Quantum Transmission via Resonant Tunneling in a Double Barrier Structure: a Path Integral Approach.

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Abstract. We study both the symmetric and asymmetric one-dimensional double barrier potential which describes the band profile of a quantum tunneling diode in the absence or the application respectively, of a constant electrical field. The semiclassical path integral theory is employed to determine the transmission amplitude, which is the Green's function for a single charge transport. The Green's function is given in an analytical form and some attributes of the transmission amplitude due to resonant tunneling are established while it is shown to exhibit maxima at the position of the resonant states. The complex spectrum of the heterostructure is revealed and the time scale for charge transport is given, both in an analytical form.

Keywords: double barrier structure, resonant tunneling diode, quasi bound states, Green's function, transmission amplitude, charge transport, transport time

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INTRODUCTION

Quantum transmission in nanostructures is in general dominated by the tunneling phenomenon. This term describes a particle transport through a classically forbidden region of motion, (barrier), meaning a region in which the potential energy exceeds the total particle energy. There is no classical analogue, since in classical mechanics the particle is totally reflected at the so called classical turning points, that is, points where the total energy equals the potential energy, and therefore no transmission ever occurs. The quantum mechanical wavefunction instead, does not vanish inside and after the barrier. Thus, according to the laws of quantum mechanics a particle incident on a potential barrier has a finite probability of appearing on the other side.

Tunneling in solids was first studied by Fowler and Nordheim [1] in the thermionic emission of electrons from metal into vacuum. Later, interest was taken in the study of tunneling through thin insulating layers, separating two metals, or a metal and a semiconductor. Zener [2] introduced the interband tunneling, describing electrons that tunnel from one energy band to another through the forbidden energy gap. The outstanding breakthroughs in the area of semiconductor device technology that followed, made possible the experimental observation of Zener tunneling in p-n junction diodes. For example, Esaki [3] introduced the so-called Esaki diode, in which the interband Zener tunneling, produces negative differential resistance in the I-V characteristics.

In most artificially engineered structures, quantum confinement may seriously reduce the dimensions of the system under study. Such confinement is usually caused by a heterojunction, (MOSFET), or simply a semiconductor- air interface, (quantum wire). For example if one thin layer of material is grown on top of another, such as the simple AlGaAs/GaAS heterostructure, the change in potential is in only the vertical growth direction, and therefore the problem practically becomes one dimensional. The ability of constructing well controlled heterostructure layers enabled Tsu and Esaki to predict at first and observe shortly after [4,5], that when bias is applied across a double barrier heterostructure we get similar to the Esaki diode current voltage characteristics. However in this case it is the resonant tunneling, which is tunneling through the barriers within the same band, that is responsible for the I/V characteristics, and not the interband tunneling. Resonant tunneling refers to the case where the transmission amplitude, which is the Green's function for electron propagation through the heterostructure, is sharply peaked about certain complex values of the energy. In fact the real parts of the above mentioned complex values are very close to these of the bound states associated with the quantum well formed between the two confining barriers. The resonant energies of such a heterostructure support a complex spectrum, due to the fact that the electron may escape away from the quantum well in either direction. Thus, there is a finite lifetime associated with the bound state. This is why these states are known as quasi-bound states. The Green's function for the lowest resonant energy may approach unity in some cases and so semiclassical methods can be applied with high accuracy.

In our days the numerical calculation of the Green's function, for systems consisting of heterostructures, can be done with a relative ease, with the aid of modern computers. However, an analytical solution is always desirable and of an instructive value. For example the analytic solution provides a direct comparison between the properties of different systems, even coming from different branches of science, as long as they can be described by the same type of potential function. In addition the application of the path integral analytic formalism seems to lack of any previous experience on these systems. Thus, our work was motivated by the need of fulfilling both the above requirements.

The purpose of this paper is to describe and further produce analytic relations for a double barrier heterostructure, via an analytic path integral formalism. Doing so we first demonstrate the importance of the double barrier structure through its close resemblance to the structure of a resonant tunneling diode. We present a widely used structure which consists of two AlGaAs barriers, (speaking more accurately we should write AlxGa1-xAs where x~0,3), separated by a thin GaAs quantum well, surrounded by heavily doped GaAs layers. Then the semiclassical path integral approach is developed and the transmission amplitude for electron transport through the heterostructure is analytically calculated. We also produce analytic relations for the complex energy spectrum supported by the double barrier structure, as well as for the time needed for charge transport.

