Quantum transport through double-dot Aharonov-Bohm interferometers

by

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Abstract

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Understanding the interplay of nonequilibrium effects, dissipation and many body interactions is a fundamental challenge in condensed matter physics. In this thesis, as a case study, we focus on the transient dynamics and the steady state characteristics of the double-dot Aharonov-Bohm (AB) interferometer subjected to a voltage and/or temperature bias.

We first consider an exactly solvable case, the noninteracting double-dot AB interferometer. The transient dynamics of this model is studied using an exact fermionic trace formula, and the analytic expressions in the long time limit are obtained using a nonequilibrium Green’s function technique. We also study the effects of elastic dephasing on the occupation-flux behaviour in this noninteracting limit. Several nontrivial magnetic flux control effects are exposed, potentially useful for the design of nanoscale devices.

The real time dynamics of the coherences and the charge current in an interacting interferometer is simulated using the numerically exact influence functional path integral (INFPI) technique. The temporal characteristics of the coherence in the weak-intermediate Coulomb repulsion case are qualitatively similar to those found in the non-interacting limit. In contrast, in the large Coulomb repulsion and the large bias limit, master equation simulations reveal notably different dynamics and steady state characteristics.

We study the effects of many body interactions on magnetoasymmetries of nonlin-
ear transport coefficients using phenomenological models, Böttiker's probes. Sufficient conditions for the diode functionality in Aharonov-Bohm interferometers are obtained analytically within the framework of Landauer-Büttiker scattering theory. Predictions of the phenomenological probes models are verified by studying a microscopic model with a genuine many body interaction, a double-dot interferometer capacitively coupled to a fermionic environment. These simulations are carried out using the INFPI technique. Some general comments about the suitability of INFPI to study nonlinear transport are presented. This work could be extended to explore nonlinear thermoelectric transport and diode behaviour in interacting many body systems.
Dedication

I would like to dedicate this thesis to my mother Savita who is not living now. She motivated me to learn science, and especially Physics.

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6.2 Magnetic field symmetries of odd and even conductance terms in centrosymmetric junctions with $\gamma_{L,R} = 0.05$. We prove that (a)-(c) $\mathcal{R}(\phi) = -\mathcal{R}(-\phi) = \Delta I(\phi)$, and (d) $\mathcal{D}(\phi) = \mathcal{D}(-\phi)$, in both transient and steady state limit. $U = 0.1$ in all cases. Other parameters are the same as in Fig. 6.1.

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6.4 Magnetic field symmetries of even (a) and odd (b) coefficients for centrosymmetric junctions for equilibrium ($\Delta \mu_F = 0$) and nonequilibrium ($\Delta \mu_F \neq 0$) environment. We use $U = 0.1$ and $\phi = \pm \pi/2$. Other parameters are the same as in Fig. 6.1.
List of symbols

A Vector potential

$B$ Magnitude of magnetic field

$\Phi_0$ Flux quantum, $\Phi_0 = h/e$

$\Phi$ Magnetic flux

$\phi$ Aharonov-Bohm phase factor, $\phi = \frac{2\pi \Phi}{\Phi_0}$

$\epsilon_1$ Energy of dot “1”

$\epsilon_2$ Energy of dot “2”

$U$ Strength of electron-electron repulsion. In model I it stands for interdot electron electron repulsion, in model III it stands for capacitive coupling to a fermionic environment

$E_d$ Shifted dot energy. It is defined as $E_d = \epsilon_{1(2)} + \frac{\nu}{2}$

$\xi_{\beta,l}$ Tunneling element of dot 1(2) to the left reservoir

$\zeta_{\beta,r}$ Tunneling of element of dot 1(2) to the right reservoir

$D$ Cutoff energy of electronic bands

$f_\nu(\omega)$ Fermi-Dirac distribution function for the $\nu^{th}$ reservoir, where $\nu = L, R$ and $\omega$ is energy of bath electrons
$\mu_\nu$ Chemical potential of the $\nu^{th}$ reservoir

$T_\nu$ Temperature of the $\nu^{th}$ reservoir

$\rho$ Total density matrix, page 17

$\sigma$ Reduced density matrix of the double-dot system, page 17

$\hat{I}$ Symmetrized charge current operator, page 68

$N_\nu$ Number operator for $\nu$ reservoir

$I_\nu$ Average current at the $\nu^{th}$ reservoir, page 17

$Q_\nu$ Average heat current at the $\nu^{th}$ reservoir, page 17

$G^+(\omega)$ Retarded Green’s function, page 20

$G^-(\omega)$ Advanced Green’s function, page 20

$\mathcal{T}_{\nu,\nu'}(\omega)$ Transmission probability from $\nu$ to $\nu'$ reservoir, page 21

$\Sigma^{\pm}(\omega)$ Retarded (advanced) self energy contribution from $\nu^{th}$ reservoir

$\Gamma^L$ Hybridization matrix to the left reservoir, page 45

$\Gamma^R$ Hybridization matrix to the right reservoir, page 45

$\Gamma^P$ Hybridization matrix to the probe reservoir, page 60
\( \gamma_{L(R)} \) Hybridization strengths to left/right reservoirs, \( \gamma_L = 2\pi \sum_l \xi_{\beta,l} \delta(\omega - \omega_l) \xi^*_{\beta',l} \), \( \gamma_R = 2\pi \sum_r \xi_{\beta,r} \delta(\omega - \omega_r) \xi^*_{\beta',r} \), see page 44

\( \gamma_p \) Hybridization to the probe reservoir, defined similarly as above, page 60

\( \Gamma \) Total diagonal decay defined as \( \Gamma = \gamma_L + \gamma_R \), page 67

\( \gamma_{\pm} \) Magnetic flux dependent decay rates, page 48

\( f_p(\omega) \) Distribution function in the dephasing probe, page 25

\( \mu_a \) Averaged chemical potential, \( \mu_a = \frac{\mu_L + \mu_R}{2} \)

\( T_a \) Average temperature, \( T_a = \frac{T_L + T_R}{2} \)

\( \Delta \mu \) Voltage bias, \( \Delta \mu = \mu_L - \mu_R \)

\( \Delta T \) Temperature bias, \( \Delta T = T_L - T_R \)

\( \delta n \) Dots' occupation difference

\( \delta t \) Time step in numerical path integral simulations

\( N_s \) Number of time slices in path integral simulations

\( \tau_c \) Correlation time in path integral simulations, \( \tau_c = N_s \delta t \)
Chapter 1

Introduction

1.1 Aharonov-Bohm effect

The Aharonov-Bohm effect is a quantum mechanical phenomenon in which a charged particle is affected by an electromagnetic field, despite being confined in a region where electric and magnetic fields are zero [1]. This is because even if the magnetic field is zero, the vector potential $\mathbf{A}$ affects the phase of the particle wavefunction. This can be illustrated from the interference effect: Consider the schematic setup in Fig. 1.1, where $S$ is an electron source, the bold arrows show two paths, and a uniform magnetic field of magnitude $B$ is introduced perpendicular to the plane of the interferometer. This field may be produced by an infinitely long thin cylinder. The vector potential $\mathbf{A}(r)$ is then given by,

$$\mathbf{A}(r) = \begin{cases} 
\frac{Br\hat{\phi}}{2} : r < R, \\
\frac{BR^2\hat{\phi}}{2r} : r > R,
\end{cases}$$

where $B$ is the magnitude of magnetic field, $\hat{\phi}$ is a unit vector along the $z$ axis, $R$ is the radius of the cylinder and $r$ is the radial coordinate. An electron passing through the lower arm will follow the direction of the vector potential, and the one in the upper arm
Figure 1.1: Aharonov-Bohm interferometer with magnetic flux $\Phi$.

will move against the vector potential. As a result, the two paths will pick up opposite phases resulting in a phase difference. The phase acquired on a given path from $r_a$ to $r_b$ (denoted by points “a” and “b” in Fig. 1.1) is,

$$\phi = \frac{2\pi}{\Phi_0} \int_{r_a}^{r_b} dr' \cdot A(r'),$$  \hspace{2cm} (1.2)

where $\Phi_0 = \hbar/e$. If two paths enclose the area $S$, the net phase difference $\Delta \phi$ is given as,

$$\Delta \phi = \frac{2\pi}{\Phi_0} \oint dS \cdot B(r') = \frac{2\pi}{\Phi_0} \int dS \cdot B(r') = 2\pi \frac{\Phi}{\Phi_0},$$  \hspace{2cm} (1.3)

where $B = \nabla \times A$. The second integral follows from Stokes’ theorem [2], and

$$\Phi = \int_S dS \cdot B(r') = BS.$$  \hspace{2cm} (1.4)

The phase difference is independent of the particular gauge chosen for $A$.

The Aharonov-Bohm effect was observed in metallic loops and later on in the semiconductor heterostructures as a periodic modulation of current with the magnetic flux, with a periodicity of $\Phi_0 = \hbar/ne$ where $n$ is an integer [3]. Specifically this effect has
Figure 1.2: Scheme of a parallel double-dot Aharonov-Bohm interferometer. The magnetic flux is denoted by $\Phi$. The lines represent two electron paths between the source (S) and drain (D) electrodes.

been demonstrated in mesoscopic rings, with a single quantum dot structure integrated into one of the arms in a ring, and in double-dot structures [4, 5]. These experiments, and others, demonstrated that charge transport in these mesoscopic systems is phase coherent.

In Fig 1.2 we include a scheme of coherently coupled parallel double-dot Aharonov-Bohm interferometer realized by Holleitner et al. [5]. The device included a two-dimensional electron gas below the surface of an AlGaAs/GaAs heterostructure. Schottky gates were built by using electron beam writing and gold evaporation. These gates form two quantum dots subjected to voltage bias applied through source (S) - drain (D) terminals. The magnetic field was applied in a direction perpendicular to the device and Aharonov-Bohm oscillations of the conductance were demonstrated.

1.2 Motivation

Aharonov-Bohm devices offer tunable systems, a natural laboratory to study the interplay of quantum interference and many body effects in solid state environments. Experimental and theoretical studies of such devices will be useful for understanding decoherence,
Chapter 1. Introduction

dissipation and transport in open quantum systems. In this work we use the double-dot AB interferometer as a case study, to explore fundamental problems such as the effect of electron-electron interactions on coherence dynamics, and transport far-from-equilibrium. In the next subsections we outline some general problems, motivating this work. In chapter 2 we present specific open questions, addressed in this thesis.

1.2.1 Coherent transport, many body interactions and decoherence

Is electron transfer through quantum dot structures phase coherent, or incoherent? How do electron-electron and electron-phonon interactions affect phase-coherent transport? From the other direction, what is the role of the interference phenomena on many body effects, such as the formation of the Kondo resonance? These questions were addressed in numerous experimental and theoretical works, detecting the presence of quantum coherence in mesoscale and nanoscale objects, using Aharonov-Bohm (AB) interferometry, see for example Refs. [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19].

In particular, oscillations in the conductance resonances of an AB interferometer, with either one or two quantum dots embedded in its arms, were experimentally demonstrated in Refs. [4, 5], indicating the presence of quantum coherence. Interestingly, AB oscillations were also manifested in the co-tunneling regime, implying that phase coherence is involved within such processes [14]. More recently, quantum transport through a parallel configuration of two coherently coupled silicon dopants forming an Aharonov-Bohm interferometer has been experimentally studied [20] demonstrating that the Kondo effect can be coherently modulated by changing the magnetic flux. This device was also shown to exhibit phase coherent transport in the sequential tunneling regime.

The steady state properties of the quantum dot Aharonov-Bohm (AB) interferometer have been intensively investigated [6, 21], with the motivation to explore coherence effects in electron transmission within mesoscopic and nanoscale structures [4, 7]. Particularly,
the role of electron-electron (e-e) interactions in AB interferometry has been considered in Refs. [8, 9, 10, 11, 12, 22, 23], revealing, e.g., asymmetric interference patterns [8] and the enhancement [12] or elimination [24] of the Kondo physics. Recent works further considered the possibility of magnetic-field control in molecular transport junctions [13, 19, 25, 26].

Considering the role of electron-electron interactions in AB interferometry, a systematic theoretical analysis carried out in Ref. [8] has argued that electron-electron repulsion effects, resulting in spin flipping channels for transferred electrons, induce dephasing. The consequence of this decohering effect was the suppression of AB oscillations and the appearance of an asymmetry in the resonance peaks. One should note however that this study has assumed infinitely strong e-e interactions and treated the system perturbatively in the dot-metals coupling strength. In other studies, e-e repulsion effects were ignored [27], incorporated using a mean-field scheme, see for example [15], or treated perturbatively using the Green’s function formalism [28, 29]. These studies, and other theoretical and numerical works [8, 25], have typically considered only the steady state limit, analyzing the conductance, a linear response quantity, or the current behavior, often in the infinite large bias case [9, 10].

The double-quantum dot Aharonov-Bohm interferometer provides an important realization of a qubit, where interference effects can be controlled by magnetic flux. Entangled states of electrons are also of interest in solid state quantum computing. The quantum dot setup can be used to design spin and charge qubits. As we have discussed in Sec 1.1, such a scheme can be realized by tunnel-coupled quantum dots, each of which contains one single (excess) electron whose spin or charge state defines the qubit. Probing the entanglement of electrons in a double-dot AB interferometer via transport noise was suggested by Loss et al. [30].

The above studies mainly focused on steady state properties of quantum dot AB interferometers. The real-time dynamics of these systems has been of recent interest,
motivated by the challenge to understand quantum dynamics, particularly decoherence and dissipation, in open nonequilibrium many body systems. Studies of electron dynamics in double-dot AB interferometers in the absence of e-e interactions have been carried out in Refs. [31, 32, 33], using a non-markovian master equation approach. The detailed non-perturbative analysis of transient dynamics of coherences and charge current for an interacting case was carried out in our work, Ref. [34].

The coherence of electron transfer processes through an AB interferometer has been typically identified and characterized via conductance oscillations in magnetic fields. However, in a double-dot AB structure, a device including two dots, both connected to biased metal leads, it is imperative that the relative phase between the two dot states (or charge states) should similarly convey information on electron coherence and decoherence.

In my thesis I focus on several different models of a double-dot Aharonov-Bohm interferometer, and demonstrate nontrivial magnetic flux dependent effects, arising from the interplay of nonequilibrium effects, quantum coherence and many body interactions. The dynamics of the interacting case is presented in Sec. 4.3 using numerically exact influence functional path integral technique (INFPI) and quantum master equations.

### 1.2.2 Nonlinear magneto-transport

The theory of linear irreversible thermodynamics provides relations between thermodynamic fluxes and thermodynamic forces,

\[ \mathbf{J} = \mathbf{LX}. \]  

(1.5)

Here \( \mathbf{J} \) is a column vector denoting the heat and particle current fluxes, \( \mathbf{X} \) denotes a column vector of thermodynamic forces related to the temperature and voltage bias, and \( \mathbf{L} \) is the Onsager matrix. Its diagonal elements are conductances, and the off-diagonal
elements are related to the Seebeck and Peltier coefficients [35, 36, 37].

*Onsager-Casimir symmetry:* Time reversal symmetry dictates reciprocal relations between linear response coefficients, \( L_{i,j} = L_{j,i} \). In the presence of a magnetic field \( B \) the reciprocity relation becomes

\[
L_{i,j}(B) = L_{j,i}(-B)
\]

(1.6)

From the above equation we can immediately see that the conductances (diagonal matrix elements) are even functions of the magnetic field. In a two-terminal Aharonov-Bohm interferometer this symmetry is known as the “phase rigidity” of linear conductance [4].

In the non-linear regime, Onsager-Casimir symmetries need not hold. A prominent example of this breakdown is the asymmetry of the differential conductance out-of-equilibrium [38, 39, 40, 41, 42]. This effect has been attributed to electron-electron interactions in the system, resulting in an asymmetric charge response under the reversal of a magnetic field, leading to a magnetoasymmetric differential conductance. Such an interaction induced asymmetry has been observed recently in carbon nanotubes and also in semiconductor quantum dots [38]. It is also of interest to investigate whether the Onsager-Casimir symmetry can be fully or partially restored beyond linear response, in the presence of many body interactions.

It is reasonable to argue that many body interactions may induce different types of phase breaking processes in a coherent transport. These include, quasi-elastic scattering and inelastic scattering. Büttiker’s probes are phenomenological tools to incorporate quasi-elastic and inelastic scattering effects. Our objective is to study systematically how many body effects and spatial asymmetries affect magnetic field symmetries and magnetoasymmetries of charge and heat current beyond linear response. The detailed discussion of different types of probes is presented in sec. 2.2.3.

*Nonlinear transport measurement:* Nonlinear transport measurements have been performed recently on Aharonov-Bohm rings connected to two leads by Leturcq *et al.* [39], reporting that the even (odd) conductance terms [coefficients of even and odd bias pow-
ers, see Eq. (2.46)] are asymmetric (symmetric) in magnetic field. It was also argued that these observations were insensitive to geometric asymmetries in the ring. Angers et al. [40] have also performed nonlinear transport measurements on GaAs/GaAlAs rings in a two-terminal configuration, reporting an antisymmetric (under the reversal of magnetic field) second order response coefficient, and attributed to e-e interactions. It should be noted that in Ref. [39] no particular symmetry of even coefficients was reported, but in Ref. [40] it was reported to be antisymmetric (under reversal of magnetic field). It is essential to understand these scenarios theoretically. In this work we analytically obtain conditions for an antisymmetric and asymmetric even coefficients, using Büttiker’s probes, Sec. 5.4.

Interaction with an external nonequilibrium environment: Magnetic field asymmetries of transport in mesoscopic conductors coupled to an environment have been theoretically studied by Kang et al. [41]. The model system used in Ref. [41] was a quantum dot conductor coupled to another conductor (treated as an environment) via a Coulomb interaction. This allows energy exchange between the conductor and the environment, without particle exchange. The environment was then driven out-of-equilibrium by applying a voltage bias. It was found that the interaction between the conductor and the environment causes magnetoasymmetry even in the linear regime, if the environment is maintained out-of-equilibrium.

Motivated by this study, we explore magnetoasymmetries of transport when a double quantum dot interferometer is coupled capacitively to an external fermionic environment. While in early studies, the capacitive interaction was either treated at the mean-field level or perturbatively [41, 43], we aim for numerically exact results. We unfold symmetry relations by calculating the current in a double-dot setup, using a numerically exact influence functional path integral method, see Sec. 2.2.4 for details. These results can be used to benchmark and validate certain perturbative non-equilibrium Green’s function schemes. Interestingly, we find that Büttiker probes obey the same symmetry relations
as those reached in a microscopic model.

1.2.3 Thermoelectric transport

The thermoelectric effect describes the conversion of a temperature gradient into a voltage, and vice versa. Strong demand for cost effective energy, and at the same time, environmentally friendly energy sources, are the driving forces for research activity in this area. Enhancing the efficiency of thermoelectric materials is one of the main themes of current research in thermoelectrics.

A general thermoelectric setup consists of a system in contact with two reservoirs, left ($L$) and right ($R$) with different temperatures and chemical potentials. In the linear response regime the performance of a bulk thermoelectric device is characterized by a single dimensionless parameter known as the figure of merit $ZT$. This quantity is given by a combination of transport coefficients, electrical conductivity $\sigma$, thermal conductivity $\kappa$, thermopower $S$, and temperature $T$. In terms of these quantities the figure of merit reads as, $ZT = (\sigma S^2 / \kappa)T$. It can be shown that the efficiency is given by,

$$\eta = \eta_c \frac{\sqrt{ZT + 1} - 1}{\sqrt{ZT + 1} + 1}$$

(1.7)

where $\eta_c = 1 - \frac{T_c}{T_H}$ is the Carnot efficiency, reached in the limit $ZT \to \infty$. The linear response approximation may be justified for bulk systems since it is possible to have large temperature difference across the sample and yet very small gradients in temperature. In nanoscale systems temperature and electrical potential gradients develop on the nanometer scale which may lead to nonlinear effects. One can still analyze the performance of nanoscale devices using an expression analogous to Eq. (1.7), [36].

Thermodynamics does not impose any upper bound on $ZT$, but the inter-relation between electric and thermal transport properties makes it extremely hard to increase the value of $ZT$ beyond 1. It was recently argued that by breaking time reversal symmetry
one may enhance thermoelectric performance [36]. This is because in broken time reversal symmetric systems the efficiency depends on (i) the magnetic field asymmetry of the thermopower and (ii) on the figure of merit. Thus, to enhance efficiency, it is important to understand how many body interactions and phase breaking processes affect transport in nanoscale systems in the nonlinear regime [36].

1.2.4 Diode behaviour in Aharonov-Bohm interferometers

Diodes are integral components in electronic circuits. The diode effect can be realized by combining many body interactions and spatial asymmetries. As an example, a theoretical model of a thermal diode using a 1-dimensional lattice exploiting anharmonicity in the form of onsite interactions and spatial asymmetry has been proposed in Refs. [44, 45, 46]. Thermal diodes were also experimentally realized in carbon and boron nitride nanotubes [46]. In this thesis, we investigate the diode effect in the AB interferometer; sufficient conditions are obtained analytically. We begin with a general two-terminal model, and then demonstrate our results numerically using a specific model of a double-dot AB interferometer, Sec. 5.6.
Chapter 2

Double-dot Aharonov-Bohm interferometer

2.1 Models

In this section we present several models of double-dot Aharonov-Bohm interferometers. These different models include distinct many body effects. We construct separate models for two reasons. First, it is technically difficult to solve the dynamics of a complex system, involving different types of many body interactions (electron-electron, electron-phonon, electron-magnetic impurities), and thus to simplify our modeling we construct several-complementary models incorporating distinct effects. Second, from the fundamental point of view, it is actually advantageous to study simplified models which allow us to isolate different many body effects.

In this work we principally focus on quantum transport through a double-dot Aharonov-Bohm interferometer. In our modeling, we include only those levels in each dot that participate in the transport process. For simplicity, we include only one level in each dot. Also, we do not consider the spin degree of freedom and focus on the dynamics and steady state characteristics of the dots’ occupation, coherences and the net charge cur-
rent. The quantum dots are connected to two metallic leads by a tunneling junction. The leads comprise noninteracting electrons in a thermodynamic equilibrium. The assumption of noninteracting electrons follows from Landau-Fermi-liquid theory \[47, 48, 49\]. The key ideas behind this theory are the notion of adiabacity and the Pauli’s exclusion principle. Consider a system of noninteracting electrons, and suppose we turn on the electron-electron interaction slowly. According to Landau-Fermi arguments, the ground state of Fermi-gas would adiabatically transform into the ground state of the interacting system. By Pauli’s exclusion principle, the ground state of Fermi gas consists of fermions occupying all momentum states corresponding to momentum \( p < p_f \), where \( p_f \) is the fermi momentum. As we turn on the interaction, the spin, charge and momentum of the fermions corresponding to occupied states remain unchanged, while the dynamical properties such as their mass, magnetic moment etc. are renormalized to new values \[50\]. Thus, there is a one-to-one correspondence between the elementary excitations of a Fermi gas and a Fermi liquid system. In the context of Fermi liquid systems, these excitations are known as “quasi-particles”. This leads to a picture of effectively noninteracting electrons. The Hamiltonian of this system has the following form,

\[ H_{AB} = H_S + H_B + H_{SB}. \] (2.1)

Here \( H_S \) comprises the isolated double-dot system, \( H_B \) represents the metallic leads, and \( H_{SB} \) includes the tunneling element between the leads and the two dots. For simplicity, we set \( \hbar = 1, k_B = 1, \) and electron charge \( e = 1 \) throughout this work.

### 2.1.1 Model I: Closed interferometer with Coulomb repulsion

In this model (spinless) electrons experience an inter-dot electron-electron (\( e-e \)) repulsion of strength \( U \), see Fig. 2.1
In second quantization the Hamiltonian of the isolated double-dot system is given by

$$ H_S = \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 + U a_1^\dagger a_1 a_2^\dagger a_2, \quad (2.2) $$

where $\epsilon_{1,2}$ are the energies of the single level dots. The third term $U a_1^\dagger a_1 a_2^\dagger a_2$ stands for the (nontrivial) inter-dot Coulomb repulsion. To keep our discussion general, we allow the states to be nondegenerate at this point. Here $a_\beta^\dagger$ and $a_\beta$ are the subsystem creation and annihilation operators, respectively, where $\beta = 1, 2$ denotes dots ‘1’ and ‘2’. The metal leads are composed of noninteracting electrons,

$$ H_B = \sum_l \omega_l a_l^\dagger a_l + \sum_r \omega_r a_r^\dagger a_r, \quad (2.3) $$

where $a_{l,r}^\dagger$ and $a_{l,r}$ are the creation and annihilation operators respectively, for an electron of energy $\omega_{l,r}$ in the left ($l$) or right ($r$) lead. The Fermi-Dirac distribution functions $f_\nu(\omega) = [e^{\beta_\nu(\omega-\mu_\nu)+1}]^{-1}$ describes the electronic occupations of the leads, where $\mu_\nu$, $\nu = L, R$ is the chemical potential and we denote by $\beta_\nu = \frac{1}{T_\nu}$ the inverse temperature for $\nu^{th}$ reservoir. The subsystem-bath coupling term is given by

$$ H_{SB} = \sum_{\beta,l} \xi_{\beta,l} a_\beta^\dagger a_l e^{i\phi_\beta_l} + \sum_{\beta,r} \zeta_{\beta,r} a_\beta^\dagger a_r e^{i\phi_\beta_r} + h.c., \quad (2.4) $$

where $\xi$ is the tunneling element of dot electrons to the left bath, and similarly $\zeta$ stands
for tunneling to the right bath. Here $\phi^L_\beta$ and $\phi^R_\beta$ are the AB phase factors, acquired by electron waves in a magnetic field perpendicular to the device plane. These phases are constrained to satisfy the following relation

$$\phi^L_1 - \phi^L_2 + \phi^R_1 - \phi^R_2 = \phi = 2\pi \Phi / \Phi_0,$$

(2.5)

where $\Phi$ is the magnetic flux enclosed by the ring and $\Phi_0 = \hbar c / e$ is the flux quantum. In what follows we adopt the gauge

$$\phi^L_1 - \phi^L_2 = \phi^R_1 - \phi^R_2 = \phi / 2.$$

(2.6)

Throughout this thesis we use the same gauge; our results are independent of this particular choice.

We apply a voltage bias $\Delta \mu \equiv \mu_L - \mu_R$, with $\mu_{L,R}$ as the chemical potential of the metals. While we bias the system in a symmetric manner, $\mu_L = -\mu_R$, the dot levels may be placed away from the so called “symmetric point” at which $\mu_L - \epsilon_\beta = \epsilon_\beta - \mu_R$. This situation may be achieved by applying a gate voltage to each dot.

### 2.1.2 Model II: Interferometer with probes; elastic and inelastic effects

Our second model allows dephasing and inelastic effects of electrons in the interferometer by using Büttiker’s probe technique, as explained in Sec. 2.2.3. The schematic setup of this model is shown in Fig. 2.2. For simplicity, in this model we do not include explicit electron-electron interactions, setting $U = 0$; the probe technique effectively introduces many body effects, from different sources. We augment the Hamiltonian (2.1) with a
Figure 2.2: Model II. The two dots are each represented by a single electronic level, which do not directly couple. The total magnetic flux is denoted by $\Phi$. The electrons of dot '1' may be susceptible to dephasing or inelastic effects, introduced here through the coupling of this dot to a Büttiker’s probe, the terminal $P$. Different types of probes are presented in Sec. 2.3

probe, adding to the system a noninteracting electron reservoir $P$,

$$H = H_{AB} + \sum_{p \in P} \omega_p a_p^\dagger a_p + \sum_{p \in P} \lambda_p a_1^\dagger a_p + h.c. \quad (2.7)$$

The parameter $\lambda_p$, assumed to be real, denotes the coupling strength of dot '1' to the $P$ terminal. The parameters of the probe terminal are determined self-consistently so as to introduce elastic dephasing or inelastic scattering of electrons as we explain in subsection 2.2.3. Note that we only allow here for local scattering events on dot '1'. One could similarly consider models in which both dots are susceptible to scattering effects, possibly from different sources.

### 2.1.3 Model III: Interferometer capacitively coupled to a fermionic environment

In our third model the double quantum dot interferometer is capacitively coupled to a fermionic environment which may be driven out of equilibrium, see Fig. 2.3. The
Hamiltonian for this model is given by

$$H = H_{AB} + H_F + H_{int}. \quad (2.8)$$

The AB Hamiltonian is given by Eq. (2.1), but for simplicity we do not include the inter-dot electron-electron interactions within the interferometer. The AB interferometer is electrostatically interacting, without exchanging particles, with a fermionic environment (FE), realized here by the junction,

$$H_F = \epsilon_p c_p^\dagger c_p + \sum_{s \in \pm} \epsilon_s c_s^\dagger c_s + \sum_{s \in \pm} g_s c_s^\dagger c_p + h.c. \quad (2.9)$$

It includes a quantum dot of energy $\epsilon_p$ coupled to two reservoirs ($s = \pm$). We distinguish between the AB interferometer and the FE by adopting the operators $c$ and $c^\dagger$ to denote creation and annihilation operators of electrons in the FE. Electrons in the AB interferometer and the FE compartment are interacting according to the form

$$H_{int} = U n_p n_1. \quad (2.10)$$

Here $n_p = c_p^\dagger c_p$, $n_1 = a_1^\dagger a_1$ are the number operators, and $U$ is the charging energy, reflecting repulsion effects when dot '1' in the AB interferometer and level $p$ in the fermionic environment are occupied. The FE may be set at equilibrium when $\mu_+ = \mu_-$ (with the Fermi energy set at zero), or biased away from equilibrium using $\Delta \mu_F \equiv \mu_+ - \mu_- \neq 0$. It introduces energy dissipation effects of electrons on dot 1, this system provides a microscopic-physical description of the probe model II.

### 2.2 Observables and methods

In this thesis we focus on following observables:
Figure 2.3: Model III. Scheme for a double-dot Aharonov Bohm interferometer coupled to a fermionic environment. This environment is made of a quantum dot (labeled $p$) itself coupled to either (a) an equilibrium sea of noninteracting electrons, or (b) two metals ($\pm$) possibly biased away from equilibrium. In both cases, the dissipative environment is introduced through a capacitive interaction of dot '1' of the interferometer to the dot $p$ in the environment.

1. The reduced density matrix: $\sigma_{\beta,\beta'}(t) = \langle a^{\dagger}_{\beta}(t)a_{\beta'}(t) \rangle = \text{Tr}[\rho(t) a^{\dagger}_{\beta}a_{\beta'}]$, where $\beta, \beta' = 1, 2$ are indices for the dots, and $\rho$ is the total density matrix.

