## Third year, assessed project report;

## Quantum mechanical scattering in a one dimensional, time dependant potential.

Investigating the transmission through a double delta potential barrier.

#### ABSTRACT

Quantum coherent transport in nanostructures has been one of the most exciting topics in 'mesoscopic physics' over the past decade. Interference and quantisation effects determine electronic properties in many phenomena like quantum Hall effect or conductance oscillations in small metallic rings. Furthermore, time-dependant coherent phenomena like the suppression of tunneling by irradiation with light have become the focus of very recent research.

In this project, we theoretically investigate the scattering of electrons from one-dimensional model potentials that change as a function of time and are of the form of a repulsive double delta function. We will perform calculations of the time-dependant Schrödinger equation to be solved numerically in a subsequent project, and compare with limiting cases that can be solved analytically.

Our aim is to make predictions for experimentally relevant quantities like e.g. the time averaged transmission coefficient.

The project is concluded upon finding the Fano resonance of the quantum dynamical case and the zero-channel transmission amplitude, involving a defined Green's function and a recursively defined self-energy, for this quantum dynamical case.

# Quantum mechanical scattering in a timedependant 1d potential.

An investigation into the transmission through a double delta potential barrier.

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# CHAPTER 1-:-INTRODUCTION TO QUANTUM MECHANICS AND ITS APPLICATION TO THIS INVESTIGATION.

#### **SECTION 1.1- INTRODUCTION**

#### 1.1.1 The Schrödinger wave equation

In any introduction to quantum mechanics, Schrödinger's wave equation must be the most important mathematical tool; Stationary Schrödinger equation;  $\hat{H}\Psi = E\Psi$ Where  $\Psi$  is the wave function corresponding to  $|\Psi|^2$  integrated over all dimensions being the representation of the probability density of the particle.  $\Psi$  completely describes the information of the particle at all points in space.

 $\hat{H}$  is the Hamiltonian operator and is functional when acting on an eigenfunction i.e. the wave function,  $\Psi$ . It contains the information of the total energy constraints on the particle and defines the idealized system of which the particle is a constituent. Consequentially, this gives an eigenvalue, E, which is usually defined in a sequence or series and is, as the physics of the microscopic world suggests, quantized into a discrete spectrum of values corresponding to the allowed energy values and is the expected value of the effect of the Hamiltonian of the system (for a simple example of energy quantization, refer to Einstein's explanation of the photoelectric effect).

#### 1.1.2 Potential barriers, the transmission coefficient and the delta function

The potential barrier function is included in the Hamiltonian of the system;  $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$  in one dimension. Where the first part of the Hamiltonian represents the effect of the kinetic energy of the incident particle wave function.

V(x) includes all the information of the potential barrier and represents the form of the potential in normal coordinate space. For an in depth look at the form of the delta function (sometimes called the Dirac delta function), see Appendix 1 of Eugen Merzbacher's Quantum

Mechanics<sup>i</sup> (third edition, Wiley, 1998). The forms of the Dirac delta potentials in this project are repulsive potentials (for a further discussion of this see the aims section of this report).

To get a grip on the problems in this project, I have chosen to point out a simple example of the effect of a repulsive square potential barrier on an incident wave function (this example is taken from chapter 2 of Franz Mandl's Quantum Mechanics<sup>ii</sup> (Wiley, 2001). Refer to this book for derivations of the results quoted here.

#### 1.1.3 Simple potential barrier problem

The potential in 1d shall have the form expressed opposite. The incident wave function,  $\varphi$ , can be expressed as a superposition of plane waves spanning from  $-\infty$  to  $+\infty$ , where k represents the wave number:-

$$V(x) = V_0(>0), for |x| < a$$
  
 $V(x) = 0, for |x| > a$ 

$$k = \sqrt{\frac{2mE}{\hbar^2}} \text{ for } E > 0$$
  
$$\phi(x < -a) = Ae^{ikx} + Be^{-ikx}$$
  
$$\phi(x > a) = Ce^{ikx}$$



 $e^{ikx}$  represents a wave function traveling in the positive x

direction and  $e^{-ikx}$  represents a wave function traveling in the negative x direction (a reflected wave function). There are no waves of the form  $e^{-ikx}$  at x > a, since there is nothing defined for the particle wave function to reflect from in this defined area of co-ordinate space. Read the first few chapters of A.P. French's Vibrations<sup>iii</sup> and wave for an introduction to the complex exponential form of a wave.

A is a constant amplitude, A' and C are constants related to A. A, A' and C are related to the particles currents. The particle current density of the incident beam is given by:-

$$j_{Incident} = \frac{\hbar k}{m} |A|^2 = j_{Transmitted} + j_{\text{Re flected}}$$

Which is obeys a conservation of particles argument. This gives the reflection and transmission coefficients as:-

$$R = \frac{j_{\text{Re flected}}}{j_{\text{Incident}}} \text{ and } T = \frac{j_{\text{Transmitted}}}{j_{\text{Incident}}} \text{ and also the relationship that } T + R = 1.$$

For this case, in the inner region |x| < a, the wave function has oscillators or real exponential character depending on the energy:

$$E > V_0 \implies \phi(|x| < a) = Be^{iqx} + B'e^{-iqx}$$
  

$$E < V_0 \implies \phi(|x| < a) = Be^{-\kappa x} + B'e^{\kappa x}$$
 where  $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$  and  $q = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$ 

The resulting transmission coefficients are found by taking into account the fact that  $\phi(x)$  and  $\phi'(x)$  have to be continuous at  $x = \pm a$ . The following transmission coefficient was derived from the above to give:-

$$T = \frac{16(k\kappa)^2}{(k+\kappa)^2} e^{-4a\kappa} where . 2a\kappa >> 1$$

The following graph is a qualitative view of what is happening before and after the potential barrier:



1.1.4 The Delta function and its properties<sup>iv</sup>

The delta function is the maths used to describe bits<sup>iv</sup>. To gain an understanding of the properties of the delta function, we first need to define a functional distribution for it to be described by. An appropriate function to use would be the

Gau $\beta$  function (in co-ordinate space), g(x) and its Fourier transform (in phase space),  $\tilde{g}(k)$ :

$$g(x) \coloneqq \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x+L)^2}{2\sigma^2}}$$
$$\widetilde{g}(k) = e^{-\frac{\sigma^2 k^2}{2}}$$



Where  $\sigma$  is a measure of how broad the distribution is in the x plane. If we now use this fact and limit  $\sigma$  to zero, we have what is called the Delta function. In co-ordinate space, this would correspond to an extremely sharp wave packet around x = - L that could serve as a model for a particle located at x = - L. We define the Delta function:

$$\delta(x+L) \coloneqq \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x+L)^2}{2\sigma^2}}$$

If the limit in the Delta function does not reach 0, but is still a very, very small number in the context of the function, the delta function can be used to describe discrete data (i.e. quanta). Conversely, if the limit does reach zero, the function will become meaningless and just describes a normal continuous data set, which is adequately described without such a delta function. The formal definition of the delta function comes from its operation on a function.

$$\int_{-\infty}^{\infty} dx \delta(x) f(x) = \lim_{\sigma \to 0} \int_{-\infty}^{\infty} dx f(x) \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} = f(0)$$

Such an operation is called a functional, which is a mapping that puts a whole function to a (complex or real) number<sup>iv</sup>. The function can, almost, be described in a piecewise way; the delta function is equal to infinity at x = 0 but is equal to zero at all other points.

Some of the properties of the delta function used in this investigation are quoted from Dr Tobias Brandes' lecture notes on Quantum Mechanics I, second year physics undergraduate course, UMIST 2003:

$$\int_{-\infty}^{\infty} dx \delta(x) f(x) = f(0)$$
$$\int_{-\infty}^{\infty} dx' \delta(x') f(x-x') = f(x)$$

The Fourier transform of the delta function is a superposition of all plane waves; the corresponding distribution of k-values in k-space is extremely broad, that is uniform from negative infinity to positive infinity. The corresponding transformation of the delta function defined by the Gau $\beta$  function gives:

$$\tilde{\delta}(x) = 1$$

i.e. this definition of the delta function is normalised.

#### 1.1.5 Harmonic oscillators

The harmonic oscillator will allow me to introduce a quantum mechanical behaviour to the potential barrier. I will now, with the help of Franz Mandl, outline the basic physics of the harmonic oscillator. For more explicit derivations, see Franz Mandl's Quantum Mechanics<sup>ii</sup>, chapter 12.5 (Wiley 2001).

I have chosen this example as it introduces the Dirac formalisation, which is used in some parts of this report. Using this formalisation also makes neat proofs that are totally explicit, yet economical with ink and paper.

The Hamiltonian for the harmonic oscillator is defined as;-

$$\hat{H} = \frac{\hat{p}}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2$$
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2$$

We now introduce two more operators that either raise or lower the state (state referring to the state function or wave function of the incident particle). These operators are named, unsurprisingly, the creation operator and the annihilation/destruction operator:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + \frac{i}{\sqrt{2m\hbar\omega}} \hat{p}$$
, are the annihilation operator and the creation operator  $\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - \frac{i}{\sqrt{2m\hbar\omega}} \hat{p}$ 

respectively.