2. THE DOUBLE BARRIER POTENTIAL AS A RESONANT TUNNELING DIODE

We consider the potential of figure 1 that follows. Potentials with such a form constitute models for resonant tunneling diodes and tunneling processes in various systems of physics and chemistry. As shown in figure 1, points ε and ζ correspond to the maximum of the barriers which they do not need to be symmetric. There are four turning points: at α and β (finite barrier, tunnelling is allowed) and at γ and δ, (again finite barrier, tunnelling is allowed), while β and γ also define the limits of the classically allowed region of motion.

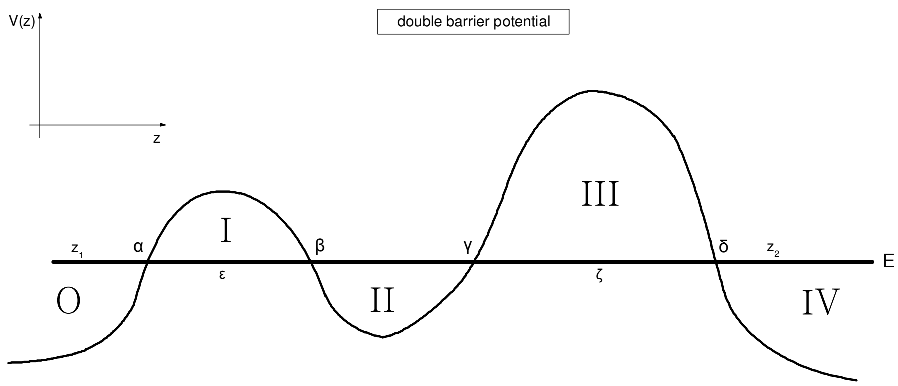

FIGURE 1: The double barrier potential *V(z)* that couples a quantum well to the continuum via two channels.

The topology of the above potential, meaning the specific permutation of classi-cally allowed and forbidden regions of motion, is the same with the one of the effective potential (band profile) of a resonant tunneling diode as this is pictured in figure 2 that follows. The barrier height is due to the conduction band offset, ΔE_c, while E_f refers to the Fermi energy of the heavily doped GaAs layers and E_o refers to the lowest resonant energy or quasibound state of the GaAs quantum well. The thickness of the AlGaAS barriers is such that allows tunneling to be significant.

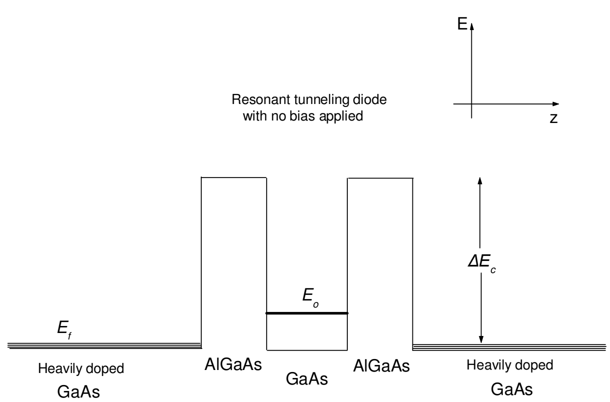

FIGURE 2: Effective potential or band profile of a resonant tunneling diode structure.

When a positive bias *V* is applied to the right contact relative to the left, the Fermi energy on the left is raised to the resonant energy E_o and a large current flows from left to right due to the maximization of the transmission amplitude. Opposite charge flow is strongly suppressed, since the carriers at the Fermi energy on the right, feel a large potential barrier, as shown in figure 3 that follows:

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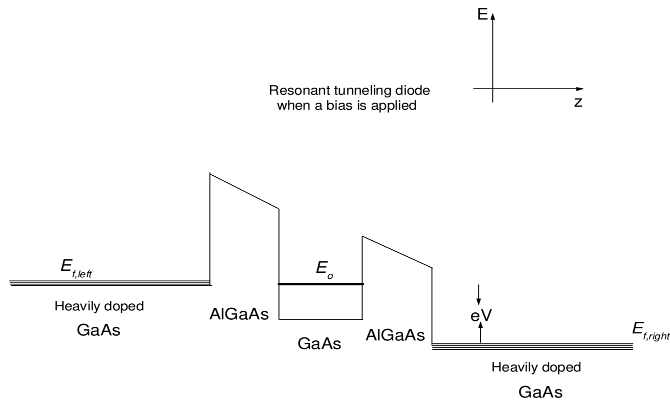

FIGURE 3: Effective potential or band profile for a resonant tunneling diode structure when a positive bias is applied to the right contact.