2. The average charge current: The charge current at left contact is given by

$$I_L = \langle I_L(t) \rangle = \text{Tr}[\rho(t) \hat{I}_L], \quad (2.11)$$

where the current operator is defined as

$$\hat{I}_L = -\frac{d\hat{N}_L}{dt} = -i[H, \hat{N}_L] \quad (2.12)$$

with the number operator $\hat{N}_L \equiv \sum_l a^{\dagger}_l a_l$. Here $H$ is the total Hamiltonian of a given model. Similarly, we can write an expression for the current at the right lead.

In what follows we denote the averaged charge current by $I$.

Ongoing miniaturization of electronic devices down to the nanoscale has triggered theoretical and computational research aiming to describe coherent transport and nonequilibrium many body effects. In perturbative analytic methods, such as the nonequilibrium Green’s function technique, the typical perturbation parameter is $U/\Gamma$, where $U$ is the
strength of the Coulomb interaction and $\Gamma$ is the coupling strength to the metallic leads. Other semi-analytic approaches, based upon the renormalization group principles are the time dependent density matrix renormalization group (TDMRG) technique, and functional renormalization group (FRG) method. The key ingredient of TDMRG is the representation of the total wavefunction in a truncated but optimized basis, instead of working in the full Hilbert space [51]. The basic idea behind FRG is the formulation of “flow equations” for the self energy accounting its full frequency dependence [52]. The starting point of this method is the exact solution in the noninteracting limit. During the flow, the self energy is continuously transformed, and the solution of the interacting problem is achieved when the flow terminates. This method can be combined with diagrammatic perturbation theory on the Keldysh contour.

As an alternative to the above methods, brute force numerical methods have been developed for studying nonequilibrium quantum transport through nanostructures. The real-time quantum Monte-Carlo (QMC) technique is well established [53], but computations are limited to short-intermediate simulation times because of the notorious sign problem. A novel method based on the QMC technique with complex chemical potentials has been recently developed in Ref. [54].

A different idea based on the deterministic iterative summation of path integrals (ISPI) was developed in Ref. [55]. This method was developed for studying the dynamics of the single impurity Anderson model, and its validity has been confirmed by a detailed comparison to other methods. A related approach, known as the “influence functional path integral” (INFPI) method is based on the deterministic iterative evaluation of the influence functional [56, 57]. This approach has been applied to the spin-fermion model and to other multi-level impurity models. It relies on the observation that in out-of-equilibrium cases bath correlations have a finite range, allowing truncation of the influence functional [56, 57].
Chapter 2. Double-dot Aharonov-Bohm interferometer

In this work, we study model I without an inter-dot Coulomb repulsion $U$ using the quantum Langevin equation approach, which is equivalent to the Green’s function technique in the $U = 0$ limit. Furthermore, we employ an exact fermionic trace formula for studying the transient dynamics of the noninteracting case. We then simulate the interacting model using (INFPI) method. This is the first time that this system is studied using a nonperturbative and deterministic technique. Model II is investigated using the nonequilibrium Green’s function method along with Büttiker’s probes. The dynamics of charge current in model III is studied using INFPI. In the next subsection we briefly explain the methods used in this work.

2.2.1 Nonequilibrium Green’s function technique

The nonequilibrium Green’s function (NEGF) technique was rigorously developed by Schwinger in a classic mathematical paper [58], treating the Brownian motion of a quantum oscillator. The next important development in this field was due to Kadanoff and Baym who derived quantum kinetic equations [59]. A diagrammatic expansion in powers of the coupling to the environment was developed by Keldysh with the key idea of contour ordering [60]. These initial developments were done in the early 1960s. Another important development in the context of quantum transport was an explicit derivation of a formula for the transmission function in terms of the Green’s function, by Caroli et al. [61].

In this work, we use the Green’s function method to obtain closed expressions for the reduced density matrix and the charge current in the case of a noninteracting ($U = 0$) double-dot AB interferometer. The treatment that we adopt is based on the quantum Langevin equation (QLE) approach [62]. We note that in the noninteracting limit ($U = 0$), quantum Langevin equation, nonequilibrium Green’s function technique, and scattering approaches, are equivalent. A detailed derivation of the QLE method is presented in section 3.2, the main expressions are included below. The reduced density
matrix for the double-dot \((\alpha, \beta = 1, 2)\) system in the noninteracting case reads \[62\],

\[
\langle \alpha^\dagger a_\beta \rangle \equiv \sigma_{\alpha,\beta} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[ (G^+\Gamma^L G^-)_{\alpha,\beta} f_L(\omega) + (G^+\Gamma^R G^-)_{\alpha,\beta} f_R(\omega) \right] d\omega. \tag{2.13}
\]

Here the matrices \(G^+\) and \(G^- = (G^+)^\dagger\) are the retarded and advanced Green’s functions, and \(f_L(\omega)\) and \(f_R(\omega)\) are the Fermi-Dirac distribution functions in the left and right reservoirs. The matrix elements of \(G^+\) are given by

\[
G^+_{\beta,\alpha}(\omega) = \frac{1}{(\omega - \epsilon_\beta)\delta_{\alpha,\beta} - \Sigma_{L,\alpha,\beta}(\omega) - \Sigma_{R,\alpha,\beta}(\omega)}.
\tag{2.14}
\]

In the above equation \(\Sigma_{L,\alpha,\beta}(\omega)\) and \(\Sigma_{R,\alpha,\beta}(\omega)\) are the self energies, see Eq. (3.6) for details.

In Eq. (2.13) \(\Gamma^{L(R)}\) are the hybridization matrices to the left and right reservoirs, with the matrix elements

\[
\Gamma^{L}_{\beta,\beta'}(\omega) = 2\pi e^{i(\phi^L_{\beta} - \phi^L_{\beta'})} \sum_l \xi_{\beta,l} \delta(\omega - \omega_l) \xi^*_{\beta',l},
\tag{2.15}
\]

and

\[
\Gamma^{R}_{\beta,\beta'}(\omega) = 2\pi e^{-i(\phi^R_{\beta} - \phi^R_{\beta'})} \sum_r \zeta_{\beta,r} \delta(\omega - \omega_r) \zeta^*_{\beta',r}.
\tag{2.16}
\]

Eq. (2.13) can be extended to describe any number of reservoirs. When a probe reservoir is included (discussed in the next section), it reads as below,

\[
\langle \alpha^\dagger a_\beta \rangle = \frac{1}{2\pi} \sum_{\nu=L,R,P} \int_{-\infty}^{\infty} (G^+\Gamma^\nu G^-)_{\alpha,\beta} f_\nu(\omega) d\omega. \tag{2.17}
\]

An expression for the charge current, in the case of noninteracting dots, is given below, see Eq. (2.18).
2.2.2 Landauer-Büttiker approach

In the scattering formalism of Landauer and Büttiker [63, 64, 65, 66], interactions between particles are neglected. Considering a multi-terminal setup, one can express the charge current from the $\nu$ to the $\nu'$ terminal in terms of the transmission probability $T_{\nu,\nu'}(\omega)$, a function which depends on the energy of the incident electron,

$$I_\nu(\phi) = \int_{-\infty}^{\infty} d\omega \left[ \sum_{\nu' \neq \nu} T_{\nu,\nu'}(\omega, \phi) f_\nu(\omega) - \sum_{\nu' \neq \nu} T_{\nu',\nu}(\omega, \phi) f_{\nu'}(\omega) \right].$$  \hspace{1cm} (2.18)

The Fermi-Dirac distribution function $f_\nu(\omega) = \left[ e^{\beta_\nu(\omega - \mu_\nu)} + 1 \right]^{-1}$ is defined in terms of the chemical potential $\mu_\nu$ and the inverse temperature $\beta_\nu$. The magnetic field is introduced via an Aharonov-Bohm flux $\Phi$ applied perpendicular to the conductor, with the magnetic phase $\phi = 2\pi\Phi/\Phi_0$. The transmission function can be written in terms of the Green’s function of the system and the self energy matrices,

$$T_{\nu,\nu'} = \text{Tr} \left[ \Gamma^\nu G^+ \Gamma^{\nu'} G^- \right].$$  \hspace{1cm} (2.19)

Explicit expressions for a particular model are included in Sec. 5.5. We consider a setup including three terminals, $L$, $R$ and $P$, where the $P$ terminal serves as the “probe”, see Fig. 2.2. The probe properties are determined by self-consistent conditions discussed in the next subsection. We focus below on the steady state charge current from the $L$ reservoir to the central system ($I_L$), and from the probe to the system ($I_P$),

$$I_L(\phi) = \int_{-\infty}^{\infty} d\omega \left[ T_{L,R}(\omega, \phi) f_L(\omega) - T_{R,L}(\omega, \phi) f_R(\omega) \right. \right.$$  
$$+ \left. T_{L,P}(\omega, \phi) f_L(\omega) - T_{P,L}(\omega, \phi) f_P(\omega, \phi) \right],$$  \hspace{1cm} (2.20)
\[ I_P(\phi) = \int_{-\infty}^{\infty} d\omega \left[ T_{P,L}(\omega, \phi)f_P(\omega, \phi) - T_{L,P}(\omega, \phi)f_L(\omega) \right. \]
\[ + \left. T_{P,R}(\omega, \phi)f_P(\omega, \phi) - T_{R,P}(\omega, \phi)f_R(\omega) \right]. \] (2.21)

Similarly, we can write the heat current at the \( \nu = L \) terminal as
\[ Q_L(\phi) = \int_{-\infty}^{\infty} d\omega (\omega - \mu_L) \left[ T_{L,R}(\omega, \phi)f_L(\omega) \right. \]
\[ -T_{R,L}(\omega, \phi)f_R(\omega) - T_{L,P}(\omega, \phi)f_L(\omega) - T_{R,P}(\omega, \phi)f_R(\omega) \right]. \] (2.22)

The heat current at the probe is given by an analogous expression. The probe distribution function is determined by the probe condition. It is generally influenced by the magnetic flux, as we demonstrate in Eqs. (2.24)-(2.27). For convenience, we simplify next our notation. First, we drop the reference to the energy of incoming electrons \( \omega \) in both transmission functions and distribution functions. Second, since the integrals are evaluated between \( \pm \infty \), we do not put the limits explicitly. Third, unless otherwise mentioned, \( f_P, \mu_P \) and all transmission coefficients are evaluated at the phase \( +\phi \), thus we do not explicitly write the phase variable. If we do need to consider e.g. the transmission function \( T_{\nu,\nu'}(-\phi) \), we write instead the complementary expression, \( T_{\nu',\nu}(\phi) \).

### 2.2.3 Büttiker’s Probes technique

Phase-breaking and energy dissipation processes arise due to the interaction of electrons with other degrees of freedom, e.g., with electrons, phonons, and defects. While an understanding of such effects, from first principles, is the desired objective of numerous computational approaches [67], simple analytical treatments are advantageous as they allow one to gain insights into transport phenomenology.

The markovian quantum master equation and its variants (Lindblad, Redfield) is simple to study and interpret [68], and as such it has been extensively adopted in studies of charge, spin, exciton, and heat transport. It can be derived systematically, from
projection operator techniques [69], and phenomenologically by introducing damping terms into the matrix elements of the reduced density matrix, to include dephasing and inelastic processes into the otherwise coherent dynamics.

Büttiker’s probe technique [66, 70, 71] and its modern extensions to thermoelectric problems [72, 35, 36, 73], atomic-level thermometry [74], and beyond linear response situations [75, 76, 77, 78, 79] present an alternative route for introducing decoherence and inelastic processes into coherent conductors. The probe is an electronic component [80], and it allows one to obtain information about local variables, chemical potential and temperature, deep within the conductor. When coupled strongly to the system, the probe can alter intrinsic transport mechanisms.

The probe technique can be exercised in several different ways, to induce distinct effects: Elastic dephasing processes are implemented by incorporating a “dephasing probe”, enforcing the requirement that the net charge current towards the probe terminal, at any given energy, vanishes [81, 82]. Inelastic heat dissipative effects are included by a “voltage probe”, by demanding that the total-net charge current to the probe terminal nullifies [66, 70, 71]. This process dissipates heat since electrons leaving the system to the probe re-enter the conductor after being thermalized. In the complementary “temperature probe” charge leakage is allowed at the probe, but the probe temperature is tuned such that the net heat current at the probe is nil [84]. The “voltage-temperature probe”, also referred to as a “thermometer”, requires both charge current and heat current at the probe to vanish. In this case inelastic - energy exchange effects are allowed on the probe, but heat dissipation and charge leakage effects are excluded.

The probe technique has been used in different applications, particularly for the exploration of the ballistic to diffusive (Ohm’s law and Fourier’s law) crossover in electronic [70, 85] and phononic conductors [86, 87, 88, 89]. More recently, the effect of thermal rectification has been studied in phononic systems by utilizing the temperature probe as a mean to incorporate effective anharmonicity [75, 76, 77, 90]. A full-counting statistics
analysis of conductors including dephasing and voltage probes has been carried out in Ref. [91]. The probe parameters, temperature and chemical potential, can be derived analytically when the conductor is set close to equilibrium [66, 80, 72]. Far from equilibrium, while these parameters can be technically defined and their uniqueness [78] allows for a physical interpretation, an exact analytic solution is missing. However, recent studies have demonstrated that iterative numerical schemes can reach a stable solution for the temperature probe [76, 79]. These techniques have been then used for following phononic heat transfer in the deep quantum limit, far from equilibrium [76, 79].

**Dephasing probe:** Elastic dephasing effects can be incorporated with the dephasing probe. A particle entering the probe is incoherently re-emitted within a small energy interval $[\omega, \omega + d\omega]$ such that $d\omega << T\nu, \Delta\mu$ [92]. It loses phase memory, but the change in energy is much smaller than the voltage bias and the temperature [92]. Since scattering processes in each energy interval are independent, the distribution function of electrons in the probe reservoir is a highly nonequilibrium one, see Eq. (2.24). Elastic dephasing effects can thus be implemented by demanding that the energy-resolved particle current vanishes in the probe,

$$I_P(\omega) = 0 \quad \text{with} \quad I_P = \int I_P(\omega)d\omega. \quad (2.23)$$

Using this condition, Eq. (2.21) provides a closed form for the corresponding (flux-dependent) probe distribution, not necessarily in the form of a Fermi function,

$$f_P(\phi) = \frac{\tau_{L,P}f_L + \tau_{R,P}f_R}{\tau_{P,L} + \tau_{P,R}}. \quad (2.24)$$

**Voltage probe:** Dissipative inelastic effects can be introduced into the conductor using the voltage probe technique. The three reservoirs ($L, R, P$) are maintained at the same inverse temperature $\beta_a$, but the $L$ and $R$ chemical potentials are made distinct, $\mu_L \neq \mu_R$. In this case the chemical potential $\mu_P$ of the probe $P$ is evaluated by demanding that
the net-total particle current flowing into the $P$ reservoir diminishes,

$$I_P = 0.$$  \hfill (2.25)

This choice allows for dissipative energy exchange processes to take place within the probe. In the linear response regime Eq. (2.21) can be used to derive an analytic expression for $\mu_P$,

$$\mu_P(\phi) = \frac{\Delta \mu}{2} \left[ \frac{\int d\omega \frac{\partial f_a}{\partial \omega} (T_{L,P} - T_{R,P})}{\int d\omega \frac{\partial f_a}{\partial \omega} (T_{P,L} + T_{P,R})} \right].$$  \hfill (2.26)

In the above equation the derivative of the Fermi function is evaluated at equilibrium. In far-from-equilibrium situations we obtain the unique [78] chemical potential of the probe numerically by using the Newton-Raphson method [161]

$$\mu_P^{(k+1)} = \mu_P^{(k)} - I_P(\mu_P^{(k)}) \left[ \frac{\partial I_P(\mu_P^{(k)})}{\partial \mu_P} \right]^{-1}. \hfill (2.27)$$

The current $I_P(\mu_P^{(k)})$ and its derivative are evaluated from Eq. (2.21) using the probe (Fermi) distribution with $\mu_P^{(k)}$. Note that the self-consistent probe solution varies with the magnetic flux.

**Temperature probe:** In this scenario the three reservoirs $L,R,P$ are maintained at the same chemical potential $\mu_a$, but the temperature at the $L$ and $R$ terminals are made different, $T_L \neq T_R$. The probe temperature $T_P = \beta_p^{-1}$ is determined by requiring the net heat current at the probe to satisfy

$$Q_P = 0.$$  \hfill (2.28)

This constraint allows for charge leakage into the probe since we do not require Eq. (2.25) to hold. We can obtain the temperature $T_P$ numerically by following an iterative
The probe temperature varies with the applied flux $\phi$.

**Voltage-temperature probe:** This probe acts as an electron thermometer at weak coupling. This is achieved by setting the temperatures $T_{L,R}$ and the potentials $\mu_{L,R}$, then demand that both

$$I_P = 0 \quad , \quad Q_P = 0 .$$

(2.30)

In other words, the charge and heat currents in the conductor satisfy $I_L = -I_R$ and $Q_L = -Q_R$, since neither charges nor heat are allowed to leak to the probe. Analytic results can be obtained in the linear response regime, see for example Refs. [72, 85]. Beyond that, equation (2.30) can be solved self-consistently, to provide $T_P$ and $\mu_P$. This can be done by using the two-dimensional Newton-Raphson method,

$$\mu_P^{(k+1)} = \mu_P^{(k)} - D_{1,1}^{-1}I_P(\mu_P^{(k)}, T_P^{(k)}) - D_{1,2}^{-1}Q_P(\mu_P^{(k)}, T_P^{(k)})$$

$$T_P^{(k+1)} = T_P^{(k)} - D_{2,1}^{-1}I_P(\mu_P^{(k)}, T_P^{(k)}) - D_{2,2}^{-1}Q_P(\mu_P^{(k)}, T_P^{(k)}),$$

(2.31)

where the Jacobean $D$ is re-evaluated at every iteration,

$$D(\mu_P, T_P) \equiv \begin{pmatrix} \frac{\partial I_P(\mu_P, T_P)}{\partial \mu_P} & \frac{\partial I_P(\mu_P, T_P)}{\partial T_P} \\ \frac{\partial Q_P(\mu_P, T_P)}{\partial \mu_P} & \frac{\partial Q_P(\mu_P, T_P)}{\partial T_P} \end{pmatrix}$$

We emphasize that besides the case of the dephasing probe, the function $f_P(\phi)$ is forced to take the form of a Fermi-Dirac distribution function in the other probe models.
2.2.4 Influence functional path integral simulations

This technique allows one to follow the nonequilibrium real-time dynamics of electrons in a subsystem-bath model (for example, the double-dot-metals) by performing exact numerical simulations [56, 57]. The principles of the INFPI approach have been detailed in Refs. [56, 57], where it has been adopted for investigating dissipation effects in the nonequilibrium spin-fermion model, and the population and the current dynamics in correlated quantum dots, by investigating the single impurity Anderson model [84] and the two-level spinless Anderson dot [93, 94]. In this thesis, we further extend this approach, examining the effect of a magnetic flux on the intrinsic coherence dynamics in Model-I. We also use this tool and study symmetries of nonlinear transport in Model III.

The INFPI method relies on the observation that in out-of-equilibrium (and/or finite temperature) cases bath correlations have a finite range, allowing for their truncation beyond a memory time dictated by the voltage-bias and the temperature. Taking advantage of this fact, an iterative-deterministic time-evolution scheme has been developed where convergence with respect to the memory time can in principle be reached [56, 57]. As convergence is facilitated at large bias, the method is well suited for the description of the real-time dynamics of devices driven to a steady state via interaction with biased leads. The INFPI approach is complementary to other numerically exact methods such as numerical renormalization group techniques [95, 96], real time quantum Monte Carlo simulations [53] and path integral methods [55]. It offers flexibility in defining the impurity subsystem and the metal band structure. The results converge well at intermediate-large voltage bias and/or high temperatures as shown in section-4.3. We outline now the technical principles of the INFPI method as developed in references [56, 57]. We begin by reorganizing the Hamiltonian, Eq. (2.1), as \( H = H_0 + H_1 \), identifying the nontrivial quartic many body interaction term in model I, Eq. (2.2) as

\[
H_1 = U \left[ n_1 n_2 - \frac{1}{2} (n_1 + n_2) \right].
\]  

(2.32)
In a similar manner, the quartic many body interaction term in model III, Eq. (2.10) can be organized. \( H_0 \) contains the remaining two-body terms, redefining the dot energies as \( E_{d,\beta} = \epsilon_\beta + U/2 \). This partitioning allows us to utilize the Hubbard-Stratonovich (HS) transformation \[154\], see Eq. (2.34) below. Formally, the dynamics of a quadratic operator, \( \hat{A} \), either given in terms of the baths (metals) or impurity degrees of freedom, can be written as

\[
\langle \hat{A}(t) \rangle = \text{Tr}[\rho(t_0)\hat{A}(t)] \equiv \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} \text{Tr}[\rho(0)e^{iH't}e^{\lambda\hat{A}}e^{-iH't}].
\] (2.33)

Here \( \lambda \) is a real number, taken to vanish at the end of the calculation, \( \rho \) is the total density matrix, and the trace is performed over both the subsystem and the reservoirs degrees of freedom. For simplicity, we assume that at the initial time \( t = 0 \) the dots and the baths are decoupled, \( \rho(0) = \sigma(0) \otimes \sigma_L \otimes \sigma_R \). The baths are prepared in a nonequilibrium biased state \( \sigma_\nu \); the subsystem is described by the (reduced) density matrix \( \sigma(0) \). We proceed and factorize the time evolution operator, \( e^{iHt} = (e^{iH_0t})^N \), further utilizing the Trotter decomposition

\[
e^{iH_0t} \approx \left( e^{iH_1\delta t/2} e^{iH_0\delta t} e^{iH_1\delta t/2} \right)^N.
\]

The many body term \( H_1 \) can be eliminated by introducing auxiliary Ising variables \( s = \pm \) via the HS transformation \[154\],

\[
e^{\pm iH_1\delta t} = \frac{1}{2} \sum_s e^{H_\pm(s)}; \quad e^{H_\pm(s)} \equiv e^{-s\kappa_\pm(n_2-n_1)}.
\] (2.34)

Here \( \kappa_\pm = \kappa' \mp i\kappa'' \), \( \kappa' = \sinh^{-1}[\sin(\delta tU/2)]^{1/2} \), \( \kappa'' = \sin^{-1}[\sin(\delta tU/2)]^{1/2} \). The uniqueness of this transformation requires \( U\delta t < \pi \). Incorporating the Trotter decomposition and the HS transformation into Eq. (2.33), the time evolution of \( \hat{A} \) is dictated by

\[
\langle \hat{A}(t) \rangle = \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} \left\{ \int ds_1^\pm ds_2^\pm ... ds_N^\pm \mathcal{I}(s_1^\pm, s_2^\pm, ..., s_N^\pm) \right\}.
\] (2.35)

The integrand, referred to as an “Influence Functional” (IF), is given by \( \langle k = 1, k + p = \)}
\[ N \),
\[
I(s_{k}^{\pm}, \ldots, s_{k+p}^{\pm}) = \frac{1}{2^{(p+1)}} \text{Tr} \left[ \sigma(0)G_{+}(s_{k+p}^{+}) \ldots G_{+}(s_{k}^{+})e^{iH_{0}(k-1)\delta t}e^{\lambda \hat{A}}e^{-iH_{0}(k-1)\delta t}G_{-}(s_{k}^{-}) \ldots G_{-}(s_{k+p}^{-}) \right]
\]  
(2.36)

Here \( G_{+}(s_{k}^{+}) = \left( e^{iH_{0}\delta t/2}e^{H_{+}(s_{k}^{+})}e^{iH_{0}\delta t/2} \right) \) and \( G_{-} = G_{+}^{\dagger} \). Eq. (2.35) is exact in the \( \delta t \to 0 \) limit. Practically, it can be evaluated by noting that in standard nonequilibrium situations, even at zero temperature, bath correlations die exponentially, thus the IF in Eq. (2.35) can be truncated beyond a memory time \( \tau_{c} = N_{s}\delta t \), corresponding to the time beyond which bath correlations may be controllably ignored [56]. Here \( N_{s} \) is an integer and the correlation time \( \tau_{c} \) is determined by the nonequilibrium situation, roughly \( \tau_{c} \sim 1/\Delta \mu \). This argument implies the following (non-unique) breakup [56]

\[
I(s_{1}^{\pm}, s_{2}^{\pm}, \ldots, s_{N}^{\pm}) \simeq I(s_{1}^{\pm}, s_{2}^{\pm}, \ldots, s_{N_{s}}^{\pm})I_{s}(s_{2}^{\pm}, s_{3}^{\pm}, \ldots, s_{N_{s}+1}^{\pm}) \ldots \\
\times I_{s}(s_{N_{s}-N_{s}+1}^{\pm}, s_{N_{s}-N_{s}+2}^{\pm}, \ldots, s_{N}^{\pm}),
\]  
(2.37)

where each element in the product, besides the first one, is given by a ratio between truncated IF,

\[
I_{s}(s_{k}, s_{k+1}, \ldots, s_{k+N_{s}-1}) = \frac{I(s_{1}^{\pm}, s_{2}^{\pm}, \ldots, s_{k+N_{s}-1}^{\pm})}{I(s_{k}^{\pm}, s_{k+1}^{\pm}, \ldots, s_{k+N_{s}-2}^{\pm})}.
\]  
(2.38)

It is useful to define the multi-time object and time-evolve it by multiplying it with the subsequent truncated IF, over the intermediate variables,

\[
R(s_{k+1}^{\pm}, s_{k+2}^{\pm}, \ldots, s_{k+N_{s}-1}^{\pm}) = \sum_{s_{1}^{\pm}, s_{2}^{\pm}, \ldots, s_{k}^{\pm}} I(s_{1}^{\pm}, s_{2}^{\pm}, \ldots, s_{N_{s}}^{\pm})I_{s}(s_{2}^{\pm}, s_{3}^{\pm}, \ldots, s_{N_{s}+1}^{\pm}) \ldots I_{s}(s_{k}^{\pm}, s_{k+1}^{\pm}, \ldots, s_{k+N_{s}-1}^{\pm}),
\]  
(2.39)
then summing over the internal variables,

$$
\mathcal{R}(s_{k+2}^\pm, s_{k+3}^\pm, \ldots, s_{k+N_s}^\pm) = \sum_{s_{k+1}^\pm} \mathcal{R}(s_{k+2}^\pm, s_{k+2}^\pm, \ldots, s_{k+N_s-1}^\pm) I_s(s_{k+1}^\pm, s_{k+2}^\pm, \ldots, s_{k+N_s}^\pm). \tag{2.40}
$$

Summation over the internal variables results in the time local expectation value,

$$
\langle e^{\lambda \hat{A}(t_k)} \rangle = \sum_{s_{k+2-N_s}^\pm, \ldots, s_{k}^\pm} \mathcal{R}(s_{k+2-N_s}^\pm, s_{k+3-N_s}^\pm, \ldots, s_{k}^\pm). \tag{2.41}
$$

This procedure should be repeated for several (small) values of $\lambda$. Taking the numerical derivative with respect to $\lambda$, the expectation value $\langle \hat{A}(t_k) \rangle$ is retrieved. The main element in this procedure, the truncated IF [Eq. (2.36)], is calculated using a fermionic trace formula [119],

$$
I = \text{Tr} \left[ e^{M_1} e^{M_2} \ldots e^{M_p} (\sigma_L \otimes \sigma_R \otimes \sigma(0)) \right] = \det \left\{ \begin{bmatrix} I_L - f_L \otimes I_R - f_R \otimes I_S - f_S + e^{m_1} e^{m_2} \ldots e^{m_p} \end{bmatrix} \right\}. \tag{2.42}
$$

Here, $\sigma_\nu$, the time-zero density matrix of the $\nu = L, R$ fermion bath and $\sigma(0)$, the subsystem initial density matrix, are assumed to follow an exponential form. Other terms $e^M$, with $M$ a quadratic operator, represent further factors in Eq. (2.36). In the determinant, $m$ is a single-particle operator, corresponding to the quadratic operator $M = \sum_{i,j} (m)_{i,j} c_i^\dagger c_j$; $c_i^\dagger$ ($c_j$) are fermionic creation and annihilation operators, either related to the system or the baths. The matrices $I_\nu$ and $I_S$ are the identity matrices for the $\nu$ space and for the subsystem, respectively. The determinant in Eq. (2.42) is evaluated numerically by taking into account $L_s$ electronic states for each metal. This discretization implies a numerical error. However, we have found that with $L_s \sim 100$ states we can reach convergence in the time interval of interest. Other sources of error, elaborated and examined in Refs. [56, 57], are the Trotter error, originating from the
approximate factorization of the total Hamiltonian into the non-commuting $H_0$ (two-body) and $H_1$ (many body) terms, and the memory error, resulting from the truncation of the IF. Convergence is verified by demonstrating that results are insensitive to the time step and the memory size, once the proper memory time is accounted for. It was shown in Ref. [34] that when the dot states are located within the bias window a shorter memory time is required for reaching convergence, in comparison to the case where the dot energies are out-of-resonance with the bias window. This could be rationalized by noting that the decorrelation time for electrons within the bias window is short relative to the characteristic timescale of decay for electrons occupying off-resonance states.

It was also noted that distinct observables may require different memory time $\tau_c$ for reaching convergence [34, 56, 57]. The dot’s occupation and the real part of the subsystem off-diagonal element, $\Re\sigma_{1,2}$, converge for $\tau_c \sim 1/\Delta\mu$. In contrast, the charge current and $\Im\sigma_{1,2}$ require a memory time at least twice longer, as these quantities are sensitive to the bias drop at each contact, rather than to the overall voltage bias. It is important to note that this scaling is approximate, and the actual memory time further depends on the subsystem (dots) energetics in a complex way. The memory time depends on $U$ in a nontrivial manner [97], and the position of the dot with respect to the left and right chemical potentials also affects the convergence behavior.

In the absence of $U$, INFPI numerical results are exact, irrespective of the memory size used in the simulation. This can be seen from Eqs. (2.36) and (2.37), where a cancellation effect takes place leaving only free propagation terms, from $t = 0$ to the current time. At infinitely large $U$ one expects again superior convergence behavior, as simultaneous occupancy is forbidden [97]. Since INFPI can not treat the infinite $U$ case in its current form, we adopted a particular quantum master equation to study this limit.
2.2.5 Master equations at $U = 0$ and $U = \infty$

Several different types of quantum master equations have been developed to study quantum transport through open systems and nanostructures [69, 98]. Given the vast literature in this field, we do not aim in reviewing it here. We only mention a specific approach of interest, the Bloch-type rate equations based on the microscopic many body Schrödinger equation as developed by Gurvitz [9]. In this thesis, we adopt master equations to complement our simulations with INFPI. The approach can be used in two different limits, (i) $U = 0$, and (ii) $U = \infty$. The main assumptions in deriving these equations are:

1. The system is subjected to a very large voltage bias, implying a unidirectional transport.

2. The reservoirs have a broad band with energy independent density of states.

3. The reservoirs are Markovian; electron relaxation in the metals is fast compared to electron dynamics in the junction.

