Time-Dependent Photomodulation of a Single Atom Tungsten Tip Tunnelling Barrier

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Abstract

There has been much work on electron emission. It has lead to the concept of the photon and new electron sources for imaging such as electron microscopes and the first formulation of holographic reconstructions [1-6]. Analytical derivations are important to gain physical insight into the problem of developing better electron sources. However, to date, such formulations have suffered by a number of approximations that have masked important physics. In this thesis, a new approach is provided that solves the Schrödinger wave equation for photoemission from a single atom tungsten tip barrier or more generally, for photoemission from a Schottky triangular barrier potential, with or without image potential effects. We describe the system, then introduce the mathematical derivation. We conclude with the applications of the theory.
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“A few minutes ago every tree was excited, bowing to the roaring storm, waving, swirling, tossing their branches in glorious enthusiasm like worship. But though to the outer ear these trees are now silent, their songs never cease.”
John Muir

“Give us insights, not numbers.” Charles A. Coulson
1 Introduction

Electron field emission is an emission of electrons induced by strong electromagnetic fields. The emission is due to the strong electric fields at the surfaces of materials that could exist in all four phases of matter. Since there is no real magnetic potential, it is the electric field only that contributes to this phenomena. Historically, emission of electrons from a surface was discovered prior to the electron discovery of J.J Thompson et al. Thermal emission due to the heating of a material was fully described by the Richardson-Dushmann equations. However, of interest was the discovery of emission when the thermodynamic temperature approached zero. The term cold field emission was coined and it has the same meaning as electron field emission. In 1744, Winkler likely observed cold field emission when studying wire electrodes. The phenomena was fully characterized only after Einstein’s work proving electrons can be emitted by a photoeffect from inside metals and not surface-adsorbed gas molecules. It is understood that there is emission due to electrons being promoted to energies above the barrier confining them to the metal and also due to electrons quantum mechanically tunneling through these barriers. In 1928, Fowler and Nordheim used the Sommerfeld model of metals and transmission probabilities to derive the Fowler-Nordheim equation describing the tunneling effect of field emission. While the equation derived by Fowler and Nordheim is experimentally valid and powerful, there are limitations associated with it. For example, the equations are only valid for a time-independent field and they neglect a second linearly independent wave solution to the Schrödinger equation describing this phenomena. This solution is valid for certain cases and can be extended to time varying electric fields. The derivation is not valid for complex band structures and does not give the distribution of electron pulses generated by these varying electric fields. However, the largest limitation of the original solution is the fact that it is only valid for time-independent field tunneling phenomena. With the advent of femtosecond laser technology and with the need to image and characterize reactions on that time order and on the scale of electron wavelengths, a full characterization of the time-dependent tunneling phenomena must be found. This paper analytically solves for the time-dependent case given any general wavefunction solution for the time-independent case for a specific barrier profile. We then calculate the total wavefunction for the emitted electrons from band structure, in a way that is adaptable for complex band structures. From the total wavefunction we then show how we could find the electron pulse’s electric field which is important in interactions with samples for applications such as electron holography. Finally, we show how we could generally analytically solve various differential equations of the form of Schrödinger’s equation using the methodology derived in this paper.

We first start with demonstrating the importance of using field emission for imaging by considering its use in electron holography and femtosecond electron diffraction. We provide detailed descriptions of these phenomena so the reader can understand the usefulness of the equations derived in this paper and the relevance of knowing the total wavefunction of the system to important phenomena that can be studied. We also introduce the derivation of the Fowler-Nordheim equation so the reader can have an understanding of the background literature describing the phenomena.

1.1 Femtosecond Electron Diffraction

Femtosecond Electron Diffraction (FED) is a new technique that has many applications in ultrafast chemical reactions and structural phase transitions. Molecular movies or the ability to see in realtime how a chemical reaction proceeds and the pathway it takes is now feasible with this technology. In order to fully characterize a chemical reaction we need resolutions on the order of one angstrom and time resolutions on the order of one hundred femtoseconds. This is accomplished by optically inducing emission by a laser femtosecond pulse from a metallic planar surface. This induces photo-absorption and transmission of electrons above the workfunction as well as thermionic transmission and finally electron tunneling. Electron tunneling comprises of lower energy electrons that can be used to image delicate structures such as proteins and this is the regime of most interest to this paper. Thus, if the Schrödinger equation is solved for the case of a femtosecond light pulse interacting with the matter and geometrical configurations that we deal with, we could create better emission devices. It becomes of utmost importance to understand the wavefunction solution for these emitted electrons. As it stands, this field is based on experimental research using an intelligent trial and error heuristic and years of experience and has yielded amazing results. Emitter design is mostly governed by ray tracing and experimental data. With the exact mathematical description of the system we could perhaps make our methods more efficient and based on a more deterministic approach.
1.2 Electron Holography

To demonstrate the importance of understanding field emission microscopy we can consider the phenomena of electron holography. This section will briefly go over the important equations and points underlying the idea of electron holography. It is merely meant to introduce the topic.

A hologram is formed when the interference pattern of a diffracted wave from an object and a reference wave are recorded on a medium[4]. Since the phase and intensity at that position in space is recorded, the object can be reproduced again by exposure to the original reference wave[4]. The technique was demonstrated to work by Haine and Mulvey[5] with electron waves as well. Electron holography relies only on the diffraction pattern recorded between a diffracted electron wave (from the sample) and a reference wave. Thus, imaging in this way does not require the need for lenses. Since the resolution limit of electron microscopes is imposed by aberration in the magnetic lenses, this means that electron holography can break through the resolution limits of conventional electron microscopes. In analogy to optical holography, electron holography can be accomplished by the use of a coherent electron source. This can be accomplished by sharpening the tip of a Tungsten filament to the width of an atom and by cooling the system to 4 Kelvin.

Electrons are emitted from the tip of a sharp Tungsten needle through field emission[4]. Electrons then encounter a barrier (such as a sample molecule) and are scattered. For demonstration let us consider electrons scattering off of a point object. We assume a monochromatic plane wave. The scattered electron wave is[4] :

\[ \psi_{\text{scattered}} = \frac{f}{r} e^{i(kr-\omega t)} \]

Where, \( f \) is the scattered amplitude and \( r \) is the distance from the point in space to the object. The intensity of electrons hitting the screen is[4]:

\[ |\psi_{\text{incident}} + \psi_{\text{scattered}}|^2 = 1 + \left( \frac{f}{L} \right)^2 - \left( \frac{2f}{L} \right) \sin \left( \frac{k(x^2 + y^2)}{2L} \right) \]

Thus, the transmitted amplitude is[4]:

\[ T(x, y) = e^{ikz}[1 + \left( \frac{f}{L} \right)^2 + i(\frac{f}{L})e^{i\frac{k(x^2 + y^2)}{2L}} - i(\frac{f}{L})e^{-i\frac{k(x^2 + y^2)}{2L}}] \]

Where we have used the identity:

\[ i(\frac{f}{L})[e^{i\frac{k(x^2 + y^2)}{2L}} - e^{-i\frac{k(x^2 + y^2)}{2L}}] = 2(\frac{f}{L})\sin(\frac{-ik(x^2 + y^2)}{2L}) \]

The first two terms correspond to the transmittance of the incident wave and do not reveal any information of the object. The third term describes the scattering due to the point object and the last term is the conjugate image[4]. The third term is used to reconstruct the image by means of an inverse Fourier transform technique[4]. Due to the conjugate image the diffraction pattern on the screen describes an object imaged through both a concave and convex lens[4].

We can create in-line electron holograms. The incident wave is in-line with the direction of propagation of the diffracted wave. If the incident wave and diffracted waves are not propagating in the same direction, then the hologram produced is named an off-axis electron hologram[6]. With in-line holograms, the conjugate diffraction pattern is inseparable from the object diffraction pattern which creates an imaging error in the object image (the meshing of both images creates undesirable effects)[4]. However, when the diffraction patterns observed are those in the Fraunhofer regime, the effects of the conjugate image are substantially reduced. The Fraunhofer regime is defined when[4]:

\[ A^2 << L\lambda \]
Where A is the aperture radius, L is the distance from sample to screen and λ is the wavelength of the electron. Another region of interest is when \[4\]:

\[ A^2 > L\lambda \]

This is the Fresnel diffraction region and a phenomena called Fresnel fringes are observed around sharp edges in the object.

### 1.3 The Fowler-Nordheim Derivation

The Fowler-Nordheim equations offer a relation between the current density and energy of electrons tunneling across a flat planar surface at 0 Kelvin. The formulation assumes an electron gas within the metal and a tunneling potential surface defined as:

\[ V(z) = E_F + \xi - eF_0 z - \frac{e^2}{4z} \]

[7] where e is the exponential function, \( \xi \) is the work function measured from the fermi energy, \( F_0 \) is the DC electric field at the surface and \( z \) is the coordinate normal to the surface.

The emitted flux is normal to the surface and is found by considering the product of a supply function for the flux of electrons impinging on the barrier and the transmission probability \( T(E_z) \). The only component of energy that matters is the coordinate normal to the surface or the \( z \)-coordinate. From the WKB approximation, \( T(E_z) \) is calculated as [7]:

\[ T(E_z) = e^{-\int \frac{\xi^2}{2m} \frac{1}{2} (V(z) - E_z) \frac{1}{2} dz} \]

Considering the fact that the electrons are assumed to tunnel in a narrow range within \( E_F \) the transmission probability function becomes [7]:

\[ T(E_z) = T_o e^{\left[ \frac{1}{2} \frac{\xi^2}{2m} \frac{1}{2} \left( \frac{E_z - E_F}{E_F} \right) \right] \left( t(w) \right)} \]

with

\[ T_o = e^{-\frac{1}{2} \frac{\xi^2}{2m} \frac{1}{2} \left( \frac{E_z - E_F}{E_F} \right)} \]

\[ w \approx 3.8 F_0 \frac{\xi}{\phi} \]

\( v \) and \( t \) are parameters that are slowly varying, derived from elliptical integrals to take into account of the image forces during the tunneling process, and range from 0.4 to 0.8 for \( v \) and approximately 1 for \( t \)[7].

The tunneling current for a given function \( T(E_z) \) is [7]:

\[ J_t = \frac{2e}{\hbar^3} \int dp_y \int dp_z \int \frac{p_x}{m} T(E_z) f(p) dp_x \]

where \( f(p) \) is the fermi dirac distribution function:

\[ f(p) = \frac{1}{1 + e^{\frac{\left( \frac{p^2}{2m} \right) - E_F}{k_B T}}} \]

This approximately yields [7]:

3
This method is experimentally valid for flat microscopic surfaces. It is not valid for nano-scale surfaces with localised band structure effects [7]. The derivation in this paper seeks to establish a general equation for the time-dependent electric field case and for more complex band structures. Also, we derive a better method to replace the WKB approximation for the transmission coefficient. We establish a general wavefunction rather than a probability current, that can be computed from the wavefunction both directly and from the transmission amplitude formulation. The wavefunction holds all the quantum dynamical information about the system and thus it is of more use.
## 2 Coordinate System and Experimental Setup

### 2.1 Assumptions used in this paper

Amongst other assumptions stated later in the paper there are four main assumptions that the reader should be aware of from the onset:

1. All emission comes from a single atom at the tip. If this is not the case than there would be diffraction across the tunneling barrier from other atoms in the vicinity that are of the order of the wavelength of the tunneling electrons apart. The diffraction integral is shown and calculated in reference [7].

2. There is no photoabsorption due to the electromagnetic pulse. We assume only modulation of the potential function. Thus, we are working with regimes in the band structure that do not have a transition moment for the optical photons we are using.

3. There are no thermal heating effects due to the emission of the electrons or from the pulse of light. We assume that the material is close to 0 Kelvin and, thus, electron-phonon coupling is at a minimum.

4. The Fourier transform and the inverse Fourier transform for the laser pulse exists.

5. Finally we are considering an ideal system from the laboratory setup. The electron pulse is propagating in a complete vacuum with no other interfering potentials and there are no space-charge effects.

### 2.2 Coordinate System

In the x-y plane there is no electric E-field since it is assumed that the polarization is perpendicular to the propagation direction (the pulse is propagating in what is assumed to be free space or an isotropic material). Thus, the potential in the x, y coordinates is unperturbed by the electric field and looks like an infinite step function.
The work function, $V_o$, is measured from the lowest energy of the well, or the zero reference potential $V_o = E_F + \xi$, where $\xi$ is the work function measured from the Fermi energy. In the z-coordinate the potential is:

Here we assume that the electric field is not seen past the tunnelling barrier (where negative z is in region 1). For all coordinates, we define region 1 as the region before the tunnelling barrier and region 2 as after the tunnelling barrier.
3 Wave Solutions in Region 1 and Region 2

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved." Paul Dirac

There are only two regions of interest as defined above, since there is only one discontinuity defined to be at z,x,y=0 of the potential function.

Before we start the derivation it is integral to note that the barrier function we use is that of a sharp triangular well without the inclusion of image potentials in the z-coordinate. There are many approximate wavesolutions to the cases where there are image effects. These solutions can be substituted into the DC case instead of the known DC solutions that we have used and the derivation method used in the paper is still valid. Thus, our assumption that the well is sharp does not inherently take away from the methodology used to derive the time dependent wavefunction solutions and the power of the physics derived in this paper remains untouched. It is also interesting to know that for cold field emission, which is the case of most interest, the triangular barrier can be approximated as sharp[7]. However, we have analytically solved and found the general solution to the problem of the tunneling barrier being defined as that used in the Fowler-Nordheim equation and with the image potential. This is given in Appendix II and is a very powerful derivation as it has always been approximated before (as with the case of the time-dependent electric field).

Thus, assuming that there are Bloch wave solutions for region 1 (the electric field does not perturb the internal band structure of the material noticeably) and assuming that within an atom the envelope function, $U_k(r)$, varies slowly and can be taken as constant we obtain in region 1:

$$\psi_I(r,t) = (A e^{i\vec{k}.\vec{r}} + B e^{-i\vec{k}.\vec{r}}) e^{-i\frac{E_k}{\hbar}t}$$

where $k$ is the wave vector of the mode and $r$ is the position $(x,y,z)$. $A,B$ are constants.

**Please note the symbol * denotes multiplication for the rest of this paper. We use it to emphasize that two quantities are being multiplied.**

3.1 Separability of Solutions

First we show that the general Schrodinger equation for region 2 is separable to three equations, one for each coordinate.

First we state the general Schrodinger equation for a particle in region 2:

$$i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (3V_0 - e\theta(t)z)\psi$$

where $e$ is the elementary charge, $m$ is the mass of the electron and $\theta$ is the time dependent electric field. We assume that the electric field is slowly varying in space due to the extremely small size of the needle tip. Thus, across the needle tip it is only a function of time. We also assume that the pulse is so fast that it is finished when electrons reach distances where the electric field of the pulse seems to vary spatially. Also, if there is another polarization along the $y$ coordinate, the Schrodinger equation of this coordinate would look the same as that of the $z$-coordinate and the same treatment would be applied. The way we apply boundary conditions to the y-coordinate would also be the same as the z-coordinate (which is outlined in section 4.1.2). Thus, we do not assume polarization in the y-coordinate for this analysis, since it is redundant. If the field were propagating in an arbitrary direction, there would be time dependent fields in all coordinates:
\[ i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (3V_0 - e\theta_z(t)z - ex\theta_x(t) - ey\theta_y(t))\psi \]

and all equations would look like the equation derived below for the z-coordinate. In the treatment of boundary conditions (in section 4.1.2), again we would follow the same procedure as outlined for the z-coordinate. Thus, treating this case is also redundant. The factor of 3 next to the one dimensional work function arises because at every point in space, the electron would have to surmount the work function potential in each coordinate (in z direction it would be the combined potential of the electric field and the work function, which in this coordinate, the work function may also be a function of time. See section 5.4). Thus, each coordinate contributes the work function potential.

