of energy $-E$ and spin $-\sigma$.

The spatial probability of localization on each of these 4 discrete levels is given by the corresponding contribution to the LDOS (see Eqs. (A.8), (A.9))

$$
|\phi_{\sigma}^\ast(n)|^2 = \frac{1}{2\sqrt{1 + \lambda^{-2}}} \left[ \sqrt{\lambda^2 + 1 - \lambda} \right]^{N(n)} \tag{A.11}
$$

where $\lambda = US/t$, and $N(n)$ is defined in (A.10). We also need to compute the contribution to the local density of states of the band (extended) states of the Mott-Hubbard bands.

**Densities of states in the bands:** $US \leq |E| \leq [(US)^2 + 4t^2]^{1/2}$

The LDOS is proportional to the imaginary part of the diagonal matrix element of the Green's function $G_{\sigma\sigma}^\ast(n, n; E)$. Using the expressions given above, this is found to be given by:

$$
G_{\sigma\sigma}^\ast(n, n; E) = \frac{i(E + \sigma US)}{2t^2 \sin 2\phi} - e^{2i(n+1)\phi} \frac{E + \sigma US}{2t^2 \sin 2\phi} \left[ i + \frac{(E + \sigma US)}{(\sigma US \cot \phi + iE)} \right]
$$
if \( n \) is even, and:

\[
G^*_{\sigma\sigma}(n, n; E) = \frac{i(E - \sigma US)}{2t^2 \sin 2\phi} - e^{2i(n+1)\phi} \left[ \frac{i(E - \sigma US)}{2t^2 \sin 2\phi} + \frac{\sqrt{E^2 - (US)^2}}{2t(\sigma US \cos \phi + iE \sin \phi)} \right]
\]

if \( n \) is odd. In both equations, the first term in the right-hand side represents the Green's function in the fundamental state \( G^0_{\sigma\sigma}(n, n; E) \). The LDOS are now simply obtained from the definition:

\[
\rho^*_{\sigma\sigma}(E) = \frac{\text{sgn}(E)}{\pi} \text{Im} \ G^*_{\sigma\sigma}(n, n; E)
\]

Using this expression it follows, by straightforward integration, that

\[
\int_{-US}^{-US} dE \left( \rho^*_{n\uparrow}(E) + \rho^*_{n\downarrow}(E) \right) = 1 - 2|\phi_\sigma(n)|^2.
\]

Since there are exactly two discrete levels for \( E < 0 \), this equation can be rewritten as:

\[
\int_{-\infty}^{0} dE \left( \rho^*_{n\uparrow}(E) + \rho^*_{n\downarrow}(E) \right) = 1.
\] (A.12)

This shows that although the electronic structure is changed in the presence of the soliton, at half-filling all the electrons will occupy levels with \( E < 0 \) (lowest energies available) and the sharp-boundary soliton is charge neutral: there is an average of one electron per site, exactly as in the ground state.

In order to test the self-consistency of the spin distribution of the sharp-boundary soliton, we calculate the expectation value of the spin at every site, and compare it with the initial parameters. The evaluation of the corresponding integrals cannot be done analytically, except for the two sites near the boundary. It can be shown that the band contribution to these expectation values is exactly zero:

\[
\frac{1}{2} \int_{-\sqrt{(US)^2 + 4t^2}}^{-US} dE \left( \rho^*_{n\uparrow}(E) - \rho^*_{n\downarrow}(E) \right) = 0, \text{ if } n = -1, 0
\]

This means that the entire contribution to the spin of these two sites comes from the two electrons in the occupied gap levels. The total spin at sites -1 and 0 is given by (see Eq. (A.11)): \( S(-1) = S(0) = \frac{-US}{2\sqrt{(US)^2 + t^2}} \)

