Transport, Tunneling, and Trajectories: Modeling Emission from Surfaces with Structure

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***Abstract*—The manner by which photo-assisted field-emitted electrons are generated, the impact of delays associated with transport to the surface, emission through and over emission barriers, and the time scales associated with accompanying tunneling / fly-over processes is complicated by conditions associated with emission from realistic surfaces. Recently studies treating transport to and emission past non-linear and resonant/reflectionless potentials motivate consideration of analytic models to be used to assess and compare characteristic time scales associated with transport to the surface, emission over and through surface wells and barriers (heterostructures), and tunneling. The formulation allows for an investigation of time-dependent effects for a class of analytically solvable models. The methods are intended to be useful for the investigation of tunneling and transmission associated with field and photoemission at short time scales.**

I. Introduction

Phenomena in narrow anode-cathode gaps are a problem of increasing importance in nanoscale studies treating quantum tunneling and time dependent behavior for field and photoemission [1]. When anode-cathode gaps are comparable to tunneling distances, or when emitter curvature is such that changes to the tunneling path are consequential [2], [3], [4], then the reliability of conventional 1D equations of electron emission (*e.g.*, Fowler Nordheim equation for field emission) are affected. The canonical electron emission equations are based on the evaluation of transmission and reflection coefficients and probabilities, which are standard problems in quantum mechanics and allow for the evaluation of current, but the problem of the time associated with tunneling remains problematic, and likely even more so for curved tunneling trajectories. For the purposes of modeling electron emission at very short time scales for the prediction of beam properties, where other processes like delayed emission after photoexcitation [5], then a trajectory interpretation that accounts for features associated with tunneling (multidimensionality and tunneling time being particularly important) is useful to develop. Progress to that end shall be presented and discussed.

An analytical model to be developed herein is based on waves incident on a Dirac delta function potential $V(x) = \Gamma\delta(x)$, where Γ governs the strength of the potential, as it provides a basis for finding a tractable Wigner distribution function. With modifications, the solutions can be used to investigate field penetration effects into a barrier and responses to sudden changes in barrier height (as would accompany the sudden application of an applied field). The demonstration of the methods are undertaken with the simplest potential profiles first so as to establish methods and quantify their behavior. The associated Wigner trajectories are presented. Afterwards, a generalization of the wave functions for modifications to the barrier, and how those wave functions evolve after sudden changes in the potential, are explored.

II. Delta Barrier Model

The one-dimensional (1D) Schrödinger's equation for a Dirac delta function potential with $\Gamma \equiv \hbar^2\gamma/2m$ becomes

$$\partial_x^2\psi(x) = \left\{\gamma\delta(x) - k^2\right\}\psi(x) \tag{1}$$

Solutions are (where an a subscript refers to the region to the left ($x < 0$) of the origin, and b to the right ($x > 0$))

$$\begin{aligned}\psi(x<0) &\equiv \psi_a(x) = Ae^{ikx} + Be^{-ikx} \\ \psi(x>0) &\equiv \psi_b(x) = A'e^{ikx} + B'e^{-ikx}\end{aligned} \tag{2}$$

Consider a box with infinite barriers at $x = \pm L/2$ with a δ-function potential at the origin: such a system is closed (no current J) and has discrete energy levels. It entails $|A|^2 - |B|^2 = |A'|^2 - |B'|^2 = 0$, satisfied by $B = Ae^{i\phi}$, $B' = A'e^{i\varphi'}$. The boundaries $\psi_a(-L/2) = \psi_b(L/2) = 0$ entail $\phi = -kL + \pi$ and $\phi' = kL + \pi$. Integrating Schrödinger's Eq. from $x = 0^-$ to $x = 0^+$ results in

$$(2k + i\gamma)e^{-ikL} + (-2k + i\gamma)e^{ikL} - 2i\gamma = 0 \tag{3}$$

The conditions result in $\psi_a(x) = 2\sin(k_j x)$ where the normalization is over the cell size $(L/2)$.