Assume a solution of the form:

\[ \psi(x, y, z, t) = \psi(x, t)\psi(y, t)\psi(z, t) = \psi_x\psi_y\psi_z \]

By substitution we obtain:

\[ i\hbar(\dot{\psi}_x\psi_y\dot{\psi}_z + \dot{\psi}_x\psi_y\psi_z + \psi_x\dot{\psi}_y\psi_z) = -\frac{\hbar^2}{2m} \nabla^2_x \psi_x\psi_y\psi_z - \frac{\hbar^2}{2m} \nabla^2_y \psi_x\psi_y\psi_z - \frac{\hbar^2}{2m} \nabla^2_z \psi_x\psi_y\psi_z + 3V_0\psi_x\psi_y\psi_z - ez\theta(t)\psi_x\psi_y\psi_z \]

We can separate the following equation to three equations:

\[ i\hbar(\dot{\psi}_x\psi_y\psi_z) = -\frac{\hbar^2}{2m} \nabla^2_x \psi_x\psi_y\psi_z + V_0\psi_x\psi_y\psi_z - ez\theta(t)\psi_x\psi_y\psi_z \]

which dividing out identical terms from the left hand side and right becomes:

\[ i\hbar(\dot{\psi}_z) = -\frac{\hbar^2}{2m} \nabla^2_z \psi_z + V_0\psi_z - ez\theta(t)\psi_z \]

which is the coordinate equation for the z-coordinate.

Similarly,

\[ i\hbar(\dot{\psi}_x) = -\frac{\hbar^2}{2m} \nabla^2_x \psi_x + V_0\psi_x \]

for the x-coordinate. And

\[ i\hbar(\dot{\psi}_y) = -\frac{\hbar^2}{2m} \nabla^2_y \psi_y + V_0\psi_y \]

for the y-coordinate.

The x and y coordinate equations have known solutions and are:

\[ \psi_x = C_{\alpha_x}e^{-\alpha_x x}e^{-i\frac{E_x}{\hbar}t} \]

Where,

\[ \alpha_x = [2m(V_0 - E_x)]^{1/2}/\hbar \]

and \( C_{\alpha_x} \) is a constant.

and,

\[ \psi_y = C_{\alpha_y}e^{-\alpha_y y}e^{-i\frac{E_y}{\hbar}t} \]

Where,

\[ \alpha_y = [2m(V_0 - E_y)]^{1/2}/\hbar \]
and $C_{\alpha\beta}$ is a constant.

$E_x, E_y$ are mode energies.

### 3.2 Wave Solution in Region 2 for the x,y Coordinates

To reiterate, for the x, y coordinates the solution in region 2 takes on the form of a decaying exponential, i.e.,

$$
\psi_{II}(\beta, t) = C_{\alpha\beta} e^{-\alpha\beta} e^{-iE_\beta t}
$$

$$
\alpha\beta = \left[2m(V_0 - E_\beta)\right]^{\frac{1}{2}} / \hbar
$$

where $\beta = x, y$ and $E$ is the mode energy. We can solve for the constant $C$ using continuity and boundary conditions. We can calculate the quantum limited beam width for a given mode energy (with no space charge effects) by finding the FWHM of this decaying exponential. In the absence of space charge effects this is found to be:

$$
\frac{|\ln(0.5)|}{\alpha}
$$

and we find that electrons at the edge of the beam waist have higher energies.

For energies greater than $V_o$ we use

$$
\psi_{II}(\beta, t) = C_{\alpha\beta} e^{-\alpha\beta} e^{-iE_\beta t}
$$

$$
\alpha\beta = \left[2m(V_0 - E_\beta)\right]^{\frac{1}{2}} / \hbar
$$

### 3.3 Wave Solution in Region 2 for the z Coordinate

#### 3.3.1 Solving for the Wavefunction

For this subsection the symbol $\psi$ refers to the wavefunction in the z-coordinate and $\nabla$, refers to differentiation with respect to (w.r.t) $z$.

To solve this problem we start by stating the electronic Schrödinger equation needed to be solved in this region for the z coordinate:

$$
i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_0 - e\theta(t)z)\psi
$$

(1)

where $e$ is the elementary charge, $m$ is the mass of the electron and $\theta(t)$ is the time dependent electric field. Sometimes $V_o$ is dependent on time. This does not change the general methodology on how we obtain solutions to this equation, please see section 5.4 for this case.

For a time independent (DC) electric field the above equation becomes,

$$
E\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_0 - e\theta z)\psi
$$

and whose general solution is known (triangular well solution):

$$
\psi = C_z Ai\left(\frac{2m}{\hbar^2} \left(\frac{1}{e\theta}\right)^\frac{3}{2} (V_0 - E - e\theta z)\right) + D_z Bi\left(\frac{2m}{\hbar^2} \left(\frac{1}{e\theta}\right)^\frac{3}{2} (V_0 - E - e\theta z)\right)
$$

where the constants precede the functions, Ai and Bi are the Airy functions [8]. In this section, $E$ means the energy contribution in the z direction for the given electron.
And,

\[ E_o = -E \]

So that this notation matches the definition of the Fourier transform shown below. This is notational to match the definition of the Fourier transform that we use in this paper.

We will now solve for the case when the potential is time dependent.

From Fourier analysis it follows straightforwardly that

\[ \psi(z, t) = \left( \frac{1}{2\pi\hbar} \right) \int_{-\infty}^{\infty} H(z, E_o) e^{i \frac{E_o t}{\hbar}} dE_o \]

(inverse Fourier transform) and

\[ H(z, E_o) = \int_{-\infty}^{\infty} \psi(z, t) e^{-i \frac{E_o t}{\hbar}} dt \]

(Fourier transform). Where \( H(z, E_o) \) is the Fourier amplitude at the given energy and spatial position. To clarify: Under the definition of the Fourier transform used, the Fourier amplitudes functions, \( H \) are the (spatial) wavefunctions for a given energy when \( E_o = -E \) where \( E \) is the given energy. Mathematically:

\[ \psi_{11}(E, z) = \int \psi_{11}(t, z) e^{-i \frac{E_o t}{\hbar}} dt \]

Or,

\[ \Lambda(z, E) = H(z, E_o) \]

Where \( \Lambda \) is the energy representation of the wavefunction. From now on the indefinite integral symbol will imply infinite limits of integration unless otherwise stated.

We know from Fourier transform theory that:

\[ \dot{\psi} = \left( \frac{1}{2\pi\hbar} \right) \int h(z, E) e^{i \frac{E t}{\hbar}} dE_o \]

where

\[ h(z, E_o) = i \frac{E_o}{\hbar} H(z, E_o). \]

(Property 1)

Therefore:

\[ h(z, E_o) = i \frac{E_o}{\hbar} \int \psi(z, t) e^{-i \frac{E_o t}{\hbar}} dt \]

Since \( h \) is the amplitude at \( E_o \), \( h \) is the quantum amplitude at an energy \( E \). There is no simple solution by just taking the Fourier transform of Eq. 1 and finding solutions for each Fourier amplitude. This is because of the mixed term of the electric field and wavefunction. Instead we apply a different set of mathematical tricks. First we state the Fourier transform of Eq. 1:

\[ -E_o H(z, E_o) = -\frac{\hbar^2}{2m} \nabla^2 H(z, E_o) + V_o H(z, E_o) - e z \int \psi(z, t) \theta(t) e^{-i \frac{E_o t}{\hbar}} dt \]  

(2)
\[ \nabla^2 H(z, E_o) \] is obtained by using the Liebnitz integral rule (we show this more in detail a few lines below). We proceed by assuming that
\[ H(z, E_o) = \int_{-\infty}^{\infty} g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt \]
where,
\[ -E_o g_{E_o}(z, t) = -\frac{\hbar^2}{2m} \nabla^2 g_{E_o}(z, t) + V_o g_{E_o}(z, t) - ezg_{E_o}(z, t)\Phi(t) \]
and \( 2\pi\Phi(-t) = \theta(t) \). Also, \( g_{E_o}(z, t) \) is a unique function per frequency. The need for using \( 2\pi\hbar\Phi(-t) = \theta(t) \) may seem bizarre but the reason will be apparent soon.

The solution to this second order differential equation is:
\[ g_{E_o}(z, t) = F_{E_o} Ai\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}(\frac{1}{e\Phi(t)})^{\frac{1}{2}}(V_o + E_o - e\Phi(t)z) + Q_{E_o} Bi\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}(\frac{1}{e\Phi(t)})^{\frac{1}{2}}(V_o + E_o - e\Phi(t)z) \]
where \( F \) and \( Q \) are constants or functions that could depend on the integration variable “\( t \)” and that depend on initial conditions (we shall come back to this) and are dependent on (functions of) \( E_o \). In fact, to insure a general solution for \( H(z, E_o) \), \( F \) and \( Q \) are composed of a function solely dependent on \( E_o \) (to satisfy the general solution to Eq. 2) multiplied by a function that could depend on both \( E_o \) and \( t \) (to satisfy the requirements of a general solution to Eq. 3).

We then proceed to prove that this assumption yields a trial solution that satisfies Eq. 1. we take the Fourier transform of Eq. 3 to obtain:
\[ -E_o H(z, E_o) = -E_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt = -\frac{\hbar^2}{2m} \int \nabla^2 g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt + V_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt - ez \int g_{E_o}(z, t)\Phi(t)e^{-i \frac{E_o}{\hbar} t} dt \]
Which is the same as:
\[ -E_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt = -\frac{\hbar^2}{2m} \int \nabla^2 (g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t}) dt + V_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt - ez \int g_{E_o}(z, t)\Phi(t)e^{-i \frac{E_o}{\hbar} t} dt \]
Thus, becoming:
\[ -E_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt = -\frac{\hbar^2}{2m} \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt + V_o \int g_{E_o}(z, t)e^{-i \frac{E_o}{\hbar} t} dt - ez \int g_{E_o}(z, t)\Phi(t)e^{-i \frac{E_o}{\hbar} t} dt \]
Since derivatives can be taken out of integrals from the Liebnitz integral rule (and the limits are not functions of the variable of the derivative-in this case not a function at all).

If we proceed by applying the inverse Fourier transform to Eq. 2 it equates to Eq. 1. Therefore, since the left hand side of Eq. 4 equates to that of Eq. 2 if we apply the inverse Fourier transform to the right side of Eq. 4 and it equates to Eq. 1 our assumption yields a working trial solution for the wave function. Thus, we have found a set of solutions to the differential equation Eq. 1. and consequently, we have found a set of solutions to Eq. 2.

By manipulation of \( F_{E_o}(t) \), \( Q_{E_o}(t) \), if we create a set of linearly independent solutions for Eq. 2, due to the fact that Eq. 2 is a second order ordinary differential equation and by the uniqueness theorem, we have found a general solution to Eq. 2. Applying the inverse Fourier transform to these solutions would give us a solution to Eq. 1. If the solutions are again linearly independent we obtain a physically relevant general solution for Eq. 1 under specified boundary conditions for Eq. 2 for each \( E_o \). This is because all physically relevant solutions to Eq. 1 are related to those of Eq. 2 by the corresponding Fourier transform, the maximum dimensionality in the basis set of physically relevant linearly independent solutions to Eq. 1 under specified boundary conditions is that of Eq. 2 which is 2 (see discussion in section 3.3.3 for proper meaning of physically relevant). Therefore, we
have to choose \( F_{E_o}(t), Q_{E_o}(t) \), carefully. Note: we do not have to necessarily find sets of linearly independent solutions for Eq. 2. If it is obvious we can directly find a set of physically relevant linearly independent equations for Eq. 1. We apply the just stated procedure to verify if we have indeed found the physically relevant general solution to Eq. 1:

Again, from Eq. 4 we obtain:

\[
-E_o \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} (t-t')} dt = -\frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt + V_o \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt - ez \int g_{E_o}(z,t) \Phi(t) e^{-i \frac{E_o}{\pi} t} dt
\]

From the convolution theorem we obtain:

\[
-E_o \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt = -\frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt + V_o \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt - ez \int G_{E_o}(E_o - E') \ast \tilde{\Phi}(E') dE'
\]

where \( G_{E_o}(E') \), \( \tilde{\Phi}(E') \) are the Fourier transforms of the respective functions. Please note that \( G_{E_o}(E') \) is really also a function of \( z G_{E_o}(E', z) \) but this is irrelevant for the analysis (for a given \( z \) all the mathematical tricks and identities hold true). It is just notationally easier to write it this way.

Applying the inverse Fourier transform to this equation yields:

\[
\frac{1}{2\pi\hbar} \int \int E_o g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} (t-t')} dtdE_o = -\frac{1}{2\pi\hbar} \frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt dE_o + \frac{1}{2\pi\hbar} V_o \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} t} dt dE_o - \frac{1}{2\pi\hbar} ez \int G_{E_o}(E_o - E') \ast \tilde{\Phi}(E') e^{i \frac{E_o}{\pi} (t')} dE'dE_o
\]

(5)

where \( t' \) is the time variable.

The last term of the equation gives:

\[
\frac{1}{2\pi\hbar} \int \int G_{E_o}(E_o - E') \ast \tilde{\Phi}(E') e^{i \frac{E_o}{\pi} (t')} dE'dE_o = \int \psi(t', z) e^{-i \frac{E_o}{\pi} t'} \ast \tilde{\Phi}(E') dE' = \psi(t', z) \ast 2\pi\hbar \Phi(-t') = \psi(t', z) \ast \theta(t')
\]

We have used the identity that \( \psi(t', z) = \frac{1}{2\pi\hbar} \int G_{E_o}(E_o)e^{i E_o (t')} dE_o \) as defined and the shift property of the Fourier transform.

Noting that: \( \psi(t', z) = \frac{1}{2\pi\hbar} \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} (t-t')} dt dE_o = \frac{1}{2\pi\hbar} \int G_{E_o}(E_o)e^{i E_o (t')} dE_o \) and after substituting this and

\( \dot{\psi}(t', z) = \frac{1}{2\pi\hbar} \int \frac{d}{dt} E_o g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} (t-t')} dt dE_o \) (property 1) into Eq. 5, the right and the left hand side of Eq. 5 are the same as Eq. 1. Thus, applying an inverse Fourier transform on Eq. 4 yields Eq. 1, verifying that we have found the general solution.

Note: \( t' = t \) (time) is used in Eq. 1. Do not confuse with the \( t \) in the above derivation used as a dummy variable. In other words, Eq. 5 is:

\[
i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_o - e\theta(t)z)\psi
\]

And,

\[
\psi(t', z) = \frac{1}{2\pi\hbar} \int g_{E_o}(z,t) e^{-i \frac{E_o}{\pi} (t-t')} dt dE_o
\]

which can be integrated numerically.

Now, we see the two linearly independent solutions to Eq. 1, forming the general solution: \( g_{E_o} \) is composed of two linearly independent functions and if we separate them out in the above double integral so we have a summation of two double integrals we notice that while the integrands themselves are linearly independent it could be that the integrals are not. However, if we choose \( F_{E_o}(t), Q_{E_o}(t) \) as constants dependent only on \( E_o \) we then come up with a set of two linearly independent functions for Eq. 2. This is because any Fourier integral of the Ai and Bi functions alone yields corresponding functions that are linearly
We have thus succeeded in finding the physically relevant general solution, given the type of boundary conditions seen in this and other physics problems to the z-coordinate wave equation. We proceed to obtain the specific overall wave function for region 2 by finding the specific solution after we apply boundary conditions. The set of boundary conditions we use is defined per $E_o$ and thus gives the exact specific wavefunction, which is composed of up to two linearly independent solutions.