We will also define the Hermitian operator  $\hat{a}^{\dagger}\hat{a} \equiv \hat{N}$ .  $\hat{a}$  and  $\hat{a}^{\dagger}$  do not commute as  $[\hat{a}, \hat{a}^{\dagger}] = \hat{a}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a} = 1 \neq 0$ The Hamiltonian for the system can be written as  $\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2})$  To find the energy eigenvalues for the Hamiltonian, we need to find the eigenvalues of  $\hat{N}$ . This is clearly an eigenvalue problem. Now we use the eigenstate of  $\hat{N}$  as  $|\lambda\rangle$  and the eigenvalue of  $\hat{N}$  as  $\lambda$ :

 $\hat{N}|\lambda\rangle = \lambda|\lambda\rangle$  where  $\langle\lambda|\lambda\rangle$  is defined to be equal to unity in a normalised situation.  $\lambda = \langle\lambda|\hat{N}|\lambda\rangle$  where  $\langle\lambda|$  is the complex conjugate of  $|\lambda\rangle$ .  $\lambda = \langle\lambda|\hat{a}^{+}\hat{a}|\lambda\rangle$   $= \langle\hat{a}^{+*}\lambda|\hat{a}\lambda\rangle$  i.e. eigenvalues of  $\hat{N}$  are non-negative and there must exist a smallest  $= \langle\hat{a}\lambda|\hat{a}\lambda\rangle \ge 0$ 

eigenvalue  $\lambda_0$ 

$$\hat{N}\hat{a}^{+}|\lambda\rangle = \hat{a}^{+}\hat{a}\hat{a}^{+}|\lambda\rangle$$

$$= \hat{a}^{+}(\hat{a}^{+}\hat{a}+1)|\lambda\rangle \quad \text{and similarly:} \quad \hat{N}\hat{a}|\lambda\rangle = \hat{a}^{+}\hat{a}\hat{a}|\lambda\rangle$$

$$= (\lambda+1)\hat{a}^{+}|\lambda\rangle \quad \text{and similarly:} \quad \hat{n}\hat{a}|\lambda\rangle = (\lambda-1)\hat{a}|\lambda\rangle$$

This shows that the operators  $\hat{a}$  and  $\hat{a}^+$  destroy or create an eigenstate  $|\lambda\rangle$ .

There exists a lowest state  $\lambda_0$ , such that  $\hat{a}|\lambda_0\rangle = 0$ . There is no lower state that exists below the lowest state (ground state).  $\hat{N}|\lambda_0\rangle = \hat{a}^+ \hat{a}|\lambda_0\rangle = 0$ , so that  $|\lambda_0\rangle$  belongs to the eigenvalue  $\lambda_0 = 0$  and the eigenvalues of  $\hat{N}$  are n = 0, 1, 2 ... $\Rightarrow \hat{N}|n\rangle = n|n\rangle$ , where  $|n\rangle$  represents the n<sup>th</sup> state of the harmonic oscillator.

Returning to our introduction to the quantum mechanics, we see that  $|n\rangle$  is analogous to  $\psi(x)$ . To take care of the quantisation previously derived, the wave function  $\psi(x) \rightarrow \psi_n(x)$ , where  $\psi_n(x)$  has a different harmonic form for each n = 0, 1, 2... and for all of our applications,  $\psi_n(x) = |n\rangle$ .

From the Schrödinger equation it can be seen that the quantisation of states also occurs in the energy eigenvalue of the system,  $E_n$ . It can be derived from our Schrödinger equation that  $E_n = \hbar \omega (n + \frac{1}{2})$  for n = 0, 1, 2 ...

I think that this section of the introduction is best summed up by a quote from Franz Mandl<sup>ii</sup>:

"... we can interpret  $|n\rangle$  as a state with n quanta present, each with energy  $\hbar\omega$ . We can see ... that  $\hat{a}^+|n\rangle$  is a state with (n + 1) quanta i.e.  $\hat{a}^+$  creates a quantum, and that  $\hat{a}|n\rangle$  is a state with (n - 1) quanta i.e.  $\hat{a}$  absorbs a quantum.  $\hat{a}$  and  $\hat{a}^+$  are accordingly known as absorption (or annihilation) and creation operators respectively. The operator  $\hat{N}$  is called the occupation number operator; its eigenvalues n = 0, 1, 2... specify the number of quanta in the state  $|n\rangle$ ."

#### SECTION 1.2- AIMS

What is the  $\delta(x)$  function? An infinite potential in the co-ordinate space. It seems to be a mirror infinitesimally thin, but still there, as to disrupt the probability amplitude of any incoming particle wave function,  $\psi(x)$ . This could be visualized as ripples on a lake that has some kind of dam system analogous to the form of the  $\delta(x)$  function. We would see this in the quantum world as ripples on the lake that seem to ignore the existence of the dam system, the only noticeable effect of the dam would be a distortion of the ripples. Considering the case

Could this  $\delta(x)$  function be a limiting case for a model? Maybe the model would consist of a region of space being a disallowed area, but since the wave function is a probability of the particle being there, it can pass the disallowed region without actually penetrating it.

The aims of this theoretical project will be to find out what this  $\delta(x)$  function is by measuring its effect on Fermion's a probability wave function (a 'particle' that obeys Fermi-Dirac statistics).

The effect of  $\delta(x)$  on the probability wave function will be found by calculating the amount of the wave function that is reflected or transmitted through the delta potential. Finding the transmission coefficient of the whole system can do this. The method used to find this will be an aim of the project.

The title of this project dictates a double delta potential barrier (see figure 1) as a previous project has already tackled a single delta potential in a classical and quantum case. For a better understanding of this project, read the report by John Robinson<sup>vi</sup> with Tobias Brandes called Transmission through a Quantum Dynamical Delta Barrier<sup>v</sup> (umist, 2002). Many

analogies can and have been made to this case, but only as far as the method that was used. The rigorous mathematical techniques involved are obviously more complicated in this project.

An aim of this project is to apply the method John Robinson used to find a static case for the system and hence the transmission coefficient. This can then be compared with a quantum case so that the quantum effect can be deduced.

The static case will use the same boundaries and initial conditions as a square potential barrier (see section 1.1.3). this is because it has no bound solutions (a repulsive barrier) and is a similar arrangement to boundaries of my problem. This approach should allow me to find the transmission coefficient at each boundary and hence find the transmission coefficient of the whole system by multiplying the two together.

To implement a quantum character to the static case, I will simulate a harmonic, oscillatory motion on one of the barriers. This will be of the form of a bosonic frequency (see figure 2) that is coupled to the incident particle wave function (see section 1.1.5). This will quantize the energy eigenvalues so that a recursive transmission coefficient can be found. Further representation of the transmission coefficient will also be implemented to make computation of these transmission coefficients the next obvious step after this project.

These methods completed, comparisons between the static and quantum (oscillator) cases can be made and concluded upon.



### SECTION 1.3- MODELED GRAPHIC DIAGRAMS

### CHAPTER 2-:-THE STATIC CASE

#### SECTION 2.1- BOUNDARY CONDITIONS

These conditions set out the form of the wave functions in the separated zones (see figure 1) and are of the same exponential form as the simple square potential barrier in section 1.1.3. Conditions set out like these assume an incident particle bean from the left.  $e^{ikx}$  represents wave functions traveling in the positive x direction and  $e^{-ikx}$  represents waves traveling in the negative x direction<sup>iii</sup>. The superposition of these states describes the form of the total wave function at any position in the one-dimensional real space.



#### SECTION 2.2- THE HAMILTONIAN AND THE SCHRÖDINGER EQUATION

The piecewise description of the bosonic potential energy variation is:  $\begin{aligned} V(-L) &= \delta(x+L) \\ V(0) &= \delta(x) \end{aligned}$ 

Where  $\delta(x - L)$  is the Dirac delta function at a position x = L, and L is the length of the gap between the two delta potential functions

The Schrödinger equation, with the applicable Hamiltonian operator inserted is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + g(\delta[x+L] + \delta[x])\psi(x) = E\psi(x)$$

#### SECTION 2.3- CONTINUITY/DISCONTINUITY CONDITIONS<sup>i</sup>

#### 2.3.1 Continuity conditions

This is a standard condition that requires the wave function not to have any discontinuous jumps in any part of its form i.e. the wave function should be smooth and continuous. All that is needed to do this is to equate the wave functions that appear at each side of a boundary (delta potentials at x = 0 & x = -L), at the boundary position.

<u>Continuity condition for wave function at x = 0;</u>

$$T_1 e^{ikx} + R_2 e^{-ikx} = T_2 e^{ikx}$$
$$T_1 + R_2 = T_2$$
$$x = 0 \Longrightarrow$$

Continuity equation for wave function at x = -L;  $Ae^{ikx} + R_1e^{-ikx} = T_1e^{ikx} + R_2e^{-ikx}$   $x = -L \Rightarrow$  $Ae^{-ikL} + R_1e^{ikL} = T_1e^{-ikL} + R_2e^{ikL}$ 

#### 2.3.2 Discontinuity conditions

This is also from a standard condition that requires the derivative of the wave function with respect to x to be continuous at all points except where the potential is infinite. One can see that from this condition, it would be intuitive to say that this gradient should be discontinuous at the places where the potential is infinite.

A method to apply this discontinuity condition is to integrate the Schrödinger equation around the delta potential position  $\pm \varepsilon$ , in the limiting case where  $\varepsilon$  is zero. This can then be equated to the small difference,  $\Delta$ , in derivatives at each side of the delta potential position  $\pm \varepsilon$ , where  $\varepsilon$ is, again, limited to zero.