III. Wigner Function

The density $\rho(x)$ for the well is given by

$$\frac{\rho(x)}{\rho_o} = \frac{3}{n^3}\sum_{n=1}^{N}(N^2 - n^2)\left[\sin(2\pi nx/L)\right]^2 \tag{4}$$

where $(N^2 - n^2)$ is from the discrete version of the supply function, and where $k_N \equiv k_F$ is the energy of the highest filled level and corresponds to $k_F = \sqrt{2m\mu}/\hbar$, where μ is the

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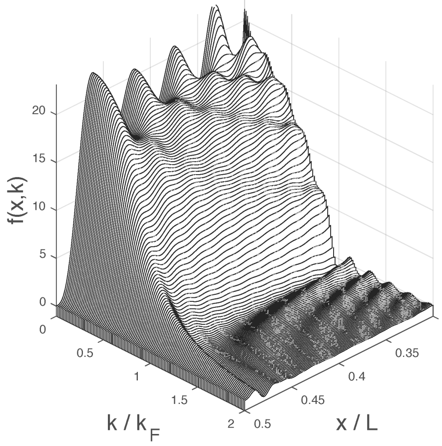

Fig. 1. Close-up of $f(x, k)$ showing the region nearest $x = L/2$.

chemical potential (or Fermi level at $T = 0$ K). Adopting the notation $\psi_n(x) \equiv \langle k_n | x \rangle$, then

$$\rho(x) = \sum_{n=1}^{N} f(k_n) \left| \langle k_n | x \rangle \right|^2 = \langle x | \hat{\rho} | x \rangle \tag{5}$$

where the density matrix $\hat{\rho}$ is defined by $\hat{\rho} \equiv \sum_{n=1}^{N} f_n |n\rangle \langle n|$. The Wigner distribution function (WDF) is obtained from the density matrix $\hat{\rho}$ by

$$f(x, k) \equiv 2 \int_{-\infty}^{\infty} dy\ e^{2iky} \langle x + y | \hat{\rho} | x - y \rangle \tag{6}$$

The Wigner function behaves much like a classical distribution, *e.g.*, the density is the first moment of the Wigner distribution, but the non-local features of quantum mechanics are made manifest in the kets $|x \pm y\rangle$ on which $\hat{\rho}$ operates. Analogous "quantum trajectories" are defined by relating the time evolution of a WDF to the classical phase space $f_c(x, t)$ defined by $\partial_t f_c + \dot{x}\partial_x f_c + \dot{k}\partial_k f_c$ if $\dot{x}$ and $\dot{k}$ are defined by the relation to the quantum version. The Wigner function and its associated trajectories are shown in Figures 1 and 2. The sudden removal of the barrier region to the right of the origin results in a time evolution of the density shown in Figure 3. The methodology behind these calculations will be described in the presentation.

IV. Summary

The groundwork for the evaluation of Wigner trajectories using analytic wave functions associated with 1D wells with infinite barriers and delta function barriers is described. For such simple systems, the trajectories are associated with the contour lines of $f(x, k)$, thereby allowing transit times to be evaluated. Modifications to the wave functions associated with multiple delta function barriers, and with a finite rightmost barrier, are discussed. The effects on density $\rho(x)$ are shown. The analytical model allowed for the consideration of the consequences of a sudden potential change wherein the region between $0 < x < L/2$ becomes accessible. The methods,

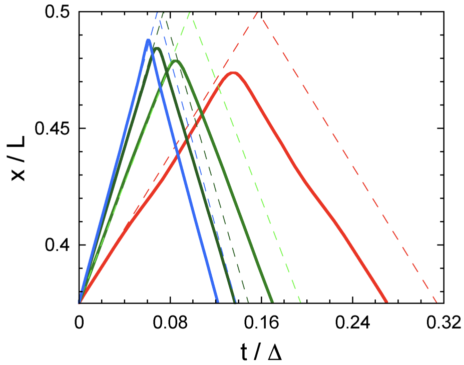

Fig. 2. Trajectories associated with Figure 1. Dashed lines are "classical".

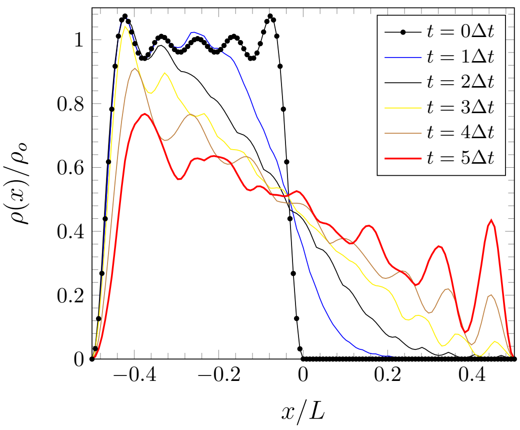

Fig. 3. First 6 steps after sudden change $V(0 < x < L/2) \to 0$, for $N = 6$.

having been established, are to be used for the investigation of more realistic barriers associated with field and photoemission separately.

Acknowledgment

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