In the large \( US/t \) limit this approaches \( -S = 1/2 \), and the picture becomes self-consistent. In this limit, the wavefunctions of the gap levels are very strongly localized near the boundary, and the two spins from the gap levels may be identified with the spins on either side of the boundary (see Fig.A.1).
The excitation energy necessary to create a sharp-boundary soliton is given by the difference between the soliton energy and the AFM background energy. This difference has two components, one coming from differences between expectation values of the electronic part $\mathcal{H}_el$, and one coming from differences between the constants part $\mathcal{H}_{\text{const}}$ (see Eq. (A.1)). For the sharp-boundary parameterization, the difference between the corresponding values of $\mathcal{H}_{\text{const}}$ is zero, so that the excitation energy is given by:

$$E^*_{\text{exc}} = \sum_{n\sigma} \int_{-\infty}^{0} dE E \Delta \rho_{n\sigma}(E) = \sum_{n\sigma} \int_{-\sqrt{(US)^2 + t^2}}^{US} dE E \Delta \rho_{n\sigma}(E) + E^+_l + \hat{E}^-_l.$$

Here,

$$\Delta \rho_{n\sigma}(e) = \rho_{n\sigma}^a(E) - \rho_{n\sigma}^b(E) = \frac{1}{\pi} \text{sgn}(E) \text{Im} (G^a_{\sigma\sigma}(n, n; E) - G^b_{\sigma\sigma}(n, n; E))$$

represents the difference in the LDOS between the sharp-boundary soliton and the AFM background. This integral is evaluated numerically as a function of $US/t$ in Fig. A.2. As expected, the energetic cost of exciting a sharp-boundary soliton decreases as $US/t \to \infty$; in this limit, the electrons are strongly localized and the interactions between them become very weak. From the equivalent Heisenberg model (valid in this limit), we know that the cost of exciting a sharp-boundary soliton must be $2JS^2 = J/2 = 2t^2/U$ (a pair of antiparallel spins becomes parallel, and $S = 1/2$ in this limit). The dotted line in Fig. A.2 shows this asymptotic value, in agreement with our mean-field theory.

As in the case of Bloch walls which separate domains of ferromagnetism in conventional materials [128] such as iron, the AFM domain wall described above has an equilibrium thickness determined by the crystal anisotropy effects on the local magnetic moment ori-
A.2.2 The FM-core and the AFM-core neutral solitons

Consider the local magnetic moments of the extended neutral soliton on one sublattice (sublattice A). We allow these magnetic moments to slowly rotate from one AFM state, (with $\vec{S} = -S\vec{e}_z$, for instance), to the second AFM state, ($\vec{S} = S\vec{e}_z$) in the $(x0z)$-plane. The $x$-direction is along the chain, and the rotation is characterized by an angle $\theta_n$ describing the expectation value of the spin at a site $n$: $\vec{S}_n = S(\cos \theta_n \vec{e}_z + \sin \theta_n \vec{e}_x)$. The angle $\theta_n$ varies from $-\frac{\pi}{2}$ to $\frac{\pi}{2}$ as $n$ goes from $-\infty$ to $+\infty$, and is described by the ansatz $\theta_n = \frac{\pi}{2} \tanh \left( \frac{n+\rho}{\rho} \right)$, where $\rho$ is the soliton core radius (in units of $a$). Here, the soliton is centered between the sites $-1$ and $0$, as in the case of the sharp-boundary soliton.

Due to the symmetry of the problem, the rotation of the second sublattice (sublattice B) is described by the same angle $\theta_n$. However, we are free to choose the sense of rotation. For the case that spins on the two sublattices rotate in the same sense (see Fig. A.3, top panel), we obtain

$$\vec{S}_n = S \left( (-1)^{bn} \cos \theta_n \vec{e}_z + (-1)^n \sin \theta_n \vec{e}_x \right)$$

(A.13)

with $b = 1$. In this case the spins remain locally antiparallel everywhere along the chain, we call this excitation an AFM-core soliton.

The second possibility is when the spins on the two sublattices rotate in opposite senses
(see Fig.A.3, lower panel). In this case we use formula (A.13) except with the choice $b = 0$. The spins in the core of the soliton become parallel and we call such an excitation a *FM-core soliton*.

The corresponding mean field Hamiltonian is given by

$$\mathcal{H}_{el}^b = -t \sum_{<i,j>} (\chi_i^\dagger \chi_j + h.c) - U S \sum_i \chi_i^\dagger \left( (-1)^b \cos \theta, \sigma_z + (-1)^i \sin \theta, \sigma_z \right) \chi_i$$  \hspace{1cm} (A.14)

where $\chi_i^\dagger = (c_{iup}^\dagger, c_{idown}^\dagger)$.

The Green's function associated with (A.14) is evaluated using Dyson's equation, with the sharp-boundary soliton as a reference case.

