SOLUTION OF THE TIME DEPENDENT SCHRÖDINGER EQUATION LEADING TO THE FOWLER-NORDHEIM ELECTRON EMISSION

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Abstract. We solve the time-dependent Schrödinger equation describing the emission of electrons from a metal surface by an external electric field E, turned on at $t=0$. Starting with a wave function $\psi(x,0)$, representing a generalized eigenfunction when $E=0$, we find $\psi(x,t)$ and show that it approaches, as $t\to\infty$, the Fowler-Nordheim tunneling wavefunction ψ_E. The deviation of ψ from ψ_E decays asymptotically as a power law $t^{-\frac32}$. The time scales involved for typical metals and fields of several V/nm are of the order of femtoseconds.

1. Introduction

The emission of electrons from a cold metal surface subjected to a constant (or oscillating) electric field is a subject of great practical and theoretical interest [Je18, Fo16, Je17]. The microscopic theory of such emissions by a constant field was developed by Fowler and Nordheim (FN) in the early days of quantum mechanics [FN28]. They considered an idealized situation in which the electrons in the conduction band are treated, a la Sommerfeld, as free independent particles. Their energies are described by a Fermi distribution with maximum energy $E_F=\hbar^2k_F^2/2m$; the deviation from this zero-temperature distribution is negligible at room temperatures. In the absence of an external field the electrons are confined by an external potential (caused by the positive ions) of magnitude $U=E_F+W$, where W is the work function, i.e. the energy necessary to extract an electron from the metal.

Considering emissions perpendicular to a flat surface at $x=0$, obtained when applying an external field E for $x\geqslant 0$, assuming that the metal occupies all space $x<0$, leads to a one-dimensional

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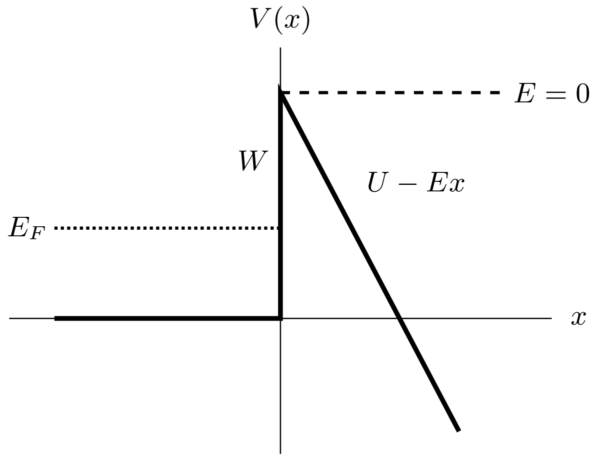

FIGURE 1. The shape of the potential $V(x)$.

tunneling problem in a triangular potential, see figure 1. The one-dimensional Schrödinger equation describing a free electron is then given by

$$i\frac{\partial \psi(x,t)}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \tag{1.1}$$

where

$$V(x) = \begin{cases} 0, & x < 0 \\ U - Ex, & x > 0 \end{cases} \tag{1.2}$$

in units $\hbar = 2m = |e| = 1$.

When $E = 0$, the potential is, simply, a step function. The Schrödinger equation (1.1) has generalized 'stationary' solutions with energies $k^2 < U$, $\psi(x,t) = e^{-ik^2 t}\psi_0(x)$, with $k > 0$ and

$$\psi_0(x) = \begin{cases} e^{ikx} + R_0 e^{-ikx} & x < 0 \\ T_0 e^{-\sqrt{U-k^2}x} & x > 0 \end{cases} \tag{1.3}$$

in which R_0 and T_0 are the *reflection* and *transmission* coefficients (we use a normalization in which the amplitude of the incoming wave with $k > 0$ is 1):

$$R_0 = \frac{ik + \sqrt{U-k^2}}{ik - \sqrt{U-k^2}}, \quad T_0 = \frac{2ik}{ik - \sqrt{U-k^2}}. \tag{1.4}$$

These constants ensure that $\psi_0(x)$ and $\partial\psi_0(x)$ are continuous at $x = 0$. Note that, in this state, the current vanishes:

$$j_0(x) = i(\psi_0 \partial_x \psi_0^* - \psi_0^* \partial_x \psi_0) = 0. \tag{1.5}$$

