A Delta Barrier In a Well And Its Generalization For Emission Studies

Kevin Jensen[1], Jeanne M. Riga[2], Andrew Shabaev[3],
Michael Osofsky[4], Joseph Prestigiacomo[3], John Petillo[1]
[1]Leidos, Tewksbury, MA; [2]Air Force Research Laboratory, Albuquerque, NM
[3]Naval Research Laboratory, Washington, DC; [4]Towson University, MD

Day 2 - 1:55-2:20 PM Wednesday Oct 4, 2023
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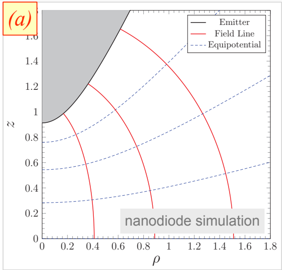
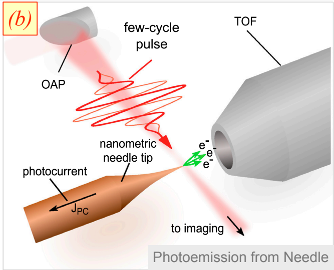
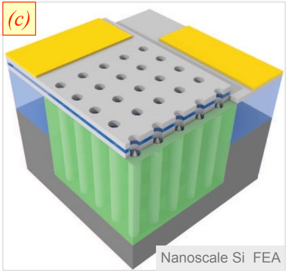
Sections Outline

Background







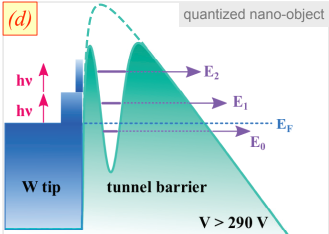
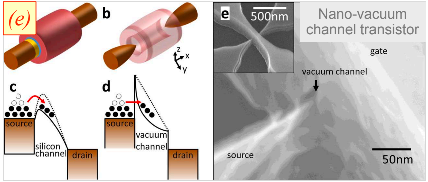


FIG. S17: Energy band diagram of tunneling barrier with a quantum dot



(*a*) Jensen et al., JAP122(6), 064501 (2017)
(*b*) Schötz et al., Nanophotonics (2021)
(*c*) Rughoobur et al., Nanotechnology 31, 335203 (2020).
(*d*) Duchet, et al., ACS photonics 8, 505 (2021)
(*e*) Han et al., Nano letters 17(4), 2146-2151 (2017)

Need for δ-function Model

Quantum Mechanics poses challenges to simulating ultra-fast and ultra-small emission conditions:

- e^- tunneling into a nanogap $\neq$ instantaneous
- e^- have a wave-behavior $\lambda = 2\pi\hbar/mv = 2\pi/k$
- non-trivial eigenstates for general barriers

δ-function barrier: agile model for charge transport

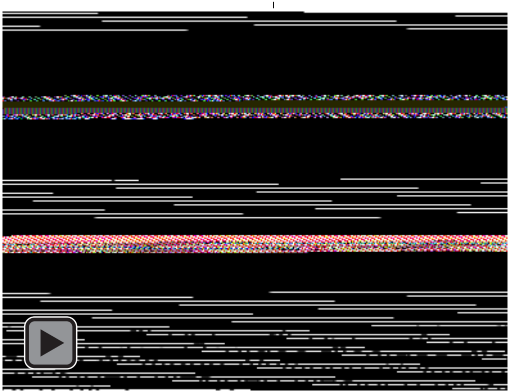
- Single parameter model (γ = strength parameter)

$$V_\delta(x) = \frac{\hbar^2}{2m}\gamma\delta(x) \quad (1)$$

- Simple analytic transmission probability

$$t(k) = \frac{2k}{2k + i\gamma}; \quad D(k) = |t(k)|^2 \quad (2)$$

Time-dependent Gaussian wave packet incident on δ-barrier (center)



Has application to specific problems of technological interest: Consider four examples