We write,

$$\mathcal{H}_{el}^b = \mathcal{H}_{el}^r + V^b$$

where $\mathcal{H}_{el}^r$ is the electronic part of the Hamiltonian of the sharp-boundary soliton. $V^b$ is a potential localized near the core of the soliton, on a region characterized by the core radius of the soliton. This potential is diagonal in the site-space, but not in the spin-space. The Dyson equation for the Green's functions are given by:

$$G_{\sigma\sigma'}^{b}(n, m; E) = \delta_{\sigma\sigma'} G_{\sigma\sigma}(n, m; E) + \sum_{\rho \sigma''} G_{\rho\sigma}(n, \rho; E) V_{\sigma\sigma''}^b(\rho) G_{\sigma''\sigma'}^{b}(\rho, m; E)$$

Here, we have used the fact that $G^b$ is diagonal in spin-space. This equation can be solved numerically. Once the values of $G_{\sigma\sigma'}^{b}(n, n; E)$ are known at any site $n$, we can calculate physical quantities such as the LDOS, the excitation energy of the soliton and the expectation value of the spin at various sites.

**Electronic states in the gap**

In the presence of a sharp-boundary soliton, 4 electronic levels split from the valence- and conduction-band, and become localized levels in the gap. For extended solitons, the number of such gap levels and their energies vary as a function of the soliton core radius. In Fig.A.4 we plot the electronic spectrum (bands and discrete levels) as a function of the soliton core radius for the two types of solitons, for a fixed value of the Mott-Hubbard gap $US/t$.

In the $\rho \to 0$ limit, both solitons show the same structure, as the sharp-boundary soliton. However, as $\rho$ increases, the behavior of the two spectra is very different. For the FM-core soliton, more and more levels split off from both bands and go deeper into the gaps. For the AFM-core soliton the tendency is opposite: the gap levels go toward and eventually re-enter the bands. These different behaviors can be understood if we analyze the $\rho \to \infty$ limit. In this limit, an AFM-core soliton is practically indistinguishable from the ground state, because the rotation angle between spins on neighboring unit cells goes to zero.
Figure A.4: Left: The lower half of the electronic spectrum of an AFM-core soliton, as a function of the soliton core-radius $\rho$. In the limit $\rho \to 0$, there are two discrete levels. In the limit $\rho \to \infty$, this soliton becomes indistinguishable from the mean-field background. As the soliton core radius $\rho$ increases, the discrete levels re-enter the bands; Right: The lower half of the electronic spectrum of a FM-core soliton, as a function of the soliton core-radius $\rho$. In the limit $\rho \to 0$, there are two discrete levels. In the limit $\rho \to \infty$, the entire chain becomes ferromagnetic and the spectrum consists of two continuum bands, the valence band corresponding to $E \in [-US - 2t, -US + 2t]$. Here $\gamma = (4t^2 + (US)^2)^{1/2}$ and $l = (t^2 + (US)^2)^{1/2}$.

Therefore, the electronic structure should become identical with that of the ground state, which consists only of the two bands. This is exactly the behavior seen in the left panel of Fig. A.4. On the other hand, in the presence of a FM-core soliton with $\rho \to \infty$, all the chain is in the core region, which is a perfect FM state. The electronic structure of a FM state can be easily calculated, and it is seen that it is made up of two bands with energies $E \in [-US - 2t, -US + 2t]$ and $E \in [US - 2t, US + 2t]$, the lower (valence) band consisting of nondegenerate levels with spins in the direction of the FM-spins (+Oz-direction, in this case), while the upper (conduction) band consists of nondegenerate levels with spins in the opposite direction. This shows that as $\rho$ increases, the initial AFM-bands containing doubly-degenerate levels with up- and down-spins in the Oz direction will spread out into the broader FM bands with spins in the Oz direction. This spreading of the bands as $\rho$ increases is shown in the right panel of Fig. A.4.