### 3.3.2 Characteristics of the Solution

Even though the potential is changing due to the added energy of the laser pulse in time, it does not smear out energy components. If there is one single energy component (amplitude) inputted in region 2, there is only a component (amplitude) for that same energy in region 2. The system cannot produce energy (frequency) components that are not in the input and it is a linear time invariant (LTI) system and can be fully characterised by an impulse response function. Therefore, from the impulse response, one can find the transfer function. This can be an easy way to find the output wavefunction in region 2. However, in the next section we solve boundary conditions algebraically. This may contradict classical claims that the system feels an external force and should account for this added energy as a function of time. Thus, smearing energy components. However, since we included this in the potential function in the Schrodinger equation, we account for this implicitly and the system becomes defined as the laser pulse and the Tungsten tip. Thus, there is no external force.

If there were only one energy component wavefunction in region 1, due to boundary conditions the functions $Q_{E_o}, F_{E_o}$ would be specified as follows. At the boundary $z=0$, the incoming time Fourier amplitude matches the time Fourier amplitude of region 2 and the spatial derivatives match as well (see section 4.1.2 for a more detailed description of this).

$$\left( \int \psi_I(z,t)e^{-i\frac{E_o-E}{\hbar}(t)} dt \right)_{z=0} = \int (Ae^{ikt} + Be^{ik't})e^{-i\frac{E_o-E}{\hbar}(t)} dt = A\delta(E_o - E^o) + B\delta(E_o - E^o)$$

where the delta function appears due to the fact that $\psi_I(z,t)$ has only one energy (frequency) component. Here $E^o = -E$, where E is the energy in region 1. A, B are the quantum amplitudes for the single energy component in region 1.

$$Q_{E_o}, \alpha f(A,B)\delta(E_o - E^o), F_{E_o}, \alpha g(A,B)\delta(E_o - E^o)$$

where A, B are the wave amplitudes of the incoming wave. $\alpha$ means direct proportionality (without any loss of generality and for the sake of the example we can assume equality) and f and g are functions of the two wave amplitudes A, B (they are derived from the boundary conditions).

and

$$\psi_z(z', t') = \frac{1}{2\pi \hbar} \int \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}(t-t')} dt dE_o = \frac{1}{2\pi \hbar} G_{E_o}(E_o, z)e^{i\frac{E_o}{\hbar}}(t')$$

where $E_o = E^o$. Thus, the wavefunction is a single energy (frequency) output at the same energy as the input.

Similarly, if A and B are both zero it is easy to see that the wavefunction for that energy would be zero for all z. Therefore, if an input energy doesn’t exist, an output energy would not exist in region 2. This fact is important in section 4 when we realise that for certain values of momenta, we obtain this case.
### 3.3.3 On Uniqueness and Boundness

Sometimes it becomes apparent that the Airy Bi function can explode for some values of $t$ and can generate discontinuities in the Fourier integrals or can generate a solution to the overall wavefunction that is exploding (for values of $z$) and is thus unphysical. This depends on the electric field function and can be an issue when the electric field becomes repulsive or zero. We can, however, always attempt to fix this by choosing the coefficient function $Q_{E_o}(t)$ accordingly. This may not solve the problem because even with an appropriate choice of $Q_{E_o}(t)$ this may destroy the linear independence of the solutions. Thus, we omit the Airy Bi function in these instances due to the physical considerations. When we cannot take the Airy Bi function Fourier transform we are not losing any physically relevant solutions, see paragraphs below. In the lab, we generally have a large DC offset voltage. Thus, in general the electric field is not repulsive or zero and the Airy Bi functions do not pose a significant problem. For the rest of the paper we assume this. However, it is easy to factor the above mentioned fact into our calculations when the electric field has times when the integrals for the Airy Bi functions explode. As stated above we ignore this term.

The particular solution obtained from the Airy function is always bound in $z$ and differentiable w.r.t $z$, and there are also no point discontinuities. Thus, we always have a physical solution. Also, the particular solution obtained from the Airy Bi function is differentiable w.r.t $z$ at all instances (this is easily seen from differentiating under the integral signs).

Please also note that when the electric field is zero the nature of the Schrodinger equation changes, and at that time, $g_{E_o}$ is composed of a different set of functions than the Airy set. In fact, it is easy to see that it would be composed of decaying exponential functions, as in the case of semi-infinite square well. Thus, the time dependent wavefunction at a time when the electric field is zero is derived from a $g_{E_o}$ being composed of a set of decaying exponential functions.

The Airy Bi function causing discontinuities in the Fourier integrals is a problem because this means that we have only found one particular solution. However, the dimensionality of Eq. 1 for a particular set of boundary conditions exceeds this. This means there may be another particular solution of relevance. It is known in physics that any physically relevant solution must have a Fourier transform to the frequency (or $E_o$ domain). By the properties of the Fourier transform and its inverse, the solution in the frequency domain also has an inverse Fourier transform to the time domain (for a given $z$). Thus, any other solution to Eq. 1 must have a representation in the $E_o$ domain, relatable through Fourier transforms. Now, without loss of generality, we can always define a function $h_{E_o}(z,t)$ for the other solution in the frequency domain, that when the Fourier integral is applied to it (in the same manner as $g_{E_o}$) it equates to the value at a certain $E_o$ and varying $z$ for the other particular solution (this is because the function in the $E_o$ domain of this solution at a constant $E_o$ and varying $z$ can always be related to $h_{E_o}$ in this fashion due to the fact that the overall solution in the $E_o$ domain has a Fourier transform.) and $h_{E_o}(z,t)$ has an inverse Fourier transform. If we apply the reverse transforms to Eq. 1 as we applied to Eq. 4 in section 3.3.1 and we apply the definition of the function $h_{E_o}(z,t)$ we recover the same equation for it as the one that has $g_{E_o}$ as a solution. Thus for this case, we obtain:

$$-E_o h_{E_o}(z) = -\frac{\hbar^2}{2m} \nabla^2 h_{E_o}(z) + V_o h_{E_o}(z) - c\varepsilon h_{E_o}(z,t)\Phi(t)$$

$h_{E_o}(z,t)$ is the same set of solutions as $g_{E_o}$. Since all physically relevant solutions to the wavefunction are obtained from Fourier transforming solutions in the energy domain, the wavefunction would be the same analytic expression as derived in section 3.3.1 but with $g_{E_o}$ replaced by $h_{E_o}$. Since $g_{E_o}$ and $h_{E_o}$ are the same, all physically relevant solutions are contained in $g_{E_o}$ even when we omit the Airy Bi function.

Also, if the potential function has distinct regions in time, we have to use the set of solutions to that region for $g_{E_o}$, as the Schrodinger equation would be different for each temporal region. Thus, for values of $t'$ in those regions we use that $g_{E_o}$ in the integrals. Again we choose constants or functions that render the overall wavefunction solutions linearly independent (sometimes we can use the same constants in all regions for one particular solution). For example:

If $\theta(t)$ is composed of the form:

$$\begin{align*}
    t &< \beta \quad \theta(t) = 0, \text{ Region 1} \\
    \beta \leq t &\leq \eta \quad \theta(t) > 0 \text{ Region 2} \\
    t &> \beta \quad \theta(t) = 0 \text{ Region 3}
\end{align*}$$
then we would have spatially decaying exponential solutions for region 1 and region 3 and the set of solutions to region 2. There are no boundary conditions for the wave function in the temporal domain, (there could be sharp energy cut-offs, etc), thus, if there are no other physical constraints, we could use the same constants throughout as long as at the end we have a set of linearly independent solutions to Eq. 1 for all regions.

Finally, if we omit the Airy Bi function we actually have a simpler problem to solve. In section 4 we solve for the wavefunction with boundary conditions. From the assumption that electrons emitted are replenished instantly in the band structure and no photoabsorption takes place, the electrons at a certain energy stay constant, and the total amount of electrons in region 1 is a constant as well. Therefore, the probability of being in a certain coordinate energy state is conserved. It is shown in section 4 that the probability is equal to the sum of the quantum amplitudes squared of the momentum states in the plane waves of region 1. This equation and the two boundary condition equations yields 3 equations. Also, if we omit the Airy Bi function we have 3 unknowns. Therefore, we completely solve for all quantum amplitudes without any additional assumptions about the state of the system (we use these additional assumptions in section 4.3.2 where we solve the z-component wavefunction).
4 Wave Solutions with Applied Boundary conditions

The geometry of the needle is that of a rectangular 3-dimensional box with dimensions $a$, $b$, $c$ for coordinates $x,y,z$ respectively attached to a few atoms.

Thus, we assume plane waves in the $x$, $y$ coordinate, in the $z$ coordinate we use the derived wavefunction in section 3.3.1.

We start by using the Bloch momentum vectors and the fact that the bulk region size is big enough that one component momentum magnitude uniquely equates to one component energy state.

For this section we assume that the bulk properties of the band structure can be applied to region 1. This is because the atom at the tip is very small so the wave function effects of the tip are small. Intuitively, the wavefunction does not have time to vary much at the atom of the tip. Due to boundary conditions (and the tunnelling barrier between region 1 at the tip and the bulk being very small), the same constants apply to the plane wavefunctions entering region 1 from the bulk. Let $\chi$ be the length of region 1. Then:

at $\beta = x, y, z$,

$$\psi_\beta = Ae^{ik_\beta(\beta+\chi)} + Be^{-ik_\beta(\beta+\chi)}$$

after the barrier of region and region 2 at the atom tip. But since $\chi \approx 0$,

$$\psi_\beta = Ae^{ik_\beta(\beta)} + Be^{-ik_\beta(\beta)}$$

The same is true for the envelope functions, $U_k$ (equating to A and B) as stated in section 3.0. Thus, wavefunctions entering the tip can be assumed to conserve their quantum amplitudes (the A’s and B’s).

This approximation generates results that support experimental results, but does not explain observed small bumps added to the energy distributions of clean microscopic tips with adsorbed atoms in field emission experiments [7]. There is usually only a slight modification but it is clear that local geometries influence electron interactions within the material at the region and deform the band structure. This band structure modification can be measured experimentally and has been done for a W atom at the apex of a (001) pyramid of height equal to 4 atomic planes above the (001) surface[7].

Thus, to be more rigorous we use that density of states function. It is clear from experiment[7] that the modification of local band structure would be primarily due to electron mobilities being influenced in the $z$-direction (the coordinate normal the apex of the tip). Transverse components of the electron electric fields from layers below cancel out leaving only the normal components in the $z$-direction.

Thus, allowed states in the $z$-direction would be modified. If we still assume that a total energy corresponds to a sphere in $k$-space and that momentum states are uniformly spaced (see explanation in section below) than we could say the spacing of the momentum states in the $z$-direction is a function of total energy and this is how we would use the above density of states. The repetition number $D$ (defined below), is only influenced by momentum states in the $x$ and $y$ coordinates and thus, will not change (we could perhaps introduce a constant $\rho$ to account for experimental discrepancy in the $D$, but we don’t do this here). Using the D.O.S derived in section 4.1.5 (in this case the volume of the box is the volume of the atom and $H$, the height of the box, is the height in the $z$-direction of the atom), we obtain for the formula for the $z$-spacing:

$$\left(\frac{D.O.S(E_{total})}{\frac{H}{2\pi}}\right) \star \Delta k_z(E_{total}) = D.O.S_{exp}(E_{total})$$

becoming,

$$\Delta k_z(E_{total}) = \frac{H}{2\pi} \frac{D.O.S_{exp}(E_{total})}{D.O.S(E_{total})}$$
Where $D.O.S_{exp}$ is the density of states obtained for the localised band structure from experiment.

Similarly, there is band structure modification when there is an applied field. We assume this band modification is minimal and we don’t treat this effect. We only assume that the primary contribution of this to the system is the field enhancement built into the electric field function $\theta(t)$ in the Schrödinger equation. Within region 1, $\theta(t)$ would be based on the polarizability of the single atom tip and would essentially be equivalent to the electric displacement field. Please see section 4.2.2 for further discussion on this topic in which we factor in electric field effects in region 1, however for the next sections we do not assume any electric field or electric displacement field in region 1.

Even with the inclusion of section 4.2.2 where we discuss electric field effects in region 1 for single atom tips, the effect deserves more study and attention and this paper does not fully cover it in its analysis.

4.1 Total Wave Function in Region 2 with Boundary Conditions

After obtaining the solution of the wavefunction of the $z$-coordinate we now have the entire wave function in region 2 (where the particle is in region 2 for all coordinates, this is assumed to be the case for all electrons outside the needle due to the fact that the tip is very small. If this is not the case than, the original functions of region 1 for those coordinates, either $x$ or $y$, will apply):

\[
\psi_{II}(x,y,z,t) = \frac{1}{2\pi\hbar} \hat{C}_\alpha^x e^{-\alpha_x x} e^{i\frac{E_x}{\hbar}t} dE_x \frac{1}{2\pi\hbar} \hat{C}_\alpha^y e^{-\alpha_y y} e^{i\frac{E_y}{\hbar}t} dE_y \frac{1}{2\pi\hbar} \hat{C}_\alpha^z e^{i\frac{E_z}{\hbar}(t-t')} dt' dE_z
\]

(here we swapped the meaning of the variables $t$ and $t'$ from the last sections for aesthetic purposes). The values $E_x$, $E_y$, $E_z$ equate to the negative energies of the respective coordinates.

4.1.1 Applying boundary conditions to the solved wavefunction, in the $x$, $y$ coordinate

The continuity and boundary conditions between region 1 and region 2 yield:

\[
\psi_I(0,t) = \psi_{II}(0,t)
\]

\[
\nabla \psi_I(0,t) = \nabla \psi_{II}(0,t)
\]

In region 1

\[
\psi_I(x,y,z,t) = \int \frac{1}{2\pi\hbar} \int \frac{1}{2\pi\hbar} \int \frac{1}{2\pi\hbar} \int A_{k_x} A_{k_y} A_{k_z} e^{i\left(k_x x + k_y y + k_z z\right)} e^{i\frac{E_{total}}{\hbar} t} \delta(k_x^2 + k_y^2 + k_z^2 - E_{total}) dk_x dk_y dk_z dE_{total}
\]

where the integral is over constant energy spheres ($E_{total} = E_x + E_y + E_z = k_x^2 + k_y^2 + k_z^2$ is a constant). Usually, however, $E_{total} = f(k_x, k_y, k_z)$ where $f$ is a constant over spheres in k-space (i.e when factoring effective mass).

