Scattering at a quantum barrier

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Abstract

Electron scattering is widely employed to determine the structures of quantum systems, with the electron interaction with the system revealing the relevant structure. In many cases the scattering potential is considered to come from an external source, one which does not interact with the system. This project aims to extend the scattering problem to a *quantum* barrier, one which has internal degrees of freedom. The electron transmission coefficients for such a system will be investigated.

Contents

1 Introduction

1.1 A Quantum Barrier

Electron scattering is well known in quantum theory, and is widely used in many areas of physics. In many cases, the potential which causes the electron to scatter is time independent, the solutions to which can be obtained by Schrdinger's formulation of wave mechanics. Even with time dependent Hamiltonians, many techniques have been well established on how to solve these types of scattering problems. In many cases, however, the potential is treated as an inherent part of the system, and not as a quantum object itself. By making the distinction between a "classical" potential and a quantum one, we are introducing the concept of a *quantum barrier*. A quantum barrier is one that has internal degrees of freedom, whereby it's potential may be perturbed by interactions with other quantum mechanical objects. As opposed to classical barriers, quantum barriers are active within the system, rather than simply providing a hurdle for other objects to overcome.

1.2 Project Objectives

It is the aim of this project to investigate electron scattering from a time dependent potential barrier. This will be achieved by treating the barrier as a quantum obstacle, thus generating its time dependence in quantum mechanically consistent manner. The special case of a delta barrier will be discussed, and it's scattering properties analyzed in depth.

2 The Static Delta Barrier

2.1 Introduction

We begin with a discussion of electron scattering from a "static" time-independent delta barrier. The Hamiltonian for such a system moving in a one dimensional potential may be written as

$$\hat{H} = \frac{\hat{p}^2}{2m} + g\delta(x)\,,$$

where g is some constant, defining the strength of the interaction potential. The Schrdinger equation therefore reads

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + g\delta(x)\right]\psi(x) = E\psi(x)\,. \tag{1}$$

The solution of this equation will yield the scattering states ($E > 0$) of the electron.

2.2 The Solution

The solution of this equation is then

$$\begin{aligned} \psi(x<0) &= Ae^{ikx} + Be^{-ikx} \\ \psi(x>0) &= Te^{ikx} \end{aligned} \tag{2}$$

where $k = \sqrt{2mE/\hbar^2}$. Here we have implemented the left incident boundary condition that there are no *left* traveling waves to the *right* of the delta potential[1]. This is an arbitrary choice and corresponds to sending in an electron beam from the *left* of the delta barrier. The requirement now is match these two equations at the barrier. To this end we impose standard boundary conditions on the wavefunction and its derivative across the barrier:

1. ψ is always continous, and

2. $\frac{d\psi}{dx}$ is continous except where the potential is infinite.

Applying the first condition to equation 2 yields

$$A + B = T\,. \tag{3}$$

The second boundary condition gives us no new information, since the potential we have is an infinite delta potential. We thus use equation 1 to derive the required condition for the derivative of $\psi(x)$ across the barrier [2]. Integrating equation 1 from $-\epsilon$ to $+\epsilon$ gives

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}\,dx+\int_{-\epsilon}^{+\epsilon}g\delta(x)\psi(x)\,dx=E\int_{-\epsilon}^{+\epsilon}\psi(x)\,dx\,.$$

In the limit, the right hand side of this function will go to zero as $\epsilon \to 0$ since it just describes the area underneath a curve of diminishing width. Employing the "sifting" property of the delta function, we can then write

$$\Delta\left(\frac{d\psi}{dx}\right)=\frac{2mg}{\hbar^2}\,\psi(0)\,, \tag{4}$$

where

$$\Delta\left(\frac{d\psi}{dx}\right)=\lim_{\epsilon\to 0}\left.\frac{d\psi}{dx}\right|_{-\epsilon}^{+\epsilon}. \tag{5}$$

This condition is now applied to the wave function, equation 2. Differentiating with respect to x and evaluating $\psi(x>0)$ at $+\epsilon$ and $\psi(x<0)$ at $-\epsilon$ gives

$$\begin{aligned}\left.\frac{d\psi}{dx}\right|_{-\epsilon} &= ik\left(Ae^{-ik\epsilon}-Be^{+ik\epsilon}\right)\,,\\ \left.\frac{d\psi}{dx}\right|_{+\epsilon} &= ikTe^{+ik\epsilon}\,,\end{aligned}$$

which, in the limit of $\epsilon \to 0$ becomes

$$\begin{aligned}\left.\frac{d\psi}{dx}\right|_{-} &= ik\left(A-B\right)\,,\\ \left.\frac{d\psi}{dx}\right|_{+} &= ikT\,.\end{aligned}$$

Therefore, using equation 5, the derivative across the barrier becomes

$$\Delta\left(\frac{d\psi}{dx}\right)=ik(T-A+B)\,. \tag{6}$$

Equating equations 4 and 6 yields the relation

$$ik(T-A+B)=\frac{2mg}{\hbar^2}(A+B)\,,$$

(using the fact that $\psi(0) = A + B$ from equation 2), which we can rearrange and write as

$$T = A(1 - 2i\beta) - B(1 + 2i\beta), \quad \text{where } \beta = \frac{mg}{\hbar^2 k}. \tag{7}$$

Again using equation 3 and eliminating B from equation 7 we find that

$$T = \frac{A}{1 + i\beta}. \tag{8}$$

The transmission coefficient $\tilde{T}$ is defined as the ratio of the outflowing probability current to the incoming current. The current density may be written as $j = \frac{\hbar}{m}\Im\left[\psi * (x)\psi'(x)\right]$ [1]. For the right flowing current, $\psi(x) = Te^{ikx}$ while for the incoming current, $\psi(x) = Ae^{ikx}$. This therefore gives the Transmission coefficient as

$$\tilde{T} = \frac{|T|^2}{|A|^2}. \tag{9}$$

Substituting equation 8 in to equation 9 gives

$$\tilde{T} = \frac{1}{1 + \beta^2}, \tag{10}$$

which, given the definition of β in equation 2 is a function of k and therefore also E:

$$\tilde{T} = \frac{1}{1 + (mg^2/2\hbar^2 E)}. \tag{11}$$

Setting $\hbar = 2m = 1$ this reduces to

$$\tilde{T} = \frac{4E}{4E + g^2}. \tag{12}$$

2.3 Discussion of Results

In figure 1 we plot the transmission coefficient, $\tilde{T}$ (henceforth $\tilde{T}$ shall be referred to as T, since the former notation is rather cumbersome) against the electron energy (which in this case is the energy of the entire system), we can see how for a fixed g, T approaches unity as $E \to \infty$ and $T \to \frac{4E}{g^2} \propto E$ as $E \to 0$.
More specifically, it can be seen that, for arbitrary g values, $T \to 1$ for $E \gg g$ and $T \propto E$ for $E \ll g$. The significance of g to E is that it defines an "energy scale" for the transmission curve. For small values of g, the curve evolves

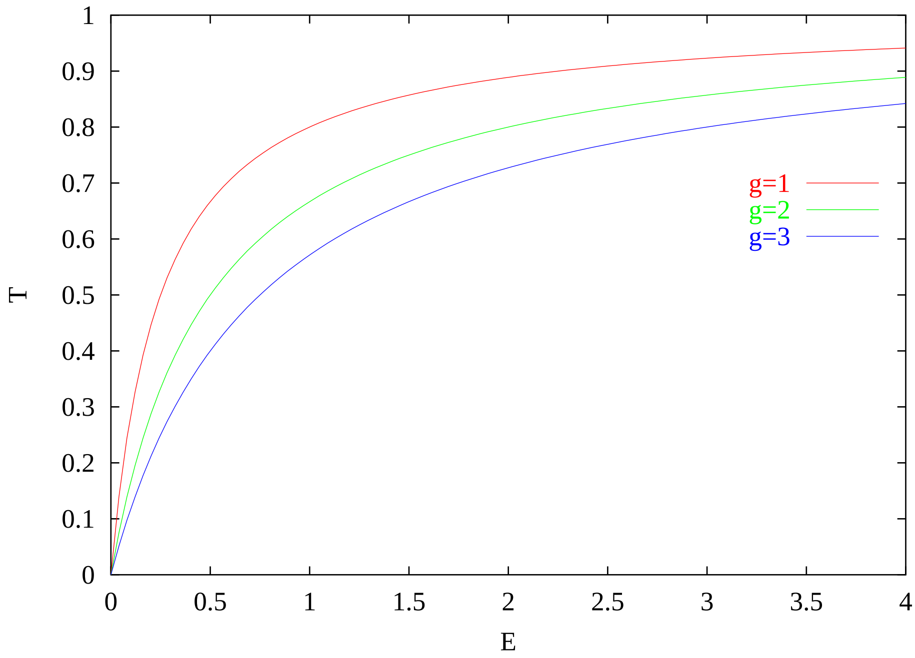

Figure 1: The transmission coefficient T as a function of energy

rapidly with energy, and quickly approaches unity. For larger values of g, however, the evolution is comparatively smaller.