However, if we further increase the applied bias, the bottom of the conduction band of the left contact is raised to the resonant energy E_o, and therefore they will not remain anymore available electrons for tunneling. This is why the current is decreased with increasing bias, which results in a region of negative differential resistance in the I/V characteristics. Comparing figures 2 and 3 it is readily seen that the application of a bias destroys the symmetry between the two potential barriers.

During the last decades, there has been a considerable volume of research into resonant tunneling diodes. Besides the fundamental physics included into this simple structure, interest also stems from the various applications in microwave systems and digital logic circuits. In these systems we may be interested in the fundamental time associated with the tunneling process, which is often taken as the lifetime of the quasi – bound state. Besides this time constant, we should also have in mind the RC time constant due to the capacitance of the structure and the transit time across the nontunneling regions of the device as well. However, when the device is properly designed these two time constants can be minimized. According to the literature the transfer- matrix method based on the discretized form of the one dimensional *Schrödinger* equation, seems to be the most popular for analyzing the double barrier structure, see [6-11] and references therein. However our approach will be different, following the semiclassical path integral method which does not involve the *Schrödinger* equation at all.

3. THE SEMICLASSICAL PATH INTEGRAL APPROACH

The path integral construction of a system's Green's function for one dimensional propagation between two points z_1 and z_2 , is accomplished by taking account of all possible changes in phase of the wavefunction. These may be due to motion inside allowed and forbidden region or due to reflection from turning points. Miller [12] developed a semiclassical periodic orbit theory, based on Gutzwiiller's trace formula [13], in his pioneering work on the application of path integrals to tunneling. This work inspired many others to improve his method and analytically solve interesting one dimensional problems.

Among those, Holstein and Swift [14] and Holstein alone [15,16] showed how *Gsc(E)* , which is the semiclassical fixed energy transmission amplitude, can be used to achieve analytic continuation of the propagator to forbidden regions, and furthermore established its connection to propagation and to reflection. Holstein's [15] central result for the calculation of the transmission amplitude via an infinite set of paths that the particle follows, connecting the initial point z_1 to the final point z_2, can be written in compact form as

$$Gsc(E) = \frac{1}{\overline{p(z_1,z_2)}} \sum_{j=1}^{\infty} \left\{ \prod_{i=1}^{N(j)} a_{ij} \right\} \quad (1)$$

In the above equation $\overline{p(z_1,z_2)}$ is a non local momentum of the particle defined by $\overline{p(z_1,z_2)} = 2\pi\sqrt{k^*(z_1)k^*(z_2)}$ where $k^*(z) = \sqrt{2\left(E - V(z)\right)}$, with E standing for the energy and $V(z)$ for the potential function, (atomic units employed throughout). In equation (1) each path is uniquely identified by an index, j, with j = 1,2,3,…..∞ , and is constructed by a set of factors α_{ij} corresponding to propagation (from α to β) in allowed regions (given by $\exp[i\int_{\alpha}^{\beta} k^*(z)dz] \equiv e^{ik}$), or in forbidden regions (given by $\exp\left[-\left|\int_{\alpha}^{\beta} \kappa^*(z)dz\right|\right] \equiv e^{-\kappa}$ where $\kappa^*(z) = \sqrt{2\left(V(z) - E\right)}$), and on the corresponding reflections from turning points ($-i$ for reflection from a turning point in an allowed region , $+ i/2$ for reflection in a forbidden region , and -1 for reflection from an infinite barrier). The product $\prod_{i=1}^{N(j)} a_{ij}$ gives the unique amplitude for each possible path for going from z_1 to z_2. For each path, j, $N(j)$ is the number of possible factors a_{ij} present in this path. In the picture that follows we schematically give the rules for the propagation-reflection factors α_{ij} that constitute the fundamental cells for constructing each individual path amplitude.

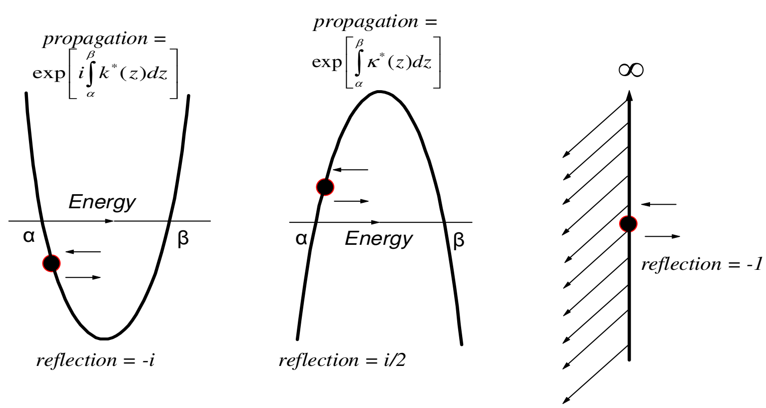

FIGURE 4: Rules for the construction of the path integral amplitudes through the α_{ij} factors. The first motion is in a classically allowed region of motion, the second in a classically forbidden region and the third motion includes reflection from an infinite barrier.