#### Discontinuity condition for gradient of wave function at x =0;

[Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ] = [Differential of the wave functions at x > 0 and -L < x < 0 and evaluated at  $+\varepsilon$  and  $-\varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ]

$$\Delta \left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^2}(T_1 + R_2) = \frac{2mg}{\hbar^2}T_2$$

$$T_2 = \frac{T_1}{\left(1 + \beta i\right)} \left[say\beta = \frac{mg}{\hbar^2 k}\right]$$

Discontinuity condition for gradient of wave function at x = -L: [Integrate Schrödinger equation around  $x = -L\pm\epsilon$ , limiting  $\epsilon \rightarrow 0$ ] = [Differential of the wave function at x< -L and -L< x< 0 and evaluated at -L+ $\epsilon$  and -L- $\epsilon$ , limiting  $\epsilon \rightarrow 0$ ]

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^2} (Ae^{-ikL} + R_1 e^{ikL}) = \frac{2mg}{\hbar^2} \left(T_1 e^{-ikL} + R_2 e^{ikL}\right)$$

$$T_{1} = \frac{A}{\left(1 + i\beta + \frac{i\beta}{\left(1 + i\beta\right)}e^{2ikL} - i\beta e^{2ikL}\right)}$$

#### SECTION 2.4- THE TRANSMISSION COEFFICIENT

The transmission coefficient of area II to area III is  $T'' = \frac{|T_2|^2}{|T_1|^2}$ 

$$T^{\prime\prime} = \frac{1}{\left(1 + \beta^2\right)}$$

Transmission coefficient of area I to area II is  $T' = \frac{|T_1|^2}{|A|^2}$ 

$$T' = \frac{1}{\left(1 - i\beta - \frac{i\beta}{(1 - i\beta)}e^{-2ikL} + i\beta e^{-2ikL}\right)\left(1 + i\beta + \frac{i\beta}{(1 + i\beta)}e^{2ikL} - i\beta e^{2ikL}\right)}$$

Transmission coefficient of the whole system is simply the multiplication of successive transmission coefficients T = T'T''

$$T = \frac{1}{1 + 2\beta^2 + 2\beta^4 + (\beta^2 - 2i\beta^3 - \beta^4)e^{2ikL} + (\beta^2 + 2i\beta^3 - \beta^4)e^{-2ikL}}$$

It would be useful to find this transmission coefficient in terms of the energy of the incident particle, T(E).

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = \frac{mg}{\hbar^2 k} = \frac{mg}{\hbar\sqrt{2mE}}$$

Using the sensible scale that corresponds to the sale of the Bohr radius, we can set  $\hbar = 2m = 1$ 

$$\Rightarrow \beta = \frac{g}{2\hbar} \sqrt{\frac{4m^2}{2mE}} = \frac{g}{2\hbar} \sqrt{\frac{2m}{E}} = \frac{g}{2\sqrt{E}}$$
$$\therefore T(E) = \frac{4E}{4E + g^2 \left( \left(\frac{1}{2E} - i\frac{g}{\sqrt{E}} - \frac{g^2}{4E}\right) e^{i2L\sqrt{E}} + \left(\frac{1}{2E} + i\frac{g}{\sqrt{E}} - \frac{g^2}{4E}\right) e^{-i2L\sqrt{E}} + \frac{g^2}{2E} \right)}$$

## CHAPTER 3-:-DISCUSSION OF THE RESULTS OBTAINED FROM CHAPTER 2

The transmission coefficient for the static case can clearly be solved analytically using a graph of T(E), since there is only a dependence of the transmission coefficient on the energy, E, of the electron and the potential constant, g. These results should be compared with the case of the single delta potential barrier<sup>vi</sup> and the case of the square potential barrier (section 1.1.3).

#### Comparison with the single delta potential

Results from reference (V) give the transmission coefficient though a Static 1d delta potential barrier to be:

$$T = \frac{4E}{4E + g^2}$$

We can see that the two differ by a variable,  $\xi$  (E), that is multiplied with  $g^2$ . This can be expressed in the form of complex variables:

$$\xi(E) = \frac{g^2}{2E} + \zeta(E) + \zeta^*(E)$$

Where  $\varsigma^*(E)$  is the complex conjugate of  $\varsigma(E)$ . The complex function of kinetic energy of the incident wave function and potential energy of the delta potential particles:

$$\zeta(E) = \left(\frac{1}{2E} - i\frac{g}{\sqrt{E}} - \frac{g^2}{4E}\right)e^{i2L\sqrt{E}}$$

This is the part of the transmission coefficient that depends on the distance L between the two delta potential barriers. When this distance is equal to zero;

$$\xi(E) = \frac{g^2}{2E}$$

Giving the transmission coefficient as  $T = \frac{4E}{4E + \frac{g^4}{2E}} = \frac{4E^2}{4E^2 + g^2}$ 

## CHAPTER 4-:-THE OSCILLATORY (QUANTUM) CASE

#### SECTION 4.1- BOUNDARY CONDITIONS

These conditions are set out in analogy with chapter 2, but taking section 1.1.5 into account. It can be seen that the quantisation of the harmonic oscillator dictates a quantisation of states also occurs in the energy eigenvalue of the system,  $E_n$ . Since the energy and wave vector, k, are related, the wave vector will also see a quantisation of states, corresponding to Fano<sup>vii</sup> type resonances. The mathematical theory behind this area of Quantum Dynamics can be found in Guido Fano's book<sup>vii</sup>, chapters 5.1-12 and 6.5.

It should be clear, after section 1.1.3, that there will be two separate cases:

When the energy is greater than the bosonic energy,  $\Omega$ n; Real wave vector,

$$k_n = \sqrt{E - \Omega n}$$

When the energy is less than the bosonic energy; Imaginary wave vector,

$$\kappa_n = \sqrt{n\Omega - E}$$

The case with the real wave vector is analogous to that of chapter 2. The case with the imaginary wave vector will need to be described by a decomposition into plane waves:

Т

CASE 1: 
$$E > \Omega n$$
  
 $\Psi_n(-L > x) = A_n e^{ik_n x} + R_{1,n} e^{-ik_n x}$   
 $\Psi_n(-L < x < 0) = T_{1,n} e^{ik_n x} + R_{2,n} e^{-ik_n x}$   
 $\Psi_n(0 < x) = T_{2,n} e^{ik_n x}$   
 $\Psi_n(0 < x) = T_{2,n} e^{ik_n x}$   
 $E < \Omega n$   
 $\Psi_n(-L > x) = R_{1,n} e^{\kappa_n x}$   
 $\Psi_n(-L < x < 0) = T_{1,n} e^{-\kappa_n x} + R_{2,n} e^{\kappa_n x}$   
 $\Psi_n(0 < x) = T_{2,n} e^{-\kappa_n x}$ 

#### SECTION 4.2- THE HAMILTONIAN AND THE SCHRÖDINGER EQUATION

The electron energy Hamiltonian  $\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ 

The interaction (coupling) Hamiltonian  $\hat{H}_{INT} = \left[g_0 + g_1\left[\hat{a} + \hat{a}^+\right]\right]\delta(x) + g_2\delta(x+L)$ 

The bosonic energy term (harmonic oscillator creating or destroying a state with photon interaction in the defined integer increments of the creation and annihilation operators, see section 1.1.5)  $\hat{H}_{B} = \Omega \hat{a}^{\dagger} \hat{a}$ 

Where  $\Omega = \hbar \omega$ , and is the bosonic frequency of the photon.

[Note that a factor of  $\Omega_2$ , the ground state of the boson, is neglected for convenience. However, it should be noted that a lowest state, the ground state, does exist and that no eigenstate can have a lower eigenvalue than E<sub>0</sub>]

The sum of these Hamiltonians for kinetic, potential and interacting energies gives the total Hamiltonian of the system:

$$\Rightarrow \hat{\mathbf{H}} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + g_0 \delta(x) + g_1 [\hat{a} + \hat{a}^+] \delta(x) + g_2 \delta(x + L) + \Omega \hat{a}^+ \hat{a}$$

Creation and Annihilation operators (defined in section 1.1.5):  $\hat{a}^+$ 

 $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$ ):  $\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$ 

Schrödinger equation (section 1.1.1);  $\hat{H}\Psi = E\Psi$ 

Where the formation of the separation ansatz of the electron wave function,  $\Psi = \psi(x)\phi(x')$  involves the separation of variables.  $\phi(x')$  is the coupled bosonic wave function, corresponding to the interacting photon.

Expand the electron wave function,  $\Psi$ , into a sum of component eigenkets,  $|n\rangle$ , from the photon in the electron frame, as a sum over all resonant states, n :

$$\Rightarrow \Psi = \sum_{n=0}^{\infty} \psi_n(x) \big| n \big\rangle$$

Where  $|n\rangle$  corresponds to  $\phi_n(x')$  and is the photon wave function traveling in the positive x direction. Conversely,  $\phi_m^*(x')$  corresponds to  $\langle m |$  and is the photon wave function traveling in the negative x direction.