The most interesting gap levels are the pair of levels closest to the midgap, because these levels accommodate the doping electrons or holes. In Fig. A.5, we show the behavior of one of these levels ($E > 0$) for different values of $US/t$, as a function of $\rho$. There are two distinct types of behavior and two different regimes for the FM-soliton. If $US/t < 2$, the level reaches the midgap, while if $US/t > 2$ the level goes to some nonzero value as $\rho \to \infty$. This is consistent with the band structure of the FM state. This state has a inner gap for energies $E \in [-US + 2t, US - 2t]$, which is consistent with the fact that if $US/2t > 1$, the gap level goes to $\pm(US - 2t) \neq 0$. If $US/2t < 1$, the gap is closed in the FM core. Therefore the gap level goes to $E = 0$ as $\rho$ increases.
Figure A.5: The energy of the near midgap \((E > 0)\) level for the undoped FM- and AFM-core solitons, for \(U_S/t = 1.3\) and 6, as a function of the soliton core radius. For the FM-core soliton this level approaches the mid-gap, while for the AFM-core soliton it approaches the band-edge. For \(U_S/t < 2\), the FM-core soliton level reaches the midgap. For \(U_S/t > 2\), this level goes to \(U_S - 2t\), the band-edge of the FM valence band.

A.2.3 Excitation energies of the neutral solitons

We now evaluate the total density of states (DOS) and the excitation energy of the FM-core and AFM-core non-self-consistent solitons. If \(\mathcal{H}_{c_i}^t\) and \(\rho^t(E)\) are the Hamiltonian and total density of states, respectively, of the sharp-boundary soliton, then the difference between the total densities of states of the chain with an extended soliton and the chain with a sharp-boundary soliton is given by[129]:

\[
\Delta \rho(E) = \rho^b(E) - \rho^t(E) = \frac{1}{\pi} \text{Im} \frac{d}{dE} \ln \det \left(1 - V^b G^t(E)\right)
\]

Since \(V^b\) has nonzero matrix elements only for a finite range of sites, the determinant can be calculated in the site-spin basis, and is equal to the determinant of the finite region with non-vanishing matrix elements of \(V^b\). Introducing the function:

\[
F(E) = \text{Im} \left\{ \ln \left[ \det \left(1 - V^b G^t(E)\right) \right] \right\}
\]

the variation of the DOS is given by:

\[
\Delta \rho(E) = \frac{1}{\pi} \frac{d}{dE} F(E)
\]

The difference between the energies of the ground-states of \(\mathcal{H}_{c_i}^t\) and \(\mathcal{H}_{c_i}^b\) can be expressed in terms of \(F(E)\):

\[
\Delta E_{gs} = \int_{\text{occ.states}} E \Delta \rho(E) dE = -\frac{1}{\pi} \int_{\text{occ.states}} F(E) dE
\]
In writing the last equality, we made use of the fact that the chemical potentials of both Hamiltonians are equal (\( \mu = 0 \) in both undoped cases). In the undoped case there is no contribution to the excitation energy coming from last term of the Hamiltonian (see Eq. (A.1)), since it has the same value for the extended solitons as for the ground state. For the doped case, the gap levels which are occupied (or empty) have to be taken into account as well.

The total excitation energy relative to the uniform AFM background is given by:

\[
E_{\text{exc}} = -\frac{1}{\pi} \int_{\text{occ. states}} F(E) dE + E_{\text{exc}}^e
\]

where \( E_{\text{exc}}^e \) is the excitation energy of the sharp-boundary soliton (see Fig. A.2). For a fixed value of \( U S/t \), the typical variation of \( E_{\text{exc}} \) with \( \rho \) is shown in Fig.A.6 In the \( \rho \rightarrow 0 \) limit, both the FM-core and AFM-core solitons behave identically and their excitation energies equal that of the sharp-boundary soliton. As \( \rho \) increases, the excitation energy of the AFM-core soliton decreases, since as \( \rho \rightarrow \infty \) this soliton merges into the AFM background. On the other hand, the excitation energy of the FM-core solitons increases with \( \rho \), since as the core size increases, more spins become parallel instead of antiparallel.

The instability of the neutral domain wall soliton is a general characteristic of 1D systems. As in the classical theory of Bloch walls separating domains of magnetization in a ferromagnet, a stable finite core size soliton can exist if crystal anisotropy energies are
included in the model. Nevertheless, the importance of these domain walls is apparent. For a doped system it is energetically advantageous to pay the cost of creating a domain wall and lower the total energy by allowing the doping electron (hole) to occupy a deep gap level than would be to let the doping electron (hole) occupy the first available level in the conduction band. In the next section, we identify two types of charged solitons on the lattice with different spin and statistics from conventional charge carriers in a metal. The lowest energy charged soliton, which is centered on a site, appears to be a spinless bosonic excitation. A charged soliton which is centered between two sites has higher energy and appears to be an unstable spin-1/2 fermion for $US/t > 2$, whereas for $US/t < 2$ it has the character of a spinless boson.