3 The Quantum Delta Barrier

3.1 Introduction

A quantum barrier is one which has internal degrees of freedom. The difference between this delta barrier and the barrier in the previous section is that now we have a potential which is *dependent* on the state of the system, rather than being simply a backdrop upon which the system evolves. We treat the barrier as a bosonic mode (a photon, or a harmonic oscillator for example), whose interaction potential is linearly proportional to it's displacement. Thus we can write the interaction potential as

$$\hat{H}_{inter} = \delta(x) \left\{ g_0 + g_1 \left[a + a^\dagger \right] \right\} , \tag{13}$$

noting that $a + a^\dagger$ is linear in the bosonic coordinates. The constants g_0 and g_1 define the strength of the interaction potential.
The energy of the boson is simply

$$\hat{H}_B = \Omega\left[a^\dagger a + \frac{1}{2}\right], \tag{14}$$

where $\Omega = \hbar\omega$ and the electron energy is as before

$$\hat{H}_0 = \frac{\hat{p}^2}{2m}. \tag{15}$$

The total hamiltonian for the system can then be written as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \delta(x)\left\{g_0 + g_1\left[a + a^\dagger\right]\right\} + \Omega\left[a^\dagger a + \frac{1}{2}\right]. \tag{16}$$

The time-independent Schrdinger equation therefore reads

$$\left\{\frac{\hat{p}^2}{2m} + \delta(x)\left\{g_0 + g_1\left[a + a^\dagger\right]\right\} + \Omega\left[a^\dagger a + \frac{1}{2}\right]\right\}\Psi = E\Psi. \tag{17}$$

3.2 The Solution

For a coupled system where the particles aren't identical, the total wave function can be written as a product of each respective particles wave function. Therefore we can make an ansatz of

$$\Psi = \psi(x)\phi(x'),$$

where $\phi(x')$ is the bosonic wave function.
The set of eigenfunctions describing the boson form the basis of a Hilbert space. We can therefore expand Ψ into a sum of these component eigenkets:

$$\Psi = \sum_{n=0}^{\infty} \psi_n(x)\left|n\right\rangle, \tag{18}$$

where $\left|n\right\rangle$ corresponds to $\phi_n(x')$.
Inserting equation 18 into the stationary Schrdinger equation (equation 17) gives

$$\begin{aligned}\textstyle\sum_{n=0}^{\infty}\left\{\frac{\hat{p}^2\psi_n(x)}{2m}\left|n\right\rangle + \delta(x)g_0\psi_n(x)\left|n\right\rangle + \delta(x)g_1\psi_n(x)\left[a + a^\dagger\right]\left|n\right\rangle\right.\\ \left. + \Omega\,\psi_n(x)\left[a^\dagger a + \tfrac{1}{2}\right]\left|n\right\rangle\right\} = \textstyle\sum_{n=0}^{\infty} E\psi_n(x)\left|n\right\rangle.\end{aligned} \tag{19}$$

Using the ladder properties of the a and $a^\dagger$ operator equation 19 becomes

$$\sum_{n=0}^{\infty}\left\{\frac{\hat{p}^2\psi_n(x)}{2m}\left|n\right\rangle + \delta(x)g_0\psi_n(x)\left|n\right\rangle + \delta(x)g_1\psi_n(x)\sqrt{n}\left|n-1\right\rangle \right.$$
$$\left. +\delta(x)g_1\psi_n(x)\sqrt{n+1}\left|n+1\right\rangle + \Omega\,\psi_n(x)\left(n+\tfrac{1}{2}\right)\left|n\right\rangle\right\} = \sum_{n=0}^{\infty} E\psi_n(x)\left|n\right\rangle . \tag{20}$$

Multiplying through by the boson state $\langle m|$, making use of the fact that $\langle m|\,n\rangle = \delta_{m,\,n}$ and making two changes of summation indices for the $|n+1\rangle$ and $|n-1\rangle$ boson states, equation 20 simplifies considerably to

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} + \delta(x)g_0\psi_n + \delta(x)g_1\sqrt{n}\psi_{n-1} + \delta(x)g_1\sqrt{n+1}\psi_{n+1}$$
$$+\Omega\left(n+\tfrac{1}{2}\right)\psi_n = E\psi_n\,. \tag{21}$$

To proceed as before, we need to make a ansatz for the electron wave function. Here, describing the wave function as running waves now has to be questioned. If we consider the electron function as a superposition of plane waves, then the wave vector should be $k_n = \sqrt{E-(n+\frac{1}{2})\Omega}$, where E is the total energy of the system, and we have set $\hbar = 2m = 1$.
The differences between this system and of that seen in section 1 is that now we have k values and coefficients which are functions of n. The wave vector k is still a continuous variable, dependent on the energy of the system, but will take on different values for different states of the boson, $|n\rangle$. This would make sense, since different boson states have different eigenenergies, thus altering the amount of energy available to the electron with a change in state. For this system, however, the wave vector for the electron, k_n, isn't necessarily real. The bosonic Hilbert space has an infinite number of dimensions. For these dimensions which are higher in energy than the total system ($(n+\frac{1}{2})\Omega > E$) the wave vector becomes imaginary. Hence we note that there are two distinct cases for the electron wave funcion:

1. $E > (n+\frac{1}{2})\Omega$, and
2. $E < (n+\frac{1}{2})\Omega$.

To proceed it is necessary to consider each case separately.

3.3 Case 1: $E > \left(n+\frac{1}{2}\right)\Omega$

Here, the electron wave vector will be purely real. We thus describe the electron wave function as a superposition of plane waves, again employing the left hand incident boundary condition.

$$\begin{aligned} \psi_n(x<0) &= A_n e^{ik_n x} + B_n e^{-ik_n x} \\ \psi_n(x>0) &= T_n e^{ik_n x} \end{aligned} \tag{22}$$

where $k_n = \sqrt{E - (n+\frac{1}{2})\Omega}$.
The same boundary conditions are applied to the wave function as in the previous section:

$$A_n + B_n = T_n\,, \tag{23}$$

which comes from the continuity of $\psi_n(x)$ across the boundary. The second boundary requirement concerning the derivative of $\psi_n(x)$ is again treated as before. We integrate equation 21 from $-\epsilon$ to $+\epsilon$:

$$-\tfrac{\hbar^2}{2m}\left[\tfrac{\partial\psi_n}{\partial x}\right]_{-\epsilon}^{+\epsilon} + g_0\psi_n(0) + g_1\sqrt{n}\psi_{n-1}(0) + g_1\sqrt{n+1}\psi_{n+1}(0) + \Omega\left(n+\tfrac{1}{2}\right)\textstyle\int_{-\epsilon}^{+\epsilon}\psi_n\,dx = E\int_{-\epsilon}^{+\epsilon}\psi_n\,dx\,.$$