Schrödinger equation as a summation over all resonant states;

$$\begin{bmatrix} -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + g_0 \delta(x) + g_1 [\hat{a} + \hat{a}^+] \delta(x) + g_2 \delta(x + L) + \Omega \hat{a}^+ \hat{a} \end{bmatrix} \Psi = \mathbf{E} \Psi$$
$$\Rightarrow \sum_{n=0}^{\infty} \begin{bmatrix} -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} |n\rangle + g_0 \delta(x) \psi_n(x) |n\rangle + g_1 [\hat{a} + \hat{a}^+] \delta(x) \psi_n(x) |n\rangle \\ + g_2 \delta(x + L) \psi_n(x) |n\rangle + \hbar \omega \hat{a}^+ \hat{a} \psi_n(x) |n\rangle \end{bmatrix}$$
$$= \sum_{n=0}^{\infty} \mathbf{E} \psi_n(x) |n\rangle$$

 $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ Creation and Annihilation operator identities:  $\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$  $\hat{a}^{+}\hat{a} \equiv \hat{N} = n$ 

$$\Rightarrow \sum_{n=0}^{\infty} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} |n\rangle + g_0 \delta(x) \psi_n(x) |n\rangle + g_1 \delta(x) \psi_n(x) \sqrt{n} |n-1\rangle \\ + g_1 \delta(x) \psi_n(x) \sqrt{n+1} |n+1\rangle + g_2 \delta(x+L) \psi_n(x) |n\rangle + \hbar \omega \psi_n(x) n |n\rangle \right]$$
$$= \sum_{n=0}^{\infty} \mathbf{E}_n \psi_n(x) |n\rangle$$

Change of summation indices so  $|n\rangle$  can be taken out as a factor

$$\Rightarrow \sum_{n=0}^{\infty} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} |n\rangle + g_0 \delta(x) \psi_n(x) |n\rangle + g_1 \delta(x) \sqrt{n} \psi_{n-1}(x) |n\rangle + g_1 \delta(x) \sqrt{n} \psi_{n-1}(x) |n\rangle + g_1 \delta(x) \sqrt{n} \psi_n(x) |n\rangle + g_2 \delta(x+L) \psi_n(x) |n\rangle + \hbar \omega \psi_n(x) n |n\rangle \right]$$
$$= \sum_{n=0}^{\infty} E_n \psi_n(x) |n\rangle$$

Multiply through by the boson state of the interacting photon  $\langle m |$ , making use of the fact that  $\langle m | n \rangle = \delta_{m,n}$ , where  $\delta_{m,n}$  is the Kronecker delta, a mathematical tool that gives a "true of false" condition for the resonance of the photon wave function with the electron wave function:

$$\delta_{m,n} = 0$$
 for  $m \neq n$   $\delta_{m,n} = 1$  for  $m = n$ 

This gives the Schrödinger equation as a recursive  $\psi_n$  equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_n}{\partial x^2} + g_0 \delta(x)\psi_n + g_1 \delta(x)\sqrt{n}\psi_{n-1} + g_1 \delta(x)\sqrt{n+1}\psi_{n+1} + g_2 \delta(x+L)\psi_n + \hbar\omega n\psi_n = \mathbf{E}_n\psi_n$$

#### SECTION 4.3- CONTINUITY/DISCONTINUITY CONDITIONS

#### Continuity conditions

These are exactly analogous to those used in chapter 2, except that there are two cases corresponding to the two different types of wave function, depending on the energy of the incident electron, see section 1.1.3.

### $_{\text{CASE 1:}} E > \Omega n$

Continuity condition for wave function at x = 0;

$$T_{1,n}e^{ik_nx} + R_{2,n}e^{-ik_nx} = T_{2,n}e^{ik_nx}$$
$$x = 0 \Longrightarrow$$
$$T_{1,n} + R_{2,n} = T_{2,n}$$

Continuity condition for wave function at x = -L;

$$T_{1,n}e^{ik_nx} + R_{2,n}e^{-ik_nx} = A_ne^{ik_nx} + R_{1,n}e^{-ik_nx}$$
$$x = -L \Longrightarrow$$
$$T_{1,n}e^{-ik_nL} + R_{2,n}e^{ik_nL} = A_ne^{-ik_nL} + R_{1,n}e^{ik_nL}$$

## CASE 2: $E < \Omega n$

Continuity condition for wave function at x = 0;

$$T_{1,n}e^{-\kappa_n x} + R_{2,n}e^{\kappa_n x} = T_{2,n}e^{-\kappa_n x}$$
$$x = 0 \Longrightarrow$$
$$T_{1,n} + R_{2,n} = T_{2,n}$$

Continuity condition for wave function at x = -L;

$$R_{1,n}e^{\kappa_n x} = T_{1,n}e^{-\kappa_n x} + R_{2,n}e^{\kappa_n x}$$
$$x = -L \Longrightarrow$$
$$R_{1,n}e^{-\kappa_n L} = T_{1,n}e^{\kappa_n L} + R_{2,n}e^{-\kappa_n L}$$

#### **Discontinuity conditions**

These are also exactly analogous to those used in chapter 2, except that there are again two cases corresponding to the two different types of wave function, depending on the energy of the incident electron, see section 1.1.3. Also, see section 1.1.4, for the properties of the delta function.

## $_{\text{CASE 1:}} E > \Omega n$

Discontinuity condition for gradient of the wave function at x =0;

Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$\Delta \left[\frac{\partial \psi_n}{\partial x}\right] = \frac{2m}{\hbar^2} \left[ g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) \right] \text{Differentiate the wave functions at } x > 0 \text{ and } -L$$

< x < 0 and evaluate at  $+\epsilon$  and  $-\epsilon;$ 

$$\Delta \left(\frac{d\psi_n}{dx}\right) = ik_n \left(T_{2,n} - T_{1,n} + R_{2,n}\right)$$

Which can be written as a sequence:

$$T_{2,n+1} = -\frac{\left(g_0(T_{2,n}) + g_1\sqrt{n}(T_{2,n-1})\right)}{g_1\sqrt{n+1}} + i\frac{\hbar^2 k_n}{m}\frac{\left(T_{2,n} - T_{1,n}\right)}{g_1\sqrt{n+1}}$$

Discontinuity condition for gradient of the wave function at x = -L;

Integrate Schrödinger equation around  $x = -L\pm\epsilon$ , limiting  $\epsilon \rightarrow 0$ ;

$$\Delta \left[\frac{\partial \psi_n}{\partial x}\right]_{-L} = \frac{2m}{\hbar^2} \left[g_2 \psi_n(-L)\right]$$

Differentiate the wave functions at x < -L and -L < x < 0 and evaluate at  $-L+\epsilon$  and  $-L-\epsilon$ ;

$$\Delta \left(\frac{d\psi_n}{dx}\right)_{-L} = ik_n \left(T_{1,n} e^{-ik_n L} - R_{2,n} e^{ik_n L} - A_n e^{-ik_n L} + R_{1,n} e^{ik_n L}\right)$$
$$T_{1,n} = \frac{A_n + \frac{img_2}{\hbar^2 k_n} T_{2,n} e^{2ik_n L}}{\frac{img_2}{\hbar^2 k_n} + 1 + \frac{img_2}{\hbar^2 k_n} e^{2ik_n L}}$$

# CASE 2: $E < \Omega n$

Discontinuity condition for gradient of the wave function at x =0; Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

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

Differentiate the wave functions at x > 0 and -L < x < 0 and evaluate at  $+\varepsilon$  and  $-\varepsilon$ ;

$$\Delta \left(\frac{d\psi_n}{dx}\right) = -\kappa_n \left(T_{2,n} + R_{2,n} - T_{1,n}\right) = -2\kappa_n \left(T_{2,n} - T_{1,n}\right)$$

Which can be written as a sequence:

$$T_{2,n+1} = -\frac{\left(g_0(T_{2,n}) + g_1\sqrt{n}(T_{2,n-1})\right)}{g_1\sqrt{n+1}} + \frac{\hbar^2\kappa_n}{m}\frac{\left(T_{2,n} - T_{1,n}\right)}{g_1\sqrt{n+1}}$$

Discontinuity condition for gradient of the wave function at x =-L;

Integrate Schrödinger equation around  $x = -L\pm\epsilon$ , limiting  $\epsilon \rightarrow 0$ ;

$$\Delta \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L} = \frac{2m}{\hbar^2} \left[ g_2 \psi_n(-L) \right]$$

Differentiate the wave functions at x < -L and -L < x < 0 and evaluate at  $-L+\varepsilon$  and  $-L-\varepsilon$ ;

$$\Delta \left(\frac{d\psi_n}{dx}\right)_{-L} = -\kappa_n \left(T_{1,n} e^{\kappa_n L} + R_{1,n} e^{-\kappa_n L} - R_{2,n} e^{-\kappa_n L}\right)$$
$$T_{1,n} = -\frac{T_{2,n} e^{-2\kappa_n L}}{\left(1 - e^{-2\kappa_n L} + \frac{\hbar^2 \kappa_n}{mg_2}\right)}$$

#### Forming of two recursive relations

The four relations above can be reduced to two separate recursive relation, corresponding to the two types of wave vector.

$$_{\text{CASE 1:}} E > \Omega n$$
.

$$mg\sqrt{n+1}(T_{2,n+1}) + mg_{1}\sqrt{n}(T_{2,n-1}) + \left(mg_{0} - i\hbar^{2}k_{n} - \frac{mg_{2}e^{2ik_{n}L}}{1 + \frac{img_{2}(1+e^{2ik_{n}L})}{\hbar^{2}k_{n}}}\right) (T_{2,n}) = -(A_{n})\frac{i\hbar^{2}k_{n}}{1 + \frac{img_{2}(1+e^{2ik_{n}L})}{\hbar^{2}k_{n}}}$$

CASE 2:  $E < \Omega n$ :

$$mg\sqrt{n+1}(T_{2,n+1}) + mg_{1}\sqrt{n}(T_{2,n-1}) + \left(mg_{0} - \hbar^{2}\kappa_{n} - \frac{mg_{2}e^{-2\kappa_{n}L}}{1 + \frac{mg_{2}(1 - e^{-2\kappa_{n}L})}{\hbar^{2}\kappa_{n}}}\right)(T_{2,n}) = 0$$

A Report and investigation by David Goodwin with Dr T. Brandes as the supervisor

#### SECTION 4.4- ASSUMPTIONS OF THE INCIDENT ELECTRON BEAM

A fundamental simplification must be made at this point, to make the previous equation the general statement that it seems. The constant amplitude for a specific state,  $A_n$ , must be simplified to make an calculations less complicated. Impose the condition that  $A_n = A \delta_{n,0}$  i.e. the boson is in its ground state for an electron incident from the left. We can also set  $A = A_0 =$  unity, corresponding to a knowledge of the incident bean intensity.