We denote the reduced density matrix of the double-dot system in the charge state basis as $\sigma_{j,j'}(t)$, $j = a, b, c, d$. Here the index $j$ labels the double-dot charge states in order of an empty dot ($a$), single occupied dot, on either the ”1” or ”2” sites ($b$ and $c$ states, respectively) and the state ($d$), with the two dots occupied. Explicitly, $|a\rangle \leftrightarrow |00\rangle$, $|b\rangle \leftrightarrow |10\rangle$, $|c\rangle \leftrightarrow |01\rangle$, and $|d\rangle \leftrightarrow |11\rangle$. The creation and annihilation operators of the dot are related to this states by $a_1^\dagger \leftrightarrow |00\rangle\langle 01| + |01\rangle\langle 11|$, $a_2^\dagger \leftrightarrow |00\rangle\langle 10| + |10\rangle\langle 11|$. Since $a_1^\dagger a_2 \leftrightarrow |01\rangle\langle 01|$, we identify the observable of interest $\sigma_{1,2}=\text{Tr}[\sigma a_1^\dagger a_2]$ by $\sigma_{b,c}$. In
the noninteracting ($U = 0$) case, the following equations hold in the infinite bias limit [9]

\[ \dot{\sigma}_{a,a} = -4\gamma_L\sigma_{a,a} + \gamma_R (\sigma_{b,b} + \sigma_{c,c} + \sigma_{b,c}e^{i\phi/2} + \sigma_{c,b}e^{-i\phi/2}) \]
\[ \dot{\sigma}_{b,b} = 2\gamma_L\sigma_{a,a} - 2(\gamma_R + \gamma_L)\sigma_{b,b} + 2\gamma_R\sigma_{d,d} + \delta\gamma e^{i\phi/2}\sigma_{b,c} + \delta\gamma e^{-i\phi/2}\sigma_{c,b} \]
\[ \dot{\sigma}_{c,c} = 2\gamma_L\sigma_{a,a} - 2(\gamma_R + \gamma_L)\sigma_{c,c} + 2\gamma_R\sigma_{d,d} + \delta\gamma e^{i\phi/2}\sigma_{b,c} + \delta\gamma e^{-i\phi/2}\sigma_{c,b} \]
\[ \dot{\sigma}_{d,d} = 2\gamma_L (\sigma_{b,b} + \sigma_{c,c} - e^{-i\phi/2}\sigma_{b,c} - e^{i\phi/2}\sigma_{c,b}) - 4\gamma_R\sigma_{d,d} \]
\[ \dot{\sigma}_{b,c} = 2\gamma_L e^{i\phi/2}\sigma_{a,a} + \delta\gamma (\sigma_{b,b} + \sigma_{c,c})e^{-i\phi/2} - 2\gamma_R\sigma_{d,d} e^{-i\phi/2} - 2(\gamma_L + \gamma_R)\sigma_{b,c} \] (2.43)

Here $\delta\gamma = (e^{i\phi}\gamma_L - \gamma_R)$. The hybridization strength, independent of the site index $\beta$, is defined as $\gamma_L = 2\pi \sum_l \xi_{l,\beta}^2 \delta(\omega - \omega_l)$, and $\gamma_R = 2\pi \sum_l \zeta_{r,\beta}^2 \delta(\omega - \omega_r)$. The equations are valid in the infinite bias limit, when $|\mu_L - \mu_R| \gg \gamma_L(R)$. The total probability, to occupy any of the four states, is unity, $\sum_{j=a,b,c,d} \sigma_{j,j} = 1$.

In the infinite $U$ regime one can again derive the system’s equations of motion in the large bias limit while excluding simultaneous occupancy at both dots, $\sigma_{d,d} = 0$. The following equations of motion are then achieved [9, 99] ($\sigma_{a,a} + \sigma_{b,b} + \sigma_{c,c} = 1$),

\[ \dot{\sigma}_{a,a} = -4\gamma_L\sigma_{a,a} + 2\gamma_R (\sigma_{b,b} + \sigma_{c,c} + \sigma_{b,c}e^{i\phi/2} + \sigma_{c,b}e^{-i\phi/2}) \]
\[ \dot{\sigma}_{b,b} = 2\gamma_L\sigma_{a,a} - 2\gamma_R\sigma_{b,b} - \gamma_R (\sigma_{b,c}e^{i\phi/2} + \sigma_{c,b}e^{-i\phi/2}) \]
\[ \dot{\sigma}_{c,c} = 2\gamma_L\sigma_{a,a} - 2\gamma_R\sigma_{c,c} - \gamma_R (\sigma_{b,c}e^{i\phi/2} + \sigma_{c,b}e^{-i\phi/2}) \]
\[ \dot{\sigma}_{b,c} = 2\gamma_L e^{i\phi/2}\sigma_{a,a} - \gamma_R e^{-i\phi/2}(\sigma_{b,b} + \sigma_{c,c}) - 2\gamma_R\sigma_{b,c} \] (2.44)

In chapter 4 we use master equations to study coherence dynamics in the $U = 0$ and $U = \infty$ limits. We extract magnetic flux dependent decay rates, and study the long time behaviour.
2.3 Open questions

2.3.1 Quantum dynamics in nonequilibrium many body systems

The double quantum dot Aharonov-Bohm interferometer offers a rich playground for studying fundamental questions of decoherence, dissipation and transport in open quantum systems. This system has been intensively investigated in the context of Kondo physics, Coulomb blockade behaviour, transmission phase lapses, coherent population trapping [6, 4, 7, 8, 9, 10, 11, 12, 13, 5, 14, 15, 16, 17, 100, 101]. From the statistical mechanics perspective, quantum dot interferometers have been used to verify quantum fluctuation theorems and derive the counting statistics in broken time reversal symmetric set-ups [91, 102]. However, the transient dynamics of this system has been mostly ignored, partially because of the lack of appropriate methodologies. The magnetic flux dependent dynamics is of a fundamental interest from the quantum information perspective. This aspect will be studied in this work. In order to achieve our objective, we will utilize the modeling tools discussed in the previous section, and address the following general questions:

1. What are the signatures of many body effects in the transient dynamics and the steady state behaviour?

2. How does a finite bias voltage affect quantum coherent transport?

3. Are there symmetries which are obeyed in the steady state limit, but are violated in the transient regime?

4. Can we understand the basic physics of transport using phenomenological models of many body interactions?
2.3.2 Transient dynamics and steady state behaviour (model I)

The behaviour of the charge current and dot occupations in nanodevices has been intensively studied in the steady state limit using markovian master equations [31]. The dynamics of coherences, the off-diagonal elements of the reduced density matrix, is of particular interest from the quantum computing perspective. This coherence dynamics was only recently studied by Tu et al. [31] who had investigated the dynamics of a noninteracting double-dot interferometer using non-markovian master equations. It was found that when the double-dot system is set at the particle-hole symmetric point $(\mu_L - \epsilon = \epsilon - \mu_R)$, and when $\phi \neq 2\pi p$ where $p$ is an integer, the real part of coherence, $\Re(\sigma_{1.2}) = 0$ and the imaginary part $\Im(\sigma_{1.2}) \neq 0$. In other words, the relative phase between the two dot states (charge states) defined as

$$\sigma_{12}(t) = |\sigma_{12}|e^{i\varphi(t)}$$

approaches $\varphi = \pm \pi/2$ in the long-time limit. It was thus argued in Ref. [31] that one can not manipulate this relative phase by changing the Aharonov-Bohm phase. This effect has been referred as the “phase localization”. Since dot energies can be tuned away from the particle-hole symmetric point by the gate voltage, it is of interest to explore if the “phase localization” effect still holds away from the symmetric point.

The noninteracting system has further revealed a wealth of intricate behavior, such as “flux-dependent level attraction” [27], and the ability to achieve decoherence control when junction asymmetry is incorporated [33]. In this thesis we study transient and steady state properties of the double quantum dot Aharonov-Bohm interferometer: population, coherence and current. First, we consider the noninteracting case ($U = 0$) and unfold novel transport characteristics induced by the interplay of magnetic flux, gate voltage, and applied bias voltage. We obtain exact analytical expressions in the steady state limit, and use an exact fermionic trace formula for the transient case, and address the
following questions:

1. What is the effect of the gate voltage and voltage bias on the dynamics of coherences, particularly away from the symmetric point?

2. How does the occupation of the dots change with the magnetic flux?

3. How does the temperature affect the occupation-flux behaviour?

4. What is the role of dephasing on the coherence behaviour?

We then focus on the dynamics of Model I with interactions ($U \neq 0$) and address the following questions:

1. What is the role of finite electron-electron repulsion effects in the “phase localization” effect, and how does it affect the charge current?

2. How does the system dynamics change in the $U = \infty$ limit, compared to the $U = 0$ case?

2.3.3 Magnetic field symmetries beyond linear response (model II)

The Onsager-Casimir symmetry relations [37] are satisfied in phase-coherent conductors, reflecting the microreversibility of the scattering matrix. For simplicity, consider a two-terminal ($L, R$) quantum-dot Aharonov-Bohm interferometer. The net current $I$ can be written as,

$$I(\phi, \Delta \mu) = G_1(\phi)\Delta \mu + G_2(\phi)\Delta \mu^2 + ...$$

(2.46)

where $G_1(\phi)$ is the linear conductance term and further terms are the non-linear conductances. According to the Onsager-Casimir symmetry relations, the linear conductance should be an even function of magnetic field. In Aharonov-Bohm interferometers with
conserved electron current this symmetry is displayed by the "phase rigidity" of the (linear) conductance oscillations with the magnetic field $B$, $G_1(B) = G_1(-B)$ [4, 21]. Beyond linear response, the phase symmetry of the conductance is not enforced, and several experiments [38, 39, 40, 106, 103, 104, 105, 107, 108, 109] have demonstrated its breakdown.

Supporting theoretical works have elucidated the role of many body interactions in the system [10, 110, 111, 112, 113, 114], typically approaching the problem by calculating the electrostatic screening potential within the conductor in a self-consistent manner, a procedure often limited to low-order conduction terms [10, 110, 112]. Magnetoasymmetries in the closed single quantum dot interferometer with strong electron-electron interactions have been analyzed beyond mean field theory by Lim et al. [107], demonstrating that in a spatially symmetric system even conductance terms are odd in the magnetic flux, and odd terms are even [107].

Although, the above studies focused on a particular realization of an Aharonov-Bohm interferometer with specific a form of many body interactions, a model independent proof of symmetry relations was missing. We show that such a proof can be constructed using Büttiker’s probe technique, as the probes offer a phenomenological means to introduce many body interactions. Our objective is to resolve the role of different scattering effects on transport symmetries beyond linear response. Specifically we focus on following questions:

1. How does pure elastic dephasing affect the Onsager symmetry?

2. What is the role of inelastic scattering processes on transport symmetries beyond linear response? Are there new symmetries beyond linear response?

3. What is the role of spatial symmetry and particle-hole symmetry on transport symmetries?

4. Can the interferometer act as a diode when the time reversal symmetry is broken,
though the device is geometrically symmetric?

2.3.4 Interferometer capacitively coupled to a fermionic environment: transient dynamics and steady state (model III)

Considering model III representing a double-dot interferometer coupled capacitively to a fermionic environment which may be out of equilibrium, see Fig. 2.3, we are interested in the transient and steady state characteristics of this model, to extract magnetic field symmetry relations. This model resembles a voltage probe in the sense that there is no charge leakage from double-dot interferometer, but energy exchange between the double-dot and the fermionic environment can occur. We particularly focus on the following questions:

1. What is the role of fermionic environment in breaking the Onsager symmetry within the AB interferometer beyond linear response?

2. Does the microscopic Hamiltonian model III support transport results as predicted by a phenomenological tool, the voltage probe?

2.3.5 Thesis organization

This thesis is centered around applying the methods discussed in sec. 2.2 to understand the various transport phenomena in models I, II and III. In chapter 3 we present the derivation of the nonequilibrium Green’s function technique using the quantum Langevin approach for model I at $U = 0$. We obtain closed expressions for the reduced density matrix of the double-dot system and expose non-trivial magnetic flux-dependent effects. We also analytically prove that in degenerate and symmetric interferometers, flux-dependent occupation difference develops. The transient dynamics of the noninteracting model I is studied using an exact fermionic trace formula.
We complement this study and consider model II, a noninteracting double-dot interferometer with a local dephasing probe. Using the nonequilibrium Green’s function method and the dephasing probe condition, we compute the occupations of the dots analytically and expose several nontrivial flux dependent effects away from the symmetric point. While at the symmetric point dot occupations are independent of magnetic flux, away from the symmetric point flux strongly affects the dots’ occupation. We further demonstrate that when the dots’ energies are aligned with the chemical potentials of leads, new coherent oscillatory patterns develop and sustain, as long as the dephasing strength is of the order of the applied voltage bias.

In chapter 4 we focus on the transient dynamics of model I with electron-electron repulsion. Coherences and the charge current are simulated using INFPI. We show that the temporal characteristics of coherences are preserved under weak-intermediate Coulomb interaction strengths. We complement our study by using Bloch-type master equations in two different limits, $U = 0$, and $U = \infty$. We show that the “phase localization” effect does not hold in the $U = \infty$ limit. We also study the temperature dependence of the coherences and the charge current. Some general observations about time scales are discussed, and a detailed convergence analysis of INFPI is presented.

In chapter 5 we continue with model II and study the role of phase breaking processes on the symmetries of nonlinear transport using Büttiker’s probe. We show that under quasi-elastic dephasing processes Onsager symmetry is maintained beyond linear response, and that there is no rectification of current. We then consider the role of inelastic scattering processes using the voltage probe technique. In this case, in the linear response regime the Onsager symmetry is maintained but beyond that we show that, it is broken. We analytically prove that for spatially symmetric systems odd conductance terms are even in magnetic flux and even conductance terms are odd. We further demonstrate that these symmetries are invalidated once spatial symmetry is broken, though at the particle-hole symmetric point these symmetries do hold irrespective of spatial asym-
metries. These observations hold for a general interferometer and we demonstrate these results using the double-dot interferometer, model II. We show that the system can act as a charge current rectifier when two conditions are met simultaneously: (i) many body effects are included in the form of inelastic scattering; and (ii) time reversal symmetry is broken. We then extend this discussion and study model II with the temperature and voltage-temperature probes. We also obtain generalized magnetic field gate voltage symmetries.

In chapter 6 we study Model III, a double-dot Aharonov-Bohm interferometer capacitively coupled to a fermionic environment. We perform simulations using INFPI and show that the magnetic flux symmetries of odd-even conductance coefficients obtained using the voltage probe, do hold for a capacitive coupling to an equilibrium or a nonequilibrium environment. In chapter 7 we conclude and discuss future directions.
Chapter 3

Model I: Noninteracting electrons

3.1 Introduction

In this chapter, we focus on a simple-minimal model, the noninteracting double quantum dot AB interferometer, and study its transient and steady state properties in biased situations. We focus on a symmetric AB setup, with a quantum dot located at each arm of the interferometer. The dots are connected to two metal leads (referred to as baths, or reservoirs) maintained in a biased state. For a scheme of this model, see Fig. 2.1. Here we consider the $U = 0$ case. In Sec. 3.2 we present the quantum Langevin approach and obtain the reduced density matrix in terms of the retarded and advanced Green’s functions. In Sec. 3.3 we obtain the steady state behaviour of the dots’ occupations, coherences and current, and study the role of a gate voltage, magnetic flux, and bias. In Sec. 3.4 we study the transient dynamics using the fermionic trace formula. Results presented here were published in Ref. [115].

3.2 Equations of motion

The steady state characteristics of the noninteracting model can be calculated exactly using the nonequilibrium Green’s function (NEGF) approach [116]. This technique has
been extensively used in the past for studying transport properties in mesoscopic systems and molecular junctions [117]. The derivation presented here follows an equation-of-motion approach [62]. In this method, the quantum Langevin equation for the subsystem is obtained by solving the Heisenberg equations of motion (EOM) for the baths’ variables, then substituting them back into the EOM for the subsystem (dots) variables. The indices \( \alpha, \beta = 1, 2 \) identify the two dots. The resulting EOM for the operators of the subsystem are [115]

\[
\frac{d a_\beta}{dt} = -i\epsilon_\beta a_\beta - i\eta^L_\beta - i\eta^R_\beta
- i \int_{t_0}^{t} d\tau \sum_{\alpha,l} \xi_{\beta,l} g_{\alpha}^+(t - \tau) \xi^*_\alpha l e^{i(\phi^L_\beta - \phi^L_\alpha)} a_\alpha(\tau)
- i \int_{t_0}^{t} d\tau \sum_{\alpha,r} \zeta_{\beta,r} g_{\alpha}^+(t - \tau) \zeta^*_\alpha r e^{i(\phi^R_\beta - \phi^R_\alpha)} a_\alpha(\tau). \tag{3.1}
\]

The (isolated) reservoirs Green’s functions are given by

\[
g_{\ell}^+(t) = -ie^{-i\omega_{\ell} t} \theta(t), \quad g_{r}^+(t) = -ie^{-i\omega_{r} t} \theta(t). \tag{3.2}
\]

In the language of the quantum Langevin approach, the terms \( \eta^L_\beta \) and \( \eta^R_\beta \) are referred to as noise, induced on the subsystem from the left and right reservoirs, respectively. Here

\[
\eta^L_\beta = i \sum_l \xi_{\beta,l} g_{\ell}^+(t - t_0) a_l(t_0) e^{i\phi^L_\beta}
\eta^R_\beta = i \sum_r \xi^*_\beta r g_{r}^+(t - t_0) a_r(t_0) e^{-i\phi^R_\beta}. \tag{3.3}
\]

As an initial condition we take a factorized state, \( \rho(t_0) = \sigma_L \otimes \sigma_R \otimes \sigma_S(t_0) \), with empty dots and the reservoirs prepared in a grand canonical state, \( \sigma_\nu = \frac{e^{-(H_\nu - \mu_\nu N)/T_\nu}}{Tr(e^{-(H_\nu - \mu_\nu N)/T_\nu})} \), \( T_\nu \) is the temperature of the \( \nu = L, R \) fermi sea and \( \mu_\nu \) stands for its chemical potential. The reduced density matrix \( \sigma_S \) denotes the state of the subsystem. Using this initial
Chapter 3. Model I: Noninteracting electrons

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condition, noise correlations satisfy

\[ \langle \eta^+_L(t) \eta^+_L(\tau) \rangle = \sum_l \xi^*_l e^{i\phi_l^L} \xi^*_l e^{i\phi_l^L} f_L(\omega_l) \]

\[ \langle \eta^+_R(t) \eta^+_R(\tau) \rangle = \sum_r \zeta^*_r e^{i\phi_r^R} \zeta^*_r e^{i\phi_r^R} f_R(\omega_r), \]  

(3.4)

with the Fermi function

\[ f_\nu(\omega) = \left[ e^{(\omega - \mu_\nu)/T_\nu} + 1 \right] \]

and expectation values evaluated in the Heisenberg representation,

\[ \langle A(t) \rangle = \text{Tr}[\rho(t_0)e^{iHt}Ae^{-iHt}] \]. steady state properties are reached by taking the limits \( t_0 \to -\infty \) and \( t \to \infty \). We now Fourier transform Eq. (3.1) using the convolution theorem with the convention

\[ \tilde{a}_\beta(\omega) = \int_{-\infty}^{\infty} dt a_\beta(t) e^{i\omega t}, \]

\[ \tilde{\eta}_\beta(\omega) = \int_{-\infty}^{\infty} dt \eta_\beta(t) e^{i\omega t}. \]  

The result, organized in a matrix form, is

\[ \tilde{a}_\beta(\omega) = \sum_\alpha G^+_{\beta,\alpha} \left[ \tilde{\eta}^L_\alpha(\omega) + \tilde{\eta}^R_\alpha(\omega) \right], \]  

(3.5)

with the Green’s function

\[ G^+_{\beta,\alpha}(\omega) = \frac{1}{(\omega - \epsilon_\beta) \delta_{\alpha,\beta} - \Sigma^L,+,\alpha(\omega) - \Sigma^R,+,\alpha(\omega)}, \]  

(3.6)

and, \( G^- = (G^+)^\dagger \). The self energies contain the phase factors,

\[ \Sigma^L,+,\alpha(\omega) = \sum_l \xi^*_l g^+_l(\omega) \xi^*_l e^{i(\phi_l^L - \phi_l^L)}, \]

\[ \Sigma^R,+,\alpha(\omega) = \sum_r \zeta^*_r g^+_r(\omega) \zeta^*_r e^{i(\phi_r^R - \phi_r^R)}. \]  

(3.7)

The real part of the self energy is a principal value integral, assumed here to vanish. This assumption holds when the metals’ density of states is energy independent and the bandwidth is large. We then define the hybridization matrix from the relation \( \Sigma^+ = \).
\[-i\gamma/2,\]

\[
\Gamma^L_{\beta,\beta'}(\omega) = 2\pi e^{i(\phi^L_\beta - \phi^L_{\beta'})} \sum_l \xi_{\beta,l}\delta(\omega - \omega_l)\xi^*_{\beta',l}. \tag{3.8}
\]

Similar expressions hold for the $R$ side. Using the steady state solution (3.5), we can write down an expression for the reduced density matrix. Back-transformed to the time domain it takes the form

\[
\langle a_\alpha^\dagger a_\beta \rangle \equiv \sigma_{\alpha,\beta} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[ (G^+\Gamma^L G^-)_{\alpha,\beta} f_L(\omega) + (G^+\Gamma^R G^-)_{\alpha,\beta} f_R(\omega) \right] d\omega. \tag{3.9}
\]

The time variable has been suppressed since the result is only valid in the steady state limit. We take $\xi_{\beta,l}$ and $\zeta_{\beta,r}$ as real constants, independent of the level index and the reservoir state, resulting in

\[
\Gamma^L_{\beta,\beta'} = \gamma_L e^{i(\phi^L_\beta - \phi^L_{\beta'})}, \quad \Gamma^R_{\beta,\beta'} = \gamma_R e^{-i(\phi^R_\beta - \phi^R_{\beta'})}, \tag{3.10}
\]

where

\[
\gamma_L = 2\pi \sum_l \xi_{\beta,l}\delta(\omega - \omega_l)\xi^*_{\beta',l}, \quad \gamma_R = 2\pi \sum_r \zeta_{\beta,r}\delta(\omega - \omega_r)\zeta^*_{\beta',r}. \tag{3.11}
\]

Using these definitions, the matrix $G^+$ takes the form

\[
G^+ = \begin{bmatrix}
\omega - \epsilon_1 + \frac{i(\gamma_L + \gamma_R)}{2} & \frac{i\gamma_L}{2} e^{i\phi/2} + \frac{i\gamma_R}{2} e^{-i\phi/2} \\
\frac{i\gamma_L}{2} e^{-i\phi/2} + \frac{i\gamma_R}{2} e^{i\phi/2} & \omega - \epsilon_2 + \frac{i(\gamma_L + \gamma_R)}{2}
\end{bmatrix}^{-1} \tag{3.12}
\]

and the hybridization matrices are given by

\[
\Gamma^L = \gamma_L \begin{bmatrix}
1 & e^{i\phi/2} \\
e^{-i\phi/2} & 1
\end{bmatrix}, \quad \Gamma^R = \gamma_R \begin{bmatrix}
1 & e^{-i\phi/2} \\
e^{i\phi/2} & 1
\end{bmatrix}. \tag{3.13}
\]
We can now calculate, numerically or analytically, the behavior of the reduced density matrix under different conditions [32]. Since in this chapter we are only concerned with symmetric dot-lead couplings, we take $\gamma_L = \gamma_R = \gamma/2$. Furthermore, we impose energy degeneracy, $\epsilon_1 = \epsilon_2 = \epsilon$. This choice simplifies the relevant matrices to

$$G^+ = \begin{pmatrix} \omega - \epsilon + \frac{i\gamma}{2} & \frac{i\gamma}{2} \cos \frac{\phi}{2} \\ \frac{i\gamma}{2} \cos \frac{\phi}{2} & \omega - \epsilon + \frac{i\gamma}{2} \end{pmatrix}^{-1},$$

$$\Gamma_L = \frac{\gamma}{2} \begin{pmatrix} 1 & e^{i\phi/2} \\ e^{-i\phi/2} & 1 \end{pmatrix}, \quad \Gamma_R = \frac{\gamma}{2} \begin{pmatrix} e^{-i\phi/2} & 1 \\ e^{i\phi/2} & 1 \end{pmatrix} \quad (3.14)$$

We present closed analytic expressions for the diagonal and off-diagonal elements of the reduced density matrix in Sec. 3.3. Complementing numerical data for the real-time dynamics are included in Sec. 3.4.

### 3.3 Stationary behaviour

#### 3.3.1 Dots’ occupation and occupation difference

We discuss here two effects that persist away from the “symmetric point”, defined as $\mu_L - \epsilon = \epsilon - \mu_R$: The occupations of the dots significantly vary with flux, and moreover, the degenerate dots acquire different occupations. After presenting general expressions away from the symmetric point, we consider other relevant cases: the finite-bias limit at the symmetric point, the limit of infinite bias (which effectively reduces to the symmetric point), and the case of $\phi = 2\pi n$, $n = 0, 1, 2...$

Analytic results are obtained from Eqs. (3.9) and (3.14), recall that $\gamma_L = \gamma_R = \gamma/2$ and $\epsilon = \epsilon_1 = \epsilon_2$. Organizing these expressions, we find that the occupation of dot '1',
\( \sigma_{1,1} \equiv \langle a_1^\dagger a_1 \rangle \), is given by two integrals,

\[
\begin{align*}
\sigma_{1,1} &= \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_L(\omega) d\omega \frac{(\omega - \epsilon)^2 + \omega_0^2 - 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2} \\
&+ \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_R(\omega) d\omega \frac{(\omega - \epsilon)^2 + \omega_0^2 + 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2},
\end{align*}
\] (3.15)

where we have introduced the short notation

\[
\omega_0 \equiv \frac{\gamma}{2} \sin \frac{\phi}{2}.
\] (3.16)

Similarly, the occupation of level '2', \( \sigma_{2,2} \equiv \langle a_2^\dagger a_2 \rangle \), is given by

\[
\begin{align*}
\sigma_{2,2} &= \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_L(\omega) d\omega \frac{(\omega - \epsilon)^2 + \omega_0^2 + 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2} \\
&+ \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_R(\omega) d\omega \frac{(\omega - \epsilon)^2 + \omega_0^2 - 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2}.
\end{align*}
\] (3.17)

In what follows we consider the zero temperature limit. The Fermi functions take then the shape of step functions and the upper limits of the integrals are replaced by the corresponding chemical potentials. We now study the contribution of the odd term in the integrand. This term is responsible for the development of occupation difference between the dots,

\[
\delta n = \sigma_{1,1} - \sigma_{2,2} = -\frac{\gamma}{4\pi} \int_{\mu_L}^{\mu_R} d\omega \frac{4\omega_0(\omega - \epsilon) \cos \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2}
\] (3.18)

We evaluate this using an integral of the form below,

\[
\mathcal{I} = \int_{d}^{c} \frac{x}{(x^2 - a^2)^2 + b^2 x^2} dx = \frac{\tan^{-1} \left[ \frac{2a^2 - b^2 - 2c^2}{b\sqrt{4a^2 - b^2}} \right] - \tan^{-1} \left[ \frac{2a^2 - b^2 - 2c^2}{b\sqrt{4a^2 - b^2}} \right]}{b\sqrt{4a^2 - b^2}}
\] (3.19)

where \( d = (\mu_R - \epsilon) \), \( c = (\mu_L - \epsilon) \), \( b = \gamma \) and \( a = \frac{\gamma}{2} \sin \frac{\phi}{2} \), leading to \( b\sqrt{4a^2 - b^2} = \pm i\gamma^2 \cos \frac{\phi}{2} \).
and

\[ 2a^2 - b^2 - 2d^2 = \gamma^2 \left[ \frac{1}{2} \sin^2 \frac{\phi}{2} - 1 \right] - 2(\mu_R - \epsilon)^2 \]
\[ 2a^2 - b^2 - 2c^2 = \gamma^2 \left[ \frac{1}{2} \sin^2 \frac{\phi}{2} - 1 \right] - 2(\mu_L - \epsilon)^2 \]

We now reorganize Eq. (3.19) using the relations \( \tan^{-1} x + \tan^{-1} y = \tan^{-1} \left( \frac{x+y}{1-xy} \right) \) and \( \tan^{-1} z = \frac{i}{2} \left[ \ln(1 - iz) - \ln(1 + iz) \right] \), to find

\[ I = \frac{\ln \left[ \frac{F_+(\phi)}{F_-(\phi)} \right]}{2\gamma^2 \cos \frac{\phi}{2}}, \]

where we define

\[ F_{\pm}(\phi) = \frac{\gamma^4}{8} \sin^4 \frac{\phi}{2} \]
\[ - (\mu_L - \epsilon)^2 \left[ \frac{\gamma^2}{2} \sin^2 \frac{\phi}{2} - (\mu_R - \epsilon)^2 - \gamma^2 \left( 1 \pm \cos \frac{\phi}{2} \right) \right] \]
\[ - (\mu_R - \epsilon)^2 \left[ \frac{\gamma^2}{2} \sin^2 \frac{\phi}{2} - (\mu_L - \epsilon)^2 - \gamma^2 \left( 1 \mp \cos \frac{\phi}{2} \right) \right]. \]

(3.21)

We can also reorganize these factors as a sum of real quadratic terms,

\[ F_{\pm}(\phi) = \frac{\gamma^4}{8} \sin^4 \frac{\phi}{2} + 2(\mu_L - \epsilon)^2(\mu_R - \epsilon)^2 \]
\[ + \frac{\gamma^2}{2} \left( \cos \frac{\phi}{2} \pm 1 \right)^2 (\mu_L - \epsilon)^2 + \frac{\gamma^2}{2} \left( \cos \frac{\phi}{2} \mp 1 \right)^2 (\mu_R - \epsilon)^2. \]

(3.22)

Attaching the missing prefactors, \( \delta n = -\frac{\gamma}{4\pi} 4\omega_0 \cos \frac{\phi}{2} I \), we simplify Eq. (3.18) to

\[ \delta n = -\frac{\sin \frac{\phi}{2}}{4\pi} \ln \left[ \frac{F_+(\phi)}{F_-(\phi)} \right]. \]

(3.23)

Inspecting Eq. (3.23), we note that it vanishes in four different cases: (i) at zero bias,
when $\mu_L = \mu_R = 0$, (ii) at infinite bias, $\mu_L \to \infty$ and $\mu_R \to -\infty$, (iii) at the symmetric point when $\mu_L - \epsilon = \epsilon - \mu_R$, particularly for $\epsilon = 0$ and $\mu_L = -\mu_R$, or when (iv) $\phi = n\pi$, $n = 0, 1, 2, \ldots$ (leading to $F_+ = F_-$. Combining Eq. (3.18) with the integration of even terms in Eq. (3.15), at zero temperature, we resolve the occupations

$$
\sigma_{1,1/2,2} = \frac{1}{4\pi} \left[ 2\pi + \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_-} \right) + \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_+} \right) + \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_-} \right) + \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_+} \right) \right] \\
\pm \frac{\sin \frac{\phi}{2}}{8\pi} \ln \left[ \frac{F_-(\phi)}{F_+(\phi)} \right].
$$

(3.24)

The positive sign corresponds to $\sigma_{1,1}$, the negative sign provides $\sigma_{2,2}$. We have also introduced the short notation for flux dependent decay rates,

$$
\gamma_\pm \equiv \frac{\gamma}{2} (1 \pm \cos \frac{\phi}{2}).
$$

(3.25)

Equation (3.24) predicts flux dependency of electron occupation at degeneracy, using symmetric hybridization constants, once the dots are tuned away from the symmetric point. Fig. 3.1 displays this behavior, and we find that as the dots energies get closer to the bias edge, $\epsilon \sim \mu_L$, the population strongly varies with $\epsilon$ (panel b).