For the $x$ and $y$ coordinate, through continuity and boundary conditions [9] in region 2:

\[
C_{\alpha_x} = \frac{2ik_x}{(ik_x - \alpha_x)} A_{k_x}
\]

\[
C_{\alpha_y} = \frac{2ik_y}{(ik_y - \alpha_y)} A_{k_y}
\]

where $A$ is the amplitude value for positive $k_x, k_y$ (the incident waves). The negative and positive $x$ momenta (same is the case for the $y$-momenta) combine to give this.
Now, in region 1 we assume the electrons are in a box of defined dimensions. For the sake of simplicity we assume that in the x and y dimensions the length of the box is the same, which we label as L. The box is aligned such that its height is parallel to the z coordinate. This is the geometry of the Tungsten needle. Modes are spaced by \( \frac{2\pi}{H} \) in the x and y plane due to the Bloch wave theory. In the z direction modes are spaced by \( \frac{2\pi}{H} \) where H is the height of the box. When dealing with a localised band structure, H and L become the dimensions of the single atom tip, and the spacing factor in the z-direction is a function of total energy. In k-space each momentum mode at the given energy lies on a constant energy sphere. The constant energy sphere's radius, \( r \), equates to:

\[
r = \sqrt{E_{\text{total}}} = \sqrt{E_x + E_y + E_z}
\]

We assume here a parabolic or near parabolic dispersion relation. For the continuation of this section \( E_x, E_y, E_z, E_{\text{total}} \) refer to energies. Note, we factor in an effective mass when dealing with the band structure. Usually, the effective mass tensor conserves the fact that in k-space the group of points lying on a sphere will still have constant energy. We assume our material to have this property. Otherwise, when dealing with other surfaces such as ellipsoids, etc the problem becomes very difficult. It is still doable, we would factor in the new surface and find the D.O.S for this, D (defined below) would be based on the cross section in the xy plane (or for D in the zy or xz plane we could have different cross sections shapes and thus would have to calculate the D’s for these shapes). If the total energy obeys the 1-1 correspondence with the k-space energy spheres but is another function than the parabolic relation, the \( E_{\text{total}} \) quantity used in D (defined below) or whenever we find total momentum magnitudes from energies will in fact be \( |k| = f^{-1}(E_{\text{total}}) \), where \( f \) is the function relation between momentum magnitudes and energy, having the restrictions outlined above. We estimate this function from the band structure diagrams obtained from experiment. Similarly, \( |k|_{xy} = g^{-1}(E_{\text{total}} - E_z) \), where this momentum is the total momentum in the xy plane and \( |k|_z = h^{-1}(E_z) \) for the z-coordinate.

Now, the modes have a spacing as defined above. The way we treat this is the following: We assume continuous modes and thus we integrate instead of summing. However, we multiply the integral by a factor inversely proportional to the mode spacing. In fact, this procedure is carried out in thermodynamics when dealing with such problems in phase space and the constant factor is usually some power of \( \frac{1}{h} \).

Let us define a quantity, D, such that D is the number of modes that lie at each latitude of the constant energy sphere per volume (between a differential of energy in the xy plane, which translates to a differential of total energy, holding the z component energy constant). Since the amount of modes per latitude is equivalent to the amount that lie on the circumference of the same circle traced in the x, y plane, it would be the density of states of a 2-D k-space surface:

\[
D(k_{xy})dk_{xy} = \frac{1}{V_{\text{box}}} \cdot \frac{1}{4} \cdot 2\pi \sqrt{E_{\text{total}}} - k_z^2 \left( \frac{L}{2\pi} \right) \left( \frac{L}{2\pi} \right) dk_{xy}
\]

Where the subscript xy denotes the magnitude of the momentum in the xy plane. Including the effective mass we obtain:

\[
D(k_{xy})dk_{xy} = \frac{1}{V_{\text{box}}} \cdot 2 \left( \frac{2m^*}{\hbar^2} \right)^{\frac{1}{2}} \cdot \frac{1}{4} \cdot 2\pi \sqrt{E_{\text{total}}} - \left( \frac{\hbar^2}{2m^*} \right) k_z^2 \left( \frac{L}{2\pi} \right) \left( \frac{L}{2\pi} \right) dk_{xy}
\]

D is called the repetition number because it represents the amount of modes that have the same value of a k-component for the z coordinate. \( V_{\text{box}} \) is the volume of the box. The factor of two in D arises from spin degeneracy. The inverse factor of 4 arises from the fact that positive and negative momentums in each coordinate occur in pairs and thus this counts as one overall state. We are adjusting D to match our definition of momentum “state” which is defined as a momentum pair (\( \beta, -\beta \)) momenta. \( \beta = x, y, z \), so that the occupation probability of that state is equal (while the occupation probability of the negative or positive momentum within that overall state is may be unequal due to the antisymmetry at the boundary of region 1 and region 2). That is why we redefine a momentum state accordingly. The “state” is really equivalently defined by the coordinate energy due to the assumed
1-1 relation. See end of this section for discussion of degenerate momentum states. Thus, the probability of finding the electron in this “state” is equivalently the probability of finding the electron at that coordinate energy.

Since they are tunnelling effects, we are adjusting the Bloch theory to factor in tunnelling at the surface of the tip and the bulk. We assume bulk solutions till this surface (or localized band structure). It is easy to understand this if we imagine the following thought experiment: Imagine that no external electric field is present. Thus, the wavefunction solutions will be the well defined Bloch equations just before the tip. At time $t=0$ when we turn on the electric field, by continuity arguments we equate the new wavefunction to the original one. By the arguments present in the beginning of the section, the amplitude of the wavefunction just before the tip will not vary much in region 1 of the tip, thus, we use this wavefunction, if it does vary due to local geometry we use the localized band structure found from experiment. Also, by what we showed in section 3.3.2, the new wavefunction does not have new energy components added to it. However, the amplitudes of the incident and reflected wave at the boundary between the tip and the bulk will change.

With this definition of momentum “state” we proceed by using probability arguments based on conventional density of state and energy occupational probability arguments. The factor of $\frac{1}{2}$ in $D$ adjusts everything to account for this. We also add a factor of $\frac{1}{2}$ and $\frac{1}{2}$ (for the definition of momentum state in the z-coordinate) in the density of states (D.O.S) function for the exact same reason (see section 4.1.5). $D$ per volume as a function of total energy in the $xy$ plane is:

$$D(E_{xy}) = D(E_{total} - E_z) = D(E_{total} - \left(\frac{\hbar^2}{2m^*}\right)k_z^2) = \frac{1}{V_{box}} \frac{1}{2} \frac{1}{4\pi} \frac{L}{2\pi} \left(\frac{L}{2\pi}\right) (\frac{m^*}{\hbar^2})$$

which is a constant as expected. Or for a more general approach as discussed above ($g$ is the transfer function between the total momentum magnitude in the $xy$ plane and the total energy of the $xy$ plane, usually, equivalent to $f$ defined above):

$$D(E_{xy}) = \frac{1}{V_{box}} \frac{1}{2} \frac{1}{4\pi} \frac{L}{2\pi} \left(\frac{L}{2\pi}\right) \frac{dg^{-1}(E_{total} - E_z)}{dE_{xy}}$$

We assume that the reflected wave in the $z$-coordinate is negligible. In other words we assume the tunnelling process a highly efficient one. This assumption is not necessary, and in other sections we resolve for cases where this does not apply (section 4.2.2). However, for simplicity we assume this property in this section.

For the $z$-momenta, the magnitude squared of the amplitude constants (the A’s) represent the probability per volume of finding an electron in that state for the $z$-momentum (note: all negative $k_z$ amplitudes are zero) at the coordinate energy (we discuss the degenerate momentum state case at the end of this section). We can equivalently say, the probability per volume of finding an electron in the given $z$-energy value (since we assumed only one magnitude $z$-momentum for a given $z$-energy). We obtain the following (where we use $D(E_{xy} = E_{total} - E_z)$, $D.O.S(E_{total})$, $dE_{total} = dE_{xy}$ in this case. Please note, $E_{k_z} = E_z$ in this notation):

$$|A_{k_z}|^2 = \frac{L}{2\pi} \int_{E_{k_z}}^{E_{max}} \left(\frac{D}{\text{D.O.S}} O.P\right) dE_{total}$$

O.P stands for the overall occupation probability of that total energy. It is not equal to the individual occupation probability of a state at an energy. See section 4.1.5. The factor beside the integral is explained in the paragraphs below. We have assumed that within the integral range of total energies, there is the specific $z$-state. However, it is possible that at a certain energy no such $z$-state is allowed, for these cases we adjust the above integral accordingly (see discussion at the end of this section on degenerate cases, the same treatment can be applied for this scenario). For the localised band structure case (i.e, when we are not using the approximation that the wavefunction in region 1 is the same as the bulk), there could be instances when the specific $z$-momentum is not allowed due to the spacing shifts in $z$-momenta at the total energy. The above equation becomes:

$$|A_{k_z}|^2 = \frac{L}{2\pi} \int_{E_{k_z}}^{E_{max}} \left(\frac{D}{\text{D.O.S}} O.P\right) Y(k_z - n\Delta k_z(E_{total})) dE_{total}$$
Where $0 \leq n \leq \frac{f-1(E_{total})}{2E_z}$, $Y$ is 1 if the argument is zero and 0 if not. As a reminder $f$ is the transfer function between total energy and total momentum. We use the D.O.S obtained by experiment. A good estimation is to assume that there is always the z-momentum state for the range of total energies used in the above two integrals, regardless of how spacing varies.

The general formula is:

$$\sum_{\text{OverallTotalEnergies}} P(\text{CoordinateEnergy}) \cdot (O.P@\text{TotalEnergy}) = \sum_{\text{OverallTotalEnergies}} \frac{\text{NumberOfStates} @ \text{CoordinateEnergy} @ \text{TotalEnergy}}{\text{TotalAmountOfStates} @ \text{TotalEnergy}} (O.P@\text{TotalEnergy})$$

Where $P$ is the probability function given a coordinate energy. Thus, equivalently (since $dE_{total} = dE_{xy}$):

$$|A_{k_z}|^2 = \frac{L}{2\pi} \int_0^{E_{max}-E_z} \left( \frac{D(E_{xy})}{D.O.S(E_{xy} + E_z)} \right) O.P(E_{xy} + E_z) dE_{xy}$$

There is a discrepancy worth mentioning in the above integral. The density of states function represents the amount of states within a small differential total energy. However, this differential energy is taken normal to the energy spheres in k-space in the calculation. $D$ represents the total amount of states within a small differential total energy in the xy plane. While, in the above integrals, the differential of the total energy is equivalent to the differential energy in the xy plane, we have to still adjust the D.O.S to count the number of states within a total differential energy that is parallel to the xy plane at a certain constant z-energy (and not normal to the k-space sphere). While having stated this, it is easy to see that they are virtually equal and this discrepancy is negligible. Please see proof of this in appendix I. Inherent to the proof in appendix I we also derived the D.O.S in the differential $dE_{xy}$ which may generate better results when used in the above type of integral. As for the $D.O.S$ by the way its defined in section 4.1.5 we factor in the same treatment as in Appendix I. Please note that if there are no x-y momenta, $D=1$. We impose this condition.

The z-coordinate of energy is held constant (at a given positive momentum). There are factors of $\frac{L}{2\pi}$ energy k-spheres between closest viable modes in the x,y plane and that’s why we have the factor, $\frac{L}{2\pi}$ (unit-less), next to the integral. If the spacing in the x and y directions are not equal then, the factor in front of the integral is the inverse of the smaller spacing. $E_{max}$ is the maximum energy of the outer most band with filled states. The spin states are already accounted for in the D.O.S and D. We assume that all probability amplitudes of the input wave are real. We can assume this without loss of generality. Since, the phase of both the amplitudes can be eliminated from both sides of the equation, and is eliminated when we take the magnitude squared value of the wave function in both regions.

Thus,

$$A_{k_z} = \frac{L}{2\pi} \int_{E_{k_z}}^{E_{max}} \left( \frac{D}{D.O.S \cdot O.P} \right) dE_{total}$$

Where $E_{k_z} = \hbar(k_z)$, this usually just equals: $(\frac{\hbar^2}{2m^*})(k_z)^2$. Given a certain momentum in the z-coordinate and a given total energy, the probability (per unit volume due to spatial normalization) for a certain momentum pair (+ve and -ve $k_z$) or “momentum state” (equivalently x-coordinate energy) in the x-coordinate is:

$$|P_{k_z|k_z|E_{total}}|^2 = \frac{2}{D}$$

where the momentum values are between $(\frac{2m^*}{\hbar^2})^{\frac{1}{2}} E_{total} - (\frac{\hbar^2}{2m^*}) k_z^2$ and 0 with effective mass effects. As discussed previously, generally, we use $g^{-1}(E_{total} - E_z)$ for these momentum values. The factor of 2 is due to spin. We assume a 1-1 correspondance
between coordinate energy and coordinate momentum here. Please see discussion at the end of this section for the degenerate momentum state case.

Now, for a given z-momentum state, one in every \( \frac{2\pi}{L} \) (or the minimum spacing in the x, y plane), total energies (or total energy k-spheres) will contain viable modes (z,x,y momentum states defined above), therefore, given a z-momentum state:

\[
|P_{k_z}|^2 = \frac{L}{2\pi} \int_{E_{k_z}}^{E_{max}} \frac{2}{D} dE_{total}
\]

(Where, \( E_{k_z} = E_x = f_x(k_x) \), \( f_x \) is the x-coordinate transfer function (usually just the normal effective mass quadratic type relation used above) between coordinate momentum and coordinate energy. Also, again, \( dE_{total} = dE_{xy} \) so we can use D derived above). For the localised band structure case we include the Y function shown above the integral.

Now, the overall probability of occupying the x,z momentum state mode is:

\[
|P_{k_x}|^2 |A_{k_z}|^2 = \frac{L}{2\pi} \bigg( \int_{E_{k_z}}^{E_{max}} \frac{2}{D} dE_{total} \bigg) \ast \frac{L}{2\pi} \bigg( \int_{E_{k_z}}^{E_{max}} \left( \frac{D}{D.O.S} O.P \right) dE_{total} \bigg)\]

and now we integrate over all z-momentum states (with the constant spacing factor) to get the overall probability of occupying a certain x-momentum state (defined above):

\[
|P_{k_x}|^2 = \left( \frac{L}{2\pi} \right)^2 \left( \frac{H}{2\pi} \right) \int_{E_{k_x}}^{E_{max}} \int_{E_{k_z}}^{E_{max}} \frac{2}{D} dE_{total} \bigg( \int_{E_{k_z}}^{E_{max}} \left( \frac{D}{D.O.S} O.P \right) dE_{total} \bigg) dk_z
\]

For the localised band structure case, the Y function inclusion in the integrals eliminates the need to include the z-spacing factor \( \left( \frac{H}{2\pi} \right) \).

Now, the probability in being in a certain coordinate momentum eigenstate (meaning \(+k_x\) or \( -k_x \)) at a certain coordinate energy equates to,

\[
|\psi_x(k_x, E_x)|^2 = |P_{k_x}|^2
\]

since these are plane waves of defined momenta for a given coordinate energy.

We have the probability of being in an overall coordinate momentum, coordinate energy state (\( |\psi_x(k_x, E_x)|^2 \)) which is given above, \( |P_{k_x}|^2 \), such that the position wavefunction is:

\[
\psi_x(x, t) = (A_{+k_x} e^{ik_x x} + A_{-k_x} e^{-ik_x x}) e^{-iE_x t}
\]

It is easy to see that the probability of occupying the positive momentum state given the probability of occupying the overall state, (which is\( |P_{k_x}|^2 \)) is:

\[
|P_{+k_x}|^2 \text{overallstateoccupied} = \frac{|A_{+k_x}|^2}{|A_{+k_x}|^2 + |A_{-k_x}|^2} = \frac{1}{2}
\]

We used the relation found from boundary conditions (for a half step potential well) that :

\[
A_{-k_x} = \frac{\alpha_x + ik_x}{ik_x - \alpha_x} A_{+k_x}
\]

And thus, the overall probability of occupying the positive momentum state is:

\[
|A_{+k_x}|^2 = \frac{1}{2} |P_{k_x}|^2
\]

Using the fact that \( A_{+k_x} \) is real,
We know that, quantum amplitudes per volume. As a reminder all factors in front of the integrals are unitless. Also, these are the limits of integration. Note, generally we use $h^{-1}(E_{\text{max}})$, where $h$ is the transfer function between $z$-momenta and $z$-energy, as discussed in previous paragraphs.