A.3 Charged domain wall solitons

By adding the energy of the first available gap level of an undoped FM/AFM-core soliton to the total excitation energy of the undoped FM/AFM-core soliton, we obtain a first estimate of the excitation energy of a doped FM/AFM-core soliton. The typical dependence with the core radius of this energy (in units of $t$), for a given $US/t$, is shown in Fig.A.7. This offers plausibility to the idea that a charged FM-core soliton is stable at a finite core radius. It suggests that the doped soliton excitation energy is indeed less than $US$ (which is the energetic cost of placing the electron (hole) on the first available level in the conduction (valence) band, in the absence of the soliton). However, this elementary consideration is not self-consistent. Adding an electron (hole) on the first available level in the gap (i.e. in a localized state) modifies the expectation values of the spin in the core of the soliton. In order to get a self-consistent model, we proceed as follows. We start with the initial parameters of an undoped soliton and calculate the corresponding Green's functions (in the way described in the previous section). The expectation values of the spin of the corresponding doped soliton at various sites are obtained by integrating, over the correct range of energies, the trace of the imaginary part of the Green's function at that site multiplied by the $\tilde{\sigma}$ operator (in spin space). This yields a new set of spin expectation values. Once these new parameters are obtained, the next iteration begins, and the process continues until it converges to a self-consistent solution.

A.3.1 The self-consistent charged solitons

Remarkably, the self-consistent, Hartree-Fock, structure of the charged soliton does not exhibit spiral twist of the magnetic background as suggested by the structure of the extended neutral solitons. Instead, the charged soliton consists of a co-linear spin alignment in which the magnitude of the local magnetic moment is suppressed within the soliton core. Using
the procedure described above, we calculate the self-consistent shape, electronic spectra and excitation energies of the charged solitons. For both self-consistent solutions, the magnitude of the spin along the chain becomes zero $S_n^z = 0$, while the spin perpendicular to the chain is suppressed in the core of the soliton. The vanishing of the component parallel to the chain has a simple interpretation. In the neutral soliton, the main contribution to the spin parallel to the chain was given by the electron on the deepest occupied gap level, and it is exactly this level which becomes empty upon hole-doping.

The two self-consistent charged solitons are depicted in Fig. A.8. The magnitude of the spin perpendicular to the chain is well approximated by $S_n^z = S \tanh (n + 0.5/\rho)$ for a doped soliton centered between two sites, and $S_n^z = S \tanh (n/\rho)$ for a doped soliton centered at a site. In Fig.A.9 we plot the self-consistent soliton core-radius for both solitons as a function of $US/t$. In the large $US/t$ limit, the localization length of the gap levels is very small and accordingly the soliton itself is very small. In the small $US/t$ limit, the bound levels are more extended, and the solitons are large. For large solitons, a continuum approximation which we discuss in the next section, recaptures the lattice results, and there is no distinction between the two types of solitons. This can be seen from Fig.A.10. and Fig.A.11. In Fig.A.10. we plot the excitation energies of the two types of solitons (in units of $t$, and defined with respect to the undoped AFM mean-field background) as a function of $US/t$. In the small $US/t$ limit, the two excitation energies are practically equal (and very well approximated by the value of $US/\sqrt{2}t$ predicted by the continuum model (dotted line)). In the intermediate and large $US/t$ regimes the size of the soliton becomes comparable to the lattice constant. In this case the doped soliton centered at a site is energetically favorable to the doped soliton centered between sites. For any value of $US/t$, the excitation energy
of both types of solitons is less than $U_S$, the energetic cost of simply adding the doping electron(hole) on the first available level in the conduction(valence) band. This suggests that charged solitons must appear automatically on the chain upon doping.