In the limit as as $\epsilon \longrightarrow 0$ we get

$$\left[\frac{\partial\psi_n}{\partial x}\right]_{-}^{+} = \frac{2m}{\hbar^2}\left[g_0\psi_n(0) + g_1\sqrt{n}\psi_{n-1}(0) + g_1\sqrt{n+1}\psi_{n+1}(0)\right]\,. \tag{24}$$

Hence

$$\Delta\left(\frac{\partial\psi_n}{\partial x}\right) = \frac{2m}{\hbar^2}\left[g_0\psi_n(0) + g_1\sqrt{n}\psi_{n-1}(0) + g_1\sqrt{n+1}\psi_{n+1}(0)\right]\,. \tag{25}$$

Taking the derivative of equation 22 and approaching the boundary from the right and the left we find that

$$\lim_{\epsilon\to 0}\left[\psi_n'(+\epsilon) - \psi_n'(-\epsilon)\right] = ik_n\left(T_n - A_n + B_n\right)\,.$$

Therefore,

$$\Delta\left(\frac{\partial\psi_n}{\partial x}\right) = ik_n\left(T_n - A_n + B_n\right)\,. \tag{26}$$

Equating 25 and 26 gives

$$ik_n\left(T_n - A_n + B_n\right) = \frac{2m}{\hbar^2}\left[g_0\psi_n(0) + g_1\sqrt{n}\psi_{n-1}(0) + g_1\sqrt{n+1}\psi_{n+1}(0)\right]. \tag{27}$$

From equation 22 we know that

$$\psi_n(0) = A_n + B_n \ ,$$

and substituting into equation 27 gives

$$\begin{aligned} T_n - A_n + B_n = -\tfrac{2im}{\hbar^2 k_n} \big[& g_0(A_n + B_n) + g_1\sqrt{n}(A_{n-1} + B_{n-1}) \\ & + g_1\sqrt{n+1}(A_{n+1} + B_{n+1})\big] \ . \end{aligned} \tag{28}$$

Using the boundary condition for continuity of ψ, equation 23, we can therefore write the coefficient of the transmitted wave in terms of T_n and A_n.

$$2(T_n - A_n) = -\tfrac{2im}{\hbar^2 k_n}\left[g_0(T_n) + g_1\sqrt{n}(T_{n-1}) + g_1\sqrt{n+1}(T_{n+1})\right] \ ,$$

This can be wrote as a sequence,

$$T_{n+1} = -\frac{(g_0 T_n + \sqrt{n} g_1 T_{n-1})}{g_1\sqrt{n+1}} + i\frac{\gamma_n\,(T_n - A_n)}{g_1\sqrt{n+1}} \ , \tag{29}$$

where $\gamma_n = \frac{\hbar^2 k_n}{m} = 2k_n$.
A solution for the set of coefficients $\{T_n\}$ can then be found provided that one of the coefficients is known. To determine this coefficient an extra condition is required.

3.4 Case 2: $E < \left(n + \frac{1}{2}\right)\Omega$

When the energy of the system is less than the boson states under consideration, the wave vector for the electron wave function becomes purely imaginary. A modification to the boundary conditions is now required, since we no longer have traveling waves.
In order to keep the wavefunction normalized (i.e. such that it doesn't blow up at $\pm\infty$) the only states which can exist are decaying modes. The electron wavefunction should now be written as

$$\begin{aligned} \psi_n(x<0) &= B_n e^{\kappa_n x} \\ \psi_n(x>0) &= T_n e^{-\kappa_n x} \end{aligned} \tag{30}$$

where $\kappa_n = \sqrt{(n+\frac{1}{2})\Omega - E}$.
From the continuity of ψ at $x = 0$, we find that

$$B_n = T_n. \tag{31}$$

Again we compare the derivatives of the wave function at some diminishing distance on either side of the barrier.

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = -2T_n\kappa_n \tag{32}$$

Equating this with the boundary condition of equation 25 gives the relation

$$-2T_n\kappa_n = \frac{2m}{\hbar^2}\left[g_0\psi_n(0) + g_1\sqrt{n}\psi_{n-1}(0) + g_1\sqrt{n+1}\psi_{n+1}(0)\right]. \tag{33}$$

From equation 30, $\psi(0) = T_n$. Inserting this into equation 33 and rearranging gives another sequence

$$T_{n+1} = \frac{-\left(\tilde{\gamma}_n + g_0\right)T_n - g_1\sqrt{n}\,T_{n-1}}{g_1\sqrt{n+1}}, \tag{34}$$

where $\tilde{\gamma}_n = \frac{\hbar^2\kappa_n}{m} = 2\kappa_n$.
We now have two sequences relating each member of the set $\{T_n\}$. Before we can combine the two separate sequences a little work is required on equation 29.

3.5 Initial Conditions

The difference between equation 29 and equation 34 is that the former contains the term A_n. To progress we need to consider what the physical meaning of this quantity is.
In our static interaction picture, we have an incoming electron beam, a reflected beam and a transmitted beam. The quantity $|A|^2$ gives the *intensity* of the incoming electron beam. In the interaction picture of the quantum barrier, things are slightly different. The quantity A now carries a subscript n. $|A_n|^2$ then corresponds to the intensity of the incoming electron beam when the boson is in it's n^{th} state (referred to as the n^{th} "channel"). If we impose the condition that the boson is *initially* in the ground state, then for an incoming electron the intensity in every channel except the zeroth channel will necessarily be zero. [1] More formally, this condition may be written as

$$A_n = A\delta_{n,0}, \tag{35}$$

[1] This is perhaps an over simplification of the problem, since in any practical situation a stream of electrons would be sent into the barrier as opposed to a single electron.

where A is some complex number, who's modulus will be taken as unity for simplicity. Applied to the sequence of equation 29 we find that we can now write these sequences in the following way:

$$g_1\sqrt{n}\,T_{n-1} + (g_0 - i\gamma_n)\,T_n + g_1\sqrt{n+1}\,T_{n+1} = -i\gamma_n A\delta_{n,0}, E > (n + \frac{1}{2})\Omega \quad (36)$$

$$g_1\sqrt{n}\,T_{n-1} + (g_0 + \tilde{\gamma}_n)\,T_n + g_1\sqrt{n+1}\,T_{n+1} = 0, \qquad E < (n + \frac{1}{2})\Omega. \quad (37)$$

Here, γ_n and $\tilde{\gamma}_n$ have their usual meaning and are both strictly real quantities. More compactly, we can allow the quantity γ_n be either real or imaginary (since $\gamma_n \propto k_n$ which can be either real or imaginary for a given E and n), and the two sequences reduce to one:

$$g_1\sqrt{n}\,T_{n-1} + (g_0 - i\gamma_n)\,T_n + g_1\sqrt{n+1}\,T_{n+1} = -i\gamma_n A\delta_{n,0}\ , \qquad E > \frac{1}{2}\,\Omega. \quad (38)$$

Note that the energy now runs continuously from $\frac{1}{2}\Omega$ (energies cannot be less than the zero point energy of the boson) , giving γ_n as a positive real quantity for channel energies less than E and as a positive imaginary quantity for channel energies greater than E.

3.6 Matrix Representation

The point about writing equation 38 in this way, is that we can neatly express each equation for every n in the form of a tridiagonal matrix as follows:

$$\begin{bmatrix} g_0 - i\gamma_0 & g_1 & 0 & 0 & \cdots & 0 \\ g_1 & g_0 - i\gamma_1 & \sqrt{2}g_1 & 0 & \cdots & 0 \\ 0 & \sqrt{2}g_1 & g_0 - i\gamma_2 & \sqrt{3}g_1 & \cdots & 0 \\ 0 & 0 & \sqrt{3}g_1 & g_0 - i\gamma_3 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \sqrt{N}g_1 \\ 0 & 0 & 0 & \cdots & \sqrt{N}g_1 & g_0 - i\gamma_N \end{bmatrix} \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ \vdots \\ T_{N-1} \\ T_N \end{bmatrix} = \begin{bmatrix} -i\gamma_0 A \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \quad (39)$$

In principle these matrices should be infinite in size, since there are an infinite number of boson states. However, we make a slight approximation of terminating the set of equations at some large $N + 1$.[2]
The point of writing the equations in the form of $BT_n = A_n$ is that now, to determine the set of T_n coefficients we simply have to apply the inverse matrix B^{-1} from the left hand side of this equation. This will yield the complete set (approximately, up to the Nth term) of T_n.
To this end, a simple matrix inversion program was used, employing the Gauss-Jordan inversion method. (A copy of the program algorithms can be found in Appendix A).