If we let  $k_n$  be real or imaginary for a given E and n, the two recursion relations can reduce to one. For simplicity, we will use  $\gamma_n = \frac{\hbar^2 k_n}{m}$ , where  $\gamma_n$  can be either real or imaginary. Again, we set  $\hbar = 2m = 1$ , to put any measurements at the scale of the Bohr radius.

$$g_{1}\sqrt{n+1}(T_{2,n+1}) + g_{1}\sqrt{n}(T_{2,n-1}) + \left(g_{0} - i\gamma_{n} - \frac{g_{2}e^{2ik_{n}L}}{1 + \frac{ig_{2}(1+e^{2ik_{n}L})}{\gamma_{n}}}\right) (T_{2,n}) = -\frac{i\gamma_{n}^{2}\delta_{n,0}}{\gamma_{n} + ig_{2}(1+e^{2ik_{n}L})}$$

This is true for and  $E > E_0$ , where  $E_0$  corresponds to the ground state energy of the boson,  $\Omega/2$ , which was noted in section 4.2. Recall the definition of  $k_n = \sqrt{E - \Omega n}$ . The above equation can now be expressed in terms of E.

$$g_{1}\sqrt{n+1}(T_{2,n+1}) + g_{1}\sqrt{n}(T_{2,n-1}) + \left(g_{0} - i\gamma_{n}(E) - \frac{g_{2}e^{2iL\sqrt{E-\Omega n}}}{1 + \frac{ig_{2}(1+e^{2iL\sqrt{E-\Omega n}})}{\gamma_{n}(E)}}\right) (T_{2,n}) = -\frac{i\gamma_{n}^{2}(E)\delta_{n,0}}{\gamma_{n}(E) + ig_{2}(1+e^{2iL\sqrt{E-\Omega n}})}$$

#### SECTION 4.5- THE STATIC QUANTUM CASE (FANO RESONANCES)<sup>vii</sup>

The above recursion relation can be compared with the static case from chapter 2 by equating  $g_0$  to  $g_2$  and  $g_1$  to zero. This should give the Fano resonances<sup>vii</sup>, of this quantum dynamical case corresponding  $\Omega \hat{a}^+ \hat{a}$  of the harmonic oscillator without any electron interaction:

$$\begin{pmatrix} g - i\gamma_n(E) - \frac{ge^{2iL\sqrt{E-\Omega n}}}{1 + \frac{ig(1+e^{2iL\sqrt{E-\Omega n}})}{\gamma_n(E)}} \end{pmatrix} (T_{2,n}) = -\frac{i\gamma_n^2(E)\delta_{n,0}}{\gamma_n(E) + ig(1+e^{2iL\sqrt{E-\Omega n}})}$$

$$\Rightarrow \left(\gamma_n(E) + ig(1+e^{2iL\sqrt{E-\Omega n}})\right) \left(g - i\gamma_n(E) - \frac{ge^{2iL\sqrt{E-\Omega n}}}{1 + \frac{ig(1+e^{2iL\sqrt{E-\Omega n}})}{\gamma_n(E)}}\right) (T_{2,n}) = -i\gamma_n^2(E)\delta_{n,0}$$

$$\Rightarrow \left(T_{2,n}\right) = \frac{\gamma_n(E)\delta_{n,0}}{ig(2+e^{2iL\sqrt{E-\Omega n}}) + \left(\gamma_n(E) - \frac{g^2}{\gamma_n(E)}(1+e^{2iL\sqrt{E-\Omega n}})\right) - \frac{i\gamma_n(E)ge^{2iL\sqrt{E-\Omega n}} - g^2(1+e^{2iL\sqrt{E-\Omega n}})e^{2iL\sqrt{E-\Omega n}})}{\gamma_n(E) + ig(1+e^{2iL\sqrt{E-\Omega n}})}$$

$$(T_{2,n}) = \frac{\gamma_n(E)\delta_{n,0}}{2ig + \gamma_n(E) - \frac{g^2}{\gamma_n(E)} - \frac{g^2}{\gamma_n(E)}} e^{2iL\sqrt{E-\Omega n}}$$

Using the definition of the transmission coefficient in section 1.1.3, and the assumption made in section 4.4, an expression for the transmission coefficient can be formulated:

$$T_{0}(E) = \frac{\gamma_{n}^{2}(E)\delta^{2}_{n,0}}{\delta^{2}_{n,0}\left(2ig + \gamma_{n}(E) - \frac{g^{2}}{\gamma_{n}(E)} - \frac{g^{2}}{\gamma_{n}(E)}e^{2iL\sqrt{E-\Omega n}}\right)\left(-2ig + \gamma_{n}(E) - \frac{g^{2}}{\gamma_{n}(E)} - \frac{g^{2}}{\gamma_{n}(E)}e^{-2iL\sqrt{E-\Omega n}}\right)}$$

Using the definition of  $\gamma_n(E) = \frac{\hbar^2}{m} \sqrt{E - \Omega n}$  and setting  $\hbar^2 = 2m = 1$  and use the equation in it's ground state (n = 0), the equation can be simplified to a similar form of the transmission coefficient found in chapter 2.

$$T_{0}(E) = \frac{4E}{4E + g^{2} \left(2 + \frac{g^{2}}{2E} + \left(\frac{g^{2}}{4E} + i\frac{g}{\sqrt{E}} - 1\right)e^{2iL\sqrt{E}} + \left(\frac{g^{2}}{4E} - \frac{ig}{\sqrt{E}} - 1\right)e^{-2iL\sqrt{E}}\right)}$$

This should now be compared with the transmission coefficient found in chapter 2:

$$T(E) = \frac{4E}{4E + g^2 \left( \left(\frac{1}{2E} - i\frac{g}{\sqrt{E}} - \frac{g^2}{4E}\right) e^{i2L\sqrt{E}} + \left(\frac{1}{2E} + i\frac{g}{\sqrt{E}} - \frac{g^2}{4E}\right) e^{-i2L\sqrt{E}} + \frac{g^2}{2E} \right)}$$

### **CHAPTER 5-:-DISCUSSION OF THE RESULTS**

### **OBTAINED FROM CHAPTER 4**

It will be useful from this point, to express the recursion relation as an infinite, tridiagonal matrix<sup>v</sup>, M:

$$M = \begin{bmatrix} \left(g_{0} - i\gamma_{n} - \frac{g_{2}\gamma_{n}e^{2ik_{n}L}}{\gamma_{n} + ig_{2}(1 + e^{2ik_{n}L})}\right) & \sqrt{1}g_{1} & 0 & 0\\ \sqrt{1}g_{1} & \left(g_{0} - i\gamma_{n} - \frac{g_{2}\gamma_{n}e^{2ik_{n}L}}{\gamma_{n} + ig_{2}(1 + e^{2ik_{n}L})}\right) & \sqrt{2}g_{1} & 0\\ 0 & \sqrt{2}g_{1} & \left(g_{0} - i\gamma_{n} - \frac{g_{2}\gamma_{n}e^{2ik_{n}L}}{\gamma_{n} + ig_{2}(1 + e^{2ik_{n}L})}\right) & \ddots\\ 0 & 0 & \ddots & \ddots \end{bmatrix}$$
  
Where MT=A if  $T = \begin{bmatrix} T_{0} \\ T_{1} \\ \vdots \\ T_{n} \end{bmatrix}$  and  $A = \begin{bmatrix} -\frac{i\gamma_{0}^{2}(E)}{\gamma_{0}(E) + ig_{2}(1 + e^{2iL\sqrt{E}})}\\ 0 & \vdots \end{bmatrix}$ 

An approximation to the solutions lay in truncating the matrix, M. alternatively one can solve this matrix recursively, with the introduction of a defined Greens function,  $G_0(E)^{viii}$ :

$$G_{0}(E) = \left[g_{0} - i\gamma_{0}(E) - \frac{g_{2}\gamma_{0}(E)e^{2iL\sqrt{E}}}{\gamma_{0}(E) + ig_{2}(1 + e^{2iL\sqrt{E}})}\right]^{-1}$$