And,

$$A_{+k_x} = \left( \frac{1}{2L} \right)^2 (\frac{H}{2\pi})^{2\pi} \int_{z_{\text{min}}}^{z_{\text{max}}} \left[ \left( \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{2}{D} dE_{\text{total}} \right) \frac{D}{D.O.S} O.P \right] dE_{\text{total}} dk_z =$$

$$\sqrt{\frac{V}{16\pi^4}} \int_{z_{\text{min}}}^{z_{\text{max}}} \left[ \left( \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{2}{D} dE_{\text{total}} \right) \frac{D}{D.O.S} O.P \right] dE_{\text{total}} dk_z$$

where $V$ is the volume of the tungsten needle. As a reminder all factors in front of the integrals are unitless. Also, these are the quantum amplitudes per volume.

We know that, $k_{\text{max}} = \sqrt{E_{\text{max}}}$ and $k_{\text{min}} = 0$ (or with effective mass effects: $k_{\text{max}} = \left( \frac{2m^*}{\hbar^2} \right)^{1/2} \sqrt{E_{\text{max}}}$ and 0 ) so these are the limits of integration. Note, generally we use $h^{-1}(E_{\text{max}})$, where $h$ is the transfer function between $z$-momenta and $z$-energy, as discussed in previous paragraphs.

Due to the invariance between the $x$ and $y$ coordinate, the quantum amplitudes for a given $y$-momentum state is (per volume):

$$A_{+k_y} = \sqrt{\frac{V}{16\pi^4}} \int_{k_{\text{min}}}^{k_{\text{max}}} \left[ \left( \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{2}{D} dE_{\text{total}} \right) \frac{D}{D.O.S} O.P \right] dE_{\text{total}} dk_z$$

$$A_{-k_y} = \sqrt{\frac{V}{16\pi^4}} \int_{k_{\text{min}}}^{k_{\text{max}}} \left[ \left( \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{2}{D} dE_{\text{total}} \right) \frac{D}{D.O.S} O.P \right] dE_{\text{total}} dk_z$$

where $k_{\text{max}} = \sqrt{E_{\text{max}}}$ and $k_{\text{min}} = 0$ (or with effective mass effects: $k_{\text{max}} = \left( \frac{2m^*}{\hbar^2} \right)^{1/2} \sqrt{E_{\text{max}}}$ and 0 ). Note, generally we use $h^{-1}(E_{\text{max}})$, where $h$ is the transfer function between $z$-momenta and $z$-energy. Also, $f_y(k_y) = E_{k_y} = E_y$. Discussed in previous paragraphs.

From these quantum amplitudes, using Eq.6 , Eq.7 we can derive the coefficient amplitudes for region 2. We only need the positive momentum amplitudes since that is all that is required for these equations.

For the highly degenerate case, we would calculate all the quantum amplitudes of the positive coordinate momentum components (this is needed for the $x,y,z$ coordinate) and the negative coordinate momentum quantum amplitudes (needed for the $z$) for a given energy. The wave function in region 2 for the coordinate would be a superposition of the individual spatial wavefunctions for each degenerate coordinate momentum state. For the $x$ and $y$ coordinate we find this from Eq. 6, 7 in region 2 and using equations derived in the next section for the $z$-coordinate in region 2.

Please note, that $A_{+k_x}$, etc is re-derived in the following paragraphs. This is an alternate way and yields an easier formula, it is just as valid as the above formulas. Equating the two formula may hold value in finding a better estimate for $D$, or the D.O.S and the spacing factors.

It is interesting to note that if for some reason, there are more coordinate momentum degeneracies for a given coordinate energy than just the negative and positive coordinate momenta, we call this a highly degenerate case. As well, we can solve for these
extra terms as we do for the case of only the 2 fold degeneracy due to positive and negative coordinate momenta. In the general case, when we have both multiple coordinate energies for a given coordinate momentum or multiple coordinate momenta for a given coordinate energy, the way to obtain the probability that a certain coordinate energy state will be occupied is not to integrate, but to sum over all total energies where for a given coordinate momentum, we obtain the coordinate energy. Thus,

\[ \sum_{\text{For } Z\text{-Momentum@CoordEnergy}} \frac{D_z}{D.O.S} \ast O.P(E_{\text{total}}) \]

We then vary the coordinate momentum and apply the same procedure. Each of the probabilities generated from this procedure is related to the respective positive coordinate momentum quantum amplitude at that coordinate energy, as:

\[ |A_{+k_z,E}|^2 = |P_{+k_z|\text{overallstateoccupied}}|^2 \ast P_i \]

Where, \( P_i \) is one probability for one coordinate momentum state at a given coordinate energy.

We can easily calculate the quantum amplitude at the coordinate energy from this (note \( |P_{+k_z|\text{overallstateoccupied}}|^2 = 1 \), if no reflected wave). Please note, we naturally assume that negative momenta equal the same energy as positive momenta due to symmetry. We can rotate region 1 by 180° and expect the same results. If we solve individual wavefunctions through the boundary conditions for each possible coordinate momentum at a given coordinate energy and then add all the results, the resulting wavefunction would be the coordinate wavefunction at that coordinate energy for region 2. Also, there may be additional phase differences between the positive momentum components for the highly degenerate case, which we can assume as non-existent for most applications. Otherwise, we would have to use additional physics outside the scope of this article. This entire procedure assumes that there is an overall function \( f \), that maps overall momentum to energy (equipotential energy spheres). Thus, the band diagram would be the same in any direction. With this assumption we can yield some results of interest, even if it is not entirely the case in reality.

For other coordinates:

Let us define

\[ D_z(E_{yz}) = D(E_{\text{total}} - E_z) = D(E_{\text{total}} - (\frac{2m^*}{\hbar^2})k_z^2) = \frac{1}{V_{\text{box}}} 2 \ast \frac{1}{4} \pi \left( \frac{H}{2\pi} \right) \left( \frac{L}{2\pi} \right) \left( \frac{m^*}{\hbar^2} \right) \]

To be rigorous, \( m^* \) represents the total effective mass in the zy plane. For localised band structure we would use \( \Delta k_z(E_{\text{total}}) \) instead of \( \left( \frac{H}{2\pi} \right) \).

Then in an analogous manner as the z-coordinate:

\[ |P_{k_z}|^2 = \frac{L}{2\pi} \int_{E_{k_z}}^{E_{\max}} (D_z D.O.S O.P) dE_{\text{total}} \]

(The constant of integration is \( \frac{L}{2\pi} \) because \( L<H \).) Also, \( |P_{k_y}|^2 \) would be the same. Deriving the quantum amplitudes for specific coordinate momentum states at the coordinate energy easily follows and was shown earlier in this section.

Thus, for the degenerate case to find the overall probability that a coordinate energy is occupied we would carry out a procedure analogous to how it was done for the z-coordinate:

\[ \sum_{\text{For } X\text{-Momentum@CoordEnergy}} \frac{D_z}{D.O.S} \ast O.P(E_{\text{total}}) \]

We then vary the coordinate momentum and apply the same procedure. We then find all degenerate quantum amplitudes as described in the previous few paragraphs. Note, \( |P_{+k_z|\text{overallstateoccupied}}|^2 = \frac{1}{2} \). We then do the same treatment to the
y-coordinate (with the appropriate $D_y$). For these coordinates (x and y) only the positive quantum amplitudes are important in eq. 6, 7. Note, we can create a better D.O.S in the same way as in Appendix I.

If there is no assumed symmetry such as the k-space spheres, anisotropic in every direction, etc, then for every coordinate momentum the probability at a given coordinate energy is:

$$\sum_{\text{All States}} \frac{\#}{E_{\text{total}}} \times O.P(E_{\text{total}})$$

Where $\#$=the numbers of states with the specific coordinate energy and coordinate momentum, O.P is the occupation probability at each total energy. This is virtually impossible to carry out practically.

Thus, if there are multiple energies for a given overall momentum state, in the form of a band structure, then we have ways to do the analysis. In nature we have complicated band structure. It is easier to assume a parabolic dispersion relationship between total momentum and energy but to assume that momentum spacing is a function of total energy. With this assumption and the above formula we can estimate emission from band structure as complicated as Tungsten or GaAs.

4.1.2 Applying boundary conditions to the solved wavefunction, in the z coordinate

For this section $E_z = -E$ where E is the z-component energy.

We now solve for $F_{E_z}$, $Q_{E_z}$. We just need to find solutions such that the continuity conditions between region 1 and region 2 are satisfied. Thus, the spatial derivatives equate and the actual value of the wave function at the barrier is the same. This yields two equations and 2 unknowns. There is a factor of $\frac{1}{2\pi\hbar}$ in front of the total wavefunction in region 2. To account for this we include them in front of $F_{E_z}$, $Q_{E_z}$. We also have to incorporate spacing factors. Eq. 8, Eq. 9 are obtained by applying the time Fourier transform to the continuity equations defined at the beginning of the section for the z component wavefunction and equating corresponding energy (frequency) components to each other.

We ignore negative momentums as the reflected wave is assumed to be small. We assume this is the only influence the laser pulse has in region 1. If this is not the case, then a better assumption would be that the system in region 1 would maintain its steady state. Therefore, it would be in the state before we introduce any degrading electric field or the state that the system in the x and y coordinate is in. Therefore, $A_{+k}$ and $A_{-k}$ would be related in the same way as their counterparts in the x and y coordinates and we could carry out a similar analysis (the proportionality factor between the amplitude squared and the probability, found when doing the analysis for the x/y coordinate would have to be accounted for here as well). In this case we can adjust the lefthand of Eq. 8, Eq. 9 accordingly. For further degeneracy (multiple z-momentums for a given z coordinate energy), using analogous calculations as outlined in the previous section, we can obtain the quantum amplitudes for each momentum state ($+k_z$, $-k_z$).

The left side of the following equations would just be a summation of the amplitudes (Eq. 9 would be a summation weighted by the momenta values). In fact, as outlined in the previous section region 2 would just be a summation of the individual wavefunctions generated from the cases where there is only that momentum state and no further momentum degeneracy (since the boundary condition equations are linear we could break them up into a set of analogous equations for each momentum pair ($+\cdot$, $-\cdot$)). Since the math is already defined for this, here we just assume that the reflected wave in the z-coordinate is zero and we continue with this assumption. However, in section 4.2.2 we treat the case where there is a reflected wave. Here we show again mathematically, which constant factor we use when replacing the summation by the integral.

$$\frac{1}{2\pi\hbar} \int H_{1E_z} e^{i\frac{E_z}{\hbar}(t)} dE_z = \frac{1}{2\pi\hbar} \int H_{2E_z} e^{i\frac{E_z}{\hbar}(t)} dE_z$$

where $H_{1E_z}$, $H_{2E_z}$, are Fourier energy components for region 1 and region 2. These integrals equate to the wave functions in the regions. Since the integral is a summation we introduce the spacing in $dk_z$ (as a reminder: instead of making $A_{+k_z} = 0$ for
values in between the spacing, we make $A_{+k_z}$continuous and introduce the spacing constant in momenta as was done above and in general phase space calculations in thermodynamics (Δ$k_z$ is defined as the spacing). Since, energies that are zero in region 1 remain zero in region 2 (shown in section 3.3.2), there would be the same amount of energies in region 2. Thus,

$$\frac{1}{2\pi}\sum_{n=0}^{\infty} A_{+n\Delta k_z} e^{i\Delta k_z(t')} \simeq \frac{H}{2\pi} \int H_{1E_z} e^{iE_z(t')} dE_z$$

where the function $f$ relates coordinate momentum to coordinate energy (here we assume a 1-1 correspondence please see previous section on how to adjust for cases without this assumption).

And,

$$\psi_{1z}(z,t) = \frac{H}{2\pi} \int H_{2E_z} e^{iE_z(t')} dE_z$$

Since there are the same energies and no added energies in region 2. Now, $H_{1E_z} A_{+k_z} e^{i k_z z}$ since no reflected wave. If we factor in a localized band structure we would not put the $z$-momenta spacing in front of the integral. Instead we would have to remain zero in region 2 (shown in section 3.3.2), there would be the same amount of energies in region 2. Thus,

$$\Delta E_k = \frac{\pi}{2\Delta k_z}$$

Then we can solve for $F_{E_z}, Q_{E_z}$

$$F_{E_z} = \frac{-M}{-\frac{M}{T} + L} A_{+k_z}$$
\[ Q_{E_z} = \frac{-\frac{L}{T} + i k_z}{-\frac{L}{T} U + M A_{+k_z}} \]  

(11)

For this section we assume that the electric field of the laser beam only contributes to electron tunneling, i.e, there is no promotion of electrons to higher energy levels due to photoabsorption nor band structure modifications due to the electric field of the pulse. This means that the pulse itself is not degraded or attenuated within the region of tunneling and we can assume the pulse profile we put in, in the calculations. This can be accomplished by studying the band structure of tungsten and using pulses centered on frequencies where the density of states in higher regions are low or where there is a bandgap. The laser pulse is very short in time and thus the absorption lifetime is much larger than the pulse itself. We assume no higher order effects such as thermal heating, scattering events and promotion of electrons to higher energies.

4.1.3 Normalization of the Wavefunction

In order for the wavefunction to be normalized such that the probability of the electrons existing is 100% over all space, all energy eigenkets of the wavefunction have to be normalized to 1. We have applied boundary conditions to already pre-normalized quantum amplitudes. Thus, within region 1 and the bulk we have an unnormalized wavefunction value of 1.

\( \Upsilon \) is the value of the unnormalized region 2 probability function.

The normalization constant for the probability function in region 1 and region 2 is:

\[ \frac{1}{\Upsilon + \Theta} \]

And thus, the overall normalization constant for the total wavefunction is:

\[ \sqrt{\frac{1}{\Upsilon + \Theta}} \]

Now, since we have found a solution in region 2 that solves the Schrodinger equation, all energy eigenkets must be orthonormal. The x and y normalization constants are easily calculated. We first focus on the z-coordinate wavefunction. If we take an arbitrary eigenket and normalize it, that normalization constant will apply for all eigenkets (due to the fact that we have orthonormal states). We take the energy eigenket: \( E_o = -\frac{V_o}{2} \) for mathematical ease. Note: \( E_o = -E_z \), where \( E_z \) is the coordinate energy.

The spatial wavefunction at this energy is:

\[ \int g_{E_o} e^{-i \frac{E_o}{\hbar} t} dt \]

We obtain for \( \Upsilon_z \):

\[ \Upsilon_z = \int_0^\infty \left| \int g_{E_o} e^{-i \frac{E_o}{\hbar} t} dt \right|^2 dz \]

Which equates to:

\[ \Upsilon_z = \int_0^\infty \left| \int [F_{E_o} Ai((\frac{2m}{\hbar^2})^{\frac{1}{2}})(\frac{1}{e\Phi(t')}^{\frac{1}{2}}(\frac{V_o}{2} - e\Phi(t') z) + Q_{E_o} Bi((\frac{2m}{\hbar^2})^{\frac{1}{2}})(\frac{1}{e\Phi(t')}^{\frac{1}{2}}(\frac{V_o}{2} - e\Phi(t') z))] e^{-i \frac{E_o}{\hbar} t} dt \right|^2 dz \]

Where, \( F_{E_o}, Q_{E_o} \) are based on the unnormalized quantum amplitudes in region 1 found in section 4.1.2. Now for the x and y coordinate, we also choose energy \( \frac{V_o}{2} \)

\[ \Upsilon_\beta = \left| C_{\alpha\beta} \right|^2 \frac{2\alpha_\beta}{2 \alpha_\beta} \]
which is what the normalization integral works out to, \( \beta = x, y \) and \( \alpha_\beta \), \( C_{\alpha_\beta} \), is evaluated at \( E = \frac{V_o}{2} \).