In Fig.A.11 we plot the lower half of the electronic spectra of the two types of solitons (these doped solitons have discrete levels only in the internal gap, and they have the usual charge-conjugation symmetry). The doped soliton centered at a site has only a doubly degenerate level at the midgap for any value of $U_S/t$. Using symmetry arguments, it is easy to see that this level is empty (or doubly occupied) for the hole(electron)-doped soliton. The spectrum of the doped soliton centered between two sites is more complicated: for $U_S/t < 2$, there are only two nondegenerate levels symmetric with respect to $E = 0$, which go to zero as $U_S/t \to 0$. Since the soliton is doped, these levels are either both occupied or both empty. For $U_S/t > 2$, a new pair of non-degenerate level splits off the inner band edges and becomes localized. The spin projections of these non-degenerate gap levels are similar to those of the sharp-boundary soliton: the two lower levels support down spins (more generally, spins pointing in the same direction as the expectation values of the spin at the two sites near the center of the soliton), while the two upper levels have the opposite projection. The appearance of this second pair of gap levels has important consequences, related to the spin of such a soliton. We discuss this issue below.
A.3.2 The spin of the charged soliton

The doped soliton centered at a site is a boson. This can be seen from its electronic spectrum: all the states in the continuum bands are spin-paired and filled, while the doubly degenerate mid-gap level is either empty or doubly occupied. This means that the total projection of the spin perpendicular to the chain is zero. Therefore this soliton is a charged boson. In the small $US/t$ limit this is confirmed by the continuum model (discussed in Chapter 3). The fact that the total spin of the doped soliton is zero can be seen also from Fig.A.8. By symmetry, the sum of the spins to the left of the core must be equal and opposite to the sum of the spins to the right of the soliton, giving a vanishing total spin.

The situation of the doped soliton centered between sites is more complicated. For $US/t < 2$, this soliton is a boson, because it has the same type of electronic structure as the other soliton. On the other hand, for $US/t > 2$, this soliton is a fermion. Since a new nondegenerate level splits from the lower band edge, this lower discrete level is occupied by one electron. While this level was still in the valence band ($US/t < 2$) its spin was delocalized over the whole chain. Therefore it did not contribute to the spin of the soliton. As this level goes deeper and deeper into the gap, the corresponding wavefunction becomes well localized in the core of the soliton, and the 1/2-spin it carries becomes the spin of the soliton. Another way to understand the fermionic character of this soliton for large $US/t$ is to start from the undoped sharp-boundary model analyzed previously, and dope it.

We have argued that in the strongly localized limit, the two electrons occupying the two discrete levels with $E < 0$ of the sharp-boundary soliton contribute equally to the spins of the two sites bordering the center of the soliton. The total spin of the undoped soliton is an integer multiple of $\hbar$. As we remove one of these electrons, in order to get a doped
soliton centered between sites, the magnitude of the spin at the two sites bordering the center decreases by half, leaving behind a total spin of $1/2$.

The bosonic charged soliton centered on a site is energetically favored and it can lower its energy further by quantum mechanical hopping along the chain. Since the structure of this soliton is unchanged as the hole moves, this type of soliton is very mobile and its total energy is lowered by an amount of the order of $t$ as it moves. The doped soliton centered between two sites is a charged fermion. This soliton, however, is relatively immobile, since motion requires changes in the magnitudes of the spins.

A.3.3 Charge density of the doped solitons

In the previous sections, we simplified the eigenvalue spectrum of the charged solitons by neglecting the charge density term $Q(i)$ in the mean-field Hamiltonian. A self-consistent treatment of the charge density leads to a loss of (charge conjugation) symmetry of the soliton eigenvalue spectrum about $E = 0$. However, the general conclusions concerning the charge and the spin of the solitons remains the same as discussed earlier. In order to take into consideration this extra charge localized in the core of the soliton, we add the term depending on $Q(i)$ in the Hamiltonian to describe the doped system. The self-consistent calculations once again yield two types of doped solitons.