Using this,  $T_0(E)$  can be defined:

$$T_{0}(E) = -\left(\frac{i\gamma_{0}^{2}(E)}{\gamma_{0}(E) + ig_{2}\left(1 + e^{2iL\sqrt{E}}\right)}\right)\left(\frac{1}{G_{0}(E) - \Sigma^{(1)}(E)}\right)$$

Where  $\Sigma^{(N)}(E)$  is the recursively defined self energy (see page 129 of E.N. Economou's Green's functions in quantum physics<sup>viii</sup>.

$$\Sigma^{(N)}(E) = \frac{Ng_1^2}{G_0^{-1}(E - \Omega N) - \Sigma^{(N+1)}(E)}$$

Using  $\gamma_n(E) = \gamma_0(E - \Omega n)$ , the self-energy can be expressed as a continued fraction:

$$\Sigma^{(1)}(E) = \frac{g_1^2}{G_0^{-1}(E - \Omega) - \frac{2g_1^2}{G_0^{-1}(E - 2\Omega) - \frac{3g_1^2}{G_0^{-1}(E - 3\Omega) - \frac{4g_1^2}{\vdots}}}$$

### CHAPTER 6-:-CONCLUSION

SECTION 6.1- THE DIFFERENCES BETWEEN THE STATIC AND QUANTUM CASES

### SECTION 6.2-POSSIBLE APPLICATIONS AND FUTURE PROSPECTS OF THIS INVESTIGATION.

### **APPENDIX-:-MATHEMATICAL DERIVATIONS**

#### SECTION A.1- THE STATIC TRANSMISSION COEFFICIENT FROM AREA II TO AREA III (SEE

#### FIG.1)

*Continuity condition for wave function at* x = 0;

$$T_1 e^{ikx} + R_2 e^{-ikx} = T_2 e^{ikx}$$
$$x = 0 \Longrightarrow$$
$$T_1 + R_2 = T_2$$

Discontinuity condition for gradient of the wave function at x = 0; Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{\partial^2\psi(x)}{\partial x^2}dx + \int_{-\varepsilon}^{+\varepsilon}g(\delta[x+L]+\delta[x])\psi(x)dx = E\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx$$
$$E\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx = 0$$
$$-\frac{\hbar^2}{2m}\Delta\left(\frac{d\psi}{dx}\right) + g\psi(0) = 0, where\Delta\left(\frac{d\psi}{dx}\right) = \lim_{\varepsilon \to 0}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{+\varepsilon}$$
$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^2}\psi(0)$$
$$\psi(0) = T_1 + R_2 = T_2$$
$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^2}(T_1 + R_2) = \frac{2mg}{\hbar^2}T_2$$

Differentiate the wave functions at x > 0 and -L < x < 0 and evaluate at  $+\varepsilon$  and  $-\varepsilon$ ;

$$\frac{d\psi}{dx}\Big|_{-\varepsilon} = ik(T_1e^{ikx} - R_2e^{-ikx})$$
$$\frac{d\psi}{dx}\Big|_{+\varepsilon} = ikT_2e^{ikx}$$
$$\lim \varepsilon \to 0$$
$$\frac{d\psi}{dx}\Big|_{-} = ik(T_1 - R_2)$$
$$\frac{d\psi}{dx}\Big|_{-} = ikT_2$$
$$\Delta\left(\frac{d\psi}{dx}\right) = ik(T_2 - T_1 + R_2)$$
$$ik(T_2 - T_1 + R_2) = \frac{2mg}{\hbar^2}(T_1 + R_2)$$
$$say\beta = \frac{mg}{\hbar^2k}$$

The transmission coefficient for area two to area three (through the delta potential at x =

$$0), T'' = \frac{|T_2|^2}{|T_1|^2}$$
$$T'' = \frac{1}{|T_1|^2} \frac{T_1^* T_1}{(1 - \beta i)(1 + \beta i)}$$
$$T'' = \frac{1}{(1 + \beta^2)}$$

#### SECTION A.2- THE STATIC TRANSMISSION COEFFICIENT FROM AREA I TO AREA II (SEE FIG.1)

Continuity equation for wave function at x = -L;  $Ae^{ikx} + R_1e^{-ikx} = T_1e^{ikx} + R_2e^{-ikx}$   $x = -L \Longrightarrow$  $Ae^{-ikL} + R_1e^{ikL} = T_1e^{-ikL} + R_2e^{ikL}$ 

Discontinuity condition for gradient of wave function at x = -L; Integrate Schrödinger equation around  $x = -L \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^{2}}{2m}\int_{-L-\varepsilon}^{-L+\varepsilon}\frac{\partial^{2}\psi(x)}{\partial x^{2}}dx + \int_{-L-\varepsilon}^{-L+\varepsilon}g(\delta[x+L]+\delta[x])\psi(x)dx = E\int_{-L-\varepsilon}^{-L+\varepsilon}\psi(x)dx$$

$$E\int_{-L-\varepsilon}^{-L+\varepsilon}\psi(x)dx = 0$$

$$-\frac{\hbar^{2}}{2m}\Delta\left(\frac{d\psi}{dx}\right)_{-L} + g\psi(-L) = 0, where\Delta\left(\frac{d\psi}{dx}\right)_{-L} = \lim_{\varepsilon \to 0}\frac{d\psi}{dx}\Big|_{-L-\varepsilon}^{-L+\varepsilon}$$

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^{2}}\psi(-L)$$

$$\psi(-L) = Ae^{-ikL} + R_{1}e^{ikL} = T_{1}e^{-ikL} + R_{2}e^{ikL}$$

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{2mg}{\hbar^{2}}(Ae^{-ikL} + R_{1}e^{ikL}) = \frac{2mg}{\hbar^{2}}(T_{1}e^{-ikL} + R_{2}e^{ikL})$$

*Differentiate the wave function at x*< -*L* and -*L*< *x*< 0 and evaluate at  $-L+\varepsilon$  and  $-L-\varepsilon$ ;

$$\begin{aligned} \left. \frac{d\psi}{dx} \right|_{-L-\varepsilon} &= ik \left( A e^{ikx} - R_{1} e^{-ikx} \right) \\ \left. \frac{d\psi}{dx} \right|_{-L+\varepsilon} &= ik \left( T_{1} e^{ikx} - R_{2} e^{-ikx} \right) \\ \lim \varepsilon \to 0 \\ \left. \frac{d\psi}{dx} \right|_{-L-} &= ik \left( A e^{-ikL} - R_{1} e^{ikL} \right) \\ \left. \frac{d\psi}{dx} \right|_{-L-} &= ik \left( T_{1} e^{-ikL} - R_{2} e^{ikL} \right) \\ \Delta \left( \frac{d\psi}{dx} \right)_{-L} &= ik \left( T_{1} e^{-ikL} - R_{2} e^{ikL} \right) \\ \Delta \left( \frac{d\psi}{dx} \right)_{-L} &= ik \left( T_{1} e^{-ikL} - R_{2} e^{ikL} - A e^{-ikL} + R_{1} e^{ikL} \right) \\ ik \left( T_{1} e^{-ikL} - R_{2} e^{ikL} - A e^{-ikL} + R_{1} e^{ikL} \right) &= \frac{2mg}{\hbar^{2}} \left( A e^{-ikL} + R_{1} e^{ikL} \right) \\ \left[ \frac{\left( T_{1} - A \right)}{e^{ikL}} + \left( R_{1} - R_{2} \right) e^{ikL} \right] &= -2i\beta\psi(-L) \\ T_{1} &= A - \left[ 2i\beta\psi(-L) e^{ikL} + \left( R_{1} - R_{2} \right) e^{2ikL} \right] \\ say\beta &= \frac{mg}{\hbar^{2}k} \\ T_{2} &= T_{1} (1 - 2\beta i) - R_{2} (1 + 2\beta i) \\ R_{2} &= T_{2} - T_{1} \\ T_{2} &= T_{1} (1 - 2\beta i) - T_{2} (1 + 2\beta i) + T_{1} (1 + 2\beta i) \\ T_{2} &= \frac{T_{1} (1 + 1 - 2\beta i + 2\beta i)}{(2 + 2\beta i)} = \frac{T_{1}}{(1 + \beta i)} \end{aligned}$$

Recall the following relationships:

$$R_{2} = \frac{T_{1}}{(1+i\beta)} - T_{1}$$

$$R_{1} = T_{1}e^{-2ikL} + R_{2} - Ae^{-2ikL}$$

$$R_{1} = T_{1}e^{-2ikL} + \frac{T_{1}}{(1+i\beta)} - T_{1} - Ae^{-2ikL}$$

Substitute into the above equation for  $T_1$ ;

$$\begin{split} T_{1} &= A - \left[ 2i\beta \left( T_{1} + R_{2}e^{2ikL} \right) + \left( R_{1} - R_{2} \right)e^{2ikL} \right] \\ &= A - 2i\beta T_{1} - 2i\beta R_{2}e^{2ikL} - R_{1}e^{2ikL} + R_{2}e^{2ikL} \\ &= A - 2i\beta T_{1} - 2i\beta R_{2}e^{2ikL} - T_{1} + A - R_{2}e^{2ikL} + R_{2}e^{2ikL} \\ &= 2A - 2i\beta R_{2}e^{2ikL} - T_{1}(1 + 2i\beta) \\ &= 2A - 2i\beta \left( \frac{T_{1}}{(1 + i\beta)} - T_{1} \right)e^{2ikL} - T_{1}(1 + 2i\beta) \\ &2A = T_{1} \left( 2 + 2i\beta + \frac{2i\beta}{(1 + i\beta)}e^{2ikL} - 2i\beta e^{2ikL} \right) \\ &T_{1} = \frac{A}{\left( 1 + i\beta + \frac{i\beta}{(1 + i\beta)}e^{2ikL} - i\beta e^{2ikL} \right)} \end{split}$$