3.7 Current Conservation

The probability current for a wave function is defined as

$$J = \frac{i\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right). \tag{40}$$

Applied to the incoming electron beam produces the equation

$$\begin{aligned} J_{In} &= \sum_{n=0}^{N'} \frac{i\hbar}{2m} A_n e^{ik_n x}(-ik_n)A_n^* e^{-ik_n x}, \\ J_{In} &= \sum_{n=0}^{N'} \frac{\hbar k_n}{2m} |A_n|^2 . \end{aligned} \tag{41}$$

where N' is the largest classically allowed boson state.
The sum over the electron states does not exceed N', since for higher boson states, the electron wave vector becomes imaginary, and there is no current flow for these states (see section 3.8).
For the reflected and transmitted parts of the beam, we have

$$\begin{aligned} J_R &= \sum_{n=0}^{N'} \frac{i\hbar}{2m} B_n e^{ik_n x}(-ik_n)B_n^* e^{-ik_n x} , \\ J_R &= \sum_{n=0}^{N'} \frac{\hbar k_n}{2m} |B_n|^2 , \\ J_T &= \sum_{n=0}^{N'} \frac{i\hbar}{2m} T_n e^{ik_n x}(-ik_n)T_n^* e^{-ik_n x} , \end{aligned} \tag{42}$$

[2]How good an approximation this is can be determined by current conservation, see section 3.7.

$$J_T = \sum_{n=0}^{N'} \frac{\hbar k_n}{2m} |T_n|^2 . \quad (43)$$

The conservation of current implies that the sum of the reflected and transmitted currents must equal the incoming current. Hence, combining equations 41, 42 and 43,

$$\begin{aligned} J_{In} &= J_R + J_T , \\ \sum_{n=0}^{N'} k_n |A_n|^2 &= \sum_{n=0}^{N'} k_n \left(|B_n|^2 + |T_n|^2 \right) . \end{aligned}$$

Using equation 23 ($A_n + B_n = T_n$),

$$\sum_{n=0}^{N'} k_n |A_n|^2 = \sum_{n=0}^{N'} k_n \left(|T_n - A_n|^2 + |T_n|^2 \right) . \quad (44)$$

We now apply the condition that the boson is initially in it's ground state, before any electron interaction, equation 35. This means that there is no incoming current in any other channel than the $n = 0$ boson state. Imposing this onto equation 44 the summation simplifies:

$$\begin{aligned} k_0 |A|^2 = k_0 \left[|T_0 - A|^2 + |T_0|^2 \right] + 2 \sum_{n=1}^{N'} k_n |T_n|^2 \\ k_0 \left[|T_0 - A|^2 + |T_0|^2 - |A|^2 \right] + 2 \sum_{n=1}^{N'} k_n |T_n|^2 = 0 . \quad (45) \end{aligned}$$

The condition outlined in equation 45 provides a useful check for accuracy in the Matrix size, $N + 1$. As N is increased, the left hand side of equation 45 should converge to zero. A tolerance threshold can be defined, t, and N increased until

$$k_0 \left[|T_0 - A|^2 + |T_0|^2 - |A|^2 \right] + 2 \sum_{n=1}^{N'} k_n |T_n|^2 \leq t. \quad (46)$$

Terminating the matrix at the smallest possible size in agreement with equation 46 will significantly reduce the amount of computational overhead in the matrix inversions.

Figure 2 shows the divergence of the total current density at the barrier as a function of the number of bosonic states, N. As can be seen, at low energy

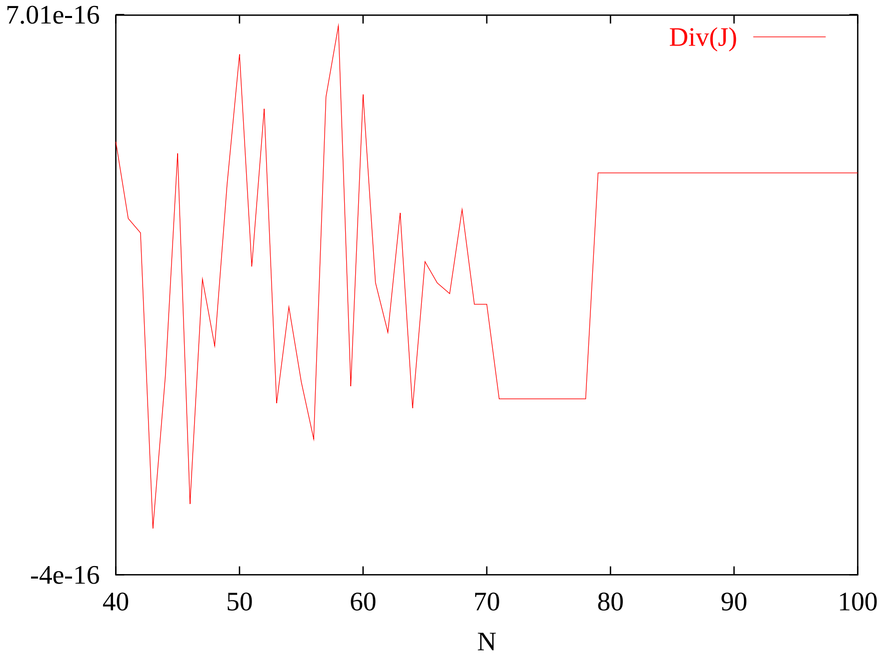

Figure 2: Current divergence for $E = 3$ and $g_1 = 1.0$

there is good convergence for quiet a small number of bosonic modes (~ 80), and weak coupling to the boson (g_1 small).
Figure 3 again shows the current divergence for stronger coupling. Here the convergence is not as fine as for the case of weaker coupling. The values of the current divergence are still of the order of 10^{-15}, however, which is a small error given that the incoming electron current is of the order of 1.
To save computational time, the bosonic Hilbert space will be terminated at approximately 250 modes. This matrix size evidently gives good accuracy for weak coupling to the boson ($g_1 < 1$), and adequate results for stronger coupling.

3.8 Partial currents

For each channel (each bosonic mode) we have different electronic modes. In the lower energy channels where $E > \left(n + \frac{1}{2}\right)\Omega$ the electron wave function is described by running waves, while for $E < \left(n + \frac{1}{2}\right)\Omega$ we have exponentially decaying electron wave functions. This is because the form of the wave function is a complex exponential, $e^{\pm i k_n x}$, where $k_n = \sqrt{E - \left(n + \frac{1}{2}\right)\Omega}$. Hence the sign of $\left[E - \left(n + \frac{1}{2}\right)\Omega\right]$ ultimately determines the form of the