It is also interesting to note that the abrupt jump at $\phi = 2\pi n$ (discussed below) disappears once the levels reside at or above the bias window, for $\epsilon \geq \mu_L$. This feature results from the strict zero temperature limit assumed in the analytic calculations.

At finite $T$, the jump at $\phi = 2\pi n$ survives even for $\epsilon > \mu_L$. However, when the temperature is at the order of the hybridization strength, $T \sim \gamma$, the modulation of the population with phase is washed out. The following parameters are used here and below: flat wide bands, dots energies at the order of $\epsilon = 0 - 0.4$, hybridization strength $\gamma = 0.05 - 0.5$, and a zero temperature, unless otherwise specified. The bias voltage is set symmetrically around the equilibrium Fermi energy, $\mu_L = -\mu_R$, $\Delta \mu \equiv \mu_L - \mu_R$. We now discuss in more details the behavior of the occupation in some special cases. First,
Figure 3.1: (a) Flux dependency of occupation for dot '1' using $\epsilon = 0$ (triangle) $\epsilon = 0.2$ (□) $\epsilon = 0.3$ (○) and $\epsilon = 0.4$ (+). Panel (b) displays results when $\epsilon$ is tuned to the bias window edge, $\epsilon \sim \mu_L$, $\epsilon = 0.29$ (□), $\epsilon = 0.3$ (diagonal), $\epsilon = 0.31$ (○), and $\epsilon = 0.31$, $T = 0.05$ (dashed-dotted line). In all cases $\mu_L = -\mu_R = 0.3$, $\gamma = 0.05$, and $T = 0$, unless otherwise stated. Reproduced from Ref. [115].

Figure 3.2: (a)-(b) Dots occupations as a function of magnetic phase $\phi$ for $\Delta \mu = 0.6$, $\epsilon = 0.2$, $T = 0$. (c) Occupation difference, $\delta n = \sigma_{1,1} - \sigma_{2,2}$. At weak coupling, $\gamma = 0.05$ (△), the dots occupations are almost identical. When the hybridization is made stronger, $\gamma = 0.5$ (○), comparable to the levels displacement from the symmetric point, $\sigma_{1,1}$ clearly deviates from $\sigma_{2,2}$. At very strong coupling, $\gamma = 2$ (+), the occupation difference reduces and asymmetries develop. For clarity, results are shown for $\phi/\pi$ between (-2, 2). Reproduced from Ref [115].
we consider the symmetric point at finite bias and $\phi \neq 2\pi n$, $n = 0, 1, 2,...$. In this case Eq. (3.24) precisely reduces to

$$\sigma_{\alpha,\alpha}(\mu_L - \epsilon = \epsilon - \mu_R) = \frac{1}{2}. \tag{3.26}$$

This result holds in the infinite bias limit, $\mu_L \to \infty$ and $\mu_R \to -\infty$, irrespective of the (finite) value of $\epsilon$. Next, the special case $\phi = 2\pi n$ should be separately evaluated. At these points we have $\omega_0 = 0$ and Eq. (3.15) provides the simple form at zero temperature

$$\sigma_{\alpha,\alpha}(\phi = 2\pi n) = \frac{\gamma}{4\pi} \int_{-\infty}^{\mu_L - \epsilon} \frac{dx}{x^2 + \gamma^2} + \frac{\gamma}{4\pi} \int_{\epsilon - \mu_R}^{\infty} \frac{dx}{x^2 + \gamma^2}$$

$$= \frac{1}{4\pi} \left[ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma} \right) + \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma} \right) \right] + \frac{1}{4}. \tag{3.27}$$

These points are reflected by abrupt jumps in the occupations-flux behavior. Specifically, at the symmetric point there is a sharp reduction of occupation number from $1/2$ [Eq. (3.26)] to $1/4$ [Eq. (3.27)], as observed earlier in Ref. [31]. Fig. 3.1 shows that at strictly zero temperature this jump disappears once the dots energies are placed at or above the bias edge, $\epsilon \geq \mu_L$. Thus, the appearance of the jump is indicative of the fact that electrons cross the junction resonantly. If only tunneling processes contribute (once the dots’ energies are placed above the bias window and the temperature is very low), the populations vary continuously with flux. The total electronic occupation of the dots, at steady state, generalizes the standard symmetric case attained in Ref. [32],

$$\sigma_{1,1} + \sigma_{2,2} = \frac{\gamma}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{[(\omega - \epsilon)^2 + \omega_0^2][f_L(\omega) + f_R(\omega)]}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2}. \tag{3.28}$$

We now highlight one of the main results of this work, the onset of occupation difference in this degenerate ($\epsilon_1 = \epsilon_2$) and spatially symmetric ($\gamma_L = \gamma_R$) setup using Eq. (3.22). The occupation difference can be controlled by manipulating the subsystem-metal
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Figure 3.3: Occupation difference as a function of bias voltage $\Delta \mu$, for different magnetic flux values, $\phi = \pi/2$ (full line), $\phi = \pi/4$ (dashed line), $\phi = \pi/8$ (dashed-dotted line). Other parameters are $\epsilon = 0.2$ and $\gamma = 0.05$, $T_\nu = 0$. The inset presents data for backward and forward biases; the main plot zooms on the positive bias regime. Reproduced from Ref. [115].

Figure 3.4: Occupation difference as a function of magnetic flux for different bias values, $\Delta \mu = 0.1$ (full line), $\Delta \mu = 0.2$ (dashed line), $\Delta \mu = 0.3$ (dashed-dotted line) and $\Delta \mu = 0.4$ (dotted line). Other parameters are $\epsilon = 0.2$, $\gamma = 0.05$ and $T_\nu = 0$. Reproduced from Ref. [115].
Figure 3.5: Finite temperature effect. Main plot: Occupation difference as a function of bias voltage for $\phi = \pi/4$. Inset: occupation of dot '1' as a function of magnetic phase for $\Delta \mu = 0.4$. In both panels $T = 0$ (dotted line), $T_\nu = 0.01$ (full line), $T_\nu = 0.05$ (dashed-dotted line) and $T_\nu = 0.1$ (dashed line). Dots parameters are $\epsilon = 0.2$ and $\gamma = 0.05$. Reproduced from Ref. [115].
hybridization energy $\gamma$, by changing the bias voltage, by applying a gate voltage for tuning the dots energies, and by modulating the phase $\phi$ through the magnetic flux. The role of these control knobs are illustrated in Figures 3.2, 3.3 and 3.4. In Fig. 3.2 we display the levels occupation in the resonant regime, $\mu_R < \epsilon < \mu_L$ while varying $\gamma$. At weak coupling $\delta n$ is insignificant. However, the occupation difference becomes large for stronger coupling strengths. More notably, Fig. 3.3 illustrates the strong controllability of $\delta n$ with applied voltage. We find that the occupation difference is maximized at the edge of the resonant transmission window, when $\mu_L - \epsilon = 0$ (or equivalently, when $\Delta\mu = 2\epsilon$). The magnetic phase affects the width and height of the peak, but not the absolute position which is only determined by the offset of $\epsilon$ from the center of the bias window. In Fig. 3.4 we further show the flux dependency of $\delta n$, which is particularly significant when $\Delta\mu = 2\epsilon$.

The effect of finite temperature on the occupation-flux dependence, and on the development of occupation difference, is displayed in Fig. 3.5. We find that the effect largely survives at finite temperature, as long as $T < \gamma$. These results were calculated numerically, based on Eqs. (3.15) and (3.17).

### 3.3.2 Coherence

It was argued that the decoherence behavior in our setup, including two noninteracting (uncoupled) quantum dots interferometer, can be suppressed when the device geometry is made asymmetric and nondegenerate, using $\epsilon_1 \neq \epsilon_2$ and $\gamma_L \neq \gamma_R$ [33].

Based on numerical simulations, we have pointed out in Ref. [34] that phase localization occurs only at the symmetric point, while at other values of $\epsilon$ the real part of $\sigma_{1,2}$ is finite and nonzero in the asymptotic limit for any phase besides $2\pi n$ [34]. This observation is established here analytically in the steady state limit, implying that decoherence could be suppressed in degenerate-symmetric systems by gating the dots, shifting their energies relative to the bias window. We derive a closed expression for the off-diagonal
system element \( \sigma_{12} \equiv \langle a_1^\dagger a_2 \rangle \) by studying Eq. (3.9),

\[
\sigma_{12} = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_L(\omega) d\omega \left\{ \frac{\cos \frac{\phi}{2} [\omega^2 - \omega_0^2]}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2} \right\} + \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} f_R(\omega) d\omega \left\{ \frac{\cos \frac{\phi}{2} [\omega^2 - \omega_0^2]}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + [\gamma(\omega - \epsilon)]^2} \right\} .
\]

(3.29)

At finite bias and zero temperature direct integration provides the real (\( \Re \)) and imaginary (\( \Im \)) parts of \( \sigma_{12} \) (\( \phi \neq 2\pi n \)),

\[
\Re \sigma_{12} = \frac{1}{4\pi} \left[ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_+} \right) - \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_-} \right) + \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_+} \right) - \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_-} \right) \right],
\]

(3.30)

and

\[
\Im \sigma_{12} = \frac{\sin(\phi/2)}{4\pi} \left[ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_+} \right) + \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_-} \right) - \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_+} \right) - \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_-} \right) \right].
\]

(3.31)

As before, we define \( \gamma_\pm = \frac{\gamma}{2}(1 \pm \cos \frac{\phi}{2}) \). We now readily confirm that at the symmetric point the real part vanishes and “phase localization” takes place [31]. In particular, in the infinite bias limit we find \( \Im \sigma_{12} = \frac{1}{2} \sin \frac{\phi}{2} \), in agreement with previous studies [34]. We also include the behavior at the special points \( \phi = 2\pi n \). Eq. (3.29) reduces then to a simple Lorentzian form, at zero temperature,

\[
\sigma_{12}(\phi = 0) = \frac{\gamma}{4\pi} \int_{-\infty}^{\mu_L - \epsilon} \frac{dx}{x^2 + \gamma^2} + \frac{\gamma}{4\pi} \int_{\epsilon - \mu_R}^{\infty} \frac{dx}{x^2 + \gamma^2}
\]

\[
= \frac{1}{4\pi} \left[ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma} \right) + \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma} \right) \right] + \frac{1}{4}.
\]

(3.32)

The sign reverses for \( \phi = \pm 2\pi \). We note that the imaginary part of the coherence identically vanishes at zero phase while the real part is finite, approaching the value 1/4 at the symmetric point. Numerical results in the steady state limit are displayed in Fig. 3.6. We find that both the real and imaginary parts of \( \sigma_{12} \) demonstrate significant
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Figure 3.6: Real and imaginary parts of the coherence as a function of the bias voltage. $\phi = \pi$ (full line), $\phi = \pi/2$ (dashed), $\phi = \pi/4$ (dashed-dotted line). Other parameters are $\epsilon = 0.2$, $\gamma = 0.05$, and $T = 0$. The oval shape marks the region of phase localization at positive bias. Reproduced from Ref. [115].

features when the dots’ levels cross the bias window, at $\Delta \mu = 2\epsilon$. The value of the real part abruptly changes sign, the imaginary part develops a step. At large bias $\Re \sigma_{1,2}$ diminishes while $\Im \sigma_{1,2}$ is finite, indicating the development of the phase localization behavior. It can be shown that the double-step structure of $\Im \sigma_{1,2}$ (as a function of $\Delta \mu$) disappears when the dots energies are set at the symmetric point.

3.3.3 Current

The electric current, flowing from the $L$ metal to the $R$ end, is obtained by defining the number operator $N_L \equiv \sum_l a_l^{\dagger} a_l$, providing the current $I_L = -\frac{dN_L}{dt} = -i[H, \hat{N}_L]$. Expectation values are calculated in the steady state limit. Using the EOM formalism as explained in Sec. 3.2, we get the standard result [116]

$$I_L = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega T_{L,R}(\omega)[f_L(\omega) - f_R(\omega)].$$

(3.33)
The transmission coefficient is defined as $T_{L,R} = \text{Tr}(\Gamma^L G^+ \Gamma^R G^-)$, where the trace is performed over the states of the subsystem (dots). In the present model, at zero temperature, we obtain

$$I_L = \frac{1}{2\pi} \int_{\mu_L}^{\mu_R} d\omega \frac{\gamma^2(\omega - \epsilon)^2 \cos^2 \frac{\phi}{2}}{[(\omega - \epsilon)^2 - \omega_0^2]^2 + \gamma^2(\omega - \epsilon)^2}$$

$$= \frac{\cos \frac{\phi}{2}}{2\pi} \left[ \gamma_+ \left\{ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_+} \right) - \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_+} \right) \right\} - \gamma_- \left\{ \tan^{-1} \left( \frac{\mu_L - \epsilon}{\gamma_-} \right) - \tan^{-1} \left( \frac{\mu_R - \epsilon}{\gamma_-} \right) \right\} \right],$$

which agrees with known results [8]. Using the NEGF formalism, we could similarly investigate the shot noise in the double-dot AB interferometer [145]. The transmission function is plotted in Fig. 3.7 displaying destructive interference pattern for $\phi = \pi$ and a constructive behavior for $\phi = 0$. For $\phi \neq n\pi$ the transmission nullifies exactly at the position of the resonant level [118]. The inset presents the current-voltage characteristics for $\phi = \pi/2$ away from the symmetric point (dashed line), and at the symmetric point...
(dotted line). We note that the double-step structure disappears at the latter case. It can be shown that the double step structure of $\Im \sigma_{1,2}$ (see Fig. 3.6) similarly diminishes at the symmetric point.

### 3.4 Transient behavior

It is of interest to investigate the development of the phase dependence of the occupancy, and the occupancy difference $\delta n$, before steady state sets. Similarly, the dynamics of coherences is nontrivial even without electron-electron interaction effects [34]. We complement the NEGF steady state expressions of Sec. 3.2 with numerical calculations of the transient behavior using an exact numerical tool that is based on the fermionic trace formula [119]

$$\text{Tr} \left[ e^{M_1} e^{M_2} \ldots e^{M_p} \right] = \det \left[ 1 + e^{m_1} e^{m_2} \ldots e^{m_p} \right].$$  \hfill (3.35)

Here $m_p$ is a single-particle operator corresponding to a quadratic operator $M_p = \sum_{i,j} (m_p)_{i,j} a_i^\dagger a_j$, where $m_p = \sum_{i,j} (m_p)_{i,j} | i \rangle \langle j |$ and $a_i^\dagger$ ($a_j$) are fermionic creation (annihilation) operators. The trace is performed over all electronic degrees of freedom. Our objective is the dynamics of a quadratic operator $B \equiv a_j^\dagger a_k$, $j, k = 1, 2$,

$$\langle B(t) \rangle = \text{Tr} \left[ \rho(t_0) e^{iHt} B e^{-iHt} \right] = \lim_{\lambda \to 0} \frac{\partial}{\partial \lambda} \text{Tr} \left[ \sigma_L \sigma_R \sigma_S(t_0) e^{iHt} e^{\lambda B} e^{-iHt} \right].$$  \hfill (3.36)

We introduce the $\lambda$ parameter, taken to vanish at the end of the calculation. The initial condition is factorized, $\rho(t_0) = \sigma_S(t_0) \otimes \sigma_L \otimes \sigma_R$, and these density operators follow an exponential form, $e^M$, with $M$ a quadratic operator. The application of the trace formula
leads to

\[
\langle e^{\lambda B(t)} \rangle = \det \left\{ [I_L - f_L] \otimes [I_R - f_R] \otimes [I_S - f_S] + e^{iht} e^{\lambda b} e^{-iht} f_L \otimes f_R \otimes f_S \right\},
\]

(3.37)

with \( b \) and \( h \) as the single-body Hilbert space matrices of the \( B \) and \( H \) operators, respectively. The matrices \( I_\nu \) and \( I_S \) are the identity matrices for the \( \nu = L, R \) space and for the subsystem (dots). The functions \( f_L \) and \( f_R \) are the band electrons occupancy \( f_\nu(\epsilon) = [e^{\beta_\nu(\epsilon - \mu_\nu)} + 1]^{-1} \). Here they are written in matrix form and in the energy representation. \( f_S \) represents the initial occupation for the dots, assumed empty, again written in a matrix form. When working with finite-size reservoirs, Eq. (3.37) can be readily simulated numerically-exactly.

Fig. 3.8 displays the evolution of the occupation difference, presented as a function of \( \Delta \mu \). In this simulation we used finite bands with a sharp cutoff, \( D = \pm 1 \). At short time \( \delta n \) shows a weak sensitivity to the actual bias. Only after a certain time, \( \gamma t \sim 2 \), the peak around the edge at \( \Delta \mu = 2\epsilon \) clearly develops. Note that since the band is not very broad, edge effects are reflected at large biases as nonzero occupation difference, in
Figure 3.9: Time evolution of the real (a) and imaginary (b) parts of the coherence $\gamma = 0.05, \epsilon = 0.2, T_\nu = 5 \times 10^{-3}, \phi = \pi/2$. Reproduced from Ref. [115].

The transient behavior of the coherences, $\Re\sigma_{1,2}$ and $\Im\sigma_{1,2}$, is included in Fig. 3.9; the corresponding steady state value are presented in Fig. 3.6. We can follow the temporal features of the phase localization effect, i.e., the disappearance of the real part of the coherence at the symmetric point or at large bias, when $\phi \neq 2\pi n$. Using $\phi = \pi/2$ we note that while at short to intermediate time ($\gamma t < 2$) significant coherence builds up, the real part of the coherence eventually survives only at small biases. Regarding timescales, we find that while $\Im\sigma_{1,2}$ reaches the steady state values at short time, $\gamma t \sim 2$, $\Re\sigma_{1,2}$ approaches its stationary limit only at longer times, for $\gamma t \sim 10$. Similar results were obtained in Ref. [34].

### 3.5 Dephasing

Phase-breaking processes arise due to the interaction of electrons with other degrees of freedom, e.g., with electrons, phonons and defects. We extend here the discussion of Sec. 3.3 and incorporate dephasing processes into our system phenomenologically, by using the well established method of Büttiker dephasing probe [66]. The schematic setup is shown...
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in Fig. 2.2. In this technique, elastic dephasing processes on the dots are emulated by including a third terminal, $P$, enforcing the requirement that the charge current towards the probe terminal, at a given electron energy, should vanish. Thus, electrons travel to the probe and return to the system with a different phase, while both electron number and electron energy are conserved. This condition sets an electron distribution within the probe. As we show below, away from the symmetric point this distribution effectively depends on the magnetic phase. Following the equations-of-motion approach as detailed in Sec. 3.2, we arrive at the steady-state expression for the reduced density matrix

$$\langle a^\dagger_\alpha a_\beta \rangle = \frac{1}{2\pi} \sum_{\nu=L,R,P} \int_{-\infty}^{\infty} (G^+ \Gamma^\nu G^-)_{\alpha,\beta} f_\nu(\omega) d\omega. \quad (3.38)$$

The probe hybridization matrix is given by

$$\Gamma^P = \gamma^P \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad (3.39)$$

and the dot’s Green’s function is written by generalizing the matrix (3.12), to include the probe self energy,

$$G^+ = \begin{bmatrix} \omega - \epsilon_1 + \frac{i(\gamma_L + \gamma_R + \gamma_P)}{2} & \frac{i\gamma_L}{2} e^{i\phi/2} + \frac{i\gamma_R}{2} e^{-i\phi/2} \\ \frac{i\gamma_L}{2} e^{-i\phi/2} + \frac{i\gamma_R}{2} e^{i\phi/2} & \omega - \epsilon_2 + \frac{i(\gamma_L + \gamma_R)}{2} \end{bmatrix}^{-1}. \quad (3.39)$$

This matrix is written here in a general form, to allow one to distinguish between the two dots and the different dots-metals hybridization terms. The dot-probe hybridization is defined as $\gamma^P = 2\pi \sum_p |\lambda_p|^2 \delta(\omega - \omega_p)$, in analogy with Eq. (5.45). In our calculations below we assume energy degenerate dots and symmetric couplings, $\epsilon = \epsilon_1 = \epsilon_2$, $\gamma_L = \gamma_R = \gamma/2$. We now derive the probe distribution by demanding that the energy resolved charge current to the $P$ terminal vanishes. The total current to $P$ is given by the sum
of the currents from the \(L\) and \(R\) terminals, generalizing Eq. (3.33),

\[
I_P = I_{L\rightarrow P} + I_{R\rightarrow P} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[ T_{L,P}(\omega, \phi) f_L(\omega) - T_{P,L}(\omega, \phi) f_P(\omega, \phi) \right] d\omega + \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[ T_{R,P}(\omega, \phi) f_R(\omega) - T_{P,R}(\omega, \phi) f_P(\omega, \phi) \right] d\omega \tag{3.40}
\]

with the transmission coefficient \(T_{\nu,\tilde{\nu}}(\omega) = \text{Tr}[\Gamma_{\nu} G^+ \Gamma_{\tilde{\nu}} G^-]\). By requiring the integrand to vanish, we arrive at the probe distribution

\[
f_P(\omega, \phi) = \frac{T_{L,P}(\omega, \phi) f_L(\omega) + T_{R,P}(\omega, \phi) f_R(\omega)}{T_{L,P}(\omega, \phi) + T_{R,P}(\omega, \phi)}. \tag{3.41}
\]

Direct evaluation of these transmission coefficients provide the electron distribution in the probe,

\[
f_P(\omega, \phi) = \frac{f_L(\omega) + f_R(\omega)}{2} + \frac{\gamma(\omega - \epsilon) \sin \frac{\phi}{2} \cos \frac{\phi}{2}}{2[(\omega - \epsilon)^2 + \omega_0^2]} [f_L(\omega) - f_R(\omega)]. \tag{3.42}
\]

As before, \(\omega_0 = \frac{\gamma}{2} \sin \frac{\phi}{2}\). This expression indicates that the magnetic flux plays a role in setting the distribution within the probe, (such that it only dephases the system and does not deplete electrons or allow energy reorganization). This dependence disappears when the dots’ energies are set at the symmetric point, since the contribution of the second term in Eq. (3.42) diminishes in the integrals of Eq. (3.43), from symmetry considerations. We now write integral expressions for the dots occupations using Eq.
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\[
\sigma_{1,1} = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta(\omega)} \left\{ (\omega - \epsilon)^2 + \omega_0^2 - 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2} \right\} f_L(\omega) \\
+ \left[ (\omega - \epsilon)^2 + \omega_0^2 + 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2} \right] f_R(\omega) \\
+ \frac{\gamma P}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta(\omega)} \left[ (\omega - \epsilon)^2 + \frac{\gamma^2}{4} \right] f_P(\omega)
\]

\[
\sigma_{2,2} = \frac{\gamma}{4\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta(\omega)} \left\{ (\omega - \epsilon)^2 + \omega_0^2 + 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2} + \omega_0\gamma P \sin \frac{\phi}{2} + \frac{\gamma^2 P}{4} \right\} f_L(\omega) \\
+ \left[ (\omega - \epsilon)^2 + \omega_0^2 - 2\omega_0(\omega - \epsilon) \cos \frac{\phi}{2} + \omega_0\gamma P \sin \frac{\phi}{2} + \frac{\gamma^2 P}{4} \right] f_R(\omega) \\
+ \frac{\gamma^2 P}{8\pi} \cos^2 \frac{\phi}{2} \int_{-\infty}^{\infty} \frac{d\omega}{\Delta(\omega)} f_P(\omega),
\]

with

\[
\Delta(\omega) = \left| (\omega - \epsilon)^2 - \omega_0^2 - \frac{\gamma^2 P}{4} + i \left( \gamma + \frac{\gamma P}{2} \right)(\omega - \epsilon) \right|^2.
\]

In the absence of dephasing these expressions reduce to Eqs. (3.15) and (3.17). In the opposite limit, at very large dephasing, \( \gamma P \gg \gamma, \gamma P > \Delta \mu \), we note that \( \sigma_{2,2} \) is dominated by \( \gamma^2 P \gamma \) terms that are flux independent, while \( \sigma_{1,1} \) is dominated by its last term, \( \propto \gamma P f_P \), which is flux dependent away from the symmetric point, resulting in \( \sigma_{1,1} \propto \sin(\phi) \). Thus, quite counter-intuitively, we find that the level that is directly susceptible to local dephasing demonstrates flux dependency of occupation at strong dephasing, while the level that indirectly suffers dephasing effects more feasibly loses its coherent oscillations.

Using numerical integration, dots occupations and their oscillation with phase are presented in Fig. 3.10. We observe the following trends upon increasing dephasing strength: At the symmetric point, panels (a)-(b), the abrupt jump at zero magnetic phase immediately disappears with the application of finite dephasing. When the dot
energies are placed away from the symmetric point, yet they buried within the bias window, panels (c)-(d), the abrupt jump at zero magnetic phase again disappears, though the oscillations of occupation with phase prevail till large dephasing, $\gamma_P \sim \Delta \mu$. More significantly, when the dots energies are tuned at the edge of the bias window, panels (e)-(f), we find that dot '1' (which is directly dephased) develops new type of oscillation with phase. Only at very large dephasing, $\gamma_P \gg \Delta \mu$, these oscillations are overly suppressed.

Thus, away from the symmetric point not only features of coherent dynamics survive even at significant dephasing strength, new type of coherent oscillations may develop as a result of the application of elastic scattering effects on the dots. It is interesting to reproduce this behavior while modeling elastic dephasing effects using other techniques [69, 120, 121, 122, 123].

Figure 3.10: The role of dephasing on the dots occupations - magnetic phase dependency, (a)-(b) $\epsilon = 0$, (c)-(d) $\epsilon = 0.2$, (e)-(f) $\epsilon = 0.3$, where $\gamma_P=0$ (dotted line), $\gamma_P = 0.01$ (dashed line), $\gamma_P = 0.05$ (dashed-dotted line) and $\gamma_P = 0.5$ (full line). Other parameters are $\gamma = 0.05$, $\Delta \mu = 0.6$, $T_\nu = 0$. Reproduced from Ref. [115].
3.6 Discussion

In this chapter, we have addressed the issue of magnetic field control on electronic occupation and coherence in the noninteracting double-dot AB interferometers, model I and model II. The system under investigation included energy degenerate dots with symmetric dot-metals hybridization strengths. However, by voltage gating the dots’ energies away from the so-called symmetric point at which $\epsilon = (\mu_L + \mu_R)/2$ we have resolved three nontrivial effects that can allow for significant controllability over dots’ occupation and their coherence: (i) Dots’ occupations may significantly vary with magnetic flux, particularly when the levels reside close to the bias edge. (ii) The dots acquire different occupations, though they are energy degenerate. This behavior is maximized at the bias edge $\epsilon \sim \mu_L$. It survives at finite temperature, as long as $T < \gamma$. (iii) Regarding the dots’ coherence, we have proven that the effect of “phase localization” [31] does not take place away from the symmetric point, allowing for coherence control in the system.

Our minimal model could be applied to describe magnetic field control in mesoscopic conducting loops and in molecular ring structures. In the latter case it was particularly noted that degeneracy is crucial for allowing controllability within realistic magnetic fields [13]. We also considered the effect of dephasing on dot occupations and demonstrated that the system can withstand dephasing under certain conditions. The results resolved here could be useful for constructing two qubit gates and long-lived memory elements.

This study was limited to the noninteracting electron model, excluding electron-electron interaction effects. In the next chapter we study the transient dynamics of coherences and the charge current, taking into account finite electron-electron repulsion. We also discuss the limit of a very strong $U$ where double occupancy is forbidden.
Chapter 4

Model I interacting case: Coherence dynamics

4.1 Introduction

The focus of this chapter is the detailed study of the dynamical role of finite electron-electron interactions on the intrinsic coherence behaviour in a biased double-dot AB interferometer, in model I. The system includes a parallel quantum dot setup for the AB interferometer, where (spinless) electrons experience an inter-dot repulsion effect. For a schematic representation, see Fig. 2.1. We focus on the dynamics of the coherences, off-diagonal elements of the double-dot reduced density matrix. Furthermore, we simulate the charge current in the system, assuming different values for the magnetic flux. Other effects considered are the role of finite temperature on the coherence pattern, and the behaviour away from the electron-hole symmetric point, a regime not considered before in a non-perturbative calculation within the AB setup [124]. Results presented in this chapter were published in Ref. [34].

Our simulations show that general dynamical characteristics of the double-dot coherence are maintained upon the application of inter-dot Coulombic interactions. In
particular, the characteristic timescale for reaching the steady state limit, the dependence of the coherence on the AB phase factors, and the form of the temporal current, similarly evolve for systems at zero or finite inter-dot interaction, for finite bias (beyond linear response), away from the electron-hole symmetric point, at low or high temperatures. We compare our data to (analytic) results based on a master equation treatment. This method can readily handle the zero electron-electron interaction case and the opposite case, the infinite interaction limit. Interestingly, in the latter Coulomb blockade limit the coherence is expected to evolve and sustain values distinctively different from its behaviour at finite interactions.