Transmission coefficient 
$$T' = \frac{|T_1|^2}{|A|^2}$$

$$\begin{split} \left| T_{i} \right|^{2} &= \frac{A^{*}A}{\left(1 - i\beta - \frac{i\beta}{(1 - i\beta)}e^{-2ikL} + i\beta e^{-2ikL}\right)\left(1 + i\beta + \frac{i\beta}{(1 + i\beta)}e^{2ikL} - i\beta e^{2ikL}\right)} \\ &\Rightarrow T' = \frac{1}{\left(1 - i\beta - \frac{i\beta}{(1 - i\beta)}e^{-2ikL} + i\beta e^{-2ikL}\right)\left(1 + i\beta + \frac{i\beta}{(1 + i\beta)}e^{2ikL} - i\beta e^{2ikL}\right)} \\ &= \frac{1}{1 + \frac{i\beta(1 - i\beta)}{(1 + \beta^{2})}e^{2ikL} - i\beta e^{2ikL} + 2\beta^{2} + \frac{\beta^{2}(1 - i\beta)}{(1 + \beta^{2})}e^{2ikL} - \beta^{2}e^{2ikL} - \frac{\beta^{2}e^{2ikL}}{(1 + \beta^{2})}e^{-2ikL} + \frac{\beta^{2}(1 + i\beta)}{(1 + \beta^{2})}e^{-2ikL} \\ &= \frac{1}{1 + 2\beta^{2} + \frac{\beta^{2}(1 + i\beta)}{(1 + \beta^{2})} + i\beta e^{-2ikL} - \beta^{2}e^{-2ikL} - \frac{\beta^{2}(1 - i\beta)}{(1 + \beta^{2})}} \\ &= \frac{1}{1 + 2\beta^{2} + \frac{(\left(i\beta + \beta^{2}\right)e^{2ikL} - \beta^{2}\right)(1 - i\beta)}{(1 + \beta^{2})} + \frac{(\left(\beta^{2} - i\beta\right)e^{-2ikL} - \beta^{2}\right)(1 + i\beta)}{(1 + \beta^{2})} + \frac{\beta^{2}}{(1 + \beta^{2})}e^{-2ikL} - \left(i\beta + \beta^{2}\right)e^{2ikL} - \beta^{2}e^{2ikL} - \beta^{2}e^{2ikL$$

### SECTION A.3- THE QUANTUM TRANSMISSION COEFFICIENT FROM AREA II TO AREA III

#### (SEE FIG.2)

 $_{CASE I:} E > \Omega n$ 

*Continuity condition for wave function at* x = 0*;* 

$$T_{1,n}e^{ik_nx} + R_{2,n}e^{-ik_nx} = T_{2,n}e^{ik_nx}$$
$$x = 0 \Longrightarrow$$
$$T_{1,n} + R_{2,n} = T_{2,n}$$

Discontinuity condition for gradient of the wave function at x = 0; Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial \psi_n}{\partial x} \right]_{-\varepsilon}^{+\varepsilon} + g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) + \hbar \omega n \int_{-\varepsilon}^{+\varepsilon} \psi_n dx = \mathbf{E}_n \int_{-\varepsilon}^{+\varepsilon} \psi_n dx Limit \ \varepsilon \to 0;$$
$$\int_{-}^{+} \psi_n dx = 0$$
$$\Rightarrow \left[ \frac{\partial \psi_n}{\partial x} \right]_{-}^{+} = \frac{2m}{\hbar^2} \left[ g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) \right]$$
$$\therefore \Delta \left[ \frac{\partial \psi_n}{\partial x} \right] = \frac{2m}{\hbar^2} \left[ g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) \right]$$

Differentiate the wave functions at x > 0 and -L < x < 0 and evaluate at  $+\varepsilon$  and  $-\varepsilon$ ;

$$\frac{d\psi_n}{dx}\Big|_{-\varepsilon} = ik_n \left(T_{1,n}e^{ik_nx} - R_{2,n}e^{-ik_nx}\right)$$
$$\frac{d\psi_n}{dx}\Big|_{+\varepsilon} = ik_n T_{2,n}e^{ik_nx}$$
$$\lim \varepsilon \to 0$$
$$\frac{d\psi_n}{dx}\Big|_{-} = ik_n \left(T_{1,n} - R_{2,n}\right)$$
$$\frac{d\psi_n}{dx}\Big|_{+} = ik_n T_{2,n}$$
$$\Delta \left(\frac{d\psi_n}{dx}\right) = ik_n \left(T_{2,n} - T_{1,n} + R_{2,n}\right)$$

$$\Rightarrow \frac{2m}{\hbar^2} \Big[ g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) \Big] = ik_n \Big( T_{2,n} - T_{1,n} + R_{2,n} \Big) \\ \psi_n(0) = T_{1,n} + R_{2,n} = T_{2,n} \\ \Rightarrow -\frac{2mi}{\hbar^2 k_n} \Big[ g_0 \Big( T_{2,n} \Big) + g_1 \sqrt{n} \Big( T_{2,n-1} \Big) + g_1 \sqrt{n+1} \Big( T_{2,n+1} \Big) \Big] = 2 \Big( T_{2,n} - T_{1,n} \Big)$$

Which can be written as a sequence:

$$T_{2,n+1} = -\frac{\left(g_0(T_{2,n}) + g_1\sqrt{n}(T_{2,n-1})\right)}{g_1\sqrt{n+1}} + i\frac{\hbar^2k_n}{m}\frac{\left(T_{2,n} - T_{1,n}\right)}{g_1\sqrt{n+1}}$$

$$CASE 2: E < \Omega n$$

*Continuity condition for wave function at* x = 0*;* 

$$T_{1,n}e^{-\kappa_n x} + R_{2,n}e^{\kappa_n x} = T_{2,n}e^{-\kappa_n x}$$
$$x = 0 \Longrightarrow$$
$$T_{1,n} + R_{2,n} = T_{2,n}$$

Discontinuity condition for gradient of the wave function at x = 0; Integrate Schrödinger equation around  $x = \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial \psi_n}{\partial x} \right]_{-\varepsilon}^{+\varepsilon} + g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) + \hbar \omega n \int_{-\varepsilon}^{+\varepsilon} \psi_n dx = \mathbf{E}_n \int_{-\varepsilon}^{+\varepsilon} \psi_n dx \, Limit \ \varepsilon \to 0;$$

$$\int_{-}^{+} \psi_n dx = 0$$

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

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

Differentiate the wave functions at x > 0 and -L < x < 0 and evaluate at  $+\varepsilon$  and  $-\varepsilon$ ;

$$\frac{d\psi_n}{dx}\Big|_{-\varepsilon} = -\kappa_n (T_{1,n}e^{-\kappa_n x} - R_{2,n}e^{\kappa_n x})$$
$$\frac{d\psi_n}{dx}\Big|_{+\varepsilon} = -\kappa_n T_{2,n}e^{-\kappa_n x}$$
$$\lim \varepsilon \to 0$$
$$\frac{d\psi_n}{dx}\Big|_{-} = -\kappa_n (T_{1,n} - R_{2,n})$$
$$\frac{d\psi_n}{dx}\Big|_{+} = -\kappa_n T_{2,n}$$
$$\Delta \left(\frac{d\psi_n}{dx}\right) = -\kappa_n (T_{2,n} + R_{2,n} - T_{1,n}) = -2\kappa_n (T_{2,n} - T_{1,n})$$

$$\Rightarrow \frac{2m}{\hbar^2} \Big[ g_0 \psi_n(0) + g_1 \sqrt{n} \psi_{n-1}(0) + g_1 \sqrt{n+1} \psi_{n+1}(0) \Big] = -2\kappa_n (T_{2,n} - T_{1,n}) \psi_n(0) = R_{2,n} + T_{1,n} = T_{2,n} \Rightarrow -\frac{m}{\hbar^2 \kappa_n} \Big[ g_0 \big( T_{2,n} \big) + g_1 \sqrt{n} \big( T_{2,n-1} \big) + g_1 \sqrt{n+1} \big( T_{2,n+1} \big) \Big] = T_{2,n} - T_{1,n}$$

#### Which can be written as a sequence:

$$T_{2,n+1} = -\frac{\left(g_0(T_{2,n}) + g_1\sqrt{n}(T_{2,n-1})\right)}{g_1\sqrt{n+1}} + \frac{\hbar^2\kappa_n}{m}\frac{\left(T_{2,n} - T_{1,n}\right)}{g_1\sqrt{n+1}}$$

#### SECTION A.4- THE QUANTUM TRANSMISSION COEFFICIENT FROM AREA I TO AREA II

<u>(SEE FIG.2)</u>

# $_{CASE 1:} E > \Omega n$

*Continuity condition for wave function at* x = -L*;* 

$$T_{1,n}e^{ik_nx} + R_{2,n}e^{-ik_nx} = A_ne^{ik_nx} + R_{1,n}e^{-ik_nx}$$
$$x = -L \Longrightarrow$$
$$T_{1,n}e^{-ik_nL} + R_{2,n}e^{ik_nL} = A_ne^{-ik_nL} + R_{1,n}e^{ik_nL}$$