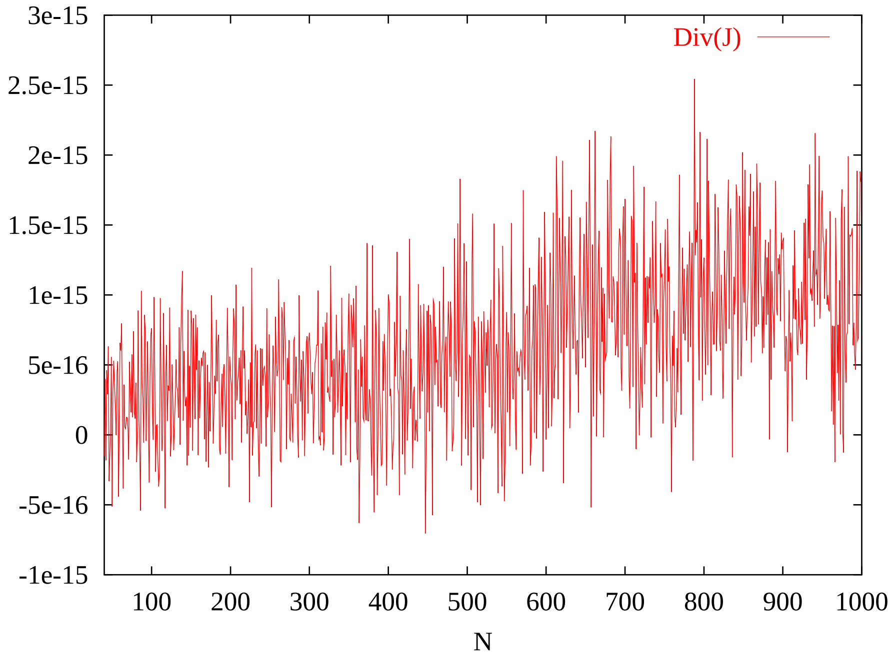

Figure 3: Current divergence for $E = 3$ and $g_1 = 1.5$

electron wave function. Since the probability current density is defined as $j = \frac{\hbar}{m}\Im\left[\psi * (x)\psi'(x)\right]$, then for purely real wave functions, $\Im\left[\Psi\right] = 0$. Therefore, only propagating (k_n real) modes will contribute to the probability current. For each specific channel, this has the implication that only if this channel energy lies within the energy of the system, E, will it contribute to the total current, J. We therefore label the largest propagating mode with the quantum numbner N', such that $\left(N' + \frac{1}{2}\right)\Omega < E < \left(N' + \frac{3}{2}\right)\Omega$.
We now define the partial outgoing current, $J_{(n)}$ for each channel,

$$J_{(n)} = \frac{\hbar k_n}{2m}|T_n|^2 \,. \tag{47}$$

The partial transmission coefficient, $T_{(n)}$ (note the distinction here between T_n and $T_{(n)}$) is then the ratio of the partial outgoing current to the incoming current,

$$T_{(n)} = \frac{\hbar k_n}{2mk_0}\frac{|T_n|^2}{|A_0|^2} \,. \tag{48}$$

Written in this way we can express the total transmission coefficient as a sum over all the partial transmission coefficients,

$$T = T_{(0)} + T_{(0)} + \ldots + T_{(N')} \,. \tag{49}$$

Such a definition of the transmission coefficient is convenient for analyzing which modes make significant contributions to the scattering process.

4 Results

The parameter g_1 determines the strength of the electron-boson coupling (namely the interaction dependent on the displacement of the boson). For $g_1 = 0$ the boson becomes transparent to the electron, and the interaction reduces to the case of a static delta barrier (this will provide a "zeroth order" check for the data obtained - see later) . For $0 < g_1 < g_0$ there is weak coupling to the boson, and the static term g_0 dominates. For $g_1 > g_0$ we have strong coupling to the boson, and g_1 becomes the dominant term. These two different cases should produce different markedly scattering curves due to the fundamentally different mechanisms by which the electron is scattered from the barrier. Here I will concentrate on the case of weak electron-boson coupling.

4.1 Weak coupling $g_1 < g_0$

In figure 4 we can see the transmission coefficient for various values of g_1 as a function of the system energy.
As can be seen, for $g = 0$ the transmission curve fits that of a static delta barrier. The only difference being that here $T(E)$ starts at a system energy value of $E = \frac{1}{2}\Omega$. This is due to the zero point energy of the boson (the total energy of the system cannot be smaller than this value). For a static delta barrier, however, the system energy is simply the electron energy, which can be zero.
As is the case for the static barrier, as $E \to 0$ (or $E \to \frac{3}{2}\Omega$), $T(E)$ becomes linear, while as $E \to \infty$, $T(E) \to 1$.
It is of interest to note here that the transmission curve of a quantum barrier lies above that of the static barrier for energies below $\frac{3}{2}\Omega$, while it lies below for energies greater than this.
Figure 5 shows the transmission curve in figure 4 between the energies $E = 1.2$ and $E = 2.8$. From this plot we can clearly see that as the energy approaches $E = \frac{3}{2}\Omega$ there is an increase of the transmission coefficient. Larger values of g_1 produce larger rates of increase of $T(E)$. As E is increases past this energy, there is a sharp drop in the transmission coefficient.
Similar effects can be seen for $E = \left(n + \frac{1}{2}\right)\Omega$. For a discussion of the physics

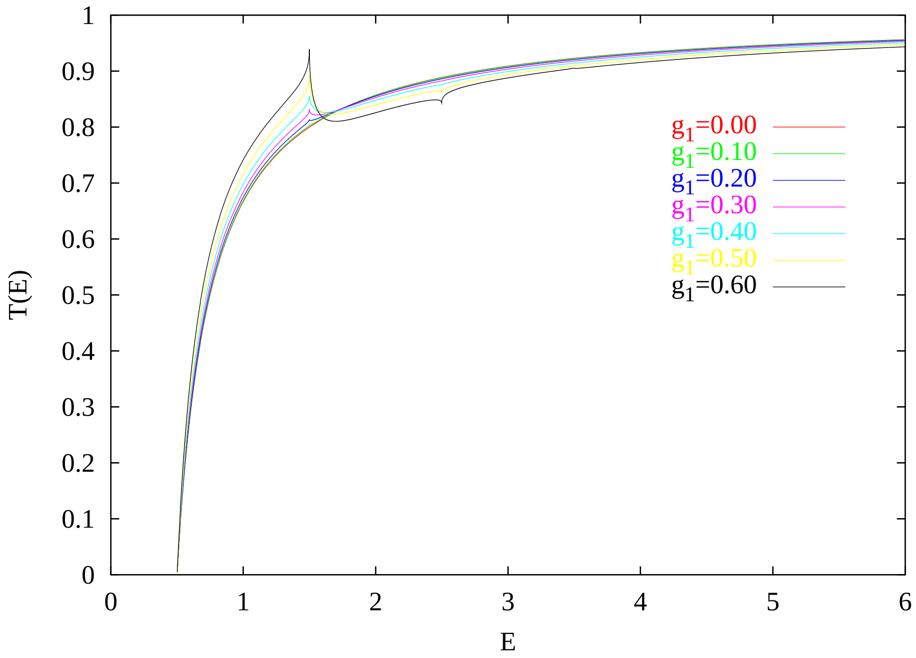

Figure 4: The transmission coefficient for various values of g_1, with $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

behind these variations in $T(E)$, we turn to the partial transmission coefficients for a fixed value of g_1.
From figure 6 it is evident that the partial currents in the $n = 0$ and $n = 1$ channels are much greater than the currents in the other channels. It is therefore these currents which dominate the total transmission coefficient. Plots can be made of the other less significant partial transmission coefficients, and similar effects can be found throughout (see figures 7 and 8).
Clearly, the $T_{(0)}$ coefficient behaves differently to all the other coefficients, which are similar in their behaviour. Typically, $T_{(n>0)} = 0$ at $E = \left(n + \frac{1}{2}\right)\Omega$ and increases rapidly over a small energy range. The coefficient then decreases slowly until E approaches $\left(n + \frac{3}{2}\right)\Omega$, where there is again a sharp increase in $T_{(n)}$. As the energy increases past this point, there is a regular decrease in $T_{(n)}$ up until $E = \left(n + \frac{1}{2}\right)\Omega$. At energies beyond this, the effect on $T_{(n)}$ becomes negligible, and as $E \to \infty$, $T_{(n)} \to 0$.
$T_{(0)}$ on the other hand increases steadily from $E = \frac{1}{2}\Omega$, and tends to 1 as $E \to \infty$.
The difference between T_0 and T_n at high energies can be explained by considering the initial conditions. That is that the boson is initially in it's