The above described method can also be found in standard textbooks of path integrals, or quantum tunneling, [17,18].

It is readily seen that the calculation of the overall transmission amplitude depends on the topology of the potential function and on the nature of the turning points. Since there is an infinity of paths traversing both the allowed and the forbidden regions, it is very crucial to include all of them in the calculation by performing correct the rather complicated combinatorics. Then, and since each path repeats itself, the infinite class of paths can be summed to constitute

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geometric progressions, from which the analytic properties of *Gsc(E)* can be recognized directly. For the present requirement of computing the overall transmission amplitude, the points z_1 and z_2 lie on the heavily doped GaAs layers, on each free side of the two barriers, as shown in figure 1.

When the potential is known explicitly, then *Gsc(E)* can be obtained analytically or numerically and its simple pole structure is revealed. Once *Gsc(E)* is known, its complex '*self-energy*' correction, namely the energy shift and width, can be extracted. This is possible by comparing the result representing the corresponding bound state problem for the inner quantum well (real energies) to the result for the resonance state problem (complex energies). As will be seen, *Gsc(E)* is a finite sum of complex poles, each representing a resonance state of the potential. The calculation leads naturally to the result that the pole of interest has a negative imaginary part, i.e. it corresponds to a decaying state, associated with the time needed for charge transport.

4. TRANSMISSION AMPLITUDE AND COMPLEX ENERGY SPECTRUM OF A DOUBLE BARRIER STRUCTURE

Considering the potential of figure 1, our objective is the calculation of the Greens function for propagation between points z_1 and z_2 via the semiclassical path integral theory. The calculation of Gsc(E) according to equation (1) entails the consideration of the phases of all possible paths, for the given total energy E. For each path, the overall phase is determined by the manner in which allowed and forbidden regions succeed one another, and by the nature of the corresponding turning points when reflection occurs. With respect to figure 1, the motion of the particle for E > 0 starts at (z_1, t_1) and ends at (z_2, t_2), at each side of the two potential barriers. So there are five regions: O (allowed), I (forbidden), II (allowed), III(forbidden), IV(allowed) and motion in O and IV is free: once the particle moves from point α to the left or from point δ to the right, it cannot be reflected. In this way we are actually interested in the calculation of the amplitude for travelling from α at the beginning of region I, to δ at the end of region III in all possible ways.

Since the sum over histories consists of calculating all possible paths connecting these points, we should spend a few lines explaining the symbolism that follows: for example $A^{III}_{\gamma\to\delta}$ means the amplitude for all the possible paths connecting γ and δ, while always staying inside region III, and $\left(I-II^{*}\right)^{\alpha\to\gamma}$ means the amplitude for all the possible paths connecting points α and γ by interchanging regions I and II, with the motion always ending inside region II, (where the asterisk goes). We can now proceed to the calculation by first dividing the problem up into smaller parts as follows:

we reach point γ without ever passing through region III by interchanging only regions I and II in all possible ways. We call this contribution C_1

$$C_1=\left(I-II^{*}\right)^{\alpha\to\gamma} \tag{2}$$

Let us give a graphical presentation of a typical path of the above contribution C_1, for the potential of figure 1. In all the graphs that follow the solid lines correspond to propagation in a classically allowed region of motion while the dash- dot lines correspond to propagation in a classically forbidden region of motion. Reflections are described by small curved lines and the succession of lines moves downwards as time passes.