Thus, the overall \( \Upsilon \) is:

\[
\Upsilon = \Upsilon_x \Upsilon_y \Upsilon_z
\]

### 4.1.4 The total wavefunction Solved with Boundary Conditions and Normalization

Barring degenerate cases or localized band effects. The total wave function for region 2 then becomes (where we use spacing constants to replace summations):

\[
\psi_{II}(x, y, z, t) = \sqrt{\frac{1}{\Upsilon + \Theta}} \frac{1}{2\pi \hbar} \frac{L}{2\pi} \int C_{\alpha_x} e^{-\alpha_x x} e^{i\frac{E_x}{\hbar}t} dE_x \frac{1}{2\pi \hbar} \frac{L}{2\pi} \int C_{\alpha_y} e^{-\alpha_y y} e^{i\frac{E_y}{\hbar}t} dE_y \frac{1}{2\pi \hbar} \frac{H}{2\pi} \int g_{E_z}(z, t') e^{-i\frac{E_z}{\hbar}(t'-t)} dt' dE_z
\]

and \( C_{\alpha_x}, C_{\alpha_y}, F_{E_z}, Q_{E_z} \) are defined by the equations derived in this section (Eq. 6, Eq. 7, Eq. 10, Eq. 11). Here, \( E_x, E_y, E_z \) represent the negatives of the respective coordinate energies. From discussion in the previous sections, we can find the total wavefunction for the degenerate momenta and energy cases or with localized band effects.

### 4.1.5 Solving for Momentum Components, D.O.S and Total Amount of Electrons Emitted.

**For this section** \( E_x, E_y, E_z, E_{total} \) are the coordinate energies.

\[
k_\beta = \frac{\sqrt{2m^*_e E_\beta}}{\hbar}
\]

\( \beta = x, y, z \) where \( m^*_e \) is the effective mass of the electron in the band.

\[
m^*_e = \hbar^2 \left( \frac{\partial^2 E}{\partial \beta^2} \right)^{-1}
\]

We assume that there is no off-diagonal elements in the tensor. Otherwise, it would be the \( \beta \)-component of the tensor product with the momentum vector.

As previously stated the Electron Occupation Probability at 0 Kelvin is 1 below the Fermi energy surface. Also, when \( A_{k_e} \) is zero the contribution \( (g_{E_z}) \) to the wave function for that energy is zero in region 2 as shown at the end of section 3.3.2.

The Density Of States or D.O.S for allowed energies (energies that satisfy the momentum spacings) defines as the number of states per total energy per volume for a rectangular box is:

\[
D.O.S = \frac{\sqrt{E_{total}} (2m^*_e)^{\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}}
\]

Or in general,

\[
D.O.S = \int \frac{f^{-1}(E_{total})^2}{2(\pi)^{2}} \frac{df^{-1}(E_{total})}{dE_{total}}
\]

where D.O.S is per volume. Here the effective mass is the total effective mass for a given magnitude of momentum. Remember that we are dealing with material where there is a unique energy for a magnitude of momentum, no matter the direction of the momentum, thus, even if the individual component effective masses vary, there is an overall effective mass only dependent on the total momentum magnitude that can be used for the D.O.S and calculating overall energy.

Leading to:
D.O.S = \[ \frac{\sqrt{E^*}}{2 \pi^2 \frac{2m^*}{\hbar^2}} \]

where the additional factors, \( \frac{1}{4}, \frac{1}{2} \), are explained in the paragraph below. And,

\[ E^* = |E_{total} - E_{max/min}| \]

It is the energy relative to the max of the valence band. If we are treating an excited state of Tungsten then we would have two cases the conduction band, where we would take energies relative to a minimum, and the valence band maximum case, where we would take energy relative to the max of the conduction band. Thus, when solving the integrals for the wave function amplitude constants, whenever we use the D.O.S, we have to change it when the energies in the integration are over different bands. Here the factor of \( \frac{1}{2} \) comes from our momentum “overall state definition” for \( k_z \) see the discussion in the beginning of section 4.1.1. The factor of \( \frac{1}{4} \) comes from our definition of “overall momentum states” (being a summation of positive and negative momenta) in the x and y coordinate. To reiterate the discussion, the states all carry the same occupation probability (however the individual positive and negative momenta don’t) so we can use the D.O.S method in general but we have to adjust the D.O.S and D functions, treating this as the definition of a state.

Now at a given time,

\[ N(t, x, y, z) = |\psi_{II}(t, z, x, y)|^2 \ast T_I \]  \hspace{1cm} (12)

Where \( N \) is the number of electrons emitted, \( T_I \) is the total amount of electrons in region 1. Please note that the distribution of electrons given a total number of electrons in region 1 is contained in the wavefunction and this is why we multiply it by the overall total number of electrons in region 1. We do not have to work in the energy domain and multiply each energy component of the wavefunction squared by the total amount of electrons in region 1 at that energy and then inverse Fourier transform it. Although, it is an alternative way.

And the total amount of electrons emitted at a certain position at a certain time is:

\[ \int_{-\infty}^{t} N(t, x, y, z) dt \]

Here we assume that the position is far enough such that if an electron is emitted it will not tunnel back. Finally,

\[ T_I = V \ast \int (D.O.S \ast f_{FD}(E_{total}))dE_{total} \]

\( V \) is the tunneling region volume, \( V \approx 10^{-36} m \), which is the volume of one Tungsten atom (at the tip). In both equations we have assumed uniform density of electrons in region 1. \( T_I \) is a function of time if region 1 has time dependent effects (as discussed in section 4.2), otherwise it is a constant from region 1. We can also find the power spectrum of \(|\psi_{II}(t, z, x, y)|^2\) (the probability per unit time per unit volume) to obtain the energy/power spectral distribution of electrons in our beam. Please note \( |\psi_{II}(t, z, x, y)|^2 \) is per volume due to the spatial normalization constraint.

The Occupation Probability function, O.P is:

\[ O.P(E_{total}) = \frac{D.O.S(E_{total}) \ast f_{FD}(E_{total})}{\int D.O.S(E_{total}) \ast f_{FD}(E_{total})dE_{total}} \]

where \( f_{FD}(E_{total}) \) is the Fermi-Dirac distribution (since we are dealing with fermions).
4.2 The time dependence of region 1

4.2.1 The Processes that Could Contribute to Time Dependence in Region 1

Please note that for the above derivation we did not bother with what was happening at the other end of the needle, the end that is attached to the laboratory apparatus. We assume that this end is connected to an infinite reservoir of electrons, and as states are unpopulated, they are instantaneously refilled. Also, we assume that the band structure is not dependent on the electric pulse in the bulk. This is the assumption that will yield the most experimental error in our design. The assumption can be restated as follows: Region 1 is time independent and is at steady state. The time dependence can occur from two factors: 1. The laser pulse effects region 1. In that case, we have to change the wavefunction and factor in the changes into the band structure (such as how it effects the D.O.S, D, O.P, effective mass, electron-electron interaction, etc). 2. If there is no infinite reservoir and the refilling of electrons doesn’t happen on a timescale much faster than the pulse. If the laser pulse is extremely short, we can assume steady state for the duration of the pulse as electron depletion would be at a minimum. The time between pulses would exceed the time electrons need to replenish the barrier. Let the amount of time that is needed to replenish the states be \( \tau \). If the amount of time it takes electrons to tunnel out at a given frequency is longer than \( \tau \) than the assumption is justified for these frequencies. Under factor 2, the wavefunctions do not change, but rather the total amount of electrons in region 1 is altered. Also if the laser pulse is extremely short, band structure changes can be assumed to be negligible as the bulk would not have time to redistribute its electrons. The electrons tunnel out on a faster time scale, analogous to a stone bouncing on water. The water molecules at the surface cannot redistribute themselves fast enough for the stone to sink, so the stone bounces or tunnels out of the water region.

The rate of electrons entering the needle tip for a given energy:

\[
\eta = \frac{R}{\tau}
\]

R is the reservoir electrons at the energy. And one could see that if the reservoir is infinite, the rate is infinite, and the filling of states is instantaneous. The total number of electrons in region 1 is given as:

\[
T_I = V \ast \int (D.O.S \ast f_{FD}(E_{total}))dE_{total}
\]

Now under factor 2, there is an overall replenishing time \( \tau_{avg} \) which describes the average time needed to replenish all states which is dependent on the overall wavefunction in region II and material properties, the rate of change of the total number of electrons in region 1 is given as:

\[
\frac{dT_I}{dt} = \eta_{avg} - (T_I \ast \int |\psi(t,z,x,y)|^2 dV)
\]

(13)

where \( dV \) is the volume past the boundary between region 1 and region 2 at the needle’s tip.

\[
\eta_{avg} = \frac{RT}{\tau_{avg}}
\]

where \( RT \) is the total amount of reservoir electrons. Solving this differential equation gives the \( T_I \) as a function of time that can be substituted back into Eq. 12. If we want a steady state in region 1 we have to choose our material and laboratory setup such that:

\[
\eta_{avg} = \frac{1}{\int |\psi(t,z,x,y)|^2 dV}
\]
For a more exact analysis we don’t factor in an average time giving:

$$\frac{\partial T_I(E)}{\partial t} = \eta - T_I \ast \int |\psi(E, z, x, y)|^2 dV$$  \hspace{1cm} (14)

Where,

$$\psi(E, z, x, y) = \int \psi(t, z, x, y) e^{-iE_0\hbar t} dt$$

$$E_0 = -E.$$ The reason why we don’t use the amount of electrons at a given energy for the wavefunction term in the above equation is because this information is contained in the wavefunction given a total number of electrons in region 1.

We then inverse Fourier transform Eq. 14 to find the total number of electrons in region 1 as a function of time, that we then use in Eq. 12. We can still use Eq. 13 if we use a $\tau$ that contains energy distribution information within it. This will work if we use:

$$\tau = \frac{1}{\int |\psi_{reservoir}(t, z, x, y)|^2 dV}$$

where the integral is over the volume of the reservoir. Under usual conditions it is extremely hard to find experimentally or analytically. This then becomes a problem of quantum dynamics factoring in reservoir thermodynamic effects and quantum control and coherence.

4.2.2 An Attempt at Solving for Laser Pulse Effects in Region 1, including photon-absorption effects (without degradation of the laser pulse)

In this section, $E_x$, $E_y$, $E_z$, $E_{total}$ are the negative value of the respective energy. Also, we do not deal with changes to the D.O.S, D, O.P or other electron-electron interaction/electron distribution effects.

The pulse would linearly degrade the potential function in Region 1 in the exact same way as in Region 2 (only in the z-direction). Thus, the solutions for region 1 would be:

$$\psi_I(x, y, z, t) = \left( \int \frac{1}{2\pi\hbar} \frac{L}{2\pi\hbar} \int \frac{1}{2\pi\hbar} \frac{L}{2\pi\hbar} A_{E_x} A_{E_y} e^{i(k_y y + k_z z)} e^{i(E_z E_{total}) t} dk_z dk_y \right) \frac{H}{2\pi\hbar} \int \int u_{E_z}(z, t') e^{-iE_z(t'-t)} dE_z dE_z$$

Where,

$$u_{E_z}(z, t) = A_{E_z} Ai\left(\frac{2m}{\hbar^2}\left(\frac{1}{e^\Phi(t')}\right)\right)^2 \left(E_z - e^\Phi(t')(L + z)\right) + B_{E_z} Bi\left(\frac{2m}{\hbar^2}\left(\frac{1}{e^\Phi(t')}\right)\right)^2 \left(E_z - e^\Phi(t')(z + L)\right)$$

where A, B could be functions of time and L is the penetration length of the electric field in region 1. This penetration depth is estimated as being 2-3 angstroms[7]. It is easy to convert the total wavefunction in region 1 to one factoring localised band effects through the discussion in section 4.1.1. Thus, we assume the above wavefunction without localised band effects for this section.

Now, we assume A, B are constants and we attempt to find a solution that matches boundary conditions. At the boundary between region 1 and region 2, the wavefunction is both spatially continuous and its derivatives are continuous. Now, in the region past the penetration depth (region 0), we should assume that the electron wavefunction is in the state prior to laser excitation. The state before laser excitation is simply the half step potential function (no electric field degradation) seen in the x or y coordinate. We equate energy wavefunctions (with spacing factors) at region 0. Therefore, we include the spacing factor $\frac{H}{2\pi}$, which is why it is included in the above equation describing the overall wavefunction. We redefine $z=0$ at the boundary between region 0 and region 1.
\[
\frac{1}{2\pi} \frac{H}{2\pi} \frac{2ik_z}{(ik_z - \alpha_z)} A_{\text{initial,}+k_z} = \\
\frac{1}{2\pi} \frac{H}{2\pi} A_{E_z}(\int Ai\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e\Phi(t')(z))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0} \\
+ \frac{1}{2\pi} \frac{H}{2\pi} B_{E_z}(\int Bi\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e\Phi(t')(z))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0}
\]

Also,

\[
-\frac{1}{2\pi} \frac{H}{2\pi} \frac{2ik_z(\alpha_z)}{(ik_z - \alpha_z)} A_{\text{initial,}+k_z} = \\
-\frac{1}{2\pi} \frac{H}{2\pi} \frac{2m}{\hbar^2} \left(\frac{1}{e}\right)^{\frac{1}{2}} A_{E_z}(\int \Phi(t')^i Ai\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e\Phi(t')(z))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0} \\
- \frac{H}{2\pi} \frac{2m}{\hbar^2} \left(\frac{1}{e}\right)^{\frac{1}{2}} B_{E_z}(\int \Phi(t')^i Bi\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e\Phi(t')(z))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0}
\]

using definitions in section 4.1.1 for the initial A (it equates to the same as the A for the x or y coordinate).