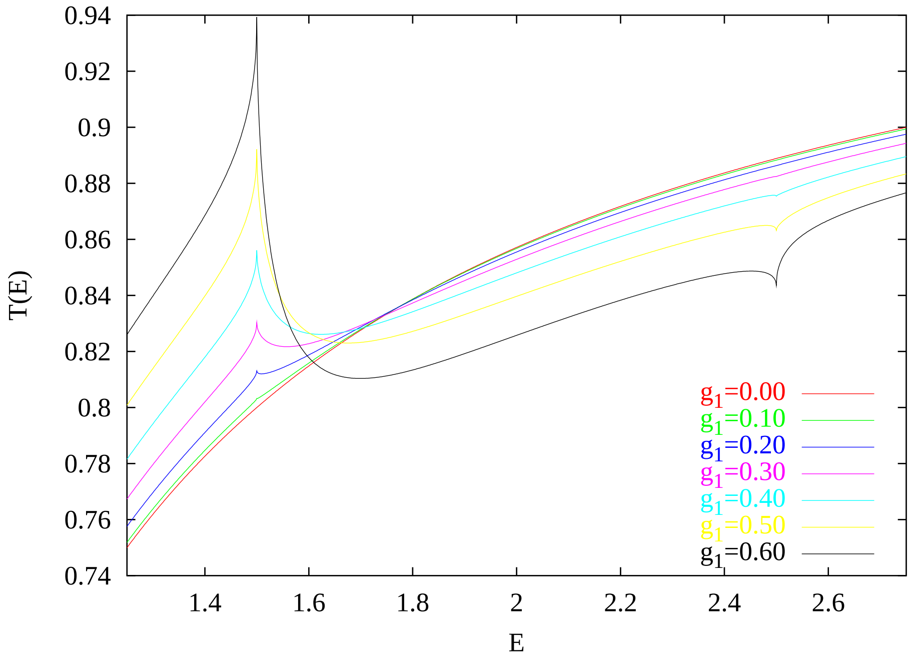

Figure 5: The transmission coefficient for various values of g_1, with $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

ground state. Hence, the incoming electron necessarily approaches in the $n = 0$ channel. At high energies, such that $E \gg g_1$, the incoming electron will effectively "see" no potential barrier, and will therefore interact weakly with the boson. This has the consequence that the electron will have a high probability of passing through the barrier unperturbed (giving $T \to 1$), and the weak interaction (weak coupling to other modes) means the electron will have a high probability of remaining in the zeroth channel. Conversely, for any other channel, the weak interaction means that there would be little chance of the boson to jump to higher states. So, for high energies, we would expect that the partial current in the $n = 0$ channel tends to unity while the partial currents in all the other channels tend to zero.

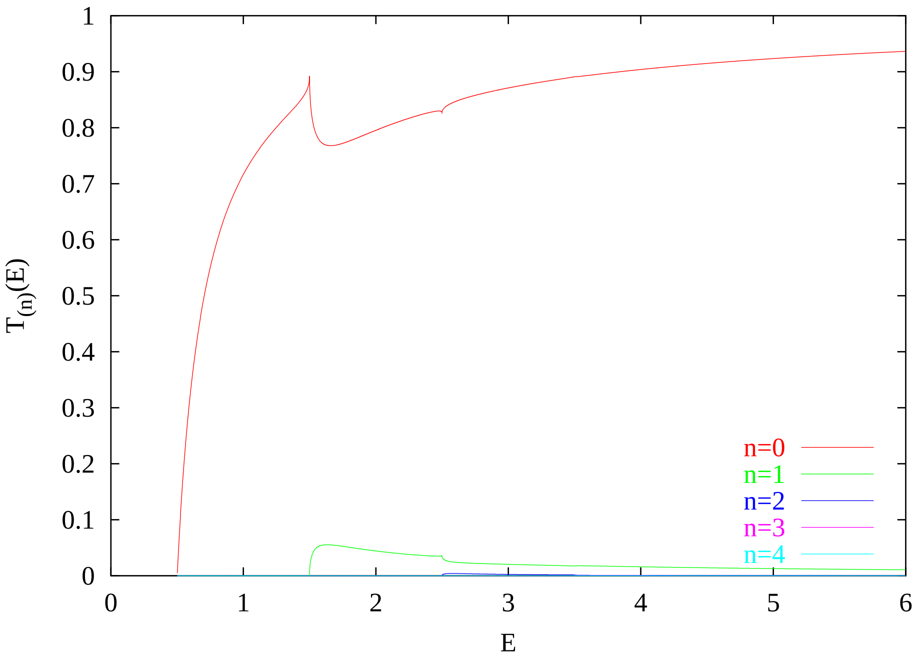

Figure 6: The partial transmission coefficients for $g_1 = 0.5$, $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

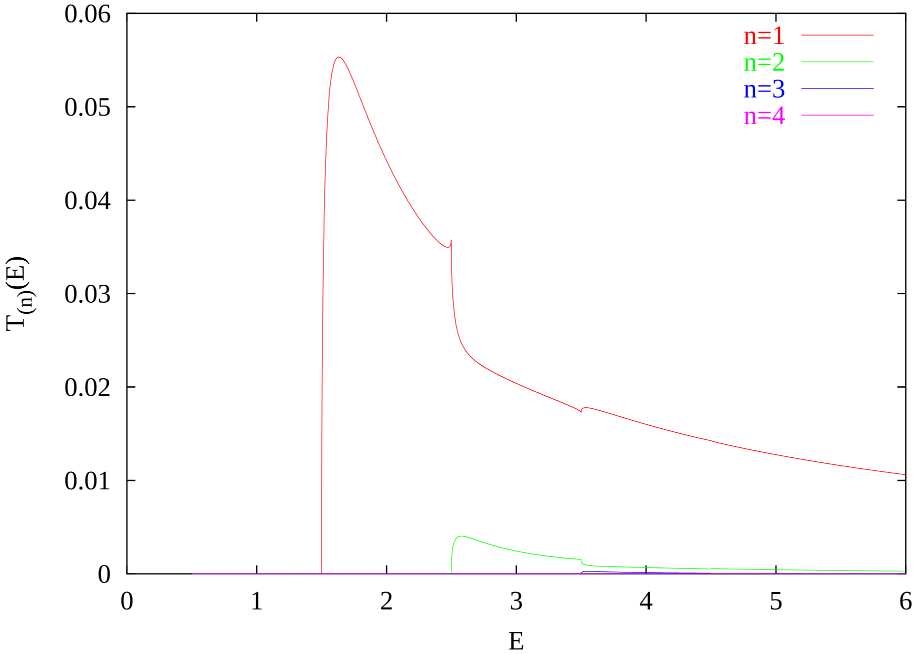

Figure 7: The partial transmission coefficients, excluding $n = 0$ for $g_1 = 0.5$, $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

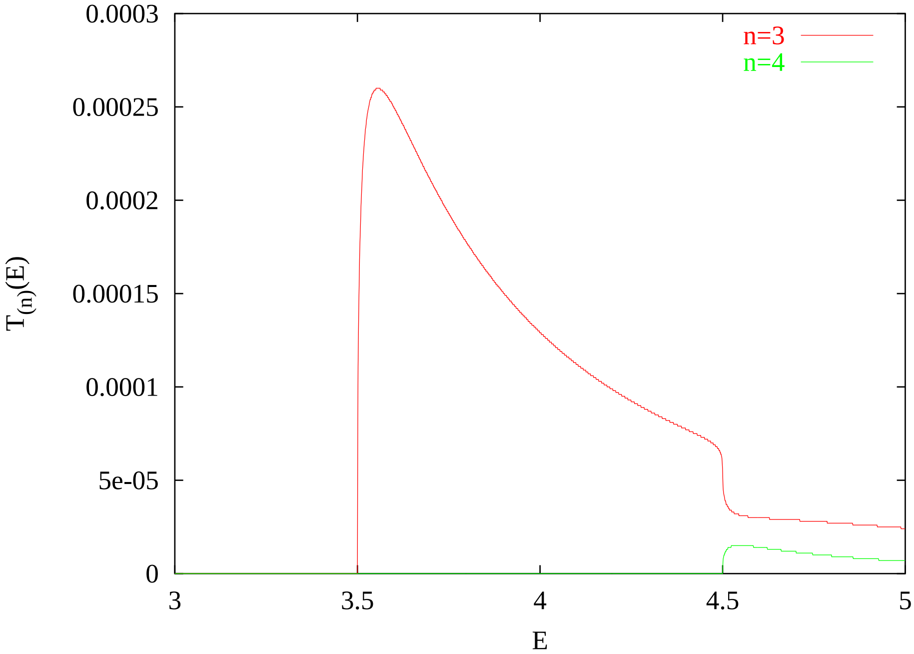

Figure 8: The partial transmission coefficients, excluding $n = 0, 1, 2$ for $g_1 = 0.5$, $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