Applications of δ-function Model

1. Modeling photoemission from e.g., GaAs, includes high and thin barrier at surface attributed to a submonolayer coating of cesium
2. Time evolution of Schrödinger equation with δ-function barrier: slow down of wave packet motion measured by transmission and reflection delay (TARD) time (paradoxical for zero-thickness barrier)
3. $I(V)$ characteristics of normal-superconducting (NS) point contacts: transition from metallic to superconducting governed by γ; able to describe crossover from metallic to small-area tunnel-junction behavior, address current and charge imbalance processes to describe quasiparticle scattering at normal-superconducting (NS) interface. For normal state, transmission probability

$$D(k_F) = \frac{1}{1+Z^2} \qquad Z \equiv \frac{\gamma}{2k_F} \tag{3}$$

$\hbar k_F$: Fermi momentum; δ-function barrier = elastic scattering at NS interface; accounts for NS microconstriction (point contact)

4. Interest in conduction, transport, and/or thermal-field emission when barriers or wells have a time dependent behavior: using steady state emission equations may be insufficient. Physics of tractable models give means to examine methods argued to be appropriate for more complex configurations.

Modification of δ-function Model: Place in Well

Tunneling and reflection delay (TARD) model: trajectory interpretation akin to Bohm trajectories

Analytical model of Well + Barrier

$$V(x) = \frac{\hbar^2}{2m}\left[k_w^2 \Theta(x^2 - L^2) + \gamma \delta_l(x)\right] \qquad (4)$$

where $k_w \rightarrow \infty$, $\Theta(s)$ is Heaviside step function, and $\delta_l(x) \rightarrow \delta$-function in limit barrier width $l \rightarrow 0$.

Wave function $\Psi(x,t) = Re^{iS}$
where $R(x,t)^2 \equiv \rho(x,t) =$ density from linear superposition of $\psi_n(x,t)$

Quantum Potential $\Omega(x)$

$$\Omega(x,t) \equiv -\frac{\hbar^2}{2mR(x,t)} \frac{d^2}{dx^2} R(x,t) \qquad (5)$$

- Width L of enclosing well modest to visualize differences due to $\delta_l(x)$
- Impact on time evolution examined & compared to δ-function limit
- $\Psi(x,t) = \sum C_n \psi_n(x,t)$: exact time evolution possible for eigenstates
- Finding $\psi_n(x,t), t(k)$ requires exact k_n for $\pm$ parity eigenstates

Sections Outline

Parameterization

- $\hbar^2 k_o^2/2m$: height of barrier in well

$$V(x) \equiv \frac{\hbar^2 \gamma}{2m}\delta(x) \tag{6}$$

- Gamow term $\theta(k)$ for $E = \hbar^2 k^2/2m$:

$$\theta(k) \equiv 2\, l\, \kappa(k) \equiv 2\, l \sqrt{k_o^2 - k^2} \tag{7}$$

Gamow factor: if $\theta \approx$ constant as $\varepsilon \to 0$, then δ-function sequence demands

$$k_o^2 = \frac{\gamma L}{\varepsilon^2} \tag{8}$$

Three regions are identified by

- Region 1: $-L/2 \leq x \leq -l/2$
  Region 3: $l/2 \leq x \leq L/2$
  $\psi_j(x) = A_j e^{ik_n x} + B_j e^{-ik_n x}$
- Region 2: $|x| \leq l/2$: $\psi_2(x) = A_2 e^{\kappa x} + B_2 e^{-\kappa x}$
- Connection between (A_j, B_j) determined by standard Transfer Matrix Approach methods

Matrix methods

$$\mathbb{P}(-l/2)|\xi_1\rangle = \mathbb{T}(-l/2)|\xi_2\rangle$$
$$\mathbb{T}(l/2)|\xi_2\rangle = \mathbb{P}(l/2)|\xi_3\rangle \tag{9}$$

$$\mathbb{P}(x) = \begin{bmatrix} e^{ik_n x} & e^{-ik_n x} \\ ike^{ik_n x} & -ike^{-ik_n x} \end{bmatrix} \quad \mathbb{T}(x) = \begin{bmatrix} e^{\kappa x} & e^{-\kappa x} \\ \kappa e^{i\kappa x} & -\kappa e^{-\kappa x} \end{bmatrix} \quad |\xi_j\rangle = \begin{bmatrix} A_j \\ B_j \end{bmatrix} \tag{10}$$

Matrix Solution I

k_n determined by boundaries (C_o chosen, and C'_o is dependent)