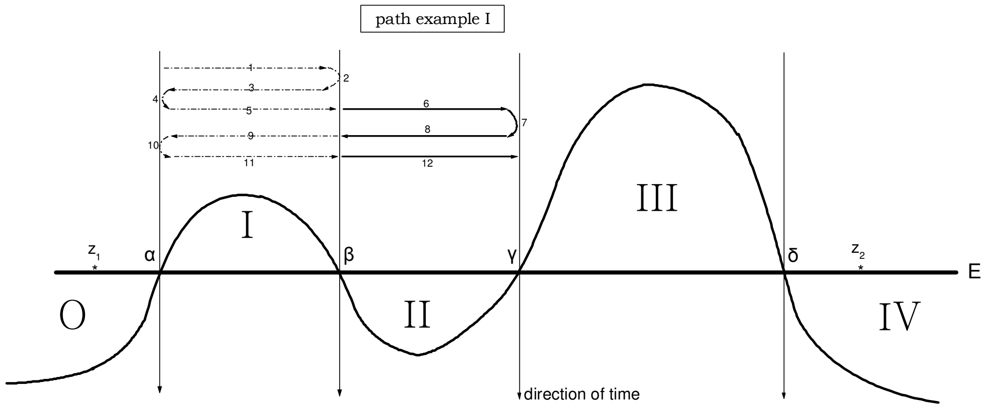

FIGURE 5: Graph representation of a typical path of contribution C_1 for the potential of figure 1. Propagation starts at α and ends at γ.

The above path is constituted by N(j)=12 propagation-reflection factors, and its contribution to the construction of the transmission amplitude is analytically given by the following time ordered product

$$a_j^{12} = e^{-\kappa_1}\frac{i}{2}e^{-\kappa_1}\frac{i}{2}e^{-\kappa_1}e^{ik}(-i)e^{ik}e^{-\kappa_1}\frac{i}{2}e^{-\kappa_1}e^{ik} = -\frac{1}{8}e^{-5\kappa_1}e^{3ik} \quad (3)$$

where $e^{ik} = \exp[i\int_\beta^\gamma k^*(z)dz]$ and where and where $e^{-\kappa_{1,2}} = \exp\left[-\left|\int_{\alpha,\gamma}^{\beta,\delta}\kappa^*(z)dz\right|\right]$ and j stands for the index of the path.

with γ as the starting point, we have the following alternatives: doing nothing, this is just a unity factor, or combine the three regions in all possible ways by keeping as last interchange i) that of regions I and II, C_2, or ii) that of regions III and II, C_3 , getting respectively

$$C_2 = \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma} + \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}\left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma} + \ldots\ldots \quad (4a)$$

and

$$C_3 = \left(III - II^*\right)^{\gamma\to\gamma} + \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}\left(III - II^*\right)^{\gamma\to\gamma} + \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}\left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}\left(III - II^*\right)^{\gamma\to\gamma} + \ldots\ldots \quad (4b)$$

It is obvious that each of the above contributions forms the infinite sum of the terms of a geometric progression, and so we can actually reduce the above sums to the following compact formulae

$$C_2 + 1 = \frac{1}{1-\left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}} \quad (4c)$$

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and

$$C_3 = \frac{\left(III - II^*\right)^{\gamma\to\gamma}}{1 - \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}} \tag{4d}$$

In fact we can also sum together C_2 +1 and C_3 to get

$$C_2 + 1 + C_3 = C_{2,3} = \frac{1 + \left(III - II^*\right)^{\gamma\to\gamma}}{1 - \left(III - II^*\right)^{\gamma\to\beta}\left(I - II^*\right)^{\beta\to\gamma}} \tag{5}$$

Let us again give a graphical presentation of a typical path of the above contribution $C_{2,3}$, for the potential of figure 1.

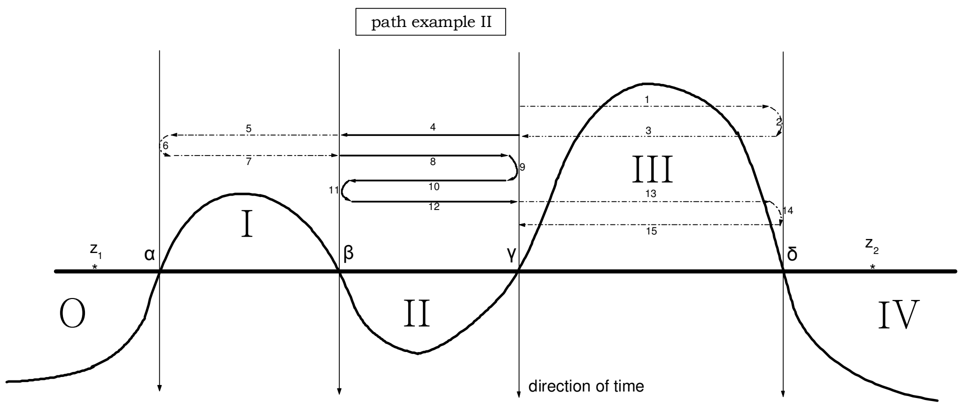

FIGURE 6: Graph representation of a typical path of contribution $C_{2,3}$ for the potential of figure 1. Propagation starts at γ and ends at γ.