Although the charged soliton centered at a site continues to have a doubly-degenerate gap level, the charged solitons centered between sites has only nondegenerate gap levels. However, their spectra are no longer symmetric with respect to $E = 0$. Instead, this symmetry manifests in a more subtle way. Let $\mathcal{H}^{\text{hole}}_d$ be the Hamiltonian of a hole-doped
soliton defined by the parameters $\vec{S}_n$ and $Q_n = 1 - \Delta \rho_n$, and $\mathcal{H}_{el}^{electron}$ the Hamiltonian of an electron-doped soliton defined by the parameters $-\vec{S}_n$ and $Q_n = 1 + \Delta \rho_n$. (This is exactly the type of correspondence expected in systems with charge-conjugation symmetry.) It is straightforward to prove that if $\Phi_{hole}(n)$ is a spinor such that $\mathcal{H}_{el}^{hole}\Phi_{hole}(n) = E\Phi_{hole}(n)$, then the spinor $\Phi_{electron}(n) = (-1)^n\Phi_{hole}(n)$ satisfies the equation $\mathcal{H}_{el}^{electron}\Phi_{electron}(n) = -E\Phi_{electron}(n)$. In other words, the electronic spectrum of the hole-doped soliton is obtained by reflection with respect to $E = 0$ from the electronic spectrum of the electron-doped soliton.

This loss of symmetry of the electronic spectrum makes the problem of determining the Fermi level non-trivial. It turns out that the chemical potential remains fixed at zero, as was the case for the undoped soliton. In other words, for a hole(electron)-doped soliton all the $2N-1$ ($2N+1$) occupied states, where $N$ is number of unit cells of the chain, are below $E < 0$. This symmetry guarantees that the "shapes" of the self-consistent electron- and hole-doped solitons are the same. The spin distribution is not greatly modified by the charge term. The tanh function still gives a good fit, and the soliton core radii have the same qualitative behavior as in the previous case. The electronic spectra of the hole-doped solitons centered between sites and centered at one site are shown in Fig. A.12 (the spectra of the corresponding electron-doped solitons are obtained by reflection with respect to $E = 0$). All the gap levels of the doped soliton centered between sites are nondegenerate, while the gap levels of the doped-soliton centered at a site are doubly degenerate.

From Fig.A.12a, we can see that the doped soliton centered at a site remains a charged boson, since only levels below $E = 0$ are occupied. For a hole-doped soliton centered at a
site, only the valence band levels are occupied and there is no possibility of a localized spin. For the electron-doped soliton centered at a site, all the degenerate gap levels are doubly occupied, and once again there is complete spin cancellation.

In the large $US/t$ limit, we find a simple analytic expression to describe the approximate position of the discrete levels of these solitons. For the hole-doped soliton centered at a site, the positions of the two doubly-degenerate gap levels are well approximated by $E = \sqrt{(US)^2 + t^2} \pm t$, while for the hole-doped soliton centered between sites, the two levels near the midgap are at $\pm t$ while the two upper levels are at $\sqrt{(US)^2 + t^2} \pm t$ (see dotted lines in Fig.A.12).

The total energies of the self-consistent electron- and hole-doped solitons are shown in Fig.A.13, left panel. The resulting excitation energy of the hole-doped solitons (lower line), which is lower than the excitation energy of the electron-doped solitons (the upper line), is an artifact of our Hamiltonian which does not contain a term describing Coulomb attraction between the electrons and the positive background nuclei. This artificially favors a hole-doped soliton. An electron-doped soliton costs more energy, in this oversimplified model, because the extra repulsive energy due to having more electrons is not compensated by attraction between the extra electron and the nuclei. The contribution of a neutralizing positive background may be estimated by simply taking the average between the excitation energies of the hole-doped soliton and the electron-doped soliton. This is shown in Fig.A.13, right panel. for the two types of doped solitons. The important observation this is that the average energy of the electron- and hole-doped soliton centered at a site, exceeds $US$. However, it should be remembered that this soliton can lower its energy by an amount $t$ by quantum mechanical hopping motion along chain. This additional mobility for the charged soliton centered on a site makes it energetically favorable compared to the soliton centered between sites.

The increase in the excitation energy of the doped-solitons when the charge terms are included is partly an artifact of the purely on-site Coulomb repulsion of the Hubbard model. For an electron-doped soliton centered at a site, the extra electron is basically localized on top of another electron, and this costs an enormous amount of energy. A more realistic model should consider a longer-range Coulomb interactions as well as a more realistic model for the positive background charge of the nuclei.
Bibliography

[10] Recent reviews of the nearly antiferromagnetic Fermi liquid approach may be found in D. Pines, Physica (Amsterdam) 235-240C, 113 (1994); in High Temperature Superconductivity and the C<sup>60</sup> Family, edited by H.C. Ren (Gordon and Breach, New York, 1995).