4.2 Discussion

To understand these effects, one must consider the mechanism by which the electron is being scattered. Ideally, we have an incoming electron, which interacts in a boson in it's *ground state*, and is then scattered by the boson. The strength of the interaction is determined by $g_1 \left[a + a^\dagger\right] \propto x'$, the bosons position. From the mathematics we have shown that these operators lead to coupling of coefficients for the electron wave function in the various channels. These coefficients, and therefore also the transmission coefficient, are now dependent not only on the energy of the system but on the state of the boson too.

We will initially consider the $n = 0$ partial transmission coefficient for $g_1 = 0.5$ compared to $g_1 = 0$, figure 9.

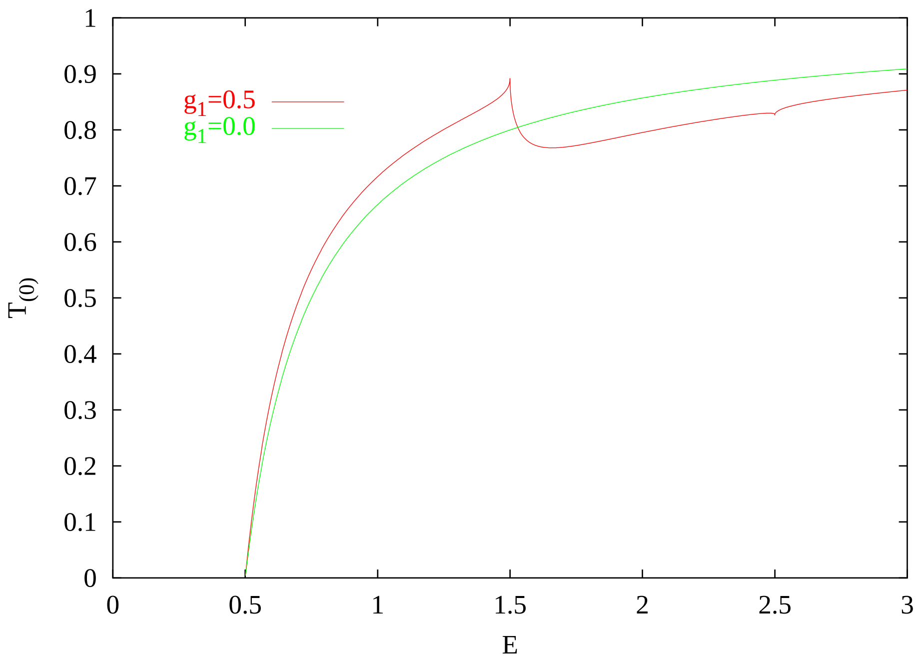

Figure 9: The partial transmission coefficients, $T_{(0)}$ for $g_1 = 0.5$, $A_0 = 1$, $\Omega = 1$ and $g_0 = 1$.

We can see that the static delta barrier, and the quantum barrier are both linear at low energies. Both transmission curves increase steadily with the energy. This is due to the fact that for energies below $\frac{3}{2}\Omega$, there is not enough energy available to excite the boson to a new state. Thus, greater system energy simply means that more energy is available to the electron, increasing the transmission coefficient. As the energy is increased further, however,

$T(E)$ becomes larger for the quantum barrier than for the static barrier, and as the energy approaches $\frac{3}{2}\Omega$ there is a sharp peak in $T(E)$. The reasons for this peak (and the deviation of $T(E)$ for the quantum barrier from the static case) are not obvious, and a theoretical derivation is necessary to account for them (see section 4.3).

As the energy is increased past $\frac{3}{2}\Omega$, there is a sharp decline in the transmission current. The reason for this is that now there is enough energy available for the boson to jump to the next energy level during the electron-boson interaction. After interacting, the boson will now sit in a superposition of these states. The probabilistic nature of the bosons state has a direct impact on the electron transmission coefficient. The electron now has an associated probability of being transmitted in either the first or the second channel. The transmission amplitude is now "shared" between these two channels. This can be seen in the plot of figure 10.

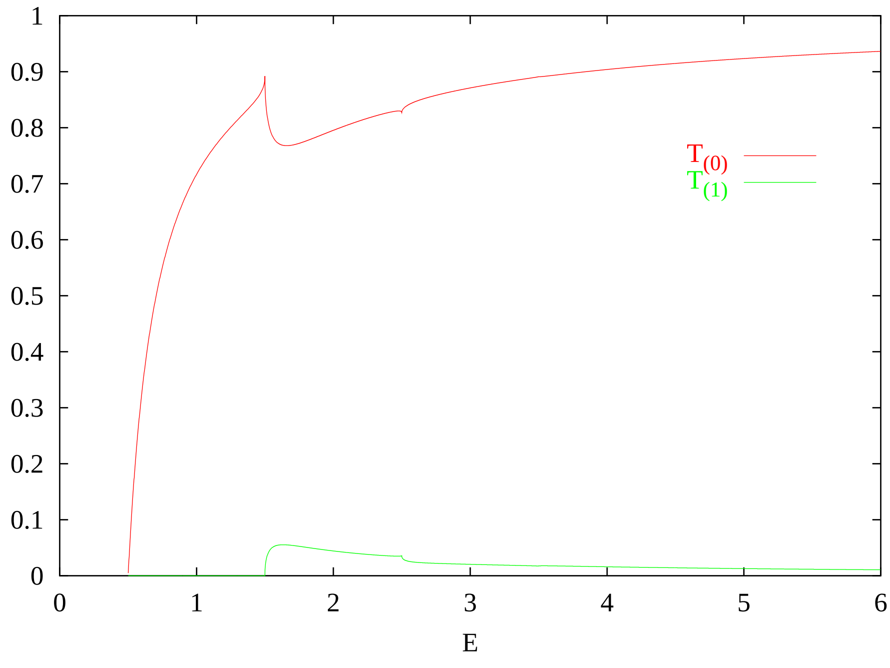

Figure 10: The partial currents "sharing" the transmission coefficient

The losses of current in the $n = 0$ channel are mirrored by the current gain in the $n = 1$ channel (although the magnitude of the losses and gains aren't necessarily equal).