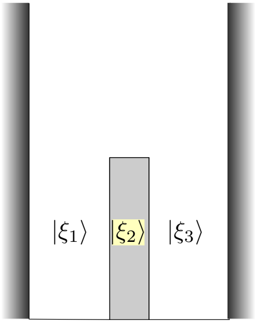
$$\begin{aligned} A_1 e^{-ik_nL/2} + B_1 e^{ik_nL/2} = 0 &\implies A_1 = C_o e^{ik_nL/2};\ \ B_1 = -C_o e^{-ik_nL/2} \\ A_3 e^{ik_nL/2} + B_3 e^{-ik_nL/2} = 0 &\implies A_3 = C'_o e^{-ik_nL/2};\ \ B_3 = -C'_o e^{ik_nL/2} \end{aligned} \quad (11)$$

Other Eigenstates: $\alpha = k_n(L-l)/2$

$$|\xi_2\rangle = \frac{iC_o}{\kappa}\begin{bmatrix} (k_n\cos\alpha + \kappa\sin\alpha)e^{\kappa l/2} \\ (-k_n\cos\alpha + \kappa\sin\alpha)e^{-\kappa l/2} \end{bmatrix} \quad (12)$$

$$|\xi_3\rangle = \begin{bmatrix} e^{-ik_nl}R_k & -iS_k \\ iS_k & e^{ik_nl}{R_k}^\dagger \end{bmatrix}|\xi_1\rangle \quad (13)$$

$$R_k = \cosh(\kappa l) - i\frac{\kappa^2 - k_n^2}{2\kappa k_n}\sinh(\kappa l);\ \ S_k = \frac{k_o^2}{2\kappa k_n}\sinh(\kappa l)$$



Two equations result: one for C'_o and another for k_n

Matrix Solution II

General Solution for finite-width center barrier, where $\kappa^2 = k_o^2 - k_n^2$

Equation for C_o'

$S_k = k_o^2 \sinh(\kappa l)/(2\kappa k_n)$

$$\frac{C_o'}{C_o} = iS_k + e^{ik_n(L-l)} \tag{14}$$

Equation for k_n

(must solve numerically)

$$\tanh(k_n l) = \frac{2\kappa k_n \sin[k_n(L-l)]}{(\kappa^2 - k_n^2)\cos[k_n(L-l)] - k_o^2} \tag{15}$$

In the limit of vanishing barrier width, a delta-sequence becomes a delta function

- $\lim_{l\to 0} \delta_l(x) \to \delta(x)$
- $\tanh(\kappa l) \to \kappa l$ as $l \to 0$
- with $k_o^2 = \gamma/l$, then Eq. (15) becomes

$$2k_n \sin(k_n L) - \gamma[1 - \cos(k_n L)] \to 0 \tag{16}$$

Eq. (16) satisfied for $k_n L = 2\pi n \;\; (\gamma \to \infty)$ or $k_n L = \pi n \;\; (\gamma \to 0)$, as expected for simple well with infinite walls

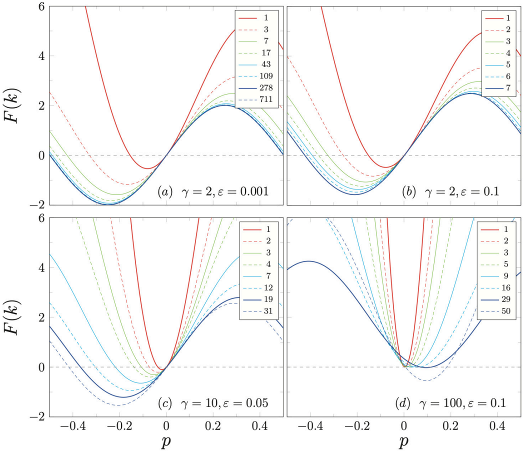
Rectangular (MIM) Barrier

General $l > 0$ case: k_n found numerically
Rewrite Eq. (15) as

$$iC_o \cosh[\kappa(k)l]\mathcal{F}(k) = 0 \tag{17}$$

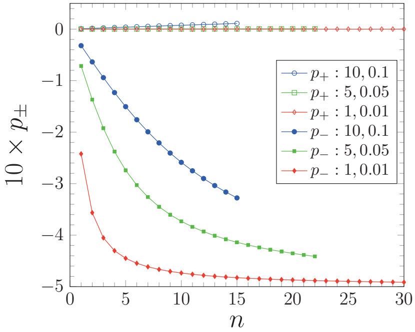
$$\begin{aligned}\mathcal{F}(k) \equiv\ & 2\sin[k(L-l)] \\ & + \frac{2k}{\kappa(k)}\cos[k(L-l)] \\ & + \frac{k_o^2}{k\kappa(k)}\{1-\cos[k(L-l)]\}\end{aligned} \tag{18}$$

- Eigen-energies such that $\mathcal{F}(k_n) = 0$: Let $k_n = 2\pi(n+p)/L$, n integer, $|p| \le 1/2$
- $\mathcal{F}(k) \rightarrow$ sequence of curves for integer n as a function of p
  as $\varepsilon \rightarrow 0$, all $p \rightarrow (0, -1/2)$

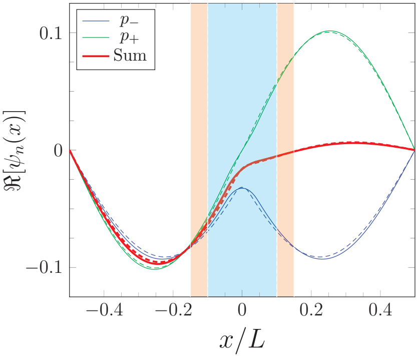


$\mathcal{F}(k)$ for $k \equiv 2\pi(n+p)/L$. Lines labeled by n

General Wave Functions



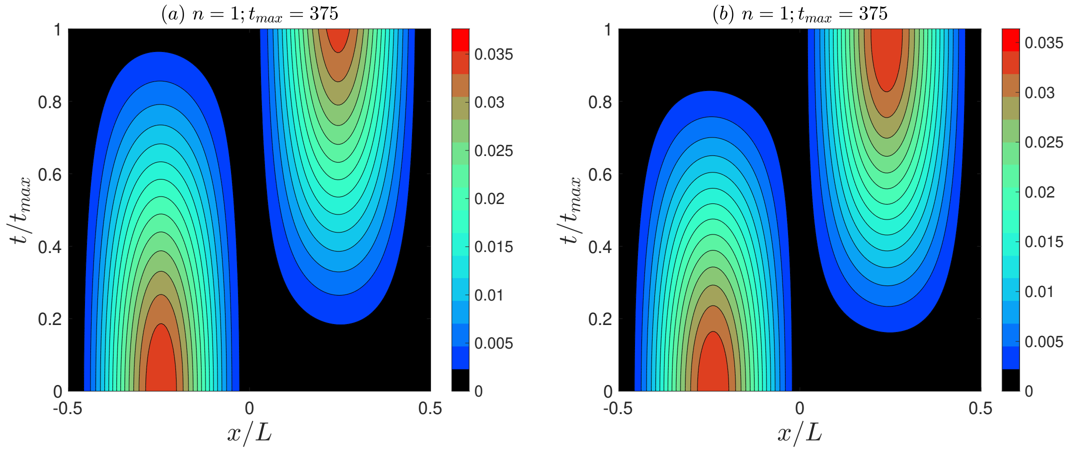
- $\mathcal{F}(k_n < k_o) = 0$ as function of n
- open symbols are larger root ($p_+ \approx 0$)
  closed are smaller root ($p_- \lesssim -0.5$)
- Legend: ($p_\pm$: γ, ε)



- $\psi_k(x)$ for $\gamma = 3$ and $n = 1$
- Shaded region is tunneling barrier
  Solid / orange: $\varepsilon = 0.3$; Dashed / blue: $\varepsilon = 0.2$
- p_+ = Antisymmetric; p_- = Symmetric