When $E > 0$, there is the possibility for an electron moving in the $+x$ direction, with kinetic energy $k^2 < U$, to tunnel through the potential barrier and be emitted. This will then produce an electron current in the $+x$-direction. To obtain the probability of tunneling, FN computed the generalized stationary solutions $\psi(x,t) = e^{-ik^2 t}\psi_E(x)$ of the Schrödinger equation (1.1) with the potential given in (1.2):

$$\psi_E(x) = \begin{cases} e^{ikx} + R_E e^{-ikx} & x < 0 \\ T_E \Phi(x) & x > 0. \end{cases}, \quad k > 0 \tag{1.6}$$

in which $\Phi(x)$ is proportional to the Airy function $\mathrm{Ai}(x)$ (or the equivalent expression in terms of Hankel or Bessel functions), which decays when $x \to \infty$, and yet has a constant positive current for all x. This solution, see also [Ro11], [Je18] yielded the tunneling probability $D(k) = 1 - |R_E|^2$ of the electron as a function of k, U and E. Integrating $kD(k)$ over the "supply function" corresponding to the density of electrons in the Fermi sea moving in the $+x$ direction with energy k^2, leads to an expression for the total steady state current j_E in a static field E. An approximate expression for j_E is [Fo08b, Je17]

$$j_E \approx c_1 E^2 e^{-\frac{c_2}{E}}. \tag{1.7}$$

The FN formula for j_E, with various corrections for the idealizations made, e.g. flat surface, independent electrons, neglect of Schottky effect, etc, serves as the backbone of cold electron emission theory and experiment. There is a vast literature on the subject (the original FN paper [FN28] has more than 6000 citations). We cite here only a few [Ro11, Fo08] and refer the reader for more information to the recent book by Jensen [Je17] and references there.

In this note we shall be concerned with a different problem, which, as far as we know, has not been investigated fully before, see, however, Yalunin et.al. [Ya11]. As an initial condition, we take a generalized stationary solution of the Schrödinger equation at $E = 0$, $\psi_0(x)$ in (1.3), and, at $t = 0$, we turn the field on, and study the time evolution. In particular, we will investigate how long it will take, if ever, for the initial state $\psi(x, 0)$ to approach the stationary state $\psi_E(x)$ in (1.6). Of course, turning on E instantaneously is an idealization, which we shall accept here.

In what follows, we shall prove that, for $\psi(x, 0) = \psi_0(x)$, $\psi(x, t)$ approaches, for long times, the $\psi_E(x)$ of (1.6), i.e.,

$$\psi(x,t) \sim e^{-ik^2 t}\psi_E(x) \tag{1.8}$$

In fact, this is still true if one takes $\psi(x, 0) = \psi_0(x) + f(x)$ where $f(x)$ is square integrable. This follows from the RAGE theorem [Ru69, AG73, En78], since the spectrum of the Hamiltonian in (1.1) is absolutely continuous. The deviation $\psi(x, t) - \psi_E(x)$ goes asymptotically as $t^{-\frac{3}{2}}$. The actual time dependence, of course, depends on the exact form of $\psi(x, 0)$. We shall calculate this for the $\psi(x, 0) = \psi_0(x)$ given in (1.3) for different values of the parameters.

Roughly speaking we find that for $U \approx 9$ eV, $\hbar^2 k^2/2m = E_F \approx 4.5$ eV and $E \approx$ 14-26 $\mathrm{V \cdot nm^{-1}}$, the time for the current $j(t)$ to approach closely its final FN value is of the order of femtoseconds, see Fig 3-6. The exact value depends on the position x where we measure the current: for larger x, the time it takes for the current to equilibrate is larger. These time scales are of practical relevance for short pulses of a few femtoseconds or less. These are now common for oscillating laser fields for which the initial value problem will be considered in a later paper. (The "steady state" solution for laser fields was investigated in detail by Faisal et al [Fa05]; see also [Zh16].)

2. Solution of the initial value problem

In order to emphasize the role of each term in the initial condition, we will split $\psi(x, 0)$ into three terms: an incoming, a reflected, and a transmitted wave.

$$\psi(x,0) = \psi^{(\mathrm{I})}(x,0) + \psi^{(\mathrm{R})}(x,0) + \psi^{(\mathrm{T})}(x,0) \tag{2.1}$$

with

$$\psi^{(\mathrm{I})}(x,0) = \Theta(-x)e^{ikx}, \quad \psi^{(\mathrm{R})}(x,0) = R_0\Theta(-x)e^{-ikx}, \quad \psi^{(\mathrm{T})}(x,0) = T_0\Theta(x)e^{-\sqrt{U-k^2}x}, \quad k > 0. \tag{2.2}$$