4.3 Theoretical Discussion

To carry out a theoretical discussion of the problem in hand, it is necessary to make a few approximations. This is necessary because, to solve the problem completely, one has to invert an infinitely large matrix (given by equation 39). The size of the matrix reflects the number of possible boson states. As a first order approximation, it is possible to terminate the boson's Hilbert space at only two boson states. The matrix then has an exact solution, and we can explain certain features of the electron scattering based on the equations we obtain.
The matrix then is as follows,

$$\begin{bmatrix} g_0 - i\gamma_0 & g_1 \\ g_1 & g_0 - i\gamma_1 \end{bmatrix} \begin{bmatrix} T_0 \\ T_1 \end{bmatrix} = \begin{bmatrix} -i\gamma_0 A \\ 0 \end{bmatrix}, \tag{50}$$

which immediately yields

$$T_1 = -\frac{g_1}{g_0 - i\gamma_1} T_0\,, \tag{51}$$

and

$$(g_0 - i\gamma_0)\, T_0 + g_1 T_1 = -i\gamma_0 A. \tag{52}$$

Eliminating T_1 gives

$$(g_0 - i\gamma_0)\, T_0 - \frac{g_1^2}{g_0 - i\gamma_1} T_0 = -i\gamma_0 A\,. \tag{53}$$

Recalling the definition $\gamma_n \propto k_n$, the parameter γ_1 can be either imaginary or real, depending on the energy of the system. For γ_1 real, i.e. $E > \frac{3}{2}\Omega$ then

$$(g_0 - i\gamma_0)\, T_0 - g_1^2 \left(\frac{g_0 + i\gamma_1}{g_0^2 + \gamma_1^2} \right) T_0 = -i\gamma_0 A\,,$$

$$T_0 \left[\left(g_0 - \frac{g_1^2 g_0}{g_0^2 + \gamma_1^2} \right) - i \left(\gamma_0 + \frac{g_1^2 \gamma_1}{g_0^2 + \gamma_1^2} \right) \right] = -i\gamma_0 A\,,$$

which gives

$$T_0 = \frac{\gamma_0 A}{\left(\gamma_0 + \frac{g_1^2 \gamma_1}{g_0^2 + \gamma_1^2} \right) + i \left(g_0 - \frac{g_1^2 g_0}{g_0^2 + \gamma_1^2} \right)}\,. \tag{54}$$

Hence, the modulus squared of T_0 becomes

$$|T_0|^2 = \frac{\gamma_0^2 |A|^2}{\left(\gamma_0 + \frac{g_1^2\gamma_1}{g_0^2+\gamma_1^2}\right)^2 + \left(g_0 - \frac{g_1^2 g_0}{g_0^2+\gamma_1^2}\right)^2} \, .$$

For the zeroth channel, the partial transmission coefficient is simply

$$T_{(0)} = \frac{|T_0|^2}{|A|^2} \, ,$$

and so,

$$T_{(0)} = \frac{\gamma_0^2}{\left(\gamma_0 + \frac{g_1^2\gamma_1}{g_0^2+\gamma_1^2}\right)^2 + \left(g_0 - \frac{g_1^2 g_0}{g_0^2+\gamma_1^2}\right)^2} \, . \tag{55}$$

For the case where γ_1 is imaginary, we need to modify equation 54, replacing γ_1 with $i\tilde{\gamma}_1$, where $\tilde{\gamma}_n$ has it's usual meaning. Proceeding as before yields

$$T_{(0)} = \frac{\gamma_0^2}{\gamma_0^2 + \left(g_0 - \frac{g_1^2}{\tilde{\gamma}_1+g_0}\right)^2} \, . \tag{56}$$

This can be conveniently written as

$$T_{(0)} = \frac{\gamma_0^2}{\gamma_0^2 + \left[c\left(\gamma_1\right) g_0\right]^2} \, , \qquad \text{where} \;\; c(\gamma_1) = \left(1 - \frac{g_1^2}{\left[\gamma_1 + g_0\right] g_0}\right) \, . \tag{57}$$

This result allows us to interpret the spikes in the transmission curve of $T_{(0)}$ at $E = \frac{3}{2}\Omega$ and other other interesting features of this graph for $E < \frac{3}{2}\Omega$. If we compare equation 57 to the transmission coefficient of a static barrier equation 12, we can see that the form of each transmission coefficient is very similar, given that $\gamma^2 \propto E$. It is evident from equation 57 that the factor of $c(\gamma_1)$ simply alters the coupling constant g_0. The modulus of the factor $c(\gamma_0$ is also always less than 1 for weak coupling. This ultimately increases the partial transmission coefficient (and hence the total transmission coefficient) to values greater than that of a static barrier.
We now wish to find the minimum value of $c(\gamma_1)$. This is obviously achieved when γ_1 is a minimum. The minimum value of γ_1 is achieved at $E = \frac{3}{2}\Omega$ (since $\gamma_1 \propto k_n = \sqrt{E - \frac{3}{2}\Omega}$ is no longer imaginary beyond this point). Therefore we expect to see a maximum in the transmission curve at $E = \frac{3}{2}\Omega$, as is observed.
It is also worth to note that as $E \rightarrow \frac{3}{2}\Omega$, the coupling "screening" constant $c(\gamma_1)$reduces to the following,

$$c(\gamma_1) \approx \left(1 - \frac{g_1^2}{g_0^2}\right) .$$

This gives the partial transmission coefficient as

$$T_{(0)} \approx \frac{\gamma_0^2}{\gamma_0^2 + \left[g_0 - \frac{g_1^2}{g_0}\right]^2} ,$$

which, for very weak coupling ($g_1 \ll g_0$) simplifies further to

$$T_{(0)} \approx \frac{\gamma_0^2}{\gamma_0^2 + g_0^2} .$$

Given that $g_0 \gg \gamma_0$ then for small E, the above transmission coefficient is linear as it approaches the peak at $E = \frac{3}{2}\Omega$.
Beyond $E = \frac{3}{2}\Omega$, we must turn to the form of the transmission coefficient given by equation 55,

$$T_{(0)} = \frac{\gamma_0^2}{\left(\gamma_0 + \frac{g_1^2\gamma_1}{g_0^2+\gamma_1^2}\right)^2 + \left(g_0 - \frac{g_1^2 g_0}{g_0^2+\gamma_1^2}\right)^2} .$$

The effect of these screening terms on both g_1 and γ_0 are not obvious. However, it is this screening which leads to the complex scattering curve between $E = \frac{3}{2}\Omega$ and $E = \frac{5}{2}\Omega$.

5 Conclusion

From the "experimental" examination of the problem, it is evident that transmission coefficient is heavily dependent on only the first three partial transmission coefficients. This is due to the fact that for weak coupling, the boson is localized around the ground state. Hence, the electron transmission will be localized around the zeroth channel. To remove the boson from this state, the system energy must be increased. Then, however, the electron "sees" no barrier, and the electron transmission is again dominated by the zeroth channel.
From the theoretical analysis, it is evident that electron transmission coefficient is dependent not only on the propagating electron modes, but also on the decaying, or "evanescent" modes. These non-propagating modes assist the electron by screening the electron-boson coupling constant, allowing a

greater probability current to flow for $E < \frac{3}{2}\Omega$, compared with a static delta barrier. For $E > \frac{3}{2}\Omega$, the screening of the coupling constant restrains the tranmission current, leading to a *reduction* in the transmission coefficient, compared to the case of a static barrier. This effect can thought of as a continuous rescaling of the system energy scale. The initial energy scale of the graph is rescaled by the screening term such that it approaches unity quite rapidly. Then, as the peak of the curve is reached at $E = \frac{3}{3}\Omega$, the scaling term changes form (due to the transition from imaginary to real of γ_1), leading to a rapid decrease in the curve.

I have shown in this report that for this type of problem therefore it is possible to apply text-book methods for electron scattering to produce physically interesting results. Perhaps a more interesting extension to the project would be to study more complex initial conditions for the boson. The current initial condition is quite idealistic, and seems to be applicable only for the case of a single incoming electron. If an electron beam were to be passed over the barrier, however, then the initial conditions for an incoming electron in the beam at some later time, t, would be determined by the scattering which has previously taken place. It would therefore be quite an interesting extension to investigate this problem using a self consistent approach for the initial conditions, such that the resulting boson state is consistent with its initial state (i.e. they should be the same). Alternatively, one could investigate how the scattering would look if the boson were in thermal equilibrium. A more complicated extension would be to investigate other types of barrier, rather than a simple delta barrier. A finite width barrier would perhaps be more realistic as a scattering model than a delta barrier.

An application for this type of electron scattering could be quantum computing. We have shown that a single incoming channel may be split into a series of channels (also known as "bands"), with the boson sitting in a superposition of these modes (it is the boson modes which define the channel). If another electron beam was then passed over the boson, and its scattering properties measured, it would be possible to deduce the state of the boson. Hence, the former interaction may be thought of as supplying the boson with information, and the second interaction may be thought of as a way recover this information. Obviously here, the boson would act as an information storing device.

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A Appendix: C++ Algorithms