To solve let the following be defined:

\[
Y = (\int Ai\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e(z)\Phi(t'))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0} \\
J = (\int Bi\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e(z)\Phi(t'))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0} \\
S = -\frac{2m}{\hbar^2} \left(\frac{1}{e}\right)^{\frac{1}{2}} (\int \Phi(t')^i Ai\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e(z)\Phi(t'))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0} \\
R = -\frac{2m}{\hbar^2} \left(\frac{1}{e}\right)^{\frac{1}{2}} (\int \Phi(t')^i Bi\left(\frac{2m}{\hbar^2}\right)^i\left(\frac{1}{e\Phi(t')}\right)^{\frac{1}{2}}(E_z - e(z)\Phi(t'))e^{-i\frac{E_z}{\hbar}(t')dt'}|_{t'=z=0}
\]

\[
A_{E_z} = \frac{-B - 2ik_z(\alpha_z)}{-\frac{2}{\pi} Y + S} \frac{2ik_z}{(ik_z - \alpha_z)} A_{k_z,\text{initial}} \\
B_{E_z} = \frac{-S - 2ik_z(\alpha_z)}{-\frac{2}{\pi} J + R} \frac{2ik_z}{(ik_z - \alpha_z)} A_{k_z,\text{initial}}
\]

And the wavefunction in region 2 also matches the exact same boundary conditions with the new wavefunctions in region 1. However, the work function is now a function of time \( V_o(t) = V_o - eL\theta(t) \). This is dealt with in section 5.4. The \( \Phi \) in region 1 and region 2 can be different and the analysis still applies, as long as within the respective regions it does not vary spatially. This is the case when we consider material electric properties at the atom tip (such as the electron displacement field and polarizability). We note that in general the influence of material electrons on the total electric field drops of sharply outside the material and in region 2 we would have only the electric field of the laser pulse. Also, within the material at region 1 due to it being small, \( \Phi \) does not vary spatially. Thus, a spatially varying \( \Phi \) is not the case in both regions to a very good approximation. Since we assume \( \Phi \) is the same, We obtain for region 2:
\[
\frac{1}{2\pi} H A e_{E_z}(\int Ai((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
+ \frac{1}{2\pi} H B e_{E_z}(\int Bi((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} = \\
\frac{1}{2\pi} H F e_{E_z}(\int Ai((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0} \\
+ \frac{1}{2\pi} H Q e_{E_z}(\int Bi((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0}
\]

Also,

\[
-e\frac{1}{2\pi} H \frac{2m}{\hbar^2} \frac{1}{e}(\frac{1}{2})^\frac{1}{2} A e_{E_z}(\int \Phi(t')^2 A i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
-e\frac{1}{2\pi} H \frac{2m}{\hbar^2} \frac{1}{e}(\frac{1}{2})^\frac{1}{2} B e_{E_z}(\int \Phi(t')^2 B i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
-e\frac{1}{2\pi} H \frac{2m}{\hbar^2} \frac{1}{e}(\frac{1}{2})^\frac{1}{2} F e_{E_z}(\int \Phi(t')^2 A i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0} \\
-e\frac{1}{2\pi} H \frac{2m}{\hbar^2} \frac{1}{e}(\frac{1}{2})^\frac{1}{2} Q e_{E_z}(\int \Phi(t')^2 B i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0}
\]

We solve for the constants. After dividing out all common constants from the LHS and RHS from each of the above equations, let the following be defined:

\[
\iota = A e_{E_z}(\int Ai((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
+ B e_{E_z}(\int Bi((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
\vartheta = A e_{E_z}(\int \Phi(t')^2 A i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
+ B e_{E_z}(\int \Phi(t')^2 B i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(E_z - e \Phi(t')(z)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=L} \\
\varpi = (\int Ai((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0} \\
\gamma = (\int Bi((\frac{2m}{\hbar})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0} \\
\lambda = (\int \Phi(t')^2 A i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0} \\
\mu = (\int \Phi(t')^2 B i'(\frac{2m}{\hbar^2})^\frac{1}{2}(\frac{1}{e \Phi(t')})^\frac{1}{2}(V_o + E_z - e \Phi(t')(z + L)))e^{-i \frac{E_z}{\hbar}(t')dt'})|_{z=0}
\]
\[ F_{E_x} = \frac{\theta - \frac{\mu}{\gamma}}{-\frac{\mu}{\gamma} + \lambda} \]

\[ Q_{E_x} = \frac{\theta - \frac{\lambda}{\omega}}{-\frac{\lambda}{\omega} + \gamma} \]

Please note,

\[ A_{hk, initial} = \sqrt{\frac{L}{4\pi} \int_{E_{kz}}^{E_{max}} \left( \frac{D}{D.O.S} \right) dE_{total}} \]

By the previous analogous arguments for the x and y coordinates in section 4.1.1 (note the inverse factor of 2 inside the root). We then normalize the wavefunction according to section 4.1.3. Technically since there is a different wave function in region 1, there is a normalization constant attributed to this region (see section 4.1.3). However, since the region is so small we can omit this integration.

Now, if we take the spatial Fourier transform of the new wave function of region 1:

\[ \int \psi_I(z, t) e^{-ikz} e^{-i\frac{E_o}{\hbar}t} dz dt = B(E, k) = B(E_o, k) \]

where \( B \) is the momentum, energy Fourier amplitude, \( E_o \) defined as in section 3.3.1. Thus, the wavefunction of region 1:

\[ \frac{1}{\hbar} \left( \frac{1}{2\pi} \right)^2 \int B(E, k) e^{ikz} e^{i\frac{E_o}{\hbar}t} dk dE_o \]

which is a linear combination of the spatial wavefunctions of the states where there is no laser pulse (note the momentum degeneracy). Therefore, we can directly obtain the probability of transitioning into another state from photoabsorption from these amplitudes and Fermi’s golden rule. This is outside the scope of this paper.

Please note that we have included the z-energy spacing factor \( \left( \frac{\hbar}{2\pi} \right) \) in \( B \).

Now, our wavefunction in region 2 accounts for some laser pulse effects for region 1. The only thing that it does not account for is the effect of the new electron distributions on the laser pulse itself (such as its degradation) and other non-linear effects from the new electron distributions. Once the effects on the pulse itself is known, the function \( \theta(t) \) of the pulse should be updated. This is where all effects such as photon absorption or multi-photon absorption come into play. Also effects such as polarization of the material, etc. As for additional band structure effects, more experimental studies need to be done.
5 Extensions

5.1 Methodology Applied to a Known Solution

We give as an example of the above method outlined in section 3.3.1 by applying it to a known solution of the time dependent Schrödinger equation. That is for a free particle:

\[
\dot{i\hbar \psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi
\]

whose solution is:

\[
\psi = \frac{1}{2\pi\hbar} \int (A_{E_o} e^{ikx} + B_{E_o} e^{-ikx}) e^{i\frac{E_o}{\hbar}t} dE_o
\]

where \( k = \sqrt{\frac{2m(E)}{\hbar}} = \sqrt{\frac{2m(-E_o)}{\hbar}} \). Here \( E_o = -E \)

We start by assuming:

\[
H(E_o, z) = \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t} dE_o
\]

where,

\[
-E_o g_{E_o} = -\frac{\hbar^2}{2m} \nabla^2 g_{E_o} \tag{15}
\]

\[
g_{E_o} = A_{E_o} e^{ikx} + B_{E_o} e^{-ikx}
\]

Applying the inverse Fourier transform to Eq. 15, yields

\[
\dot{i\hbar \psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi
\]

Thus,

\[
\psi(x, t) = \frac{1}{2\pi\hbar} \int \int g_{E_o}(z, t)e^{-i\frac{E_o}{\hbar}(t-t')} dtdE_o = \frac{1}{2\pi\hbar} \int G_{E_o}(E_o) e^{i\frac{E_o}{\hbar}t} dE_o = \frac{1}{2\pi\hbar} \int (A_{E_o} e^{ikx} + B_{E_o} e^{-ikx}) e^{i\frac{E_o}{\hbar}(t-t')} dE_o
\]

Thus, we obtain the same solution with this method.

5.2 Calculating the Electric Field of the Electron Pulse

We know from Maxwell’s Equations:

\[
\nabla \cdot E_{\text{pulse}}(x, y, z, t) = \frac{\rho(x, y, z, t)}{\epsilon_o}
\]

where E is the electric field and \( \rho \) is the electron density.

From Eq. 12, we get the amount of electrons per volume-the density

\[
\rho(x, y, z, t) = \text{NumberOfElectronsEmmitted}(t, x, y, z) = (|\psi_{\text{region1}}(t, x, y)|^2 \ast \text{TotalNumberElectrons}_{\text{region1}})
\]

Thus,
\[ \nabla \cdot \mathbf{E}_{\text{pulse}}(x, y, z, t) = \frac{(\psi_{\text{region1}}(t, z, x, y))^2 \ast \text{TotalNumberElectrons}_{\text{region1}}}{\epsilon_0} \]

This can be calculated numerically using a computer. By holding coordinates constant, one can calculate the electric field surface around the pulse. From this one can obtain the potential surface by integrating along an easy path of the electric field surface for a constant time.

### 5.3 Generalizing the Method

We generalise the method in section 3.3.1. This means that we find all relevant solutions in the general wavefunction whose frequency (or Fourier variable) representation exists for a given differential equation of the form:

\[
\sum_{n=0}^{\infty} A_n \psi^{(n)} = \sum_{n=0}^{\infty} \theta_n(t) \nabla^n \psi + \theta_\alpha(t, \text{allothervariables}) \psi
\]

where \((n)\) indicates the \(n\)th time derivative (we label the variable on the left of this equation as time). \(n\) also indicates the gradient order and also is a label for the \(t\) dependent function \(\theta\) in front of each gradient. We assume that all \(\theta\) have Fourier and inverse Fourier transforms.

with the assumption that the general solution, \(g_\omega\), to:

\[
\sum_{n=0}^{\infty} A_n \omega^n g_\omega = \sum_{n=0}^{\infty} \theta_n \nabla^n g_\omega + \sum_{\alpha=0}^{\infty} \theta_\alpha(\text{allothervariables}, t = \text{const}) g_\omega
\]

is known, \(\theta_\alpha, \theta_n\) are constants, \(\omega\) is an angular frequency, \(\nabla\) is a gradient over all other variables (or any subset of all other variables). In fact, \(\nabla\) can represent any function of the gradients of the “other” variables.

Now, let’s define \(q_\omega\) as the same function save the fact that the constants \(\theta_\alpha, \theta_n\), are replaced by the functions \(2\pi \phi_n(-t) = \theta_n(t)\), \(2\pi \phi_\alpha(-t) = \theta_\alpha(t)\).

The general solution \(g_\omega\), is made up of the sum of specific solutions. For each specific solution we multiply by a coefficient function that has input variables: \(t\) and \(\omega\), these functions have the same form and the same reason for their form as in section 3.3.1. Let’s redefine \(g_\omega\) as being the sum of these new specific solutions.

It is easy to see that by assuming:

\[ H_\omega = \int g_\omega e^{-i\omega t} dt \]

where \(H\) is the Fourier amplitude of \(\psi\)

and by applying the inverse Fourier transform and the convolution theorem as outlined in section 3.3.1 and by the generalised identity:

\[ \psi^{(n)} = \frac{1}{2\pi} \int \omega^n H_\omega e^{i\omega t} d\omega \]

and \(\omega^n H_\omega = h_\omega^{(n)}\) where \(h_\omega^{(n)}\) indicates the Fourier amplitude of the \(n\)th time derivative \(\psi\), we obtain Eq. 16 in the exact same way as outlined in section 3.3.1. We could create a basis of linearly independent solutions by choosing the coefficient functions as we did for section 3.3.1 that are relevant to the problem (whether experimental or purely mathematical).

and for \(\psi\) we obtain as a solution:

\[ \psi(t', \text{allothervariables}) = \frac{1}{2\pi} \int \int g_\omega(\text{allothervariables}, t) e^{-i\omega(t-t')} dtd\omega \]
5.4 Another Useful Example: Pertaining to a time dependent work function $V_o$

In practice, the work function is also affected by the laser pulse, and thus, is also a function of time. The methodology outlined in section 3.3.1 and the above section easily solves this situation. Here we show this, reiterating section 3.3.1 but with $V_o(t)$, which is the symbol we use for the time dependent work function.

For this subsection the symbol $\psi$ refers to the wavefunction in the z-coordinate, $\nabla_z$ refers to differentiation w.r.t. z.

To solve this problem we start by stating the electronic Schrödinger equation needed to be solved in this region for the z coordinate:

$$i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_0(t) - e\theta(t)z)\psi$$

(17)

where $e$ is the elementary charge, $m$ is the mass of the electron and $\theta(t)$ is the time dependent electric field.

For a time independent (DC) electric field the above equation becomes,

$$E\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_0 - e\theta z)\psi$$

and whose general solution is known (triangular well solution):

$$\psi = C_z Ai\left(\frac{2m}{\hbar^2} \frac{1}{e\theta} \left( \frac{1}{e\theta} \right)^2 \right) (V_o - E - e\theta z) + D_z Bi\left(\frac{2m}{\hbar^2} \frac{1}{e\theta} \left( \frac{1}{e\theta} \right)^2 \right) (V_o - E - e\theta z)$$

where the constants precede the functions. In this section, $\mathit{E}$ means the energy contribution in the $z$ direction for the given electron.

And,

$$E_o = -E$$

By definition. This is notational to match the definition of the Fourier transform that we use in this paper.

We will now solve for the case when the potential is time dependent.

From Fourier analysis it follows straightforwardly that

$$\psi(z,t) = \left( \frac{1}{2\pi\hbar} \right)^\frac{1}{2} \int_{-\infty}^{\infty} H(z,E)e^{\frac{E_o}{\hbar}t} dE_o$$

and

$$H(z,E_o) = \int_{-\infty}^{\infty} \psi(z,t)e^{-\frac{E_o}{\hbar}t} dt$$

where $H(z,E_o)$ is the Fourier amplitude at the given energy and spatial position. To clarify : Under the definition of the Fourier transform used, the Fourier amplitudes functions, $H$ are the (spatial) wavefunctions for a given energy when $E_o = -E$ where E is the given energy. Mathematically:

$$\psi_{II}(E,z) = \int \psi_{II}(t,z)e^{-\frac{E_o}{\hbar}t} dt$$

Or,
\[ \Lambda(z, E) = H(z, E_o) \]

Where \( \Lambda \) is the energy representation of the wavefunction. From now on the indefinite integral symbol will implicitly imply infinite limits of integration else otherwise stated.

We know from Fourier transform theory that:

\[ \psi = \left( \frac{1}{2\pi\hbar} \right) \int h(z, E_o) e^{i\frac{E_o}{\hbar}t} dE_o \]

where

\[ h(z, E_o) = i\frac{E_o}{\hbar}H(z, E_o). \]

(Property 1)

Therefore:

\[ h(z, E_o) = i\frac{E_o}{\hbar} \int \psi(z, t) e^{-i\frac{E_o}{\hbar}t} dt \]

There is no simple solution by just taking the Fourier transform of Eq. 17 and finding solutions for each Fourier amplitude. This is because of the mixed term of the electric field and wavefunction. Instead we apply a different set of mathematical tricks. First we state the Fourier transform of Eq. 17:

\[ -E_o H(z, E_o) = -\frac{\hbar^2}{2m} \nabla^2 H(z, E_o) + \int \psi(z, t) V_o(t) e^{-i\frac{E_o}{\hbar}t} dt - ez \int \psi(z, t) \theta(t) e^{-i\frac{E_o}{\hbar}t} dt \]  \hspace{1cm} (18)

We proceed by assuming that

\[ H(z, E_o) = \int_{-\infty}^{\infty} g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt \]

where,

\[ -E_o g_{E_o}(z, t) = -\frac{\hbar^2}{2m} \nabla^2 g_{E_o}(z, t) + V_o(t) g_{E_o}(z, t) - ez g_{E_o}(z, t) \Phi(t) \]  \hspace{1cm} (19)

and \( 2\pi\hbar\Phi(-t) = \theta(t), \) \( 2\pi\hbar V_o(-t) = V_o(t). \) Also, \( g_{E_o}(z, t) \) is a unique function per frequency. The need for using \( 2\pi\hbar\Phi(-t) = \theta(t) \)

, \( 2\pi\hbar V_o(-t) = V_o(t) , \) may seem bizarre but the reason will be apparent soon.

The solution to this second order differential equation is:

\[ g_{E_o}(z, t) = F_{E_o} Ai((\frac{2m}{\hbar^2})^{\frac{1}{2}} (\frac{1}{e\Phi(t)})^\frac{3}{2} (V_o(t) + E_o - e\Phi(t)z)) + Q_{E_o} Bi((\frac{2m}{\hbar^2})^{\frac{1}{2}} (\frac{1}{e\Phi(t)})^\frac{3}{2} (V_o(t) + E_o - e\Phi(t)z)) \]

where \( \Phi \) and \( Q \) are defined as in section 3.3.1.