4.2 Model I

We focus on the symmetric AB setup, with a quantum dot located at each arm of the interferometer, see Fig. 2.1. The dots are each connected to two metal leads, maintained in a biased state. The dots '1' and '2' are represented by the electronic levels $\epsilon_1$, and $\epsilon_2$, respectively, described by the creation (annihilation) operators $a_\beta^\dagger (a_\beta)$, where $\beta = 1, 2$. These levels are coupled in an AB geometry to two metal leads ($\nu = L, R$) with chemical potentials $\mu_\nu$. For a schematic representation see Fig. 2.1. Here we include the Hamiltonian of model I and the definitions, since we use slightly different convention for the hybridization. The total Hamiltonian, $H_{AB}$, has the form,

$$H_{AB} = H_S + H_B + H_{SB},$$

where $H_S$ corresponds to the isolated dot Hamiltonian,

$$H_S = \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 + Ua_1^\dagger a_1 a_2^\dagger a_2.$$
$H_B$ include the left and right leads,

$$
H_B = \sum_l \omega_l a_l^\dagger a_l + \sum_r \omega_r a_r^\dagger a_r, \quad (4.3)
$$

and $H_{SB}$ stands for the dot-lead tunneling term,

$$
H_{SB} = \sum_{\beta,l} \xi_{\beta,l} a_\beta^\dagger a_l e^{i\phi_{\beta,l}} + \sum_{\beta,r} \zeta_{\beta,r} a_\beta^\dagger a_r e^{i\phi_{\beta,r}} + h.c. \quad (4.4)
$$

Here $\xi_{\beta,l}$ and $\zeta_{\beta,r}$ are real numbers. The hybridization matrix elements between the dot and the left/right leads are,

$$
\Gamma_{L,\beta,\beta'}(\omega) = 2\pi e^{i(\phi_{\beta,l} - \phi_{\beta'l})} \sum_l \xi_{\beta,l} \delta(\omega - \omega_l) \xi_{\beta',l}^*, \quad (4.5)
$$

$$
\Gamma_{R,\beta,\beta'}(\omega) = 2\pi e^{-i(\phi_{\beta,r} - \phi_{\beta'r})} \sum_r \zeta_{\beta,r} \delta(\omega - \omega_r) \zeta_{\beta',r}^*. \quad (4.6)
$$

We assume that level one and two couple identically with left ($L$) lead and write the diagonal element of hybridization matrix $\Gamma^L$ as,

$$
\gamma_L = \pi \sum_l (\xi_{l,\beta})^2 \delta(\omega - \omega_l), \quad (4.7)
$$

and similarly to the right ($R$),

$$
\gamma_R = \pi \sum_r (\zeta_{r,\beta})^2 \delta(\omega - \omega_r). \quad (4.8)
$$

The total diagonal decay is identified by $\Gamma = \gamma_L + \gamma_R$. Further, in what follows we only consider a degenerate situation with $\epsilon \equiv \epsilon_{\beta}$, and the dots are symmetrically coupled to both the leads. Using the INPFI approach, the following observables could be followed: the dots’ occupation, $\langle n_{\beta} \rangle \equiv \text{Tr}[a_{\beta}^\dagger a_{\beta} \rho]$, the coherence, $\sigma_{1,2} \equiv \text{Tr}[a_{1}^\dagger a_{2} \rho]$, and the total
current passing through the interferometer. The trace is performed over all degrees of freedom, metals and impurity. The charge current presented will be the symmetrized current, $\langle I \rangle \equiv \text{Tr}[\hat{I}\rho]$. It is accessed by defining the symmetrized current operator, extending the definitions in Sec. 2.2, Eq. (2.12).

$$\hat{I} = \frac{\hat{I}_L - \hat{I}_R}{2}. \quad (4.9)$$

Within INFPI, these observables are simulated in the Heisenberg representation assuming an initial density matrix $\rho(0)$ describing a nonequilibrium-biased situation. Please refer to Sec. 2.2.4 for general description of INFPI.

### 4.3 INFPI numerical results

We present here the coherence dynamics $\sigma_{1,2}(t) = \langle a_1^\dagger(t)a_2(t) \rangle$ and the charge current $\langle I_e \rangle$ within the interacting double-dot AB interferometer. As we show below, we find that finite e-e interactions do not destroy the general characteristics of the coherence behaviour, for the cases $U/\Gamma \leq 4$ considered here.

We focus on the following set of parameters: The double-dot subsystem includes two degenerate states with $\epsilon \equiv \epsilon_\beta$ ($\beta = 1, 2$). The dynamics is studied away from the electron-hole symmetric point, $E_d = \epsilon + U/2 = 0.2$. The metals’ band structure is taken identical at the two ends, and we use leads with constant density of states and a sharp cutoff at $D = \pm 1$. The inter-dot repulsion is taken at the range $U = 0 - 0.2$, whereas the system-bath hybridization strength is taken as $\Gamma = 0.05$. As we demonstrate below, our results generally converge for $U/\Gamma \leq 4$. The bias voltage is applied in a symmetric manner, $\mu_L = -\mu_R$, and we take $\mu_L - \mu_R = \Delta \mu \sim 0.6$. The temperature is varied, where $\beta_{\nu} = 1/T_{\nu} = 200$ corresponds to the low-$T$ case, and $\beta_{\nu} = 5$ reflects a high-$T$ situation. The numerical parameters of INFPI adopted are $L_s \sim 100$ states per bath, time step of $\delta t \sim 0.8 - 1.6$ and a memory time $\tau_c \sim 3 - 10$. This choice of
bath states suffices for mimicking a continuous band structure [56, 57]. Also, recurrence effects are not observed before $\Gamma t \sim 10$. For simulating dynamics beyond that time larger reservoirs are constructed, as necessary. The time step was selected based on two (contrary) considerations: (i) It should be made short enough, for justifying the Trotter breakup, $\delta t U < 1$. (ii) For computational reasons, it should be made long enough, to allow coverage of the system memory time with few terms, $N_s < 8$, recalling that $\tau_c = \delta t N_s$.

Before presenting our results, we explain the initial condition adopted. At time $t = 0$ the double-dot levels are both empty, while the (decoupled) reservoirs are separately prepared with occupation functions obeying the Fermi-Dirac statistics at a given temperature and bias.

![Figure 4.1: Left panel: Time evolution of the states coherence, in the absence of electron repulsion effects. Shown is the real part of $\sigma_{1,2}(t)$, plotted for the phases $\phi$ ranging from 0 to $2\pi$, top to bottom. $E_d = 0.2$, $\Gamma = 0.05$, $U = 0$, $\Delta \mu = 0.6$, $\beta \nu = 200$, $L_s = 240$. Right panel: The corresponding steady state values as a function of $\phi/\pi$, calculated using a Green’s function method with a band cutoff $D = \pm 1$ (full line) and $D = \pm 20$ (dashed line). The arrow indicates the value at $\phi = \pi/2$. Reproduced from Ref. [34].](image)

**4.3.1 Coherence dynamics at $U = 0$**

We begin by considering the noninteracting case, $U = 0$. The left panels in Figures 4.1 and 4.2 display the time evolution of the real and imaginary parts of $\sigma_{1,2}(t)$, respectively, for relatively large bias $\Delta \mu = 0.6$ and at low temperature. We find that $\Re \sigma_{1,2}$ decays at...
Figure 4.2: Left panel: Time evolution of the imaginary part of $\sigma_{1,2}(t)$, in the absence of electron repulsion effects. The phase factors $\phi$ range between $-\pi$ to $\pi$, bottom to top. Other parameters are the same as in Fig. 5.3. Right panel: The corresponding steady state values as a function of $\phi/\pi$, calculated using a Green’s function method. Reproduced from Ref. [34].

a flux dependent rate after the initial rise. The imaginary part, displayed in Fig. 4.2, saturates with a time scale $1/\Gamma$ [31]. Defining $\sigma_{1,2}(t) = |\sigma_{1,2}(t)|e^{i\varphi(t)}$, it was argued in Ref. [31] that this relative phase localizes to the values $\varphi = -\pi/2$ or $\pi/2$ in the long time limit when $\phi \neq 2p\pi$, $p$ is an integer. This localization behaviour is expected only when the (degenerate) dot levels are symmetrically placed between the chemical potentials, i.e., for $\epsilon = 0$. Away from this symmetric point, using $\epsilon = 0.2$, the left panel of Fig. 4.1 shows that the real part of $\sigma_{1,2}$ is finite and nonzero in the asymptotic limit for any phase, besides $\pi$. This reflects that though the bias is large, it still does not represent an “infinite bias limit”, as its “finiteness” is tractable in the steady state value.

We establish the validity of our results in the noninteracting limit by comparing the long time behaviour of INFPI with exact steady state values generated from the nonequilibrium Green’s function (GF) method [62]. The right panels in Figs. 4.1 and 4.2 display GF data for the real and imaginary parts of $\sigma_{1,2}$, respectively. For $\Re \sigma_{1,2}$, its long-time value shows a weak phase dependent behaviour, sensitive to the cutoff used, $D = \pm 1$ or $D = \pm 20$, the latter mimicking an infinite band. We compare INFPI data at $\phi = \pi/2$ to GF calculations, noting a discrepancy of less that 5%: At this phase
\[ \Re \sigma_{1,2}(t\Gamma = 15) = -0.041 \] with INFPI, whereas GF calculations (arrow) yield \(-0.043\). The behaviour of \( \Im \sigma_{1,2} \) was found to be practically insensitive to the cutoff used, \( D = \pm 1 \) or \( D = \pm 20 \). Overall, Green’s function simulations and INFPI results agree within 1.5\% for \( \Im \sigma_{1,2} \). Deviations between the methods should diminish when running INFPI simulations with more states per electronic bath.

![Figure 4.3: Time evolution of \( \sigma_{1,2} \) for \( U = 0 \) (full line), \( U = 0.1 \) (dashed line) and \( U = 0.2 \) (dotted line). Main: Real part of \( \sigma_{1,2}(t) \). The three top lines were simulated for \( \phi = 0 \). The bottom lines were obtained using \( \phi = \pi/2 \). The numerical parameters are \( \delta t = 1, N_s = 6 \) and \( L_s = 120 \). Inset: Imaginary part of \( \sigma_{1,2}(t) \) when \( \phi = \pi \). Numerical parameters are \( \delta t = 1.6, N_s = 6 \) and \( L_s = 120 \). Other parameters are \( E_d = 0.2, \Gamma = 0.05, \Delta \mu = 0.6 \) and \( \beta_\nu = 200 \). Reproduced from Ref. [34].](image)

### 4.3.2 Coherence and current at finite \( U \)

We now investigate the role of e-e repulsion effects on the coherence behaviour. Fig. 4.3 displays the real part of \( \sigma_{1,2}(t) \) for two phases, \( \phi = 0 \) and \( \phi = \pi/2 \), and its imaginary part for \( \phi = \pi \) (inset), for three values of \( U \). Data for \( \Im \sigma_{1,2}(t) \) at \( U = 0.2 \) has not converged for the \( \tau_c \) adopted, see text following Fig. 4.9. In comparison to the \( U = 0 \) case, we find that general trends are maintained, though the long time coherences are larger in the finite \( U \) case. Note our convention: the parameter \( E_d = \epsilon + U/2 \) is taken as fixed between simulations with different values of \( U \). The trajectory simulated extends up to \( \Gamma t = 3 \), where convergence is satisfactory. Different memory times were used for
simulating the real part of the coherence or its imaginary part. We adopted $\tau_c \sim 5$ when simulating $\Re \sigma_{1,2}$ whereas $\tau_c \sim 10$ was used for acquiring $\Im \sigma_{1,2}$. A more detailed discussion of convergence issues is given in Sec. 4.3.3.

Fig. 4.4 presents $\sigma_{1,2}(t)$ for several phases $\phi$, at $U = 0.1$. By comparing the data to the $U = 0$ case (see Figs. 4.1 and 4.2), we conclude that the symmetry of the off-diagonal elements is preserved in the presence of interactions. Naturally, one would be interested to follow this dynamics to the steady state limit. There are however two practical reasons why we cannot extend our finite-$U$ simulations to longer times. First, to eliminate recurrences, one needs to include more electronic states in each metal. Second, in order to gain correct results at long times the time step should be made shorter, so as to minimize the Trotter error buildup. The latter point is usually hard to overcome: Decreasing the time step while maintaining the overall memory time implies a larger $N_s$ value, with exponentially more permutations to sum up. More details about the computation time and memory size are given in Sec. 4.3.3.

The general pattern of the coherence is displayed in Figs. 4.5 and 4.6, plotting the behaviour of $\sigma_{1,2}$ as a function of the phase factor, at a particular time, $\Gamma t = 2$, for
$U = 0$, $0.1$, and $0.2$, at different temperatures. It should be noted that by this time the real part of the coherence has not yet reached its steady state value. We find that the coherence symmetry around $\phi = \pi$ (for $\Re \sigma_{1,2}$) or $\phi = 0$ (for $\Im \sigma_{1,2}$) is maintained, though the absolute numbers change. Interestingly, while the effect of the temperature is significant for $\Im \sigma_{1,2}$, showing a visible reduction in values at high $T$, the real part of $\sigma_{1,2}$ is only lightly affected by the temperature. The decrease of $\Im \sigma_{1,2}$ with temperature is also reflected in the behaviour of the charge current, as we show next.

![Figure 4.5: Effect of finite $U$ on the coherence. $\Re \sigma_{1,2}$ is plotted as a function of the phase factor $\phi$ at a particular time, $\Gamma t = 2$, for different $U$-values and temperatures, $T = 1/\beta$. Other parameters are the same as in Fig. 4.4. Reproduced from Ref. [34].](image-url)

![Figure 4.6: Effect of finite $U$ on the coherence. $\Im \sigma_{1,2}$ is plotted as a function of $\phi$ at a particular time, $\Gamma t = 2$, at finite $U$ and for different temperatures, $T = 1/\beta$. Other parameters are the same as in Fig. 4.4. Reproduced from Ref. [34].](image-url)

We study the behaviour of the charge current at different phases, for different e-e repulsion strengths and temperatures. Fig. 4.7 shows, as expected, a destructive
interference pattern for electron current in the long time limit when $\phi = \pi$, irrespective of the value of $U$. This perfect destructive interference indicates that charge transport is fully coherent in this model. The temporal behaviour does show however a sensitivity to the value of $U$, manifesting that systems with variable $U$ differently respond to the initial condition. However, these variations concurrently die around $\Gamma t \sim 1$, indicating on a common mechanism for approaching steady state.

In the steady-stat limit the current scales like $\langle I_e \rangle \propto [1 + \cos(\phi)]$, for finite $U$ [8]. This relation does not hold in the short time limit. It is interesting to note that irrespective of $U$ and the phase factor, the current approaches the steady state limit on a relatively short timescale, $\Gamma t \sim 2$, similarly to the behaviour of $\Im \sigma_{1,2}$. At high temperatures, Fig. 4.7 manifests that the system is still fully coherent, while temporal oscillations are washed out. The reduction of the current at high temperatures can be attributed to the softening of the contacts’ Fermi functions from the sharp step-like form at low temperatures. The electronic states at the right lead in the bias window are not fully empty any longer. Similarly, at the left lead electronic states overlapping with $E_d$ may be empty. Overall, this results in the reduction of the current at high $T$.

Figure 4.7: Charge current through an AB interferometer at low temperatures, $\beta = 200$ (left panel) and high temperatures $\beta = 5$ (right panel) for $\phi = 0$, $\pi/2$, and $\pi$, top to bottom with $U = 0.2$ (full line), $U = 0.1$ (dashed line), $U = 0$ (dotted line). Other parameters are the same as in Fig. 4.4. In our convention we fix the shifted dot energies $E_d = \epsilon + U/2$. The current increases with increasing $U$ since given our convention and choice of parameter, $\epsilon$ is pushed into the bias window for $U = 0.1$. Numerical parameters are $\delta t = 1$, $N_s = 6$ and $L_s = 120$. Reproduced from Ref. [34].
4.3.3 Convergence analysis

We exemplify here the convergence behaviour of the real and imaginary parts of $\sigma_{1,2}$ at low temperatures, as well as the behaviour of the current. Fig. 4.8 demonstrates that $\Re \sigma_{1,2}$ nicely converges for $U = 0.2$, for $\tau_c \geq 5$. The asymptotic limit is practically reached, within $\sim 1.5\%$ error, already for $\tau_c \sim 1/\Delta \mu$. We confirm that the results are insensitive to the particular time step selected (inset). We have also verified (not shown) that simulations performed with different phase factors similarly converge.

The convergence of $\Im \sigma_{1,2}$ is generally slower, as we show in Fig. 4.9. While $\Re \sigma_{1,2}$ converges for $\tau_c \gtrsim 1/\Delta \mu$, we find that $\Im \sigma_{1,2}$ requires memory time at least twice longer for achieving convergence. For $U = 0.1$ $\Im \sigma_{1,2}$ is converging. In contrast, at stronger interactions, $U = 0.2$, the large time step adopted results in a Trotter error buildup, and the results seem to diverge around $\tau_c \sim 10 - 12$ (inset). The challenge in simulating large-$U$ systems is that a short time step should be employed, for controlling the Trotter-$\delta t U$ error. However, a short time step implies that the memory time $\tau_c$ is covered with a large $N_s$, i.e., exponentially more permutations need to be summed up when calculating the influence functional. This issue is non-trivial and may be tracked down by sampling the paths that are mostly contributing to the overall dynamics.

We also present the behaviour of the charge current at different $\tau_c$ values, see Fig. 4.10. It generally converges when $\tau_c \sim 6$, irrespective of the phase factor (not shown), for $U/\Gamma \leq 4$, in agreement with earlier studies [57].

Overall, we conclude that we can faithfully simulate the time evolution of the coherence $\sigma_{1,2}$ and the current for $\Delta \mu = 0.6$ and $U/\Gamma = 2$. For larger $U$, the real part of $\sigma_{1,2}$, the dot occupation, and the current can be still converged [56, 57]. The simulation of $\Im \sigma_{1,2}$ requires longer $\tau_c$ and a shorter time step at $U/\Gamma > 2$. Roughly, these observations can be rationalized noting that the dynamics of $\Re \sigma_{1,2}$ is influenced by the full potential drop, $\mu_L - \mu_R$, similarly to the dots occupation $\langle n_m \rangle$ [31]. In contrast, the dynamics of $\Im \sigma_{1,2}$ is sensitive to the bias drop at each contact [31], resulting in longer decorrelation.
Figure 4.8: Convergence behaviour of $\Re \sigma_{1,2}$ for $\phi = 0$ and $U=0.2$. Other physical parameters are the same as in Fig. 4.4. Numerical parameters are $\delta t = 0.8$ and $N_s = 2$ (+), $N_s = 3$ (dashed-dotted line), $N_s = 4$ (dashed line), $N_s = 5$ (full line) and $N_s = 6$ (dotted line). The inset shows the convergence behaviour at a particular time, $\Gamma t = 2$, as a function of the memory time $\tau_c = N_s \delta t$, using three different values for the time steps, $\delta t = 0.8$ (o), $\delta t = 1$ (□) $\delta t = 1.6$ (*). Reproduced from Ref. [34].

Figure 4.9: Convergence behaviour of $\Im \sigma_{1,2}$ for $\phi = \pi$ and $U=0.1$. Other physical parameters are the same as in Fig. 4.4. Numerical parameters are $\delta t = 1.6$ and $N_s = 2$ (+), $N_s = 3$ (dashed-dotted), $N_s = 4$ (dashed line), $N_s = 5$ (full line) and $N_s = 6$ (dot), $N_s = 7$ (dotted line). The inset presents $\Im \sigma_{1,2}$ at a particular time, $\Gamma t = 2$, for $U = 0.1$ and $U = 0.2$, as a function of the memory time $\tau_c = N_s \delta t$, using three different time steps, $\delta t = 0.8$ (o), $\delta t = 1$ (□) $\delta t = 1.6$ (*). Reproduced from Ref. [34].
Figure 4.10: Convergence behaviour of the charge current, $\phi = \pi/2$ and $U=0.2$. Other physical parameters are the same as in Fig. 4.4. Numerical parameters are $\delta t = 1$ and $N_s = 2$ (+), $N_s = 3$ (dashed-dotted), $N_s = 4$ (dashed line), $N_s = 5$ (full line) and $N_s = 6$ (dot), $N_s = 7$ (dotted line). The inset presents the data at a particular time, $\Gamma t = 2$, for $U = 0.1$ (bottom) and $U = 0.2$ (top), as a function of the memory time $\tau_c = N_s \delta t$, using $\delta t = 1$ (□) and $\delta t = 1.6$ (*). Reproduced from Ref. [34].

times. Details of simulation times are presented in [34].

4.4 Master equation analysis: $U = 0$ and $U = \infty$

We compare the noninteracting case ($U = 0$) and the finite $U$ case with $U = \infty$ limit. In order to simulate the dynamics in this limit, we use the master equations described in Sec. 2.2.5. Here we study the dynamics of reduced density matrix $\sigma_{j,j'}$ in the charge state basis, where $j = a, b, c, d$ denotes the double-dot charge states. Explicitly, $|a\rangle \leftrightarrow |00\rangle$, $|b\rangle \leftrightarrow |10\rangle$, $|c\rangle \leftrightarrow |01\rangle$, and $|d\rangle \leftrightarrow |11\rangle$.

$U = 0$ case: In the steady state limit we demand that $d\vec{\sigma}/dt = 0$, the vector $\vec{\sigma}$ includes the matrix elements $\sigma_{j,j'}$ of Eq. (2.43), and obtain the stationary solution, valid for $\phi \neq 0$,

$$\sigma_{b,c}(t \rightarrow \infty) = \frac{i}{2} \sin(\phi/2).$$ (4.10)

This expression holds in the symmetric setup, $\gamma_L = \gamma_R$, for $\phi \neq 2\pi p$, $p$ is an integer. The real part is identically zero leading to the “phase localization”, Eq. (2.45). The
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Results of Figs. 4.1 and 4.2 demonstrate the breakdown of the “phase localization” effect at finite bias. There, the real part is finite, yet small, approaching a fixed value. The imaginary part slightly deviates from the prediction of Eq. (4.10) due to the finite bias used. One could also get hold of the characteristic rates from the dynamical equation, by diagonalizing the matrix $M$ in $d\vec{\sigma}/dt = M\vec{\sigma}$. We obtain five rates, with two phase dependent rates, $\propto [1 \pm \cos(\phi/2)]$. For small $\phi$, the smallest rate is $\propto [1 - \cos(\phi/2)]$, in agreement with [31]. It can be also proved that in this noninteracting case the steady state current scales with $\langle I_e \rangle \propto [1 + \cos(\phi)]$ [9].

The dynamics of the coherence, attained from the master equation (2.43), is displayed in Fig. 4.11 for $\phi = \pi/2$. In the long time limit the real part approaches zero; the imaginary part reaches $\frac{1}{2} \sin(\pi/4) = 0.354$. INFPI results at zero $U$ are also included in dotted lines. Deviations of INFPI simulations from master equation results can be traced to the finite band used within INFPI, in comparison to the infinite-flat band assumed in the master equation approach. For finite $U$, we have found that at large bias, $\Delta \mu = 2D$, INFPI data overlaps with the $U = 0$ case (not shown) as the system basically stands on the symmetric point.

$U = \infty$ case: For a spatially symmetric junction, $\gamma_L = \gamma_R$, the steady state solution for the coherence in the $U = \infty$ limit becomes,

$$\sigma_{b,c}(t \to \infty) = -\frac{1}{2}e^{-i\phi/2}$$

$$= -\frac{1}{2} \cos(\phi/2) + \frac{i}{2} \sin(\phi/2). \tag{4.11}$$

While the imaginary part predicted is identical to the $U = 0$ case, see Eq. (4.10), the real part is finite and phase dependent. The dynamics in infinite $U$ limit is presented in Fig. 4.11 (dashed lines). We find that the imaginary part is weakly sensitive to the onset of $U$. In contrast, the real part significantly deviates from the $U = 0$ case already at $\Gamma t \sim 1$.

By analyzing the eigenvalues of the rate matrix (2.44), we note that phase dependent
relaxation rates in the infinite $U$ regime are the same as for noninteracting electrons, see also Fig. 4.11. It would be interesting to explore this evolution within the INFPI approach. However, as we are currently limited to $U/\Gamma \leq 4$ values, this would require an algorithmic improvement of the INFPI technique. We believe that such an extension could be achieved since the $U = \infty$ case should converge faster than the intermediate $U$ limit [97].

Figure 4.11: Master equation analysis: Real and imaginary parts of $\sigma_{b,c}$ at $\phi = \pi/2$, for $U = 0$ and $U = \infty$, obtained by simulating Eq. (2.43) and Eq. (2.44), respectively. Results from INFPI method with $U=0$ are represented by dotted lines, practically overlapping with $U = 0$ master equation curves. Reproduced from Ref. [34].

4.5 Discussion

In this chapter our goal has been to address the effect of e-e interactions on the intrinsic coherence behaviour of an open quantum system. As a case study, the coherence dynamics in a double quantum dot AB interferometer, away from the symmetric point, has been simulated using an exact numerical technique. While the specific time evolution described here depends on the particular initial conditions employed, decoupled system-bath, we can still draw some general conclusions: (i) Coherence timescales. The real and imaginary parts of the coherence approach the steady state limit in differing ways: $\Re \sigma_{1,2}$ reaches the steady state limit with (strong) magnetic-flux dependent rates. In particular,
the timescale to reach the asymptotic limit is very slow for small $\phi$. In contrast, $\Im \sigma_{1,2}$ approaches steady state within a time scale that is \textit{flux-independent}. This observation is valid away from the symmetric point, at finite interaction strengths and at low or high temperatures. (ii) Transport properties and subsystem dynamics. Comparing the time evolution of the coherences in Figs. 4.1 and 4.4 to the evolution of the current as depicted in Fig. 4.7, we note that the charge current approaches steady state around $\Gamma t \sim 2 (\beta_\nu = 200)$, in a phase independent rate, similarly to the behaviour of $\Im \sigma_{1,2}$. It can be also shown, at least at the symmetric point, that the double-dot occupancy is proportional to $\Re \sigma_{1,2}$ in the asymptotic long-time limit [31]. These relations suggest that the current dynamics, or more generally, transport coefficients, connect to the dynamics concealed within $\Im \sigma_{1,2}$. The dot occupation, an impurity property, correlates in some limit with $\Re \sigma_{1,2}$. Understanding the correspondence between transport properties, e.g., current, current noise, Seebeck coefficient, and impurity properties such as population and coherences, is a topic of fundamental interest in nonequilibrium open quantum systems [95]. Our results here demonstrate a nontrivial connection between the current and $\Im \sigma_{1,2}$. It is of interest to further explore these relations analytically.

More particular observations include the following points: (i) Coherence symmetry, with respect to the magnetic flux, observed at $U = 0$ and at low temperatures, is maintained even when e-e interactions are turned on, and at high temperatures. (ii) The charge current displays the effect of perfect destructive interference in the long time limit for $\phi = \pi$, irrespective of the onset of e-e interactions, see Fig. 4.7, indicating that “phase rigidity” is obeyed in symmetric and degenerate double-dot interferometer beyond linear regime even with many-body interactions. While temporal characteristics are sensitive to the actual $U$-value employed, the different curves concurrently merge around $t\Gamma \sim 1$. (iii) At finite interactions, $U/\Gamma \leq 4$, at low or high temperatures, we have found that the coherence evolves similarly to the $U = 0$ case, showing related characteristic timescales and long time values. Specifically, for $\phi = \pi/2$ the real part of $\sigma_{1,2}$ approaches a small
number (zero at the symmetric point), while the imaginary part is larger, $\sim 0.35$. On the other hand, a master equation treatment in the infinite $U$ regime predicts a significantly different behaviour: The magnitude of $\Re \sigma_{1,2}$ and $\Im \sigma_{1,2}$ should be the same, $\sqrt{2}/4$, for the $\phi = \pi/2$ phase factor.

We have discussed so far only coherent dynamics in double-dot AB interferometer. It is interesting to study how phase breaking processes affect phase rigidity. In the next chapter we include quasi-elastic dephasing effects by means of Büttiker dephasing probes using nonequilibrium Green’s functions. We also discuss the role of inelastic scattering and capacitive coupling to equilibrium and nonequilibrium environments.
Chapter 5

Symmetries of nonlinear transport

5.1 Introduction

In previous chapters we studied the dynamics of the reduced density matrix and the charge current in interacting systems using different techniques: a numerically exact influence functional path integral method, master equations valid in the infinite $U$ limit. We also discussed magnetic flux control of dot occupations with and without elastic dephasing effects, using a probe. In this chapter we focus on magnetic field symmetries of nonlinear transport coefficients in the presence of many body effects, taken into account by a phenomenological technique, the probe reservoir, discussed in chapter 2.

Our objective here is to provide a systematic and comprehensive analysis of the role of different types of probes on transport symmetries in nonlinear conductors. We want to understand the role of elastic dephasing, heat dissipation, and charge leakage processes on symmetries of charge current, rectification, and heat current in two-terminal conductors, with respect to the magnetic field, temperature bias, and voltage bias. Specifically, our main goal is to develop, and analyze the breakdown, of magnetic field symmetry relations for nonlinear transport beyond the Onsager-Casimir result in the presence of incoherent
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effects. Expanding the charge current in powers of the bias $\Delta \mu$ we write [162]

$$I(\phi) = G_1(\phi) \Delta \mu + G_2(\phi)(\Delta \mu)^2 + G_3(\phi)(\Delta \mu)^3 + ...$$

(5.1)

with $G_{n>1}$ as the nonlinear conductance coefficients. We incorporate many body effects using Büttiker probes. (i) We confirm the validity of Onsager-Casimir symmetry of linear conductance ($G_1(\phi) = G_1(-\phi)$) using an approach based on quantum mechanical equations of motion while allowing for elastic and inelastic effects. (ii) We obtain magnetic field symmetries and magnetoasymmetries of higher order conductance coefficients.