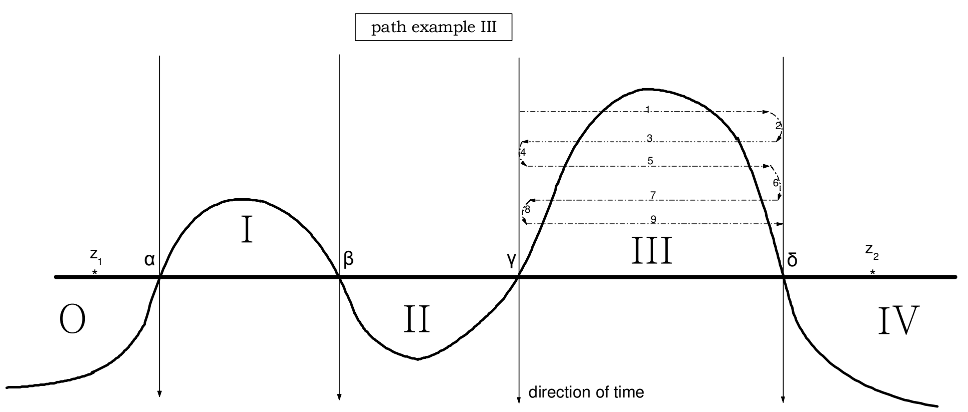

FIGURE 7: Graph representation of a typical path of contribution C_4 for the potential of figure 1. Propagation starts at γ and ends at δ.

The above path is constituted by *N(j)*=15 propagation-reflection factors, and its contribution to the construction of the transmission amplitude is analytically given by the following time ordered product

$$b_j^{15} = e^{-\kappa_2} \frac{i}{2} e^{-\kappa_2} e^{ik} e^{-\kappa_1} \frac{i}{2} e^{-\kappa_1} e^{ik} (-i) e^{ik} (-i) e^{ik} e^{-\kappa_2} \frac{i}{2} e^{-\kappa_2} = \frac{i}{8} e^{-2\kappa_1} e^{-4\kappa_2} e^{4ik} \tag{6}$$

the last contribution involves only region *III* and no other, so it is simply the amplitude

$$C_4 = A^{III}_{\gamma\to\delta} \tag{7}$$

We give a last graphical presentation of a typical path of the contribution C_4, for the potential of figure 1.

The above path is constituted by *N(j)*=9 propagation-reflection factors, and its contribution to the construction of the transmission amplitude is analytically given by the following time ordered product

$$c_j^9 = e^{-\kappa_2} \frac{i}{2} e^{-\kappa_2} \frac{i}{2} e^{-\kappa_2} \frac{i}{2} e^{-\kappa_2} \frac{i}{2} e^{-\kappa_1} = -\frac{1}{16} e^{-5\kappa_2} \tag{8}$$

We can now proceed to the calculation of the above contributions in terms of simpler amplitudes and transmission reflection factors.

$$C_1 = \left(I - II^*\right)^{\alpha\to\gamma} = A^I_{\alpha\to\beta} A^{II}_{\beta\to\gamma} \begin{Bmatrix} 1 + (-i) e^{ik} A^I_{\beta\to\beta} A^{II}_{\beta\to\gamma} + \\ (-i) e^{ik} A^I_{\beta\to\beta} A^{II}_{\beta\to\gamma} (-i) e^{ik} A^I_{\beta\to\beta} A^{II}_{\beta\to\gamma} + \dots \end{Bmatrix} \tag{9}$$

Again we recognize the sum of a geometric progression and we can write the above expression in the closed form that follows

$$\begin{aligned} C_1 = \left(I - II^*\right)^{\alpha\to\gamma} &= A^I_{\alpha\to\beta} A^{II}_{\beta\to\gamma} \frac{1}{1 + ie^{ik} A^I_{\beta\to\beta} A^{II}_{\beta\to\beta}} \\ &= \frac{A^I_{\alpha\to\beta} A^{II}_{\beta\to\gamma}}{1 - A^I_{\beta\to\beta} A^{II}_{\beta\to\beta}} \end{aligned} \tag{10}$$

It is then straightforward to prove that the following relation also holds

$$\left(I - II^*\right)^{\beta\to\gamma} = \frac{A^I_{\beta\to\beta} A^{II}_{\beta\to\gamma}}{1 - A^I_{\beta\to\beta} A^{II}_{\beta\to\beta}} \tag{11}$$