We then proceed to prove that this assumption yields a trial solution that satisfies Eq. 17.

we then take the Fourier transform of Eq. 19 to obtain:

\[ -E_o H(z, E_o) = -E_o \int g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt = -\frac{\hbar^2}{2m} \int \nabla^2 g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt + \int V_o(t) g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt - ez \int g_{E_o}(z, t) \Phi(t) e^{-i\frac{E_o}{\hbar}t} dt \]

Which is the same as:

\[ -E_o \int g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt = -\frac{\hbar^2}{2m} \int \nabla^2 (g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t}) dt + \int V_o(t) g_{E_o}(z, t) e^{-i\frac{E_o}{\hbar}t} dt - ez \int g_{E_o}(z, t) \Phi(t) e^{-i\frac{E_o}{\hbar}t} dt \]
Thus, becoming:

$$-E_o \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt = -\frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt + \int V_o(t)g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt - e\int g_{E_o}(z,t)\Phi(t)e^{-i\frac{E_o}{\hbar}t}dt$$

(20)

Since derivatives can be taken out of integrals.

If we proceed by applying the inverse Fourier transform to Eq. 18 it equates to Eq. 17. Therefore, since the left hand side of Eq. 20 equates to that of Eq. 18 if we apply the inverse Fourier transform to the right side of Eq. 20 and it equates to Eq. 17 our assumption yields a working trial solution for the wave function. Thus, we have found a set of solutions to the differential equation Eq. 17. And consequently, we have found a set of solutions to Eq. 18.

By manipulation of $F_{E_o}(t), Q_{E_o}(t)$, if we create a set of linearly independent solutions for Eq. 18, due to the fact that Eq. 18 is a second order ordinary differential equation and by the uniqueness theorem, we have found a general solution to Eq. 2. Applying the inverse Fourier transform to these solutions would give us a solution to Eq. 17. If the solutions are again linearly independent we obtain a general solution for Eq. 17 under specified boundary conditions for Eq. 18 for each $E_o$. This is because all physically relevant solutions to Eq. 17 are related to those of Eq. 18 by the corresponding Fourier transform, the maximum dimensionality in the basis set of physically relevant linearly independent solutions to Eq. 17 under specified boundary conditions is that of Eq. 18 which is 2 (see discussion in section 3.3.3 for proper meaning of physically relevant). Therefore, we have to choose $F_{E_o}(t), Q_{E_o}(t)$, carefully. Note: we do not necessarily find sets of linearly independent solutions for Eq. 18. If it is obvious we can directly find a set of linearly independent equations for Eq. 17. We apply the just stated procedure to verify if we have indeed found the general solution to Eq. 17:

Again, from Eq. 20 we obtain:

$$-E_o \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt = -\frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt + \int g_{E_o}(z,t)V_o(t)e^{-i\frac{E_o}{\hbar}t}dt - e\int g_{E_o}(z,t)\Phi(t)e^{-i\frac{E_o}{\hbar}t}dt$$

From the convolution theorem we obtain:

$$-E_o \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt = -\frac{\hbar^2}{2m} \nabla^2 \int g_{E_o}(z,t)e^{-i\frac{E_o}{\hbar}t}dt + \int g_{E_o}(z,t)V_o(t)e^{-i\frac{E_o}{\hbar}t}dt - e\int G_{E_o}(E_o - E')^* \tilde{\Phi}(E')dE'$$

where $G_{E_o}(E'), \tilde{\Phi}(E')$ are the Fourier transforms of the respective functions. Please note that $G_{E_o}(E')$ is really also a function of $z$ $G_{E_o}(E', z)$ but this is irrelevant for the analysis (for a given $z$ all the mathematical tricks and identities hold true). It is just notionally easier to write it this way.

Applying the inverse Fourier transform to this equation yields:

$$-\frac{1}{2\pi\hbar} \int \int E_o g_{E_o}(z,t)e^{-\frac{i}{\hbar}E_o(t-t')}dtdE_o = -\frac{1}{2\pi\hbar} \nabla^2 \int \int g_{E_o}(z,t)e^{-\frac{i}{\hbar}E_o(t-t')}dtdE_o$$

$$+\frac{1}{2\pi\hbar} \int \int G_{E_o}(E_o - E'')^* \tilde{V}_o(E'')e^{\frac{i}{\hbar}E_o(t-t')}dE'dE_o - \frac{1}{2\pi\hbar} e\int \int G_{E_o}(E_o - E')^* \tilde{\Phi}(E')e^{\frac{i}{\hbar}E_o(t-t')}dE'dE_o$$

(21)

where $t'$ is the time variable.

The last terms of the equation gives:

$$\frac{1}{2\pi\hbar} \int \int G_{E_o}(E_o - E')^* \tilde{\Phi}(E')e^{\frac{i}{\hbar}E_o(t-t')}dE'dE_o = \int \psi(t', z)e^{-\frac{i}{\hbar}E_o(t-t')} \tilde{\Phi}(E')dE' = \psi(t', z) * 2\pi\hbar \Phi(-t') = \psi(t', z) * \theta(t')$$

$$\frac{1}{2\pi\hbar} \int \int G_{E_o}(E_o - E'')^* \tilde{V}_o(E'')e^{\frac{i}{\hbar}E_o(t-t')}dE'dE_o = \int \psi(t', z)e^{-\frac{i}{\hbar}E_o(t-t')} \tilde{V}_o(E'')dE'' = \psi(t', z) * 2\pi\hbar V_o(-t') = \psi(t', z) * V_o(t')$$

We have used the identity that $\psi(t', z) = \frac{1}{2\pi\hbar} \int G_{E_o}(E_o)e^{\frac{i}{\hbar}E_o(t-t')}dE_o$ as defined and the shift property of the Fourier transform.
Noting that: 
\[ \psi(t', z) = \frac{1}{2\pi\hbar} \int g_{E_o}(z, t)e^{-i\frac{\hbar}{2m}(t-t')}dtdE_o = \frac{1}{2\pi\hbar} \int G_{E_o}(E_o)e^{i\frac{\hbar}{2m}(t')}dE_o \]
and after substituting this and 
\[ \dot{\psi}(t', z) = \frac{1}{2\pi\hbar} \int \frac{i}{2} E_o g_{E_o}(z, t)e^{-i\frac{\hbar}{2m}(t-t')}dtdE_o \] (property 1) into Eq. 21, the right and the left hand side of Eq. 21 are the same as Eq. 17. Thus, applying an inverse Fourier transform on Eq. 20 yields Eq. 17, verifying that we have found the general solution (note: \( t' = t \) used in Eq. 17, do not confuse with the \( t \) in the above derivation used as a variable of integration). In other words, Eq. 21 is:

\[ i\hbar \dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (V_0(t) - e\theta(t)z)\psi \]

Therefore,

\[ \psi(t', z) = \frac{1}{2\pi\hbar} \int \int g_{E_o}(z, t)e^{-i\frac{\hbar}{2m}(t-t')}dtdE_o \]

which can be integrated numerically.

For the exact same reasons as stated in section 3.3.1 we choose \( F_{E_o}, Q_{E_o} \) as being functions dependent only on \( E_o \).

It is physically relevant to use:

\[ V_o(t) = V_o - e^{\frac{3}{2}}\theta(t)^{\frac{3}{2}} \]

[7]

### 5.5 Emission From a Flat Thin Surface

This case is very simple. The tunnelling atoms at the surface become the “tip” atoms. The wavefunctions in the x and y coordinate are normal Bloch wavefunctions (the plane wavefunctions present without the effects of tunnelling). The z-wavefunction analysis is the same. The only difference is the fact that the x and y wavefunctions in region 2 are the same as in the bulk.
6 Summary

We have effectively shown that the analytic methods existing today in the scientific community for field emission need to be updated. There is a need to effectively develop the theory for both a complex band structure and a time-variant electric field. The applications of field emission technology warrant this development, as we could obtain time-resolved structural data on the femtosecond scale and on structures in the angstrom scale. In section 3, we derive the general solution to the wavefunction in the tunneling and emitted regions for a time-variant electric field. We then factor in specific boundary conditions to obtain the complete wavefunction. The boundary conditions are obtained from the band structure of the material itself and the procedure is outlined in section 4. Within this section, we also discuss additional effects such as time dependent effects in region 1 due to the electric field and how that can influence our calculations. Finally, we conclude with generalizing the method found in solving the Schrodinger equation for this system to solving the class of similar second order partial differential equations. We also find an analytic form for the solution to the Schrodinger equation with the imaging potential term. This is shown in Appendix II. Thus, we have obtained analytic solutions to all versions of the Schrodinger equation used in literature for the field emission phenomena.
7 Appendix I

We can estimate

\[ dk = \frac{dk_{xy}}{\cos \sigma} \]

where \( k_{xy} \) is the total momentum in the x-y plane and \( \sigma \) is the angle between the total momentum and the xy plane.

Now,

\[ \cos \sigma = \frac{k_{xy}}{k} \]

and the density of states, D.O.S in terms of the differential \( dk_{xy} \) becomes:

\[ D.O.S(k)dk_{xy} = \frac{1}{(2\pi)^2} \frac{1}{4} \frac{1}{2} (4\pi)k^2 \frac{dk_{xy}}{\cos \sigma} = \frac{1}{(2\pi)^2} \frac{1}{4} \frac{1}{2} (4\pi) \frac{k_{xy}^2}{\cos^3 \sigma} dk_{xy} \]

Now, the D.O.S in terms of xy-energy is:

\[ D.O.S(E_{total})dE_{xy} = \frac{1}{2(\pi)^2} \frac{1}{4} \frac{1}{2} \frac{1}{2} \frac{1}{2} (\frac{2m^*}{\hbar^2})^\frac{3}{2} \frac{1}{4} \frac{1}{2} \frac{1}{2} \frac{1}{2} E_{total}^\frac{3}{2} dE_{xy} \]

And,

\[ \frac{D}{D.O.S} = \frac{1}{\sqrt{\frac{1}{2}(\pi)^2} \frac{1}{2} \frac{1}{2} \frac{1}{2} (\frac{2m^*}{\hbar^2})^\frac{3}{2} \frac{1}{4} \frac{1}{2} \frac{1}{2} \frac{1}{2} E_{total}^\frac{3}{2} E_{xy}^\frac{3}{2} \}

Where, we state again as a reminder:

\[ E_{total} = E_{xy} + E_z \]

Now, since the integral is carried out to the maximum energy, the \( E_{xy} \) term starts dominating and we obtain:

\[ \frac{D}{D.O.S} = \frac{1}{\sqrt{\frac{1}{2}(\pi)^2} \frac{1}{2} \frac{1}{2} \frac{1}{2} (\frac{2m^*}{\hbar^2})^\frac{3}{2} \frac{1}{4} \frac{1}{2} \frac{1}{2} \frac{1}{2} E_{total}^\frac{3}{2} E_{xy}^\frac{3}{2} \}

which is what we have already. Thus, the difference is negligible. However, for a better result, one should use the ratio derived in this appendix whenever we have this ratio in the integral over the differential \( dE_{xy} \).
8 Appendix II

To find the solution to the Schrodinger equation defined by:

\[ V(z) = E_F + \xi - eF_o z - \frac{e^2}{4z} \]

We apply the same procedure as outlined in section 3.3.1 and 7.3. We swap \( z \) for \( t \) and \( E \) for \( E_o \) and solving this potential becomes almost trivial. \( F_o \) is a DC electrical field.

The symbol \( \nabla_t \) denotes a derivative w.r.t to time.

Now, we have from the time-dependent Schrodinger equation:

\[ i\hbar \nabla_t \psi(z,t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(z,t) + V_o \psi(z,t) - eF_o z \psi(z,t) - \frac{e^2}{4z} \psi(z,t) \]

We define the spatial Fourier transform as:

\[ \psi(z,t) = \left( \frac{1}{2\pi} \right) \int_{-\infty}^{\infty} H(t,k)e^{ikz}dk \]

(inverse Fourier transform) and

\[ H(t,k) = \int_{-\infty}^{\infty} \psi(z,t)e^{-ikz}dz \]

(Fourier transform). Where \( H(t,k) \) is the Fourier amplitude at the given wavevector, \( k \), and time.

Now, we assume:

\[ H(t,k) = \int_{-\infty}^{\infty} g_k e^{-ikz}dz \]

with,

\[ -\frac{\hbar^2}{2m} k^2 g_k(t,z) = i\hbar \nabla_t g_k - V_o g_k + eF_o l(z)g_k + f(z)g_k \] (22)

And \( l(z) = -2\pi z \), \( f(z) = -2\pi \frac{e^2}{4z} \).

The general solution of \( g_k \), i.e., the two linearly independent solutions are:

\[ g_k = C(k,z)e^{\frac{i\hbar z^2}{2m} - V_o + eF_t l(z) + f(z)t} + D(k,z) \]

where \( C \) and \( D \) are functions over \( kz \). We already know that if we take \( C \) and \( D \) as only depending on \( k \) we have to linearly independent solutions, and thus, thats all thats necessary (by the same arguments as in 3.3.1).

Now, we know from the convolution theorem, the identities for \( \psi \) concerning the spatial Fourier transforms and the method present in section 3.3.1 and 5.3 that Eq. 22 will transform into the Schrodinger equation stated in the beginning of this Appendix. Thus, the general solution for \( \psi(z,t) \) becomes:

\[ \psi(z,t) = \frac{1}{2\pi} \int \int g_k e^{-ik(z-z')}dzdk \]
Where \( z' \) is the position. Now, using the identity: 
\[
E[k] = -\frac{\hbar^2 k^2}{2m} + V_o
\]
we have:
\[
\psi(z, t) = \frac{1}{2\pi} \int e^{-iE[k]t} \int [C(k) e^{i[\epsilon F_o(z) + f(z)]t} + D(k) e^{iE_o t}] e^{-ik(z-z')} dz dk
\]

If there is no choice of C, D for which the above integral exists, than there are no spatially bound solutions or solutions that have momentum representations. The only solutions that remain are ones that remain spatially unbound. For many applications, this means only unphysical solutions would remain. In the above integral \( f(z) \) explodes at \( z = 0 \). If we recall that \( C(k) \) can also be a function of \( z \) and if we define it as not varying with \( z \) except for being zero at \( z = 0 \) and/or values around that point, with the proper choice of D we overcome this problem. Note, our choices of C and D have to also create a wavefunction that has an energy representation in order for it to be physically relevant.

Let us choose \( D(k) = D_o \) where \( D_o \) is a constant and \( C(k) = -\frac{\hbar^2}{m} k C_o (\frac{-\hbar^2 k^2}{2m} + V_o) \) Where \( C_o \) is a function of \( k \). It is easy to see that under this choice we have two linearly independent solutions to the Fourier spatial amplitude (whose basis set dimension is 2). Also we have two linearly independent solutions to the wavefunction that have energy representations. Therefore, we have a physically relevant general solution under validating boundary conditions.

Under this choice the wavefunction becomes:
\[
\psi(z, t) = \frac{1}{2\pi} \int e^{-iEo t} \int [C_o(E) e^{i[\epsilon F_o(z) + f(z)]t}] e^{-i(k-z') dz dE} + D_o
\]

Where we recover \( D_o \) by the fact that we applied a Fourier transform and then its inverse. This is the general wavefunction for a specific case of boundary conditions to illustrate the point that we have a separate energy term (thus, the boundary conditions that is used for each energy can easily apply to solving for each C and D and we have the most specific wavefunction possible). We choose specific linearly independent solutions to obtain more experimentally relevant general solutions, for example, keeping \( D \) as a function of \( k \) (or \( D \) as a function with the same form as \( C(k) \), etc.). We could use this method in sync with that in section 3.3.1. Also, we could use this method instead of section 3.3.1 if we know the solution to the time differential equation given a pulse profile. They are alternate methods.
References


Additional References: