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Interaction of Particle Beams with One-Dimensional Potential Barriers

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Interaction of Particle Beams with One-Dimensional Potential Barriers

Introduction

The objective of this project was to model particle beams in a number of 1-*D* potential systems and to create generalized Mathematica programs that can later be added on to continue further research into more complicated systems involving electric fields across nanowires. The project was mainly used to investigate how the transmission coefficients (i.e., percentage transmission) of these beams dynamically varied with changing parameters and to visualize in real time how exactly resonance peaks and band structures arose and changed as certain parameters (such as number and height of barriers) changed values.

Methods & Techniques Used

The standard procedure was to follow the method introduced by Walker and Gathright in their 1993/1994 paper "Exploring one-dimensional quantum mechanics with transfer matrices", which uses different matrices to displace the particle beam over various potential discontinuities and structures (Walker and Gatheright 1994). The discontinuity, propagation, and delta matrices can be used to derive any number of complicated shapes.

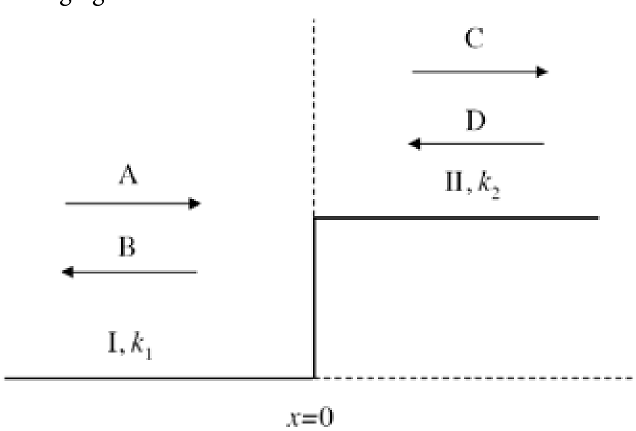
We wrote programs using Mathematica code that modeled different barrier systems, beyond those considered in the Walker paper, ranging from a simple double barrier to an *N*-barrier system. The main equation used was Schrödinger's time-independent equation,

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} = (E - V_0)\psi$$

The solution to the above equation (for $E > V_0$) is the generalized 1-*D* wave equation,

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

The generalized potential discontinuity used corresponds to the following figure:



with *A*, *B*, *C*, *D* corresponding to the coefficients of the approaching and reflected wave on each side of the discontinuity.

The coefficients on either side can be related to each other through the following discontinuity matrix (Walker 1992),

$$\mathbf{d}(v_1, v_2) = \frac{1}{2}\begin{pmatrix} 1+\frac{\sqrt{e-v_1}}{\sqrt{e-v_2}} & 1-\frac{\sqrt{e-v_1}}{\sqrt{e-v_2}} \\ 1-\frac{\sqrt{e-v_1}}{\sqrt{e-v_2}} & 1+\frac{\sqrt{e-v_1}}{\sqrt{e-v_2}} \end{pmatrix}$$

where $k_i = \frac{\sqrt{2mV_0}}{\hbar}\sqrt{e - v_i}$ and k_1 and k_2 are the respective wavenumbers on each part of the potential and $\begin{pmatrix} A \\ B \end{pmatrix} = \mathbf{d}(v_1, v_2)\begin{pmatrix} C \\ D \end{pmatrix}$. All potential and energy terms are scaled by a reference potential V_0. Therefore $e = E/V_0$ and $v_i = V_i/V_0$ where *E* and V_i are the energy of the particle beam and the potential of the system respectively.

If the discontinuity does not occur at $x = 0$, the coordinate system can be translated by the use of a propagation matrix [2] ρ (Walker 1992). This allows the discontinuity and propagation operators to remain independent of each other and allows for a "cleaner" handling of the system.

If the unprimed coordinate system is translated into the primed coordinate system with $x = x' + a$ with no change in potential, then

$$\begin{aligned} \psi'(x') &= \psi(x) \\ &= \psi(x' + a) \\ &= Ae^{ikx'}e^{ika} + Be^{-ikx'}e^{-ika} \\ &= A'e^{ikx'} + B'e^{-ikx'} \end{aligned}$$

Therefore, $\begin{pmatrix} A' \\ B' \end{pmatrix} = \mathbf{p}\begin{pmatrix} A \\ B \end{pmatrix}$, where

$$\mathbf{p} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}$$

Using these, transfer matrices of a large number of complicated systems were modeled very efficiently and the transmission graphs of up to 1 000 barriers could be generated within the order of a minute. The transfer-matrix approach also has the advantage of being an exact representation of the system, with numerical calculations done only when calculating the final transmission coefficient graphs.

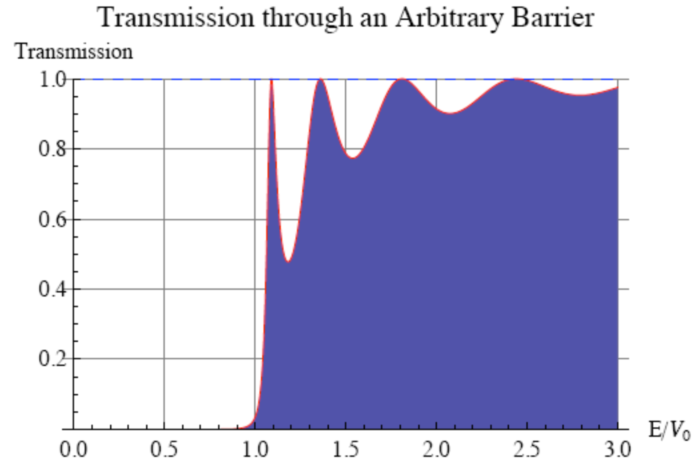


Figure 1
Transmission through an arbitrary barrier with $V_1 = 0$, $V_2 = 1$, $V_3 = 0.5$, *barrier strength* = π/0.9 and *barrier length* = 3.

Conclusion

Standard tunneling effects were replicated through the codes which clearly showed Ramsauer peaks[1] when a small number of barriers were considered. As the number of barriers were increased, bands of unit transmission formed (a precursor to the electron energy band structure found in solids) (Griffiths and Steinke 2001), with the number of peaks alternating between N and N - 1 between odd and even bands respectively.

Implications and Further Work

These Mathematica codes provide the basis for modeling a large number of complicated systems. Since the codes used were built from scratch and are completely different from those used by Walker to generate the graphs in his paper, they are versatile in different ways. Also, unlike Walker's programs, the ones created for this project are real-time interactive, allowing the user to graphically change all the parameters without resorting to modifying the code. we will continue to keep building on these codes, eventually adding the effects of external electric fields simulating those in real one-dimensional systems such as nanowires. This would let us investigate phenomena such as Fano Resonances.[2]

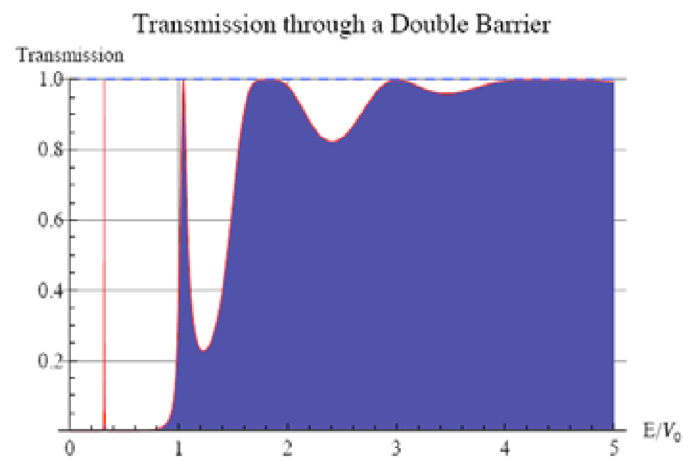


Figure 2
Transmission through a double barrier with $V_1 = 0$, $V_2 = 1$, *barrier strength* = π/0.9, *barrier length* = 1 and *barrier separation* = 1.

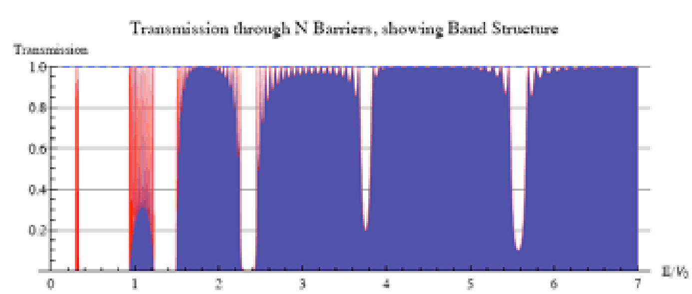


Figure 3
Transmission through 20 barriers with $V_1 = 0$, $V_2 = 2$, *barrier strength* = π/0.9, *barrier length* = 1 and *barrier separation* = 1. Distinct band structure can be seen.

Notes

[1] Ramsauer peaks are peaks of unit transmission in symmetrical barriers when an integral number of half-wavelengths fit in the barrier. The effect of this is to make the barrier seem transparent. For non-symmetrical barriers, the peaks still occur, but do not reach unit transmission but follow the envelope formed by the transmission through the discontinuity without the barrier.

[2] All potentials are scaled using an arbitrary factor of V_0 and all lengths are scaled by a factor of a_0. Barrier strength is a dimensionless quantity. All of these values depend on the particular system being studied and the specific particle used in the beam.

References

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