We can now proceed to the combination of regions II and III and calculate the following contributions

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$$\left(III-II^{*}\right)^{\gamma\to\gamma} = A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}\begin{Bmatrix}1+A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}+ \\ A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}+....\end{Bmatrix} = \frac{A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}}{1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}} \tag{12}$$

where again it is straightforward to also calculate

$$\left(III-II^{*}\right)^{\gamma\to\beta} = \frac{A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\beta}}{1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}} \tag{13}$$

We now take in account of all of the above contributions by multiplying the factors C_1 $C_{2,3}$ and C_4, since they correspond to statistically independent events, and get the final result

$$C_{total} = C_1 \text{ x } C_{2,3} \text{ x } C_4 =$$

$$\frac{A^{I}_{\alpha\to\beta}A^{II}_{\beta\to\gamma}}{1-A^{I}_{\beta\to\beta}A^{II}_{\beta\to\beta}} \text{ x } \frac{1+\dfrac{A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}}{1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}}}{1-\dfrac{A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\beta}}{1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}}\dfrac{A^{I}_{\beta\to\beta}A^{II}_{\beta\to\gamma}}{1-A^{I}_{\beta\to\beta}A^{II}_{\beta\to\beta}}} \text{ x } A^{III}_{\gamma\to\delta} = \tag{14}$$

$$\frac{A^{I}_{\alpha\to\beta}A^{II}_{\beta\to\gamma}A^{III}_{\gamma\to\delta}}{\left(1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}\right)\left(1-A^{I}_{\beta\to\beta}A^{II}_{\beta\to\beta}\right)-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\beta}A^{I}_{\beta\to\beta}A^{II}_{\beta\to\gamma}}$$

In order to complete the above formula we should also include the initial propagation from z_1 to α which is simply the $A^{O}_{z_1\to a}$ and the last propagation from δ to z_2 which is the $A^{IV}_{\delta\to z_2}$. In this way equation (1) of the Green's function is written as follows

$$G_{sc}(E) = \frac{A^{O}_{z_1\to a}A^{IV}_{\delta\to z_2}}{\overline{p(z_1,z_2)}}\frac{A^{I}_{\alpha\to\beta}A^{II}_{\beta\to\gamma}A^{III}_{\gamma\to\delta}}{\left(1-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\gamma}\right)\left(1-A^{I}_{\beta\to\beta}A^{II}_{\beta\to\beta}\right)-A^{III}_{\gamma\to\gamma}A^{II}_{\gamma\to\beta}A^{I}_{\beta\to\beta}A^{II}_{\beta\to\gamma}} \tag{15}$$

Since we have given the general expression of the Green's function we can now discuss the type of symmetry between the two potential barriers. We should note that independently of the type of symmetry it is always true that $A^{II}_{\gamma\to\gamma} = A^{II}_{\beta\to\beta}$, $A^{II}_{\beta\to\gamma} = A^{II}_{\gamma\to\beta}$ and $A^{II}_{\beta\to\beta} = A^{II}_{\gamma\to\gamma}$.

Symmetric barriers case:

It is clear that if we are dealing with symmetric potential barriers then it is true that $A^{III}_{\gamma\to\gamma} = A^{I}_{\beta\to\beta}$ and $A^{I}_{\alpha\to\beta} = A^{III}_{\gamma\to\delta}$. The total path contribution from α to δ can then be written as

$$C_{sym} = \frac{A^{I}_{\alpha\to\beta} A^{II}_{\beta\to\gamma} A^{III}_{\gamma\to\delta}}{\left(1 - A^{III}_{\gamma\to\gamma} A^{II}_{\gamma\to\gamma}\right)^2 - \left(A^{III}_{\gamma\to\gamma} A^{II}_{\beta\to\gamma}\right)^2} \tag{16a}$$

Let us define $1 - A^{III}_{\gamma\to\gamma} A^{II}_{\gamma\to\gamma} \equiv e$ and $A^{III}_{\gamma\to\gamma} A^{II}_{\beta\to\gamma} \equiv d$. We then have

$$A^{I}_{\alpha\to\beta} A^{II}_{\beta\to\gamma} A^{III}_{\gamma\to\delta} = A^{I}_{\alpha\to\beta}\left[A^{II}_{\beta\to\gamma} A^{III}_{\gamma\to\delta} \frac{i}{2} e^{-\kappa}\right] \frac{2}{i} e^{\kappa} = -2ie^{\kappa} A^{I}_{\alpha\to\beta} d \tag{16b}$$

where

$$e^{-\kappa} = \exp\left[-\left|\int_{\alpha}^{\beta} \kappa^*(z)dz\right|\right] = \exp\left[-\left|\int_{\gamma}^{\delta} \kappa^*(z)dz\right|\right] \tag{16c}$$