Sections Outline

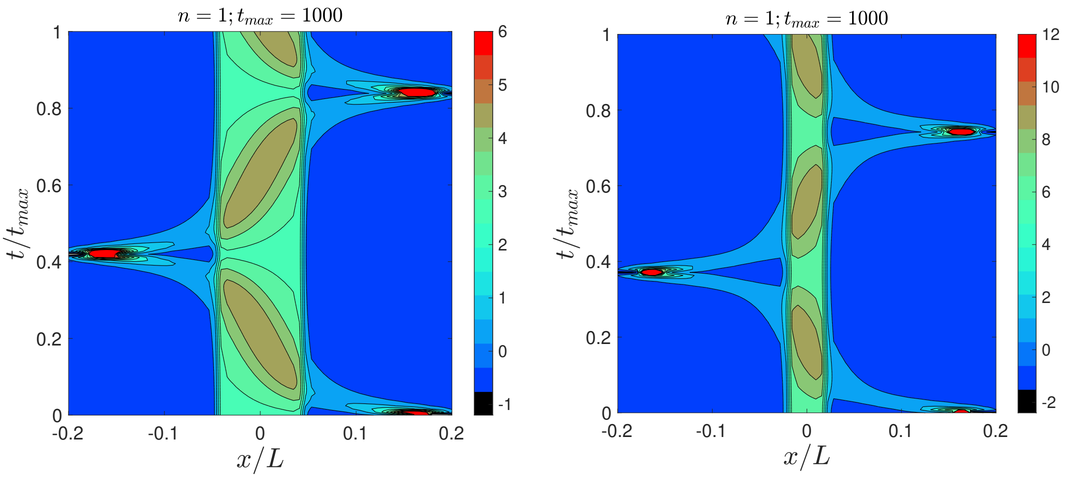
Exact Evolution of Eigenstates



Time evolution of probability density using solid curve $\psi_n(k)$: $\varepsilon = 0.3$

Time evolution of probability density using dashed curve $\psi_n(k)$: $\varepsilon = 0.2$

Comparison to Delay Times



Quantum potential $\Omega(x, t)$ for $\varepsilon = 0.3$ Quantum potential $\Omega(x, t)$ for $\varepsilon = 0.2$

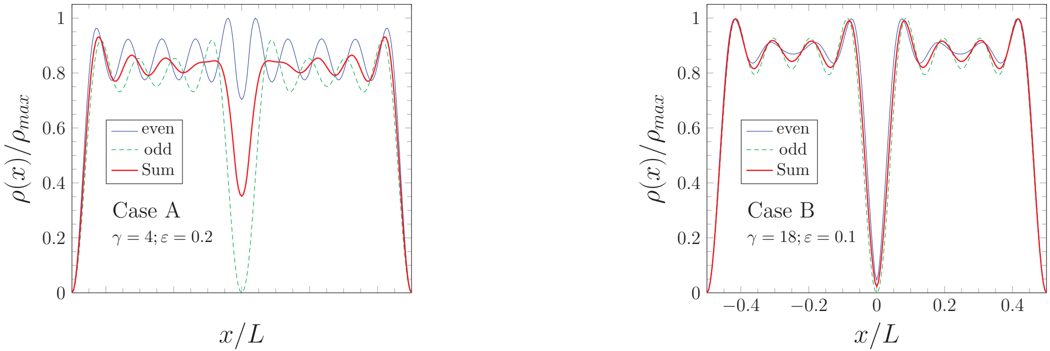
Density Profiles

Case A Low, wide $V(x)$, ρ coupled through barrier region

Case B High, narrow $V(x)$, ρ looks distinct, but is coupled

legend Even/odd = parity, sum = superposition of $\psi_n^{\pm}(x)$

$$\rho(x) = \sum_{j=1}^{n_f} f(k_j) \left|\psi_j(x)\right|^2 \qquad (19)$$



Superposition of $n_f = 6$ lowest $\psi_n(x)$ with metal-like weighting $f(k_n) \propto n_f^2 - n^2$

Concluding Remarks

Findings

1. Wave functions for rectangular barrier in confining well examined and solved exactly
2. Limit of vanishing barrier width, eigen-momenta k_n for ± parity $\psi_n(k)$ converge in $\gamma \to \infty$ limit
3. Change of tunneling time related to singularities in time-evolution of quantum potential $\Omega(x,t)$
4. $\rho(x)$ with metal-like weighting for shorter, wider barrier and taller, thinner barrier: as $\varepsilon \to 0, \gamma \to \infty$, then $\rho(x) \to$ two adjacent wells, but $\psi_n^{\pm}(x)$ span both wells, are coupled: $\Omega(x)$ for each case is finite near origin and allows transfer of energetic Bohmian trajectories.

Future Work

Model / Methodology suitable for

- Develop extension of Z-parameter characterization of NS interfaces proposed by Blonder, *et al.*
- Provide analytic framework for examining time dependent potential barrier on evolution of electron density (superposition of wave functions) in quantum wells and electron emission sources