To obtain $\psi(x, t)$ we will first solve for $\hat{\psi}_p(x)$, the Laplace transform of $\psi(x, t)$, which we will obtain in closed form. We will then compute, by inverting the Laplace transform, the long time asymptotics analytically, and the short time behavior numerically. This method gives exact results which can be computed with high accuracy. It is thus better for our purposes than direct computations of the solution of(1.1). The latter requires cutoffs for the non-square integrable functions we are dealing with and cannot be used for long times. The Laplace transform of ψ is

$$\hat{\psi}_p(x) := \int_0^\infty dt\ e^{-pt}\psi(x,t) \tag{2.3}$$

It satisfies the equation

$$(-\partial_x^2 + \Theta(x)(U - Ex) - ip)\hat{\psi}_p(x) = -i\psi(x,0). \tag{2.4}$$

We solve this equation:

$$\hat{\psi}_p(x) = \begin{cases} C_1(p)e^{\sqrt{-ip}x} + F_p^{(\mathrm{I})}(x) + R_0 F_p^{(\mathrm{R})}(x) & \text{if } x < 0 \\ \\ C_2(p)\varphi_p(x) + T_0 F_p^{(\mathrm{T})}(x) & \text{if } x > 0 \end{cases} \tag{2.5}$$

where R_0 and T_0 are given in (1.4),

$$F_p^{(\mathrm{I})}(x) := -\frac{ie^{ikx}}{-ip + k^2}, \quad F_p^{(\mathrm{R})}(x) := -\frac{ie^{-ikx}}{-ip + k^2} \tag{2.6}$$

$$F_p^{(\mathrm{T})}(x) := 2\pi\left(\varphi_p(x)\int_0^x dy\ \eta_p(y)e^{-\sqrt{U-k^2}y} + \eta_p(x)\int_x^\infty dy\ \varphi_p(y)e^{-\sqrt{U-k^2}y}\right) \tag{2.7}$$

and

$$\varphi_p(x) = \mathrm{Ai}\left(e^{-\frac{i\pi}{3}}\left(E^{\frac{1}{3}}x - E^{-\frac{2}{3}}(U - ip)\right)\right), \quad \eta_p(x) = e^{-\frac{i\pi}{3}}\mathrm{Ai}\left(-\left(E^{\frac{1}{3}}x - E^{-\frac{2}{3}}(U - ip)\right)\right) \tag{2.8}$$

are the two solutions of $(-\partial_x^2 + U - Ex - ip)f = 0$. They both decay as $x^{-\frac{1}{4}}$ when $x \to \infty$ and have the correct behavior for large p. The phases $e^{-\frac{i\pi}{3}}$ and -1 are cube roots of -1. The constants $C_1(p)$ and $C_2(p)$ are set so that $\hat{\psi}_p$ and $\partial\hat{\psi}_p$ are continuous at $x = 0$:

$$C_1(p) = -\frac{iT_0}{\sqrt{-ip}\varphi_p(0) - \partial\varphi_p(0)}\left(\frac{\sqrt{U-k^2}\varphi_p(0) + \partial\varphi_p(0)}{-ip + k^2} + \int_0^\infty dy\ \varphi_p(y)e^{-\sqrt{U-k^2}y}\right) \tag{2.9}$$

and

$$C_2(p) = -\frac{iT_0}{\sqrt{-ip}\varphi_p(0) - \partial\varphi_p(0)}\left(\frac{\sqrt{U-k^2} + \sqrt{-ip}}{-ip + k^2}\right.$$
$$\left. -2i\pi(\sqrt{-ip}\eta_p(0) - \partial\eta_p(0))\int_0^\infty dy\ \varphi_p(y)e^{-\sqrt{U-k^2}y}\right). \tag{2.10}$$

The square root is defined with a branch cut along the positive imaginary axis, in such a way that $\sqrt{-ip}$ has a branch cut along the real negative axis.

A simple calculation shows that, as expected,

$$\lim_{\substack{|p|\to\infty \\ \mathcal{R}e(p)>0}} p\hat{\psi}_p(x) = \psi(x,0) \tag{2.11}$$

which confirms that $\hat{\psi}_p(x)$ is, indeed, the Laplace transform of a function whose initial condition is $\psi(x,0)$. We then invert the Laplace transform:

$$\psi(x,t) = \frac{1}{2i\pi}\int_{\gamma-i\infty}^{\gamma+i\infty} dp\ e^{pt}\hat{\psi}_p(x) \tag{2.12}$$

in which $\gamma > 0$ is an arbitrary small parameter taken close to 0.