Discontinuity condition for gradient of the wave function at x = -L; Integrate Schrödinger equation around  $x = -L \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L-\varepsilon}^{-L+\varepsilon} + g_2 \psi_n (-L) + \hbar \omega n \int_{-L-\varepsilon}^{-L+\varepsilon} \psi_n dx = \mathbf{E}_n \int_{-L-\varepsilon}^{-L+\varepsilon} \psi_n dx$$
$$Limit \ \varepsilon \to 0; -\int_{-L-}^{-L+} \psi_n dx = 0$$
$$\Rightarrow \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L-}^{-L+} = \frac{2m}{\hbar^2} [g_2 \psi_n (-L)]$$
$$\therefore \Delta \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L}^{-L+\varepsilon} = \frac{2m}{\hbar^2} [g_2 \psi_n (-L)]$$

Differentiate the wave functions at x < -L and -L < x < 0 and evaluate at  $-L+\varepsilon$  and  $-L-\varepsilon$ ;

$$\frac{d\psi_n}{dx}\Big|_{-L-\varepsilon} = ik_n \left(A_n e^{ik_n x} - R_{1,n} e^{-ik_n x}\right)$$

$$\frac{d\psi_n}{dx}\Big|_{-L+\varepsilon} = ik_n \left(T_{1,n} e^{ik_n x} - R_{2,n} e^{-ik_n x}\right)$$

$$\lim \varepsilon \to 0$$

$$\frac{d\psi_n}{dx}\Big|_{-L-} = ik_n \left(A_n e^{-ik_n L} - R_{1,n} e^{ik_n L}\right)$$

$$\frac{d\psi_n}{dx}\Big|_{-L+} = ik_n \left(T_{1,n} e^{-ik_n L} - R_{2,n} e^{ik_n L}\right)$$

$$\Delta \left(\frac{d\psi_n}{dx}\right)_{-L} = ik_n \left(T_{1,n} e^{-ik_n L} - R_{2,n} e^{ik_n L}\right)$$

$$\Rightarrow \frac{2m}{\hbar^2} [g_2 \psi_n (-L)] = ik_n (T_{1,n} e^{-ik_n L} - R_{2,n} e^{ik_n L} - A_n e^{-ik_n L} + R_{1,n} e^{ik_n L})$$

$$\psi_n (-L) = A_n e^{-ik_n L} + R_{1,n} e^{ik_n L} = T_{1,n} e^{-ik_n L} + R_{2,n} e^{ik_n L}$$

$$R_{2,n} = T_{2,n} - T_{1,n}$$

$$\Rightarrow \psi_n (-L) = T_{1,n} e^{-ik_n L} + T_{2,n} e^{ik_n L} - T_{1,n} e^{ik_n L}$$

$$\Rightarrow -\frac{2img_2}{\hbar^2 k_n} (T_{1,n} e^{-ik_n L} + T_{2,n} e^{ik_n L} - T_{1,n} e^{ik_n L}) = (T_{1,n} e^{-ik_n L} - R_{2,n} e^{ik_n L} - A_n e^{-ik_n L} + R_{1,n} e^{ik_n L})$$

$$R_{1,n} e^{ik_n L} - R_{2,n} e^{ik_n L} = T_{1,n} e^{-ik_n L} - A_n e^{-ik_n L}$$

$$\Rightarrow -\frac{2img_2}{\hbar^2 k_n} (T_{1,n} e^{-ik_n L} + T_{2,n} e^{ik_n L} - T_{1,n} e^{ik_n L}) = 2e^{-ik_n L} (T_{1,n} - A_n)$$

$$\Rightarrow \frac{img_2}{\hbar^2 k_n} T_{1,n} = (A_n - T_{1,n}) + \frac{img_2}{\hbar^2 k_n} (T_{2,n} - T_{1,n}) e^{2ik_n L} = A_n + \frac{img_2}{\hbar^2 k_n} T_{2,n} e^{2ik_n L} - T_{1,n} \left(1 + \frac{img_2}{\hbar^2 k_n} e^{2ik_n L}\right)$$

$$\Rightarrow \frac{img_2}{\hbar^2 k_n} T_{1,n} + T_{1,n} \left(1 + \frac{img_2}{\hbar^2 k_n} e^{2ik_n L}\right) = A_n + \frac{img_2}{\hbar^2 k_n} T_{2,n} e^{2ik_n L}$$

$$\Rightarrow T_{1,n} = \frac{A_n + \frac{img_2}{\hbar^2 k_n}}{\hbar^2 k_n} T_{2,n} e^{2ik_n L}$$

### CASE 2: $E < \Omega n$

*Continuity condition for wave function at* x = -L*;* 

$$R_{1,n}e^{\kappa_n x} = T_{1,n}e^{-\kappa_n x} + R_{2,n}e^{\kappa_n x}$$
$$x = -L \Longrightarrow$$
$$R_{1,n}e^{-\kappa_n L} = T_{1,n}e^{\kappa_n L} + R_{2,n}e^{-\kappa_n L}$$

Discontinuity condition for gradient of the wave function at x = -L; Integrate Schrödinger equation around  $x = -L \pm \varepsilon$ , limiting  $\varepsilon \rightarrow 0$ ;

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L-\varepsilon}^{-L+\varepsilon} + g_2 \psi_n (-L) + \hbar \omega n \int_{-L-\varepsilon}^{-L+\varepsilon} \psi_n dx = \mathbf{E}_n \int_{-L-\varepsilon}^{-L+\varepsilon} \psi_n dx$$
$$Limit \ \varepsilon \to 0; -\int_{-L-}^{-L+} \psi_n dx = 0$$
$$\Rightarrow \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L-}^{-L+} = \frac{2m}{\hbar^2} [g_2 \psi_n (-L)]$$
$$\therefore \Delta \left[ \frac{\partial \psi_n}{\partial x} \right]_{-L}^{-L+\varepsilon} = \frac{2m}{\hbar^2} [g_2 \psi_n (-L)]$$

Differentiate the wave functions at x < -L and -L < x < 0 and evaluate at  $-L + \varepsilon$  and  $-L - \varepsilon$ ;

$$\begin{aligned} \left. \frac{d\psi_n}{dx} \right|_{-L-\varepsilon} &= \kappa_n R_{1,n} e^{\kappa_n x} \\ \left. \frac{d\psi_n}{dx} \right|_{-L+\varepsilon} &= -\kappa_n (T_{1,n} e^{-\kappa_n x} - R_{2,n} e^{\kappa_n x}) \\ \lim \varepsilon \to 0 \\ \left. \frac{d\psi_n}{dx} \right|_{-L-} &= \kappa_n R_{1,n} e^{-\kappa_n L} \\ \left. \frac{d\psi_n}{dx} \right|_{-L-} &= -\kappa_n (T_{1,n} e^{\kappa_n L} - R_{2,n} e^{-\kappa_n L}) \\ \Delta \left( \frac{d\psi_n}{dx} \right)_{-L} &= -\kappa_n (T_{1,n} e^{\kappa_n L} + R_{1,n} e^{-\kappa_n L} - R_{2,n} e^{-\kappa_n L}) \\ \end{array} \\ \left. \Rightarrow \frac{2m}{\hbar^2} [g_2 \psi_n (-L)] = -\kappa_n (T_{1,n} e^{\kappa_n L} + R_{1,n} e^{-\kappa_n L} - R_{2,n} e^{-\kappa_n L}) \\ \psi_n (-L) &= R_{1,n} e^{-\kappa_n L} = T_{1,n} e^{\kappa_n L} + R_{2,n} e^{-\kappa_n L} \\ \end{array} \right. \\ \left. \frac{T_{1,n} = -\frac{T_{2,n} e^{-2\kappa_n L}}{\left(1 - e^{-2\kappa_n L} + \frac{\hbar^2 \kappa_n}{mg_2}\right)} \end{aligned}$$

<sup>&</sup>lt;sup>i</sup> E.Merzbacher, Quantum Mechanics (third edition), Wiley 1998.

<sup>&</sup>lt;sup>ii</sup> F. Mandl, Quantum Mechanics, Wiley 2001.

<sup>&</sup>lt;sup>iii</sup> A.P. French, Vibrations and waves, Chapman & Hall 1998.

<sup>&</sup>lt;sup>iv</sup> T. Brandes, Lectures on Quantum Mechanics I, second year physics undergraduate course, UMIST 2003. <sup>v</sup> Based on a report by John Robinson<sup>vi</sup> with T. Brandes as the co-author, Transmission through a Quantum Dynamical Delta Barrier, phys. Stat. Sol. (b) **234**, No. 1, 378-384 (2002), department of physics UMIST 2002.

<sup>&</sup>lt;sup>vi</sup> J. Robinson, Scattering at a quantum barrier, third year project, department of physics UMIST 2002.

<sup>&</sup>lt;sup>vii</sup> G. Fano, Mathematical methods of quantum mechanics, McGraw-Hill 1971.

<sup>&</sup>lt;sup>viii</sup> E.N. Economou, Green's Functions in Quantum Physics, Springer-Verlag Berlin Heidelberg 1979.