Our study of transport behaviour beyond linear response further exposes sufficient conditions for the onset of the charge current rectification (diode) effect, referring to the situation where the magnitude of the current differs when the bias polarity is reversed. This effect, of fundamental and practical interest, is realized by combining many body interactions with a broken symmetry: broken spatial inversion symmetry or a broken time reversal symmetry. Rectifiers of the first type have been extensively investigated theoretically and experimentally, including electronic rectifiers, thermal rectifiers [44] and acoustic rectifiers [126]. In parallel, optical and spin rectifiers were designed based on a broken time reversal symmetry, recently realized e.g. by engineering parity-time metamaterials [127]. The model system investigated in this work, a double-dot AB junction, offers a feasible setup for devising broken time reversal rectifiers.

We consider here four different probes (dephasing, voltage, temperature and voltage-temperature) and demonstrate with numerical simulations a stable solution and a facile convergence for the probe parameters far from equilibrium. We discuss the operation of the double-dot interferometer, susceptible to inelastic effects, as a charge rectifier, when time reversal symmetry is broken. We derive symmetry relations for nonlinear heat transfer in the presence of charge leakage. This chapter is organized as follows. In Sec. 5.2 we introduce the main observables of interest and summarize our principal
results. In Sec. 5.3 we discuss situations that fulfill phase rigidity. Magnetic field symmetry relations in a spatially symmetric setup are derived in Sec. 5.4. Magnetic field–gate voltage symmetries, valid for generic double-dot AB interferometer models, are presented in Sec. 5.5. Supporting numerical simulations are included in Sec. 5.6. In Sec. 5.7 we discuss relation of our results to other treatments. In Sec. 5.8 we present all the conclusions. The words “diode” and “rectifier” are used interchangeably in this work, referring to a dc-rectifier.

5.2 Symmetry measures and main results

In the main body of this chapter we restrict ourselves to voltage-biased junctions, \( \mu_L \neq \mu_R \), while setting \( T_a = \beta_1 = T_L = T_R \). We also limit our focus to charge conserving systems satisfying

\[
I(\phi) \equiv I_L(\phi) = -I_R(\phi),
\]  

and study the role of elastic dephasing (dephasing probe) and dissipative (voltage probe) and non-dissipative (voltage-temperature probe) inelastic effects on the charge transport symmetries with magnetic flux. We complement this analysis by considering a temperature-biased heat-conserving junction, \( T_L \neq T_R, \mu_a = \mu_L = \mu_R \) and \( Q_L = -Q_R \). We then study the phase symmetry of the heat current, allowing for charge leakage in the probe. We do not study the thermoelectric effect in this work.

We now define several measures for quantifying phase symmetry in a voltage-biased three-terminal junction satisfying Eq. (5.2). In this work we study relations between two quantities: a measure for the magnetic field asymmetry

\[
\Delta I(\phi) \equiv \frac{1}{2}[I(\phi) - I(-\phi)],
\]
and the dc-rectification current,

\[
\mathcal{R}(\phi) \equiv \frac{1}{2} [I(\phi) + \bar{I}(\phi)]
\]

\[
= G_2(\phi)(\Delta \mu)^2 + G_4(\phi)(\Delta \mu)^4 + ... \quad (5.4)
\]

with \( \bar{I} \) defined as the current obtained upon interchanging the chemical potentials of the two terminals. We also study the behaviour of odd conductance terms,

\[
\mathcal{D}(\phi) \equiv \frac{1}{2} [I(\phi) - \bar{I}(\phi)]
\]

\[
= G_1(\phi)\Delta \mu + G_3(\phi)(\Delta \mu)^3 + ... \quad (5.5)
\]

For a non-interacting system we expect the relation

\[
I(\phi) = -\bar{I}(-\phi) \quad (5.6)
\]

to hold. Combined with Eq. (5.1) we immediately note that \( G_{2n+1}(\phi) = G_{2n+1}(-\phi) \) and \( G_{2n}(\phi) = -G_{2n}(-\phi) \) with \( n \) as an integer. We show below that these relations are obeyed in a symmetric junction even when many body interactions (inelastic scattering) are included. This result is not trivial since the included many body interactions are reflected by probe parameters which depend on the applied bias in a nonlinear manner and the magnetic phase in an asymmetric form, thus, we cannot assume Eq. (5.6) to immediately hold. Our analysis below relies on two basic relations. First, the transmission coefficient from the \( \xi \) to the \( \nu \) reservoir obeys reciprocity, given the unitarity and time reversal symmetry of the scattering matrix,

\[
\mathcal{T}_{\xi,\nu}(\omega, \phi) = \mathcal{T}_{\nu,\xi}(\omega, -\phi). \quad (5.7)
\]
Second, the total probability is conserved,
\[
\sum_{\xi \neq \nu} T_{\xi,\nu}(\omega, \phi) = \sum_{\xi \neq \nu} T_{\nu,\xi}(\omega, \phi). \tag{5.8}
\]

Using Eq. (2.20), we express the deviation from the magnetic field symmetry as
\[
\Delta I = \frac{1}{2} \int [T_{L,R} - T_{R,L}] (f_L + f_R) d\omega + \frac{1}{2} \int [T_{L,P} - T_{P,L}] f_L d\omega
+ \frac{1}{2} \int [T_{L,P} f_P(-\phi) - T_{P,L} f_P(\phi)] d\omega \tag{5.9}
\]

For the sake of simplicity we write \( T_{\nu,\xi}(\omega, \phi) \) as \( T_{\nu,\xi} \). We use the probability conservation, Eq. (5.8), and simplify this relation,
\[
\Delta I = \frac{1}{2} \int [T_{L,R} - T_{R,L}] f_R d\omega + \frac{1}{2} \int [T_{L,P} f_P(-\phi) - T_{P,L} f_P(\phi)] d\omega. \tag{5.10}
\]

Since \( I_L = -I_R \), the rectification current can be written in two equivalent forms,
\[
\mathcal{R} = \frac{1}{2} \int T_{P,L}(f_L + f_R - f_P(\phi) - \bar{f}_P(\phi)) d\omega
= -\frac{1}{2} \int T_{P,R}(f_L + f_R - f_P(\phi) - \bar{f}_P(\phi)) d\omega, \tag{5.11}
\]

with \( \bar{f}_P \) as the probe distribution when the biases \( \mu_L \) and \( \mu_R \) are interchanged. We can also weight these expressions and adopt a symmetric definition
\[
\mathcal{R} = \int \frac{T_{P,L} - T_{P,R}}{4} (f_L + f_R - f_P(\phi) - \bar{f}_P(\phi)) d\omega \tag{5.12}
\]

The behaviour of odd conductance terms can be similarly written as
\[
\mathcal{D}(\phi) = \frac{1}{2} \int \left\{ [T_{L,R} + T_{L,P} + T_{R,L}] (f_L - f_R) - T_{P,L}[f_P(\phi) - \bar{f}_P(\phi)] \right\} d\omega
= -\frac{1}{2} \int \left\{ [T_{L,R} + T_{R,P} + T_{R,L}] (f_R - f_L) - T_{P,R}[f_P(\phi) - \bar{f}_P(\phi)] \right\} d\omega \tag{5.13}
\]
Our results are organized by systematically departing from quantum coherent scenarios, the linear response regime, and spatially symmetric situations. This chapter includes four parts, and we now summarize our main results:

(i) \textit{Phase Rigidity.} In Sec. 5.3 we discuss two scenarios that do obey the Onsager-Casimir symmetry relation $I(\phi) = I(-\phi)$: It is maintained in the presence of elastic dephasing effects even beyond linear response. This relation is also valid when inelastic scatterings are included, albeit only in the linear response regime. While these results are not new [64], we include this analysis here so as to clarify the role of inelastic effects in breaking the Onsager symmetry, beyond linear response.

(ii) \textit{Magnetic field (MF) symmetry relations beyond linear response.} In Sec. 5.4 we derive magnetic-field symmetry relations that hold beyond linear response in \textit{spatially symmetric} junctions susceptible to inelastic effects, $\mathcal{R}(\phi) = \Delta I(\phi) = -\mathcal{R}(-\phi)$ and $\mathcal{D}(\phi) = \mathcal{D}(-\phi)$. In other words, we show that odd (even) conductance terms are even (odd) in the magnetic flux. Note that “spatial” or “geometrical” symmetry refers here to the left-right mirror symmetry of the junction. Below we refer to these symmetries as the “MF symmetry relations”.

(iii) \textit{Magnetic field-Gate voltage (MFGV) symmetry relations beyond linear response.} In Secs. 5.5-5.6 we focus on geometrically \textit{asymmetric} setups, adopting the double dot AB interferometer as an example. While we demonstrate, using numerical simulations, the breakdown of the MF relations under spatial asymmetry, we prove that charge conjugation symmetry entails magnetic field-gate voltage symmetries: $\mathcal{R}(\epsilon_d, \phi) = -\mathcal{R}(-\epsilon_d, -\phi)$, and $\mathcal{D}(-\epsilon_d, -\phi) = \mathcal{D}(\epsilon_d, \phi)$, with $\epsilon_d$ as the double-dot energies. We refer below to these symmetries as the “MFGV symmetry relations”.

(iv) we also prove that the heat current (within a heat-conserving setup) satisfies relations analogous to (i)-(iii).
5.3 Phase rigidity and absence of rectification

In this section we adopt a formalism based on quantum mechanical equations of motion and demonstrate that, consistent with the theory of irreversible thermodynamics: (i) The symmetry $I(\phi) = I(-\phi)$ is preserved under quasi-elastic dephasing effects, implemented via a dephasing probe (ii) Onsager-Casimir symmetry is obeyed in the presence of inelastic effects implemented using the voltage probe technique. These results have already been discussed in e.g., Ref. [64]. We detail these steps here so as to provide closed expressions for the probe parameters in the linear response regime. We also show that the quasi-elastic dephasing does not lead to diode behaviour.

5.3.1 Dephasing effects beyond linear response

Implementing the dephasing probe (2.23) we obtain the respective distribution

$$f_P(\phi) = \frac{\mathcal{T}_{L,P} f_L + \mathcal{T}_{R,P} f_R}{\mathcal{T}_{P,L} + \mathcal{T}_{P,R}}. \quad (5.14)$$

We substitute this function into Eq. (5.10), the measure for phase asymmetry, and obtain

$$\Delta I = \frac{1}{2} \int \left[ \mathcal{T}_{L,R} - \mathcal{T}_{R,L} \right] f_R d\omega + \frac{1}{2} \int \mathcal{T}_{L,P} \frac{\mathcal{T}_{P,L} f_L + \mathcal{T}_{P,R} f_R}{\mathcal{T}_{L,P} + \mathcal{T}_{R,P}} d\omega$$

$$- \frac{1}{2} \int \mathcal{T}_{P,L} \frac{\mathcal{T}_{L,P} f_L + \mathcal{T}_{R,P} f_R}{\mathcal{T}_{P,L} + \mathcal{T}_{P,R}} d\omega. \quad (5.15)$$

The denominators in these integrals are identical, see Eq. (5.8), thus we combine the last two terms into

$$\Delta I = \frac{1}{2} \int \left[ \mathcal{T}_{L,R} - \mathcal{T}_{R,L} \right] f_R d\omega + \frac{1}{2} \int \frac{\left[ \mathcal{T}_{L,P} \mathcal{T}_{P,R} - \mathcal{T}_{P,L} \mathcal{T}_{R,P} \right] f_R}{\mathcal{T}_{P,R} + \mathcal{T}_{P,L}} d\omega. \quad (5.16)$$
Utilizing Eq. (5.8) in the form $\mathcal{T}_{L,P} = \mathcal{T}_{P,L} + \mathcal{T}_{P,R} - \mathcal{T}_{R,P}$, we organize the numerator of the second integral, $(\mathcal{T}_{P,R} - \mathcal{T}_{R,P})(\mathcal{T}_{P,R} + \mathcal{T}_{P,L})f_R$. This results in

$$\Delta I = \frac{1}{2} \int [\mathcal{T}_{L,R} - \mathcal{T}_{R,L} + \mathcal{T}_{P,R} - \mathcal{T}_{R,P}] f_R d\omega$$

$$= \frac{1}{2} \int f_R \left[ \sum_{\nu \neq R} \mathcal{T}_{\nu,R} - \sum_{\nu \neq R} \mathcal{T}_{R,\nu} \right] d\omega, \quad (5.17)$$

which is identically zero, given Eq. (5.8). This concludes our proof that dephasing effects, implemented via a dephasing probe, cannot break phase rigidity even in the nonlinear regime. Following similar steps we show that elastic dephasing effects cannot bring about the effect of charge rectification even when the junction acquires spatial asymmetries. We substitute $f_P$ into Eq. (2.20) and obtain

$$I_L = \int [F_L f_L - F_R f_R] d\omega$$

$$\quad (5.18)$$

with

$$F_L = \frac{\mathcal{T}_{L,R}(\mathcal{T}_{P,L} + \mathcal{T}_{P,R}) + \mathcal{T}_{L,P}\mathcal{T}_{P,R}}{(\mathcal{T}_{P,L} + \mathcal{T}_{P,R})}. \quad (5.19)$$

$F_R$ is defined analogously, interchanging $L$ by $R$. We now note the following identities,

$$\mathcal{T}_{L,P}\mathcal{T}_{P,R} = [\mathcal{T}_{P,L} + \mathcal{T}_{P,R} - \mathcal{T}_{R,P}]\mathcal{T}_{P,R}$$

$$= (\mathcal{T}_{P,R} - \mathcal{T}_{R,P})(\mathcal{T}_{P,R} + \mathcal{T}_{P,L}) + \mathcal{T}_{P,L}\mathcal{T}_{R,P}$$

$$= (\mathcal{T}_{R,L} - \mathcal{T}_{L,R})(\mathcal{T}_{P,R} + \mathcal{T}_{P,L}) + \mathcal{T}_{P,L}\mathcal{T}_{R,P} \quad (5.20)$$

Reorganizing the first and third lines we find that

$$\mathcal{T}_{L,R}(\mathcal{T}_{P,R} + \mathcal{T}_{P,L}) + \mathcal{T}_{L,P}\mathcal{T}_{P,R} = \mathcal{T}_{R,L}(\mathcal{T}_{P,R} + \mathcal{T}_{P,L}) + \mathcal{T}_{P,L}\mathcal{T}_{R,P} \quad (5.21)$$
which immediately implies that $F_L = F_R$. This is turn leads to $I = -\bar{I}$, thus $\mathcal{R} = 0$. We conclude that the current only includes odd (linear and nonlinear) conductance terms under elastic dephasing, $I = \mathcal{D}(\phi) = \mathcal{D}(-\phi)$, and that phase rigidity is maintained even if spatial asymmetry is presented. This conclusion in valid under both applied voltage and temperature biases.

### 5.3.2 Inelastic effects in linear response

We introduce inelastic effects using the voltage probe technique. In the linear response regime we expand the Fermi functions of the three terminals around the equilibrium state

$$f_a(\omega) = \left[ e^{\beta_a(\omega - \mu_a)} + 1 \right]^{-1},$$

$$f_\nu(\omega) = f_a(\omega) - (\mu_\nu - \mu_a) \frac{\partial f_a}{\partial \omega}.$$  \hspace{1cm} (5.22)

The three terminals are maintained at the same temperature $T_a$. The derivative $\frac{\partial f_a}{\partial \omega}$ is evaluated at the equilibrium value $\mu_a$. For simplicity we set $\mu_a = 0$. We enforce the voltage probe condition, $I_P = 0$, demanding that

$$\int \left[ (\mathcal{T}_{P,L} + \mathcal{T}_{P,R}) f_P(\phi) - \mathcal{T}_{L,P} f_L - \mathcal{T}_{R,P} f_R \right] d\omega = 0.$$  \hspace{1cm} (5.23)

In linear response this translates to

$$0 = \int \left[ (\mathcal{T}_{P,L} + \mathcal{T}_{P,R}) \left( f_a - \mu_P(\phi) \frac{\partial f_a}{\partial \omega} \right) \right. \left. - \mathcal{T}_{L,P} \left( f_a - \mu_L \frac{\partial f_a}{\partial \omega} \right) - \mathcal{T}_{R,P} \left( f_a - \mu_R \frac{\partial f_a}{\partial \omega} \right) \right] d\omega.$$  \hspace{1cm} (5.24)
For convenience, we apply the voltage in a symmetric manner, \( \mu_L = -\mu_R = \Delta \mu / 2 \). We organize Eq. (5.24) and obtain the probe chemical potential, a linear function in \( \Delta \mu \),

\[
\mu_P(\phi) = \frac{\Delta \mu}{2} \int d\omega \frac{\partial f_a}{\partial \omega} \frac{(\mathcal{T}_{L,P} - \mathcal{T}_{R,P})}{(\mathcal{T}_{P,L} + \mathcal{T}_{P,R})}.
\]  

(5.25)

We simplify this result by introducing a short notation for the conductance between the \( \nu \) and \( \xi \) terminals,

\[
G_{\nu,\xi}(\phi) \equiv \int d\omega \left( -\frac{\partial f_a}{\partial \omega} \right) \mathcal{T}_{\nu,\xi}(\omega, \phi).
\]  

(5.26)

This quantity fulfills relations analogous to Eqs. (5.7) and (5.8). For brevity, we do not write next the phase variable in \( G \), evaluating it at the phase \( \phi \) unless otherwise mentioned. The probe potential can now be compacted,

\[
\mu_P(\phi) = \frac{\Delta \mu}{2} \frac{G_{L,P} - G_{R,P}}{G_{P,L} + G_{P,R}}.
\]  

(5.27)

Furthermore, in geometrically symmetric systems \( \mathcal{T}_{R,P}(\omega, \phi) = \mathcal{T}_{P,L}(\omega, \phi) \), resulting in \( G_{R,P}(\phi) = G_{P,L}(\phi) \) and

\[
\mu_P(\phi) = \frac{\Delta \mu}{2} \frac{G_{L,P}(\phi) - G_{L,P}(-\phi)}{G_{L,P}(\phi) + G_{L,P}(-\phi)}.
\]  

(5.28)

Thus \( \mu_P(\phi) = -\mu_P(-\phi) \) in linear response. Below we show that this symmetry does not hold far from equilibrium. We now expand Eq. (5.10) in the linear response regime

\[
\Delta I = \frac{1}{2} \int (\mathcal{T}_{L,R} - \mathcal{T}_{R,L}) \left( f_a - \mu_R \frac{\partial f_a}{\partial \omega} \right) d\omega
\]

\[
+ \frac{1}{2} \int \left\{ \mathcal{T}_{L,P} \left[ f_a - \mu_P(-\phi) \frac{\partial f_a}{\partial \omega} \right] - \mathcal{T}_{P,L} \left[ f_a - \mu_P(\phi) \frac{\partial f_a}{\partial \omega} \right] \right\} d\omega.
\]  

(5.29)
Utilizing the definition (5.26) we compact this expression,

\[
\Delta I = \frac{1}{2} (G_{L,R} - G_{R,L}) \mu_R
- \frac{1}{2} [G_{P,L} \mu_P(\phi) - G_{L,P} \mu_P(-\phi)].
\] (5.30)

Using Eq. (5.8), the first line can be rewritten as

\[
I_1 = \frac{\Delta \mu}{4} (G_{L,P} - G_{P,L}).
\] (5.31)

The second line in Eq. (5.30) reduces to

\[
I_2 = -\frac{\Delta \mu}{4} G_{P,L} \frac{G_{L,P} - G_{R,P}}{\mathcal{N}} + \frac{\Delta \mu}{4} G_{L,P} \frac{G_{P,L} - G_{P,R}}{\mathcal{N}}
= -\frac{\Delta \mu}{4} \frac{G_{P,L} G_{P,R} - G_{P,L} G_{R,P}}{\mathcal{N}},
\] (5.32)

where we have introduced the short notation \( \mathcal{N} \equiv G_{P,L} + G_{P,R} \). Now, we substitute \( G_{L,P} = G_{P,L} + G_{P,R} - G_{R,P} \), and this allows us to write

\[
I_2 = -\frac{\Delta \mu}{4} \frac{(G_{P,R} - G_{R,P})(G_{P,R} + G_{P,L})}{\mathcal{N}}
= -\frac{\Delta \mu}{4} (G_{P,R} - G_{R,P}).
\] (5.33)

Combining \( \Delta I = I_1 + I_2 \), we reach

\[
\Delta I = -\frac{\Delta \mu}{4} (G_{P,R} - G_{R,P} - G_{L,P} + G_{P,L})
= -\frac{\Delta \mu}{4} \left( \sum_{\nu \neq P} G_{P,\nu} - \sum_{\nu \neq P} G_{\nu,P} \right)
\] (5.34)

which is identically zero given the conductance conservation (5.8). It is trivial to note that no rectification takes place in the linear response regime, \( \mathcal{R} = 0 \).
5.4 Beyond linear response: spatially symmetric setups

In this section we consider the role of inelastic effects on the current symmetry in an AB interferometer, beyond the linear response regime. The probe condition $I_P = 0$ translates Eq. (2.21) into three relations,

$$
\int d\omega (\mathcal{T}_{P,L} + \mathcal{T}_{P,R}) f_P(\phi) = \int d\omega (\mathcal{T}_{L,P} f_L + \mathcal{T}_{R,P} f_R)
$$

$$
\int d\omega (\mathcal{T}_{L,P} + \mathcal{T}_{R,P}) f_P(-\phi) = \int d\omega (\mathcal{T}_{P,L} f_L + \mathcal{T}_{P,R} f_R)
$$

$$
\int d\omega (\mathcal{T}_{P,L} + \mathcal{T}_{P,R}) \bar{f}_P(\phi) = \int d\omega (\mathcal{T}_{L,P} f_R + \mathcal{T}_{R,P} f_L).
$$

(5.35)

First, we consider the situation when time reversal symmetry is protected, with the magnetic phase given by multiples of $2\pi$. Then, $\mathcal{T}_{\nu,\xi} = \mathcal{T}_{\xi,\nu}$, and particularly we note that $\mathcal{T}_{L,P} = \mathcal{T}_{P,L}$. Furthermore, in the model considered in Sec. 5.5, $\mathcal{T}_{P,L} = \chi \mathcal{T}_{P,R}$, with $\chi$ as an energy independent parameter, reflecting spatial asymmetry, see for example the discussion around Eq. (5.45). Using the voltage probe condition (5.35) we find that

$$
\int (\mathcal{T}_{P,L} + \mathcal{T}_{P,R})(f_P(\phi) + \bar{f}_P(\phi))d\omega = \int (\mathcal{T}_{P,L} + \mathcal{T}_{P,R})(f_L + f_R)d\omega,
$$

(5.36)

Given the linear relation between $\mathcal{T}_{L,P}$ and $\mathcal{T}_{R,P}$, this equality holds separately for each transmission function,

$$
\int \mathcal{T}_{\nu,\nu}(f_P(\phi) + \bar{f}_P(\phi))d\omega = \int \mathcal{T}_{\nu,\nu}(f_L + f_R)d\omega \quad \nu = L, R,
$$

(5.37)

providing $\mathcal{R} = 0$ in Eq. (5.12). Thus, if $\mathcal{T}_{P,L} = \mathcal{T}_{L,P} = \chi \mathcal{T}_{P,R}$, rectification is absent. In physical terms, the junction conducts symmetrically for forward and reversed direction, though many body effects are presented, if we satisfy two conditions: (i) Spatial asymmetry is included in an energy-independent manner, for example using different broad-band
hybridization parameters at the two ends. (ii) Time reversal symmetry is protected.

We now derive symmetry relations for left-right symmetric systems with broken time-reversal symmetry. In this case the mirror symmetry $T_{P,L}(\phi) = T_{P,R}(-\phi)$ applies, translating to

$$T_{P,L}(\phi) = T_{R,P}(\phi). \tag{5.38}$$

When used in Eq. (5.35), we note that the distributions should obey

$$\bar{f}_P(\phi) = f_P(-\phi), \tag{5.39}$$

leading to $\bar{\mu}_P(\phi) = \mu_P(-\phi)$. We emphasize that $\mu_P(\phi)$ itself does not posses a phase symmetry.

Since the leakage of charge into the probe is prohibited, the deviation from phase rigidity, Eq. (5.10), can be also expressed in terms of the current $I_R$, to provide (note the sign convention)

$$\Delta I(\phi) = \frac{1}{2} \int d\omega [(T_{L,R} - T_{R,L})f_L - T_{R,P}f_P(-\phi) + T_{P,R}f_P(\phi)]. \tag{5.40}$$

We define $\Delta I$ by the average of Eqs. (5.10) and (5.40),

$$\Delta I(\phi) = \frac{1}{4} \int d\omega \left[(T_{L,R} - T_{R,L})(f_L + f_R) + (T_{L,P} - T_{R,P})f_P(-\phi) + (T_{P,R} - T_{P,L})f_P(\phi) \right].$$

We proceed and make use of two relations: $T_{L,R} - T_{R,L} = T_{P,L} - T_{L,P}$, and Eq (5.38), valid in geometrically symmetric junctions. With this at hand we write

$$\Delta I(\phi) = \frac{1}{4} \int (T_{P,L} - T_{P,R})(f_L + f_R - f_P(\phi) - \bar{f}_P(\phi))d\omega = R(\phi) = -R(-\phi), \tag{5.41}$$
This concludes our derivation of the MF symmetries,

$$\Delta I(\phi) = R(\phi) = -R(-\phi), \quad D(\phi) = D(-\phi). \tag{5.42}$$

In spatially symmetric systems odd conductance terms acquire even symmetry with respect to the magnetic field, as noted experimentally [39, 107], while even conductance terms, constructing $R$, are odd with respect to $\phi$. This result was also obtained analytically in a two-terminal AB interferometer, when strong electron-electron interactions were taken into account in the quantum dot, beyond the mean-field approach [113]. The relation $\Delta I(\phi) = R(\phi)$ could be exploited in experimental studies: One could determine whether a quantum dot junction is $L$-$R$ symmetric by testing this equality.

We now emphasize the following points: (i) Eq. (5.42) does not hold when a spatial asymmetry is introduced, by coupling the scattering centers unevenly to the leads. (ii) The derivation of Eq. (5.42) does not assume a particular form for the density of states of either the $L$ and $R$ leads, or the probe reservoir, as long as Eq. (5.38) is satisfied. (iii) The symmetry relations obtained here are valid under the more restrictive (non-dissipative) voltage-temperature probe, Eq. (2.30). (iv) The analysis in this section reveals sufficient conditions for charge rectification for structurally symmetric junctions: $R(\phi) \neq 0$ when time-reversal symmetry is broken, $\phi \neq 2\pi n$, and inelastic scatterings (effective anharmonicity) are allowed.

### 5.5 Beyond linear response: model II

In this section we demonstrate our analytical results. We adopt a double-dot AB model with a probe coupled to dot ‘1’, see Fig. 2.2, to allow for inelastic effects. The Hamilto-
nian has the following form,

\[ H = H_{AB} + \sum_{p \in P} \omega_p a_p^\dagger a_p + \sum_{p \in P} \lambda_p a_1^\dagger a_p + h.c. \]  

(5.43)

We voltage-bias the system, \( \Delta \mu \equiv \mu_L - \mu_R \), with \( \mu_{L,R} \) as the chemical potential of the metals, and use the convention that a positive current is flowing left-to-right. While we bias the system in a symmetric manner, \( \mu_L = -\mu_R \), this choice does not limit the generality of our discussion since the dots may be gated away from the so-called “symmetric point” at which \( \mu_L - \epsilon_\beta = \epsilon_\beta - \mu_R \).

### 5.5.1 Transmission functions

Our model does not include interacting particles, thus its steady-state characteristics can be written exactly using the nonequilibrium Green’s function approach [116, 117]. In terms of the Green’s function, the transmission coefficient is defined as

\[
T_{\nu,\xi} = \text{Tr} [\Gamma^\nu G^+ \Gamma^\xi G^-],
\]  

(5.44)

where the trace is performed over the states of the subsystem (dots). In our model the matrix \( G^+ \) (\( G^- = [G^+]^\dagger \)) takes the form

\[
G^+ = \begin{bmatrix}
\omega - \epsilon_1 + \frac{i(\gamma_L + \gamma_R + \gamma_D)}{2} & \frac{i\gamma_L}{2} e^{i\phi/2} + \frac{i\gamma_R}{2} e^{-i\phi/2} \\
\frac{i\gamma_L}{2} e^{-i\phi/2} + \frac{i\gamma_R}{2} e^{i\phi/2} & \omega - \epsilon_2 + \frac{i(\gamma_L + \gamma_R)}{2}
\end{bmatrix}^{-1},
\]
with the hybridization matrices satisfying
\[
\begin{align*}
\Gamma^L &= \gamma_L \begin{bmatrix} 1 & e^{i\phi/2} \\ e^{-i\phi/2} & 1 \end{bmatrix}, \\
\Gamma^R &= \gamma_R \begin{bmatrix} 1 & e^{-i\phi/2} \\ e^{i\phi/2} & 1 \end{bmatrix} \\
\Gamma^P &= \gamma_P \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}
\end{align*}
\]
\hspace{1cm} (5.45)

The coupling energy between the dots and leads is given by
\[
\gamma_\nu(\epsilon) = 2\pi \sum_{j \in \nu} |v_j|^2 \delta(\omega - \omega_j).
\hspace{1cm} (5.46)
\]

In the wide-band limit adopted in this work \(\gamma_\nu\) are taken as energy independent parameters. We now assume that the dots are energy-degenerate, \(\epsilon_d \equiv \epsilon_1 = \epsilon_2\), but allow for a spatial asymmetry in the form \(\gamma_L \neq \gamma_R\). The transmission functions are given by
\[
\begin{align*}
T_{L,R}(\omega, \phi) &= \frac{\gamma_L \gamma_R}{\Delta(\omega, \phi)} \left[4(\omega - \epsilon_d)^2 \cos^2 \frac{\phi}{2} + \frac{\gamma_P^2}{4} + \gamma_P(\epsilon_d - \omega) \sin \phi \right] \\
T_{L,P}(\omega, \phi) &= \frac{\gamma_L \gamma_P}{\Delta(\omega, \phi)} \left[(\omega - \epsilon_d)^2 + \frac{\gamma_R^2}{4} \sin^2 \frac{\phi}{2} + \gamma_R(\omega - \epsilon_d) \sin \phi \right] \\
T_{R,P}(\omega, \phi) &= \frac{\gamma_R \gamma_P}{\Delta(\omega, \phi)} \left[(\omega - \epsilon_d)^2 + \frac{\gamma_L^2}{4} \sin^2 \frac{\phi}{2} - \gamma_L(\omega - \epsilon_d) \sin \phi \right]
\end{align*}
\hspace{1cm} (5.47)
\]

with the denominator an even function of \(\phi\),
\[
\Delta(\omega, \phi) = \left[ (\omega - \epsilon_d)^2 - \gamma_L \gamma_R \sin^2 \frac{\phi}{2} - \frac{(\gamma_L + \gamma_R)\gamma_P}{4} \right]^2 \\
+ \left( \gamma_L + \gamma_R + \frac{\gamma_P}{2} \right)^2 (\omega - \epsilon_d)^2.
\hspace{1cm} (5.48)
It is trivial to confirm that in the absence of the probe, an even symmetry of the current with $\phi$ is satisfied, beyond linear response [27].

\[
I_L(\phi) = \int d\omega \frac{4\gamma_L\gamma_R(\omega - \epsilon_d)^2 \cos^2 \frac{\phi}{2} [f_L(\omega) - f_R(\omega)]}{[(\omega - \epsilon_d)^2 - \gamma_L\gamma_R \sin^2 \frac{\phi}{2}]^2 + (\gamma_L + \gamma_R)^2(\omega - \epsilon_d)^2}
\]

With the probe, inspecting the transmission functions in conjunction with Eq. (5.27), we immediately conclude that under spatial asymmetries the probe chemical potential does not obey a particular symmetry, even in linear response when phase rigidity is trivially obeyed, see Sec. 5.3.2. We now discuss the properties of the probe when the interferometer is $L$-$R$ symmetric, $\gamma/2 = \gamma_L = \gamma_R$. The transmission functions satisfy $T_{R,P}(\omega, \phi) = T_{P,L}(\omega, \phi)$. We substitute these expressions into Eq. (5.14) and resolve the distribution of a dephasing probe [115].

\[
f^D_P(\omega, \phi) = \frac{f_L(\omega) + f_R(\omega)}{2} + \frac{\gamma(\omega - \epsilon_d) \sin \phi}{4[(\omega - \epsilon_d)^2 + \omega_0^2]} [f_L(\omega) - f_R(\omega)]
\]  

(5.49)

with $\omega_0 = \frac{\gamma}{2} \sin \frac{\phi}{2}$. The nonequilibrium term in this distribution is odd in the magnetic flux. Similarly, when a voltage probe ($V$) is implemented, analytic results can be obtained in the linear response regime,

\[
\mu^V_P(\phi) = \Delta \mu \sin \phi \frac{\int d\omega \frac{\partial f_a}{\partial \omega} \frac{\gamma(\omega - \epsilon_d)}{\Delta(\omega, \phi)}}{\int d\omega \frac{\partial f_a}{\partial \omega} \frac{2(\omega - \epsilon_d)^2 + \frac{1}{2} \gamma^2 \sin^2 \frac{\phi}{2}}{\Delta(\omega, \phi)}}.
\]  

(5.50)

Here $f_a$ stands for the equilibrium (zero bias) Fermi-Dirac function. This chemical potential is an odd function of the magnetic flux, though phase rigidity is maintained in the linear response regime.
5.5.2 Generalized magnetic field-gate voltage symmetries

The MF symmetry relations (5.42) are not respected when the spatial mirror symmetry is broken. Instead, in Sec 5.6.5 we prove that in a generic model for a double-dot interferometer susceptible to inelastic effects the following result holds

\[ \mathcal{R} = -\mathcal{C}(\mathcal{R}), \quad \mathcal{D} = \mathcal{C}(\mathcal{D}). \]  

(5.51)

Here \( \mathcal{C} \) stands for the charge conjugation operator, transforming electrons to holes and vice versa. In terms of the parameters of our AB interferometer model, this relation reduces to the following magnetic flux-gate voltage (MFGV) symmetries,

\[ \mathcal{R}(\epsilon_d, \phi) = -\mathcal{R}(-\epsilon_d, -\phi), \]
\[ \mathcal{D}(\epsilon_d, \phi) = \mathcal{D}(-\epsilon_d, -\phi). \]  

(5.52)

Since the energies of the dots can be modulated with a gate voltage [109], these generalized symmetries can be examined experimentally.

5.6 Numerical simulations

Using numerical simulations we demonstrate the behaviour of the voltage and the voltage-temperature probes far from equilibrium, and the implications on phase rigidity and magnetic field symmetries.

5.6.1 Probe parameters

We consider the model Eq. (2.1) and implement inelastic effects with the dissipative voltage probe, by solving the probe condition (2.25) numerically-iteratively, using Eq. (2.27), to obtain \( \mu_P \). We also investigate the transport behaviour of the model under
the more restrictive dissipationless voltage-temperature probe, by solving Eq. (2.31) to obtain both $\mu_P$ and $T_P$.

![Figure 5.1](image)

Figure 5.1: Self-consistent parameters of the voltage probe (full) and the voltage-temperature probe (dashed), displaying disparate behaviour far from equilibrium: (a) Probe chemical potential, (b) temperature. We also show (c) the magnitude of net charge current from the probe and (d) net heat current from the conductor towards the probe. The interferometer consists two degenerate levels with $\epsilon_{1,2} = 0.15$ coupled evenly to the metal leads $\gamma_{L,R} = 0.05$. Other parameters are $\gamma_P = 0.1$, $\phi = 0$, and $T_L = T_R = 0.1$. The probe temperature is set at $T_P = 0.1$ in the calculations of the voltage probe. Reproduced from Ref. [125].

Fig. 5.1 displays the self-consistent probe parameters $\mu_P$ and $T_P$ for $\phi = 0$ when heat dissipation is allowed at the probe (full line), and when neither heat dissipation nor charge leakage take place within $P$ (dashed line). We find that the probe parameters largely vary depending on the probe condition, particularly at high biases when significant heat dissipation can take place [panel (d)]. We also verify that when Newton-Raphson iterations converge, the charge current to the probe is negligible, $|I_P/I_L| < 10^{-12}$. Similarly, the heat current in the voltage-temperature probe is negligible once convergence is reached.

Uniqueness of the parameters of the voltage and temperature probes has been recently proved in Ref. [78]. We complement this analytical analysis and demonstrate that the parameters of the voltage-temperature probe are insensitive to the initial conditions adopted, see Fig. 5.2. Convergence has been typically achieved with $\sim 5$ iterations.
While the voltage probe had easily converged even at large biases, we could not manage to converge the voltage-temperature probe parameters at large biases $\Delta \mu > 1$ and low temperatures $T_{L,R} < 1/50$ since eliminating heat dissipation within the probe requires extreme values, leading to numerical divergences within the model parameters adopted.

### 5.6.2 Nonlinear transport with dissipative inelastic effects

In this subsection we examine the nonlinear transport behaviour of an AB interferometer coupled to a voltage probe. In Fig. 5.3 (a) we display the measure $\Delta I$ as a function of bias for a spatially symmetric system using two representative phases, $\phi = \pi/2$ and $\pi/4$. We confirm numerically that in the linear response regime $\Delta I = 0$. More generally, the relation $\Delta I = R$ is satisfied for all biases, as expected from Eq. (5.42). Our conclusions are intact when an “up-down” asymmetry is implemented in the form $\epsilon_1 \neq \epsilon_2$ [128]. The corresponding chemical potential of the probe is shown in Fig. 5.3(b)-(c) for $\phi = \pi/4$. In the linear response regime it grows linearly with $\Delta \mu$ and it obeys an odd symmetry relation, $\mu_P(\phi) = -\mu_P(-\phi)$. Beyond linear response $\mu_P$ does not follow neither an even
Figure 5.3: (a) MF symmetry and rectification in spatially symmetric junctions. (b) Chemical potential of the probe in the linear response regime. (c) Chemical potential of the probe beyond linear response. The junction’s parameters are $\epsilon_1 = \epsilon_2 = 0.15$, $\gamma_P = 0.1$, $\beta_a = 50$ and $\gamma_L = \gamma_R = 0.05$. Reproduced from [125].

Figure 5.4: Breakdown of the MF symmetry relations for spatially asymmetric junctions, $\gamma_L = 0.05 \neq \gamma_R = 0.2$. (a)-(b) $\Delta I$ (dashed) and $R$ (square) for $\phi = \pi/4$ and $\pi/2$. The corresponding probe potential is displayed in panel (c) for $\phi = \pm \pi/4$ and in panel (d) for $\phi = \pm \pi/2$. Other parameters are $\epsilon_1 = \epsilon_2 = 0.15$, $\gamma_P = 0.1$ and $\beta_a = 50$. Reproduced from Ref. [125].
nor an odd phase symmetry, but at large enough biases it is independent of the sign of the phase.

Fig. 5.4 displays results when spatial asymmetry in the form $\gamma_L \neq \gamma_R$ is implemented. Here we observe that $\Delta I \neq R$, and that the probe chemical potential does not satisfy an odd symmetry with the magnetic phase, even in the linear response regime.

As the breakdown of the MF symmetries (5.42) occurs under a spatial asymmetry in the presence of inelastic effects, we study next the role of $\gamma_P$, $\Delta \gamma \equiv \gamma_R - \gamma_L$ and the metals temperature $\beta_a$ on these relations.

In Fig. 5.5 (a)-(b) we extract $\mathcal{D}$, and present it along with $\mathcal{R}$ as a function of $\Delta \gamma$. We note that the symmetry of $\mathcal{R}$ is easily broken with small spatial asymmetry, while $\mathcal{D}$ is more robust. The role of the coupling strength $\gamma_P$ is considered in Fig. 5.6. First, in spatially symmetric systems we confirm again that the MF relations (5.42) are satisfied, and we note that as $\gamma_P$ increases, the variation of $\mathcal{D}$ and $\mathcal{R}$ with phase is fading out. Quite interestingly, the rectification contribution $\mathcal{R}$ may flip sign with $\gamma_P$, for a range of phases. (The sign of $\mathcal{R}$ reflects whether the total current has a larger magnitude in the forward or backward bias polarity). Second, when a spatial asymmetry is introduced
we note a strong breakdown of the MF phase symmetry for $R$, while the coefficient $D$ still closely follows the MF symmetry [39]. Interestingly, with increasing $\gamma_P$ the variation of $D$ with phase is washed out (panel d), but even conductance terms show a stronger alteration with $\phi$ (panel c). Thus, even and odd conductance terms respond distinctively to decoherring and inelastic processes.

In Fig. 5.7 we consider the role of the reservoirs temperatures on the conductance coefficients. With increasing temperature a monotonic erosion of the amplitude of all conductance terms with phase takes place. This should be contrasted to the non-monotonic role of $\gamma_P$ on $R$, as exposed in Fig. 5.6.

Inspecting e.g., Fig. 5.7 we point out that in our construction $R(\phi = 0) = 0$, even in the presence of geometrical asymmetry, see discussion following Eq. (5.37). We recall that many body effects are presented here effectively, thus this observation is not trivial given the common expectation that the combination of many body interactions and spatial asymmetry should bring in the current rectification effect [44]. Indeed, extended models in which the system is connected to the reservoirs indirectly, through “linker” states,
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Figure 5.7: Temperature dependence of even and odd conductance terms. (a)-(b) Spatially symmetric system, $\gamma_L = \gamma_R = 0.05$. (c)-(d) Spatially asymmetric system, $\gamma_L = 0.05 \neq \gamma_R = 0.2$. In all panels $\beta_a = 50$ (dots), $\beta_a = 10$ (dashed line) and $\beta_a = 5$ (dashed-dotted line). The light dotted lines mark symmetry lines. Other parameters are $\Delta \mu = 0.4$, $\gamma_P = 0.1$ and $\epsilon_1 = \epsilon_2 = 0.15$. Reproduced from Ref. [125].

Figure 5.8: MF symmetries at the symmetric point $\epsilon_d = \epsilon_1 = \epsilon_2 = 0$. (a) Even $R$ (b) odd $D$ conductance terms for spatially symmetric $\gamma_L = \gamma_R = 0.05$ (dots) and asymmetric situations $\gamma_L = 0.05$, $\gamma_R = 0.2$ (dashed lines). Other parameters are $\Delta \mu = 0.4$, $\gamma_P = 0.1$ and $\beta_a = 50$. Reproduced from Ref. [125].
Figure 5.9: (a)-(b) Chemical potential of the probe at the symmetric point, for spatially symmetric $\gamma_L = \gamma_R = 0.05$ (circles), and asymmetric $\gamma_L = 0.05 \neq \gamma_R = 0.2$ cases (dots). (a) Bias dependence of $\mu_P$. The lines contain the overlapping $\phi = \pm \pi/4$ results. (b) Magnetic flux dependency of $\mu_P$ for $\Delta \mu = 0.4$. Other parameters are $\beta_a = 50$ and $\gamma_P = 0.1$. Reproduced from Ref. [125].

present rectification even at zero magnetic field, as long as both spatial asymmetry and inelastic effects are introduced [76].

### 5.6.3 Symmetries of nonlinear heat transport

In this section we study symmetry relations of the electronic heat current under nonzero magnetic flux and a temperature bias $T_L \neq T_R$, in the absence of a potential bias, $\mu_a = \mu_L = \mu_R = \mu_P$. Using the temperature probe (2.28), we demand that heat dissipation at the probe vanishes, $Q_P = 0$, but allow for charge leakage in the probe. We now express the $L$ to $R$ heat current $Q_{\Delta T} \equiv Q_L = -Q_R$ in powers of the temperature bias as

$$Q_{\Delta T}(\phi) = K_1(\phi)\Delta T + K_2(\phi)(\Delta T)^2 + K_3(\phi)(\Delta T)^3 + \ldots,$$

where $K_{n>1}$ are the nonlinear conductance coefficients. These coefficients depend on the junction parameters: energy, hybridization and possibly the temperature $T_a = (T_L + T_R)/2$. We define next symmetry measures for the heat current $Q_{\Delta T}$, parallel to Eqs.
First, we collect even conductance terms into $R_{\Delta T}$,

$$R_{\Delta T}(\phi) \equiv \frac{1}{2}[Q(\phi) + \bar{Q}(\phi)]$$

$$= K_2(\phi)(\Delta T)^2 + K_4(\phi)(\Delta T)^4 + ...$$

$$= \int \frac{T_{P,L} - T_{P,R}}{4} (f_L + f_R - f_P(\phi) - \bar{f}_P(\phi))(\omega - \mu_a) d\omega$$

(5.53)

Here $\bar{Q}$ is defined as the heat current obtained upon interchanging the temperatures of the $L$ and $R$ terminals. We also study the behaviour of odd conductance terms,

$$D_{\Delta T}(\phi) \equiv K_1(\phi)\Delta T + K_3(\phi)(\Delta T)^3 + ...$$

(5.54)

In the absence of the probe and in the linear response limit the heat current satisfies an even phase symmetry,

$$Q_{\Delta T}(\phi) = Q_{\Delta T}(-\phi).$$

(5.55)

Deviations from this symmetry are collected into the measure

$$\Delta Q_{\Delta T} = \frac{1}{2}[Q_{\Delta T}(\phi) - Q_{\Delta T}(-\phi)]$$

$$= \frac{1}{2} \int [T_{L,R} - T_{R,L}] (\omega - \mu_a) f_R d\omega$$

$$+ \frac{1}{2} \int [T_{L,P} f_P(-\phi) - T_{P,L} f_P(\phi)] (\omega - \mu_a) d\omega.$$  

(5.56)

*Linear response regime*. We repeat the derivation of Sec. 5.3, and find that in the linear response regime, $\delta T_\nu/T_a \ll 1$, $T_L = T_a + \delta T_L$, $T_R = T_a + \delta T_R$, the probe temperature $T_P = T_a + \delta T_P$ obeys

$$\delta T_P(\phi) = \frac{\int d\omega \left( -\frac{\partial f_a}{\partial \omega} \right) \frac{(\omega - \mu_a)^2}{T_a} (\delta T_L T_{L,P} + \delta T_R T_{R,P})}{\int d\omega \left( -\frac{\partial f_a}{\partial \omega} \right) \frac{(\omega - \mu_a)^2}{T_a} (T_{P,L} + T_{P,R})}$$

(5.57)
Using this relation, one can readily repeat the steps in Sec. 5.3 and prove that $\mathcal{R}_{\Delta T} = 0$, thus $Q_{\Delta T}(\phi) = D_{\Delta T}(\phi) = Q_{\Delta T}(-\phi)$.

**Symmetry relations far from equilibrium:** We discuss here symmetry relations for spatially symmetric junctions. We adapt the temperature probe condition (2.28) to three situations. First, the standard expression is given by

\[
\int d\omega (T_{P,L} + T_{P,R}) f_P(\phi)(\omega - \mu_a) = \int d\omega (T_{L,P} f_L + T_{R,P} f_R)(\omega - \mu_a). \tag{5.58}
\]

We reverse the magnetic phase and get

\[
\int d\omega (T_{L,P} + T_{R,P}) f_P(-\phi)(\omega - \mu_a) = \int d\omega (T_{P,L} f_R + T_{P,R} f_L)(\omega - \mu_a). \tag{5.59}
\]

Similarly, when interchanging the temperatures $T_L$ and $T_R$ we look for the probe distribution $\tilde{f}_P$ which satisfies

\[
\int d\omega (T_{P,L} + T_{P,R}) \tilde{f}_P(\phi)(\omega - \mu_a) = \int d\omega (T_{L,P} f_R + T_{R,P} f_L)(\omega - \mu_a). \tag{5.60}
\]

Note that $f_P(\phi)$, $f_P(-\phi)$ and $\tilde{f}_P(\phi)$ are required to follow a Fermi-Dirac form. The temperature $\beta_P$ should be obtained so as to satisfy the probe condition. If the junction is left-right symmetric, the mirror symmetry $T_{P,L}(\phi) = T_{R,P}(\phi)$ applies. We use this relation in Eqs. (5.59) and (5.60) and conclude that the probe distribution obeys,

\[
\tilde{f}_P(\phi) = f_P(-\phi). \tag{5.61}
\]
This directly implies that ($\mu_a = \mu_L = \mu_R = \mu_P$)

\[ \bar{\beta}_P(\phi) = \beta_P(-\phi). \] (5.62)

Note that $\beta_P(\phi)$ does not need to obey any particular magnetic phase symmetry. The deviation from phase rigidity, Eq. (5.56), can be expressed using the heat current flowing into the $R$ terminal,

\[ \Delta Q_{\Delta T} = \frac{1}{2} \int \left[ (\omega - \mu_a)([T_{L,R} - T_{R,L}]f_L \\
- T_{R,P}f_P(-\phi) + T_{P,R}f_P(\phi)) \right] d\omega. \] (5.63)

We define $\Delta Q_{\Delta T}$ as the average of Eqs. (5.56) and (5.63),

\[ \Delta Q_{\Delta T} = \frac{1}{4} \int d\omega (\omega - \mu_a) \left[ (T_{L,R} - T_{R,L})(f_L + f_R) \\
+ (T_{L,P} - T_{R,P})f_P(-\phi) + (T_{P,R} - T_{P,L})f_P(\phi) \right]. \]

Using the identities $T_{L,R} - T_{R,L} = T_{P,L} - T_{L,P}$ and $T_{P,L} = T_{R,P}$, the latter is valid in

Figure 5.10: Magnetic field symmetries of (a) even and (b) odd electronic heat conductance terms. Spatially symmetric system (dashed dotted), $\gamma_L = \gamma_R = 0.05$. Spatially asymmetric junction (dashed), $\gamma_L = 0.05 \neq \gamma_R = 0.2$. Light dotted lines represent the symmetry lines. Other parameters are $T_L = 0.15$, $T_R = 0.05$, $\epsilon_1 = \epsilon_2 = 0.15$, $\gamma_P = 0.1$, $\mu_a = \mu_L = \mu_R = \mu_P = 0$. Reproduced from Ref. [125].
geometrically symmetric junctions, we get

\[ \Delta Q_{\Delta T}(\phi) = \frac{1}{4} \int (T_{P,L} - T_{P,R})(f_L + f_R - f_P(\phi) - \bar{f}_P(\phi))(\omega - \mu_a)d\omega \]
\[ = R_{\Delta T}(\phi) = -R_{\Delta T}(-\phi). \]  

(5.64)

This concludes our derivation that under a temperature bias even (odd) heat conductance coefficients satisfy an odd (even) magnetic field symmetry,

\[ R_{\Delta T}(\phi) = -R_{\Delta T}(-\phi) = \Delta Q_{\Delta T}(\phi), \]
\[ \mathcal{D}_{\Delta T}(\phi) = \mathcal{D}_{\Delta T}(-\phi), \]  

(5.65)

as long as the junction acquires a spatial mirror symmetry. We adopt the double-dot model (2.1) presented in Sec. 5.5 and study its heat current behaviour. In the absence of the probe, assuming for simplicity degeneracy and spatial symmetry, \( \gamma/2 = \gamma_{L,R} \), we obtain

\[ Q_L(\phi) = \int d\omega(\omega - \mu_a)\frac{\gamma^2(\omega - \epsilon_d)^2 \cos^2 \frac{\phi}{2}}{[(\omega - \epsilon_d)^2 - \frac{\gamma^2}{4} \sin^2 \frac{\phi}{2}]^2 + \gamma^2(\omega - \epsilon_d)^2}[f_L(\omega) - f_R(\omega)], \]

satisfying the Onsager symmetry. Fig. 5.10 displays the MF symmetries, and their violation. Deviations from phase symmetry for \( \mathcal{D}_{\Delta T} \) are small, of the order of \( 10^{-5} \).

5.6.4 Nonlinear transport with non-dissipative inelastic effects

The simulations presented throughout Figs. 5.3-5.9 were obtained under the voltage probe condition, thus heat dissipation takes place at the probe. In Fig. 5.11 we show that the breakup of the MF symmetries occurs in spatially asymmetric setups under the more restrictive voltage-temperature probe, when non-dissipative inelastic effects are allowed. We again note that the breakdown of the phase symmetry of \( \mathcal{D} \) is small, one
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Figure 5.11: Voltage-temperature probe. (a) $R$ and (b) $D$ in spatially symmetric case (dashed-dotted lines) $\gamma_{L,R} = 0.05$ and asymmetric setups (dashed lines) $\gamma_L = 0.05 \neq \gamma_R = 0.2$. $\beta_a = 10$, $\gamma_P = 0.1$, $\epsilon_{1,2} = 0.15$. Reproduced from Ref. [125].

order of magnitude below the variation in $R$.

5.6.5 Magnetic field-gate voltage symmetries

We derive the MFGV symmetry relations by considering a double-dot interferometer model which does not necessarily acquire a spatial symmetry. Given the Hamiltonian in Eq. (5.43), we introduce a charge conjugation operator $\mathcal{C}$ that acts to replace an electron by a hole [129],

\[
\mathcal{C}(\epsilon_d) = -\epsilon_d, \quad \mathcal{C}(\omega_k) = -\omega_k, \\
\mathcal{C}(v_{n,j}e^{i\phi_n}) = -v_{n,j}^*e^{-i\phi_n}, \quad \mathcal{C}(\langle a^\dagger a \rangle) = 1 - \langle a^\dagger a \rangle. \tag{5.66}
\]

Here $a^\dagger$ and $a$ are fermionic creation and annihilation operators, respectively. Note that in our model the transmission function satisfies $T(\omega, \epsilon_d, \phi) = T(-\omega, -\epsilon_d, -\phi)$, i.e. it is invariant under charge conjugation. First, we need to find what symmetries does the probe chemical potential obey. Our derivation below relies on the following identity for the Fermi function,

\[
f(\epsilon, \mu) = \left[ e^{\beta(\epsilon - \mu)} + 1 \right]^{-1} = 1 - f(\epsilon, -\mu). \tag{5.67}
\]
Since we use the convention \( \mu_L = -\mu_R \), we conclude that \( f_L(-\omega, \mu_L) = 1 - f_R(\omega, \mu_R) \). Next we omit the direct reference to the energy \( \omega \) within \( T \) and the Fermi functions. Also, we do not write the phase \( \phi \) in the transmission function, unless necessary to eliminate confusion. We now study the probe condition (5.35) as is, under reversed bias voltage, and under charge conjugation,

\[
\int d\omega (T_{P,L} + T_{P,R}) f_P(\mu_P(\epsilon_d, \phi, \mu_L, \mu_R)) = \int d\epsilon (T_{L,P} f_L + T_{R,P} f_R) 
\]

(5.68)

\[
\int d\omega (T_{P,L} + T_{P,R}) f_P(\mu_P(\epsilon_d, \phi, \mu_L, \mu_R)) = \int d\epsilon (T_{L,P} f_R + T_{R,P} f_L). 
\]

(5.69)

\[
\int d\omega (T_{P,L} + T_{P,R}) [1 - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R))] = \int d\omega (T_{L,P} [1 - f_R] + T_{R,P} [1 - f_L]) 
\]

(5.70)

For clarity, we explicitly noted the dependence of \( f_P \) on the chemical potential \( \mu_P \), itself obtained given the set of parameters \( \epsilon_d, \phi, \) and \( \mu_{L,R} \). Equation (5.70) now reduces to

\[
\int d\omega (T_{P,L} + T_{P,R}) f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R)) = \int d\omega (T_{L,P} f_R + T_{R,P} f_L). 
\]

(5.71)

Comparing it to Eq. (5.69) we immediately note that

\[
f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R)) = f_P(\mu_P(\epsilon_d, \phi, \mu_R, \mu_L)).
\]

This result should be compared to Eq. (5.39), valid for spatially symmetric systems. Since the three reservoirs \( L, R, P \) are maintained at the temperature \( T_a \), this relation implies that

\[
\mu_P(\epsilon_d, \phi, \mu_L, \mu_R) = -\mu_P(-\epsilon_d, -\phi, \mu_R, \mu_L). 
\]

(5.72)
We now utilize Eq. (5.72) and derive symmetry relations for $R$ and $D$. We recall the explicit expressions for these measures, see the definitions (5.11) and (5.13) in Sec. 5.2.

The charge-conjugated expressions satisfy

$$
\mathcal{C}(R) = \frac{1}{2} \int d\epsilon T_{p,l} \left\{ [1 - f_R] + [1 - f_L] - [1 - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R))] \\
- [1 - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_R, \mu_L))] \right\}
= -\frac{1}{2} \int d\epsilon T_{p,l} \left\{ f_R + f_L - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R)) - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_R, \mu_L)) \right\}
= -R
$$

(5.73)

The last equality is reached by using Eq. (5.72). Similarly, we obtain the symmetry of odd conductance terms as

$$
\mathcal{C}(D) = \frac{1}{2} \int d\epsilon \left\{ (T_{l,R} + T_{l,P} + T_{R,L})(1 - f_R - 1 + f_L) \\
- T_{p,l} [1 - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R)) - 1 + f_P(-\mu_P(-\epsilon_d, -\phi, \mu_R, \mu_L))] \right\}
= \frac{1}{2} \int d\epsilon \left\{ (T_{l,R} + T_{l,P} + T_{R,L})(f_L - f_R) \\
+ T_{p,l} [f_P(-\mu_P(-\epsilon_d, -\phi, \mu_L, \mu_R)) - f_P(-\mu_P(-\epsilon_d, -\phi, \mu_R, \mu_L))] \right\}
= D
$$

(5.74)

In the double-dot interferometer model these relations translate to the MFGV symmetries,

$$
\mathcal{R}(\epsilon_d, \phi) = -\mathcal{R}(-\epsilon_d, -\phi), \\
\mathcal{D}(\epsilon_d, \phi) = \mathcal{D}(-\epsilon_d, -\phi).
$$

(5.75)

In words, these relations show that even conductance terms flip sign when the magnetic flux is reversed and the gate is applied such that the dot energies $\epsilon_d$ switch position with respect to the equilibrium Fermi energy. Odd conductance terms are invariant under this
transformation. For compactness, the derivation above has been performed assuming 
\( \epsilon_d = \epsilon_1 = \epsilon_2 \). It is trivial to extend our results beyond degeneracy. The scan of the 
current with \( \epsilon_d = \epsilon_{1,2} \) is presented in Fig. 5.12. When \( \epsilon_d > \Delta \mu \), Onsager symmetry is 
practically respected since the linear response limit is practiced, providing \( \Delta I \sim R \sim 0 \). More significantly, this figure reveals the MFGV symmetry (5.52), valid irrespective 
of spatial asymmetries and many body (inelastic) effects. This symmetry immediately 
implies that at the so-called “symmetric point”, when \( \epsilon_d = 0 \) (set at the Fermi energy), 
\( R(\phi) \) is an odd function of the magnetic flux irrespective of spatial asymmetries. This 
behaviour is displayed in Fig. 5.8. We also note that at the symmetric point the probe 
chemical potential is identically zero (Fermi energy) in symmetric setups, and it satisfies 
\( \mu_P(\phi) = \mu_P(-\phi) \) far from equilibrium for setups with a broken inversion symmetry, see 
Fig. 5.9.

\[
\begin{array}{ll}
(a) & \text{(a)} \\
(b) & \text{(b)} \\
(c) & \text{(c)} \\
(d) & \text{(d)}
\end{array}
\]

Figure 5.12: Magnetic field–gate voltage (MFGV) symmetries. (a)-(b) Even and odd 
conductance terms for a spatially symmetric junction with \( \gamma_L = \gamma_R = 0.05 \). (c)-(d) 
Even and odd conductance terms for a spatially asymmetric system with \( \gamma_L = 0.05 \), 
\( \gamma_R = 0.2 \), demonstrating that \( R(\epsilon_d, \phi) = -R(-\epsilon_d, -\phi), D(\epsilon_d, \phi) = D(-\epsilon_d, -\phi) \). In all 
cases \( \phi = -\pi/4 \) (small dots) and \( \phi = \pi/4 \) (empty circle), \( \Delta \mu = 0.4, \gamma_P = 0.1 \) and 
\( \beta_a = 50 \). Reproduced from Ref. [125].
5.7 Relation of results to other treatments

Magnetic field symmetries of nonlinear transport were analyzed in several other papers by including electron-electron interactions at different levels: mean field, Coulomb blockade, Kondo limit [110, 111, 112, 113]. Particularly, in Ref. [110] and more recent studies [42] electron-electron interactions were taken into account by considering the nonlinear response of the electronic potential landscape in the conductor to the applied voltage. This is done by adopting scattering theory: The argument is that in a nonequilibrium situation the charge density in the conductor piles up in response to the applied voltage. The scattering matrix then becomes bias dependent through its dependence on the potential landscape in the conductor. Nonlinear conductance terms contain information about charge response in the system, effects that are non-even in the magnetic field, and this leads to deviations from Onsager’s reciprocity relation beyond linear response.

In our approach, we include interaction effects in the interior of the conductor within an alternative approach, the probe. We recall that this tool emulates (electron-electron, electron-phonon) interactions in the conductor as follows: First, we apply a bias and set the temperatures at the two boundaries, $\mu_\nu$, $\beta_\nu$. We then include many body effects at the conductor, e.g., inelastic effects, using a voltage probe, by demanding that the charge current towards it vanishes. This constraint sets the probe parameters $\mu_P$ and $\beta_P$, describing charge distribution at the interior of the device. With these statistical measures, chemical potentials and temperatures, we can calculate the charge current in the Landauer picture. Our calculations provide us with the self-consistent probe chemical potential, and this measure is generally neither even nor odd in the magnetic field, even in linear response. Fig. 5.4 indeed shows that $\mu_P$ depends on the applied bias and the magnetic flux, generally missing magnetic field symmetries. We can interpret the probe potential as the local-internal potential in the conductor. We highlight that in our approach we do not set it by hand. Rather, by setting boundary conditions for the $L$ and $R$ terminals, and by imposing the probe constraint, we find the probe potential as a
We now argue that our analysis here, based on the probe technique, has a comparable status to the treatment of Ref. [110], and related studies, which are based on the behaviour of the screening potential under bias. The screening potential is an electrostatics-theory property; it responds to interactions between microscopic degrees of freedom. Similarly, the probe potential is an effective statistical measure, describing the internal potential, enclosing effects of microscopic scattering processes in the conductor. Both the screening potential and the probe potential can be interpreted as the effects of many body interactions and while these measures are not necessarily equivalent, they both consistently incorporate effects beyond linear response: The screening potential is written as an expansion in voltage, the probe potential is determined self consistently, at arbitrarily large applied voltage.

In a recent study the wave-packet propagation in a top-down asymmetric Aharonov-Bohm ring has been studied numerically by using the nonlinear Schrödinger equation [130]. It has been shown that this Aharonov-Bohm ring can act as a diode even when it is mirror symmetric and that it satisfies symmetry relations identical to those in our work. Note that the inelastic voltage probe effectively introduces nonlinearity. In real systems such nonlinearities may occur due to interactions: $e$-$ph$, $e$-$e$ and interactions with other impurities.

Fluctuation theorems and full counting statistics of nonlinear heat transport in a three terminal system have been studied by means of a temperature probe in Ref. [131], extracting leading order nonlinear thermal conductance term. The main argument in this work is based on the assumption of separation of time scales; assuming that charge fluctuations in the probe are much slower compared to the electron relaxation in the probe, and the time-scales for transport in the conductor. Under this assumption, magnetic field symmetries of leading-order nonlinear thermal conductance coefficients were obtained, and the presence of an antisymmetric (under the reversal of magnetic field)
thermal conductance term has been demonstrated for a triple quantum dot Aharonov-Bohm interferometer. This work supports our general proof of symmetry relations for nonlinear heat transport, presented in Sec. 6.6.3.

We conclude this discussion by emphasizing that the derivation of symmetries beyond linear response should be eventually done beyond phenomenological approaches and mean field treatments, by adopting model Hamiltonians with genuine many body interactions [113], and by using exact quantum techniques [132]. This will be the focus of the next chapter.

5.8 Discussion

We have studied the role of elastic and inelastic scattering effects on magnetic field symmetries of nonlinear conductance terms using Büttiker’s probe technique. For spatially symmetric junctions we proved the validity of the MF symmetries for charge transport, $D(\phi) = D(-\phi)$ and $R(\phi) = -R(-\phi)$, though many body inelastic effects, introduced via the probe, are asymmetric in the magnetic flux. We demonstrated the breakdown of these MF symmetries when the junction has a left-right asymmetry, in the presence of inelastic effects. Using a double-dot AB interferometer model we showed that it respects more general MFGV symmetry relations, $R(\epsilon_d, \phi) = -R(-\epsilon_d, -\phi)$ and $D(\epsilon_d, \phi) = D(-\epsilon_d, -\phi)$.

We now recall that these sets of symmetries were derived only based on the symmetry of the probe distribution function $f_P$, upon reversal of the applied bias. Considering a conductor coupled to a voltage probe and placed under both an applied temperature bias and a voltage bias, we write the formal expansion $I_L = -I_R = \sum_{n,m} G_{n,m} \Delta\mu^n \Delta T^m$ and identify $R = \sum_{n+m=2k} G_{n,m} \Delta\mu^n \Delta T^m$, to contain even conductance terms, and the complementing term $D = \sum_{n+m \neq 2k} G_{n,m} \Delta\mu^n \Delta T^m$. Following the discussion of Secs. 5.4-5.5, we can immediately confirm the validity of the MF and the MFGV symmetries implying that e.g. $G_{1,1}(\phi) = -G_{1,1}(-\phi)$ for spatially symmetric setups.
The rectification effect, of fundamental and practical interest, is realized by combining many body interactions with a broken symmetry: broken spatial inversion symmetry or a broken time reversal symmetry. Rectifiers of the first type have been extensively investigated theoretically and experimentally, including electronic rectifiers, thermal rectifiers [44] and acoustic rectifiers [126]. In parallel, optical and spin rectifiers were designed based on a broken time reversal symmetry, recently realized e.g. by engineering parity-time meta-materials [127].

The model system investigated in Secs. 5.5-5.6, the double-dot AB interferometer, offers a feasible setup for devising rectifiers based on broken time reversal symmetry: We found that $R \neq 0$, when two conditions are simultaneously met: (i) the magnetic flux obeys $\phi \neq 2\pi n$, $n$ is an integer, (ii) and the probe introduces inelastic effects. However, when time reversal symmetry is maintained (when the flux obeys $\phi = 2n\pi$) our model does not bring about the rectification effect, even if the spatial mirror symmetry is broken. The technical reason is that in our minimal construction both dots are coupled to the $L$ and $R$ metals directly, with an energy independent hybridization constant. In extended models when the ring is coupled indirectly to the $L$ and $R$ metals, through a spacer state, geometrical rectification may develop even in the absence of the threading magnetic flux. It is of interest to verify the results of this work by adopting a microscopic model with genuine many body interactions [133, 121, 123], by modeling a quantum point contact [41, 43] or an equilibrated phonon bath, exchanging energy with the junction’s electronic degrees of freedom. This could be done by extending numerical and analytic studies, e.g., Refs. [101, 134, 25], to the nonlinear regime.

We conclude this work by highlighting potential applications of the probe technique to far-from-equilibrium situations. In the linear response regime this self-consistent tool has been proven extremely useful for investigating the ballistic to diffusive crossover in electron [70, 85] and phonon transport [87, 88, 89]. While explicit analytic results are missing beyond linear response, we have demonstrated here that one could still adopt
this approach far from equilibrium and infer general transport symmetries, by analyzing the properties of the probe. Our simulations confirm the stability of the self-consistent numerical approach to far-from-equilibrium scenarios, and its utility for exploring transport properties. As this technique is no longer limited to the linear response limit or to weak (probe-conductor) coupling problems, it is now possible to explore its predictions (e.g., the rectification behaviour) alongside quantum master equation approaches and other treatments incorporating genuine elastic dephasing and inelastic effects. Future studies will be devoted to the analysis of the thermoelectric effect under broken time reversal symmetry [35, 36, 73, 25, 42, 135, 136] in the far-from-equilibrium regime, and to the study of quantum transport, far from equilibrium, in networks with broken time reversal symmetry [137].
Chapter 6

Microscopic approach: model III

6.1 Introduction

In the previous chapter, we obtained symmetry relations of nonlinear transport using phenomenological probe models within the Landauer-Büttiker scattering formalism. We argued that the probes effectively emulate many body ineractions. Here we focus on model III, a double-dot interferometer capacitively coupled to an equilibrium or a nonequilibrium fermionic environment. This setup is related to Büttiker’s voltage probe; energy exchange processes are allowed, but particle leakage between the double-dot interferometer and the fermionic environment is blocked. The main objectives of our work here are (i) To study a genuine many body model and quantify magnetic field symmetries and magnetoasymmetries of nonlinear transport. (ii) To test the qualitative predictions of inelastic probe models studied in the previous chapter.

6.2 Model

The Hamiltonian of model III is written as

\[ H = H_{AB} + H_F + H_{\text{int}}. \]  

(6.1)
where $H_{AB}$ is the double-dot system, Eqs (2.1)-(2.4), $H_F$ represents a fermionic environment which consists of a single level coupled to two metallic leads, refer to Eq. (2.9) and Fig. 2.3, and $H_{int}$ is the interaction term between electrons in the double-dot and the fermionic environment, assuming the form

$$H_{int} = U n_p n_1.$$  \hspace{1cm} (6.2)

Here $n_p = c_p^\dagger c_p$, $n_1 = a_1^\dagger a_1$ are the number operators of a special level ($p$) in the fermionic environment and dot ‘1’ in the AB interferometer; $U$ is the charging energy. The coupling energy between the two dots (in the AB interferometer) and the leads can be absorbed into the hybridization energy,

$$\gamma_L = 2\pi \sum_l \xi_{\beta,l} \delta(\omega - \omega_l) \xi_{\beta',l}, \quad \gamma_R = 2\pi \sum_r \zeta_{\beta,r} \delta(\omega - \omega_r) \zeta_{\beta',r}.$$  \hspace{1cm} (6.3)

Note that in our simulations, described below, we set the parameters $\gamma_{\nu}$ and the electron density of states in the metals, assumed to be a constant up to a sharp cutoff. We again define the dot-reservoir hybridization energies for the fermionic environment system from Eq. (2.9),

$$\gamma_s = 2\pi \sum_{s=\pm} |g_s|^2 \delta(\omega - \omega_s).$$  \hspace{1cm} (6.4)

Here $s \in \pm$ represents left (+) and right (-) leads in the fermionic environment.

The main observable of interest in this work is the charge current $\langle I(t) \rangle$ flowing across the AB interferometer. We could separately simulate the currents at the $L$ and $R$ terminals, but we choose to directly compute the expectation value of the averaged current from a certain initial state up to the steady state limit. This measure satisfies certain symmetries in the transient regime, as we show in Sec. 6.3.2. Simulations are carried out using the numerically exact INFPI method. Our starting point is the formal
expression for the current,

\[ \langle I(t) \rangle = \text{Tr}[\rho \hat{I}] = \text{Tr}[\rho(0)e^{iHt}\hat{I}e^{-iHt}] \tag{6.5} \]

Here \( \rho \) is the total density matrix, and the trace is performed over all degrees of freedom (AB and FE). As an initial condition, we select for convenience a factorized initial state \( \rho(0) = \sigma_F(0) \otimes \sigma_{AB}(0) \) with \( \sigma_{AB} \) as the density matrix of the interferometer. We further assume that \( \sigma_{AB}(t = 0) = \sigma_S(0) \otimes \sigma_L \otimes \sigma_R \), with \( \sigma_S(0) \) as the reduced density matrix of the double-dot within the AB interferometer. The FE is similarly prepared in a factorized state with \( \sigma_F(0) = \sigma_p(0) \otimes \sigma_+ \otimes \sigma_- \). The four reservoirs \( \xi = L, R, \pm \) are all prepared in a grand canonical state with a given chemical potential and temperature,

\[ \rho_\xi = e^{-\beta_\xi (H_\xi - \mu_\xi N_\xi)}/\text{Tr}[e^{-\beta_\xi (H_\xi - \mu_\xi N_\xi)}] \].

In what follows we set all reservoirs at the same temperature \( \beta^{-1} \).

## 6.3 Numerical results

### 6.3.1 Charge current

The charge current in the interferometer, considering either an isolated case \((U = 0)\) or a dissipative case \((U = 0.1)\) is presented in Fig. 6.1. We confirm that the former, a fully coherent system, obeys phase rigidity, \( I(\phi) = I(-\phi) \), at all times. In contrast, when the AB setup is coupled to a FE, the transient current and the steady state value do not transparently expose any symmetry. This was indeed an early observation in several relates studies: many body effects generate an internal potential that is not necessarily phase symmetric, leading to the breakdown of linear response symmetries [110]. It can be seen from Fig. 6.1 that the current through the AB interferometer increases when the interferometer is capacitively coupled to a fermionic environment. This could be reasoned by noting that the capacitive coupling modifies the interference pattern. Due
Chapter 6. Microscopic approach: model III

to the Coulomb energy shift of the bare dot energies (within a perturbative language) the dots are not degenerate for nonzero $U$. Depending upon the position of dot levels relative to the fermi energy of the metallic leads, opposite trends may be observed. Before discussing the underlying magnetic field symmetries and magnetoasymmetries of transport coefficients, we present an example of the convergence analysis in panel (c). Here we display the current as a function of $\tau_c = \delta t N_s$ in the transient regime, and after steady state has been established. In both cases we confirm that results converge around $\tau_c \sim 1/\Delta \mu$. It should be noted that to approach the exact limit should control the time step and the memory size, concurrently. This is because if we only increase the memory length $\tau_c$ to infinity but maintain a fixed-finite timestep $\delta t$, the time discretization error (Trotter) will accumulate as we add more terms into the truncated IF, deviating from the exact limit. Thus, one should carefully monitor both the time-step and the memory size for achieving reliable results, as was noted in the related QUAPI method [138].

6.3.2 Magnetic field dependence of transport coefficients

We now explore the underlying symemtries of the current using the data of Fig. 6.1, by separating the current into its odd and even conductance terms. For the sake of convienence we present the symmetry measures,

$$\Delta I(\phi) \equiv \frac{1}{2}[I(\phi) - I(-\phi)],$$  \hspace{1cm} (6.6)

$$\mathcal{R}(\phi) \equiv \frac{1}{2}[I(\phi) + \bar{I}(\phi)],$$ \hspace{1cm} (6.7)

$$\mathcal{D}(\phi) \equiv \frac{1}{2}[I(\phi) - \bar{I}(\phi)],$$ \hspace{1cm} (6.8)

where $\bar{I}(\phi)$ is the current obtained upon interchanging the chemical potentials of the left-right leads in the double-dot AB interferometer. From the power series expansion of the current, Eq. (5.2), one can see that $\mathcal{R}(\mathcal{D})$ are even(odd) conductance terms. We
Figure 6.1: (a) Charge current in the AB interferometer. $U = 0$ with $\phi = \pm \pi/2$ (dot and circles, overlapping) and $U = 0.1$ with $\phi = \pi/2$ (dashed-dotted), $\phi = -\pi/2$ (dashed). (b) Zooming on the long time limit of the $U = 0.1$ case. (c) Confirming convergence for the $U = 0.1$ data set at short and long times. The different symbols correspond to different timesteps: $\delta t = 0.6$ (○), $\delta t = 1.0$ (□), and $\delta t = 1.2$ (+). The quantum dots in the AB interferometer are set at $\epsilon_{1,2} = 0.15$ and $\gamma_{L,R} = 0.05$. The FE is set at equilibrium ($\mu_F = 0$) with $\epsilon_p = -0.5$ and $\gamma_{\pm} = 0.2$. All reservoirs are prepared at low temperature with $\beta = 50$. Numerical parameters in (a)-(b) are $\delta t = 0.6$, $N_s = 4$ and $L_s = 120$. The bands extend between $D = \pm 1$. 
resolve these measures by studying the dynamics with a reversed bias.

In Fig. 6.2 we demonstrate that in a geometrically symmetric double-dot interferometer, $\gamma_L = \gamma_R$, the symmetries obtained in Eq. (5.42) are satisfied in both the transient and the steady state limit. Deviations from the relation (5.42) are small, $(R(\phi) + R(-\phi))/2R(\phi) \sim (1 + i) \times 10^{-6}$. Since the real and imaginary parts (the latter reflects computing errors) are of the same order, we conclude that deviations from the symmetry (5.42) originates from computing errors.

![Figure 6.2: Magnetic field symmetries of odd and even conductance terms in centrosymmetric junctions with $\gamma_{L,R} = 0.05$. We prove that (a)-(c) $R(\phi) = -R(-\phi) = \Delta I(\phi)$, and (d) $D(\phi) = D(-\phi)$, in both transient and steady state limit. $U = 0.1$ in all cases. Other parameters are the same as in Fig. 6.1.](image)

In Fig. 6.3 we present the magnetic flux dependence of $R(D)$ in the steady state limit, and in Fig. 6.4, we study the effect of a nonequilibrium fermionic environment ($\Delta \mu_F \neq 0$). Our main observations are:

- For a spatially symmetric double-dot AB interferometer ($\gamma_L = \gamma_R$), even conductance coefficients are antisymmetric under the reversal of magnetic flux, $R(\phi) = -R(-\phi)$, and odd conductance coefficients are symmetric, $D(\phi) = D(-\phi)$. For the
Figure 6.3: (a) $R(\phi)$ (b) $D(\phi)$, $U = 0.1$ in all cases. Centrosymmetric junctions (Red circles, $\gamma_L = \gamma_R = 0.05$) $R(\phi) = -R(-\phi)$, $D(\phi) = D(-\phi)$. Noncentrosymmetric junctions (black squares, $\gamma_L = 0.05 \neq \gamma_R = 0.2$). Other parameters are the same as in Fig. 6.1.

- The above symmetries of $R(D)$ are broken once the left-right asymmetry ($\gamma_L \neq \gamma_R$) is introduced in a double-dot interferometer. The symmetry breaking effect is pronounced in even coefficients, while the symmetries of odd coefficients are very weakly broken, see Fig. 6.3, panels (a)-(b) black squares.

- The previous observations qualitatively agree with the results obtained using B"uttiker’s probes. However, Fig. 6.3 (a) (black squares), shows a significant effect distinctive from B"uttiker’s probe prediction: In the case of a voltage probe, for a spatially asymmetric case, (Fig. 5.6 (c)), rectification does not occur at $\phi = 0$. However,
it is nonzero for the model III even when $\phi = 0$. Since the capacitive coupling alters the charge state of a double-dot system, it may induce an energy dependent asymmetry in the transmission, leading to the rectification of current.

![Graph showing magnetic field symmetries](image)

Figure 6.4: Magnetic field symmetries of even (a) and odd (b) coefficients for centrosymmetric junctions for equilibrium ($\Delta \mu_F = 0$) and nonequilibrium ($\Delta \mu_F \neq 0$) environment. We use $U = 0.1$ and $\phi = \pm \pi/2$. Other parameters are the same as in Fig. 6.1.

### 6.4 Discussion

We studied magnetic field symmetries of nonlinear transport using a numerically exact path integral technique. Our simulations are in a qualitative agreement with those of Büttiker’s voltage probe. There are three significant advantages for adopting INFPI over other numerical and analytical techniques, to the study of transport symmetries far-from-equilibrium. First, analytic considerations and numerical simulations suggest that the memory time scales as $\tau_c \sim 1/\Delta \mu$ [56, 57, 139, 138]. Thus, the method quickly converges
to the exact limit at large bias. Since we are specifically interested here in beyond-linearresponse situations, INFPI is perfectly suitable for the present situation. Second, our objective here is in testing magnetic field symmetries in nonlinear transport, rather than in studying particular features in the current-voltage curve. This task fits INFPI since it is a deterministic time propagation scheme. Thus, even if simulation results deviate from the exact limit to some extent, our conclusions are intact since $I(\phi)$ and $I(-\phi)$ deviate from the exact limit in an equivalent way. In contrast, methods that rely on stochastic sampling of diagrams may accumulate distinct errors in the evaluation of $I(\pm\phi)$, thus one may need to approach the exact limit for validating the symmetries (5.42). Finally, INFPI is a flexible tool. We can readily test the nonlinear symmetry relations in the class of models where the interacting part is given by the form $H_{int}$, Eq. (2.10). Future work will focus on the study of magnetotransport in other correlated models.
Chapter 7

Conclusions and future directions

7.1 Summary

In this thesis we studied the transient dynamics and steady state properties of a double-dot AB interferometer. In chapter 1, we introduced the physical realization of a parallel double-dot setup, and outlined the general motivations behind this work. Three models were introduced in chapter 2: (i) A double-dot interferometer with electron-electron interactions, (ii) the case with Büttiker probes, and (iii) a double-dot setup capacitively coupled to a fermionic environment. We also briefly presented the numerical and analytical techniques used in this work and discussed several open questions addressed in this thesis.

The steady state properties and the transient dynamics of the noninteracting double-dot interferometer were presented in chapter 3. Quantum Langevin equations were derived, we solved these equations using the Green’s functions method, and resolved an expression for the reduced density matrix in the steady state limit. We also followed the transient dynamics using an exact fermionic trace formula. Using these tools we exposed several non-trivial magnetic flux dependent effects: (i) flux dependent occupation difference at degeneracy, (ii) breakdown of phase localization away from the particle-hole
symmetric point, and (iii) non-trivial transient features in the coherence dynamics. We also studied the effect of temperature on the occupation difference.

We incorporated *quasi-elastic* dephasing effects in coherent dynamics using Büttiker’s dephasing probe, obtained analytical expressions for dot occupations, and exposed several magnetic flux dependent effects away from the symmetric point. For example we demonstrated the development of new coherent oscillatory patterns when dot energies are aligned with the Fermi energies of left/right leads. We also showed that at the symmetric point the dots occupations are independent of the magnetic flux.

We incorporated an electron-electron repulsion term in chapter 4. Using INFPI, we followed the transient dynamics of the reduced density matrix and charge current for small-intermediate Coulomb interaction strengths. The dynamics in the infinite $U$ limit was studied using quantum master equations revealing fundamental deviations from the finite $U$ case.

In chapter 5 we focused on magnetic field symmetries and magnetoasymmetries of nonlinear transport coefficients. We showed that Onsager symmetries are obeyed beyond the linear response when elastic dephasing effects are in place, irrespective of spatial asymmetries. We also proved the absence of the diode effect in this case. We introduced inelastic effects using Büttiker’s voltage probe, and showed that the Onsager symmetries are obeyed in the linear regime, though the probe chemical potential need not be an even function of the magnetic field. Using the voltage probe condition, exploiting the conservation of transmission probabilities, we analytically showed that for a mirror symmetric system, odd conductance terms (coefficients of odd powers in bias) are even in magnetic flux while even terms (coefficients of even powers in bias) are odd.

We demonstrated these results using a model of double-dot interferometer. We also proved that the same symmetries hold at the particle-hole symmetric point irrespective of spatial asymmetries. This analysis was also extended to describe a temperature and a voltage-temperature probe. Away from the particle-hole symmetric point, introducing
spatial asymmetries breaks the odd-even behaviour. We found that the symmetry breaking is more pronounced in even terms and the symmetries of odd terms are only weakly broken. We established that the double-dot interferometer can act as a diode when two conditions are met simultaneously: (i) many body effects are included, here in the form of inelastic scattering, and (ii) time reversal symmetry is broken.

In chapter 6, we studied the dynamics and the steady state behaviour of magnetic field symmetries and magnetoasymmetries in a double quantum dot interferometer capacitively coupled to a fermionic environment. Interestingly, we found that the results obtained using inelastic probes do hold in this case. Our conclusions remain intact even when the fermionic environment is driven out of equilibrium by applying a voltage bias.

7.2 Observations

We first focused on the dynamics and steady state behaviour of the reduced density matrix and the charge current in the noninteracting case and exposed the nontrivial interplay of magnetic flux, nonequilibrium effects and coherences:

- The occupations of the dots can be controlled by a magnetic flux away from the symmetric point, and strong modulations are observed when the dots’ energies are aligned with the fermi energy of the left/right leads. An abrupt jump in dot occupations is observed when the magnetic flux takes values $\phi = 0, 2\pi n$, where $n$ is an integer.

- The abrupt jump disappears at zero $T$ only when the dot levels are positioned far outside the bias window. Increasing the temperature, the jump reappears, indicating the broadening of the resonance. Hence we can conclude that the abrupt jump is a consequence of resonant tunneling.

- The energy degenerate and symmetrically coupled dots can have different occupations in the presence of magnetic flux ($\phi \neq 2\pi n$) when placed away from the
symmetric point. The development of occupation difference is a generic finite-bias effect, it disappears in the infinite bias limit when the transport is strictly unidirectional. Increasing the temperature gradually reduces the occupation difference, though it persists as long as the temperature is smaller than the system-bath hybridization energy.

- The phase localization effect occurs when (i) the dots are placed at the symmetric point, and (ii) in the infinite bias limit, when the dot levels are effectively at the center of the bias window.

Büttiker probes offer an elegant phenomenological tool to introduce dephasing in coherent transport. The dephasing probe condition allows one to compute the reduced density matrix analytically. This simple system offers an interesting insights into how a quasi-elastic dephasing affects the coherent transport. Considering the model of a double dot interferometer, where one of the dots is coupled to a dephasing probe, we found that away from the symmetric point the dot occupations can be controlled using a magnetic flux, even in the presence of dephasing sources. we exposed the following nontrivial effects:

- The abrupt jump observed in the occupation-flux behaviour disappears when dephasing effects are introduced.

- Away from the symmetric point, the occupations of the dots show flux dependent modulations.

- When the dot levels are tuned at the edge of bias window, we find that the dot which is coupled to a probe develops new types of coherent oscillations with magnetic flux. The above phenomenon persists as long as the coupling to a dephasing probe is smaller than the applied voltage bias.
The dynamics of the interacting case is simulated using INFPI, and we have rigorously established the utility of this method to study the long-time magnetic flux dependent dynamics. At low temperatures the method does not converge if the bias is much smaller than the strength of the Coulomb interaction. In the intermediate bias regime ($\Delta \mu > \Gamma$), and in weak-intermediate Coulomb interaction strengths ($U/\Gamma \sim 4$) the dynamics of coherences and charge current can be faithfully simulated. Our main findings are:

- The real part of the subsystem coherence $\Re(\sigma_{1,2})$ decays with magnetic flux dependent rate $\Gamma(1 \pm \cos(\phi/2))$ when $\phi \neq 2\pi n$, while the imaginary part of the coherence $\Im(\sigma_{1,2})$ settles to the steady state with a flux independent rate.

- The $\Re(\sigma_{1,2})$ is $4\pi$ periodic in magnetic flux and $\Im(\sigma_{1,2})$ is $2\pi$ periodic.

- Under a small-intermediate Coulomb interaction strengths ($U/\Gamma \sim 4$), qualitative characteristics of coherence dynamics are similar to the noninteracting case, while in the $U = \infty$ limit the the transient dynamics significantly deviates from the noninteracting case, and the phase-localization effect breaks down.

- At $\phi = \pi$ destructive interference nullifies the charge current in the steady state limit, irrespective of $U$ and temperature of the leads.

Magnetic field symmetries of nonlinear transport were studied using the probe techniques incorporating many body interactions. Our main findings are:

- Onsager symmetries are obeyed beyond linear response with quasi-elastic dephasing irrespective of spatial asymmetries.

- The quasi-elastic dephasing probe does not allow for the diode effects, though the time reversal symmetry and spatial symmetry are broken.

- Beyond linear response, inelastic interactions break the Onsager symmetries and hence the phase rigidity.
• Beyond the linear regime, the even conductance terms (coefficients of even bias powers) are odd under the reversal of magnetic flux, while the odd terms (coefficients of odd bias powers) are even if the setup is spatially and/or particle-hole symmetric. These symmetries are broken away from the symmetric point, when the spatial asymmetries are introduced.

• Our proof of symmetry relations for the mirror symmetric setups is general and we did not assume any particular system Hamiltonian.

• In spatially asymmetric systems, the symmetry breaking is pronounced in even conductance terms and the symmetries of odd terms are weakly broken.

• The double-dot interferometer acts as a diode when two conditions are simultaneously meet: (i) broken time reversal symmetry, and (ii) many body interactions included in the form of inelastic scattering.

We studied magnetic field symmetries of the double-dot Aharonov-Bohm interferometer capacitively coupled to a fermionic environment which may be out-of-equilibrium. We argued that this setup is analogous to the voltage probe introducing inelastic effects. Numerical results for the transient and steady state magnetic field symmetries were obtained using INFPI technique. We found that the observations derived from the voltage probe do remain intact, irrespective of whether the fermionic environment is in equilibrium or out-of-equilibrium.

7.3 Future work

Algorithmic improvements of INFPI: In this work we studied the transient dynamics of a double-dot system using numerically exact path integral algorithm. We treated the many body interaction term using the Hubbard Stratonovich (HS) transformation, the quartic interaction is decomposed into quadratic terms by introducing an auxillary spin variable
The main drawback of this procedure is that the time translation invariance of the influence functional is lost, and it must be updated at every iteration. Such a scheme is computationally expensive, limiting the practical applicability of the method. The HS transformation is unique if \( U\delta t < \pi \), where \( U \) is the strength of the electron-electron interaction and \( \delta t \) is the time step chosen. If \( U \) is very large, then the time step should be made very small, implying long simulation times.

INFPI technique without the HS transformation was theoretically formulated using the Hubbard basis in Ref. [56]. In this case the evaluation of the resulting trace is challenging since matrix elements of nonquadratic operators enter the calculation. Future efforts will be concentrated on resolving this issue so that one can study the dynamics in the \( U = \infty \) case and in the Kondo regime.

**Thermoelectricity.** Future research will focus on nonlinear thermoelectric transport in broken time reversal symmetric systems with many body interactions. Specifically, we will study how various scattering mechanisms affect the maximum power efficiency. This problem can be addressed using Büttiker’s probes. We will also attempt to modify exact path integral methods to incorporate electron-phonon interactions. Such an extension will be paramount for the study of thermoelectric transport in interacting systems, as much work is done either using phenomenology or within the perturbative Green’s function technique.

**The effect of spatial asymmetries on coherence dynamics.** In chapter 4 we focused on the dynamics of coherences in degenerate and symmetric junctions. In a future project we will focus on non-degenerate and spatially asymmetric systems, and study the effects of many body interactions. Results from exact numerical calculations will be compared to perturbative approaches.

**Noise and correlations.** It is of interest to compute current-current correlations and higher order cumulants in interacting quantum dot networks using INFPI, comparing the results with perturbative Keldysh techniques.
Though this is a formal conclusion of the thesis, it is just the beginning of a long and rich effort to understand nonequilibrium phenomena which makes our life interesting. It is not surprising that the understanding of nonequilibrium many body quantum phenomena is a daunting task, but what is rather astonishing is our ability to create simplified theoretical models to capture the essence of those effects.

I salute the imagination and ingenuity of Prof. Markus Büttiker who came up with the interesting and valuable probe technique. It is sad that Prof. Büttiker is no longer living with us, a huge intellectual loss for the field of quantum transport. Let him be in a peace, and we should keep his legacy to advance this field, so that it will be always full of excitement.
Bibliography


[113] J. S. Lim, D. Sanchez, and R. Lopez, Phys. Rev. B 81, 155323 (2010). Note that in this work the authors used a different convention for the current expansion with voltage, \( I = G_0 \Delta \mu + G_1 \Delta \mu^2 + \ldots \).


[162] Persistent currents exist in at thermal equilibrium due to the absence of time-reversal symmetry. In our work here we consider only net charge transport. However, since persistent currents are antisymmetric in the magnetic field, we could add them to the definition of $\mathcal{R}(\phi)$, and our observations would be still valid.