As is well known the integral on the right hand side of (2.12) can be computed by studying the singularities, poles and branch points of $\hat{\psi}_p(x)$, lying in the half plane $\mathcal{R}e(p) \le 0$. In particular,

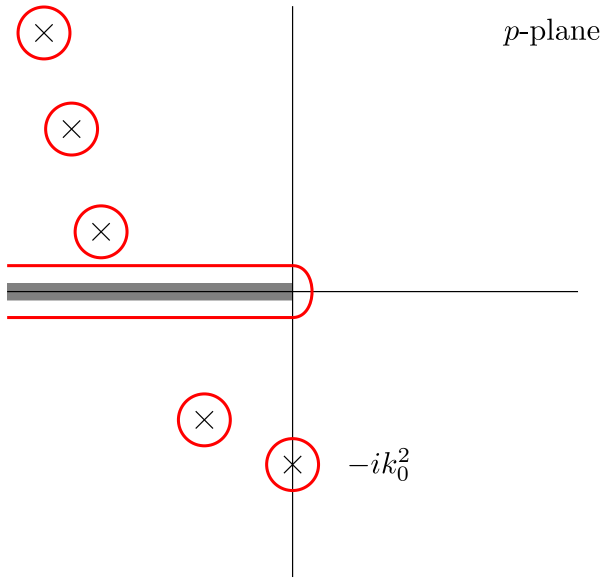

FIGURE 2. The deformed integration contour goes around the poles (one of which is on the imaginary axis, at $-ik^2$, while the others are in the negative real half-plane) and goes along the branch cut on the real negative axis.

the only terms which do not decay as $t \to \infty$ come from poles on the imaginary p-axis. Analyzing-(2.5)-(2.10) we find that the singularities of $\hat{\psi}_p(x)$ are, for $k > 0$,

- a pole on the imaginary axis, located at $-ik^2$, coming from (2.6), (2.10) and (2.11)
- poles with strictly negative real parts corresponding to the roots of $\sqrt{-ip}\varphi_p(0) - \partial\varphi_p(0)$ appearing in the denominators of C_1 and C_2,
- a branch cut along the negative real axis coming from $\sqrt{-ip}$.

We deform the integration contour as in figure 2. The residues of the poles with a negative real part decay exponentially in time (because of the factor e^{pt} in (2.12)). The integral along the branch cut yields, by Taylor expansion, a term which decays as $t^{-\frac{3}{2}}$. Finally, the residue at $-ik^2$ yields the only term which does not decay in time. All in all, we find that

$$\psi(x,t) = e^{-ik^2 t}\psi_E(x) + \left(\frac{t}{\tau_E(x)}\right)^{-\frac{3}{2}} + O(t^{-\frac{5}{2}}). \tag{2.13}$$

where ψ_E is the FN solution (1.6) and

$$\tau_E(x) = \begin{cases} (c_E(\varphi_0(0) + x\partial\varphi_0(0)))^{\frac{2}{3}} & \text{if } x < 0 \\ (c_E\varphi_0(x))^{\frac{2}{3}} & \text{if } x > 0 \end{cases} \tag{2.14}$$

with

$$c_E = -\frac{T_0 e^{\frac{i\pi}{4}}}{2\sqrt{\pi}(\partial\varphi_0(0))^2}\left(\frac{\sqrt{U-k^2}\varphi_0(0) + \partial\varphi_0(0)}{k^2} + \int_0^\infty dy\ \varphi_0(y)e^{-\sqrt{U-k^2}y}\right). \tag{2.15}$$

Therefore, the wave function tends to the Fowler-Nordheim solution, with a rate $t^{-\frac{3}{2}}$.

Concluding Remarks.

1. All the contributions which do not decay as $t \to \infty$ come from the incident wave $\psi^{(I)}(x,0)$. There are no poles on the imaginary axis coming from the other parts of $\psi(x,0)$. In fact, as already

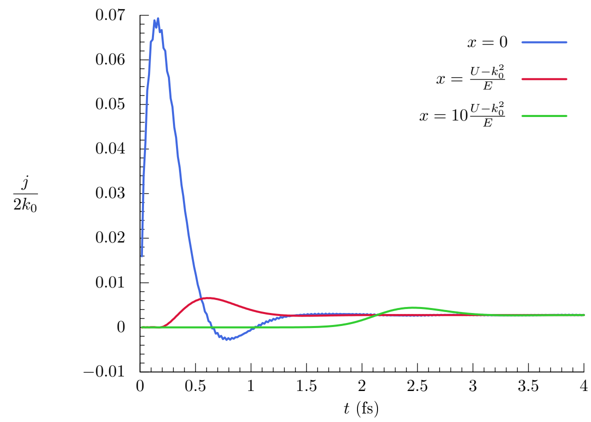

FIGURE 3. $E = 14V \cdot \mathrm{nm}^{-1}$, $x_0 = \frac{U - k^2}{E} = 4.5/14\,\mathrm{nm}$.

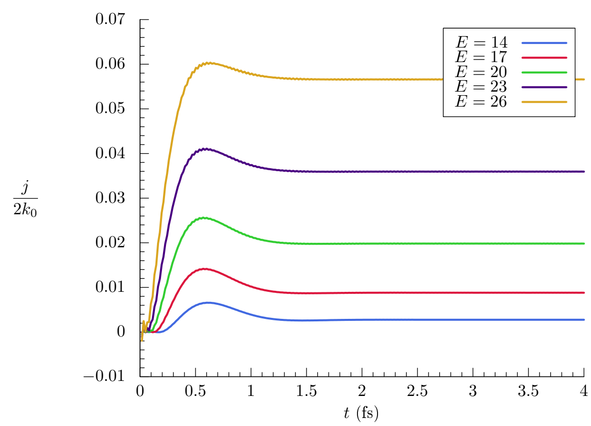

FIGURE 4. $x = 4.5/E$ nm.

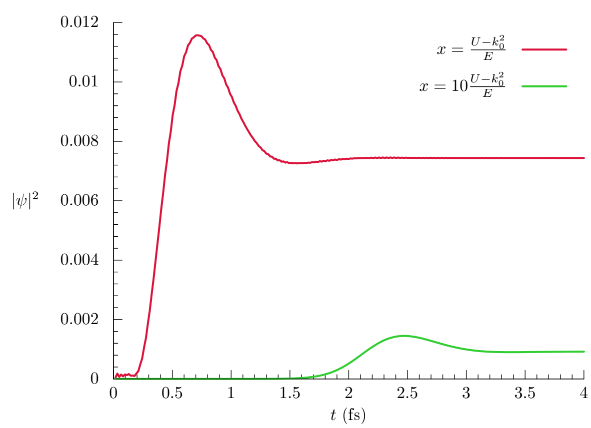

FIGURE 5. $E = 14\,V/\mathrm{nm}$, $x = 0.321\,\mathrm{nm}$.

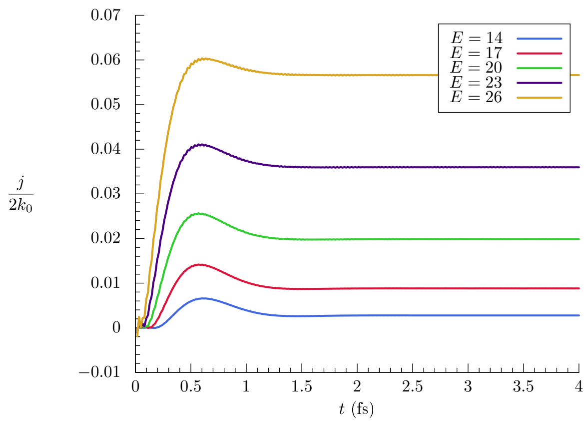

FIGURE 6. $x = 4.5/E$ nm.

noted, the asymptotic value of $\psi(x,t)$ would be unchanged if we added any square-integrable function to the initial condition. Furthermore the asymptotics would be unchanged if we added a wave moving away from the origin (e.g. a term e^{-ik_1x} with $k_1 > 0, x < 0$ or e^{ik_1x} with $k_1 > 0, x > 0$).

2. While the time scale of the approach to the FN solution is clearly of order of femtoseconds we have not attempted to compute a "tunneling time". This is, as is well known, a tricky business, with many definitions [Landauer & Martin [La94], Landsman & Keller [Lan15]]. Defining such a time in terms of the approach of the initial state to some steady state was investigated by McDonald et. al. [Mc13], see also [Pf95].

3. We are currently analyzing the initial value problem for the case of oscillating laser fields. The corresponding "steady state" problem was studies by Faisal et. al. [Fa05].

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