In this way the overall contribution can be written as

$$C_{sym.} = -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{1}{e-d} - \frac{1}{e+d}\right) \tag{17}$$

In order to further construct analytic relations we should calculate the fundamental amplitudes that appear in the above formulae in terms of the transmission factors.

$$\begin{aligned} A^{I}_{\alpha\to\beta} &= e^{-\kappa}\left(1 + \frac{i}{2}e^{-\kappa}\frac{i}{2}e^{-\kappa} + \ldots\right) \\ &= \frac{e^{-\kappa}}{1 + e^{-2\kappa}/4} \end{aligned} \tag{18a}$$

$$\begin{aligned} A^{II}_{\beta\to\gamma} &= e^{ik}\left(1 + (-i)e^{ik}(-i)e^{ik} + \ldots\right) \\ &= \frac{e^{ik}}{1 + e^{2ik}} \end{aligned} \tag{18b}$$

$$\begin{aligned} A^{II}_{\gamma\to\gamma} &= e^{ik}(-i)e^{ik}\left(1 + (-i)e^{ik}(-i)e^{ik} + \ldots\right) \\ &= -i\frac{e^{2ik}}{1 + e^{2ik}} \end{aligned} \tag{18c}$$

$$\begin{aligned} A^{III}_{\gamma\to\gamma} &= e^{-\kappa}\frac{i}{2}e^{-\kappa}\left(1 + \frac{i}{2}e^{-\kappa}\frac{i}{2}e^{-\kappa} + \ldots\right) \\ &= \mathrm{i}/2\frac{e^{-2\kappa}}{1 + e^{-2\kappa}/4} \end{aligned} \tag{18d}$$

We can now proceed to the calculation the denominators of equation (17). We will have

$$\begin{aligned} &e \mp d = 1 - A^{III}_{\gamma\to\gamma} A^{II}_{\gamma\to\gamma} \mp A^{III}_{\gamma\to\gamma} A^{II}_{\beta\to\gamma} = \\ &1 - \mathrm{i}/2\left(\frac{e^{-2\kappa}}{1 + e^{-2\kappa}/4}\right) \mathrm{x} \left(-i\frac{e^{2ik}}{1 + e^{2ik}}\right) \mp \mathrm{i}/2\left(\frac{e^{-2\kappa}}{1 + e^{-2\kappa}/4}\right) \mathrm{x} \left(\frac{e^{ik}}{1 + e^{2ik}}\right) \end{aligned} \tag{19}$$

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We introduce the following two symbols, corresponding to the forbidden and the allowed region of motion respectively:

$$\rho \equiv e^{-2\kappa}/4 \qquad \text{and} \qquad \sigma \equiv e^{2ik} \tag{20}$$

and write the overall contribution as

$$C_{sym.} = -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{(1+\rho)(1+\sigma)}{(1+\rho)(1+\sigma)-2\rho\sigma-2i\rho\sigma^{1/2}} - \frac{(1+\rho)(1+\sigma)}{(1+\rho)(1+\sigma)-2\rho\sigma+2i\rho\sigma^{1/2}}\right) \tag{21}$$

Direct remarks can be expressed concerning the structure of the above formulae:

a) It is obvious that when $\rho << 1$ which is equivalent to say that we have strong barriers confining the inner classically allowed region, and so practically no interaction with the continuum appears, we get

$$C_{sym.} \cong -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{(1+\sigma)}{(1+\sigma)} - \frac{(1+\sigma)}{(1+\sigma)}\right) = 0 \tag{22}$$

b) It is easy to see that the condition $1+\sigma=0$ determines the eigenvalues of the classically allowed region of motion, since we can actually write $e^{2ik} = e^{\pm i\pi} \Rightarrow k = n\pi + \pi/2, \quad n = 0,1,2,..$ which is the Bohr Sommerfield quantization rule. For example if the area of confinement is a harmonic potential of the form $U(x) = \frac{1}{2}\omega^2 x^2$ with turning points at α and –α, meaning $\mathrm{E} = \frac{1}{2}\omega^2\alpha^2$, k is equal to the quantity $\sqrt{2}\int_{-\alpha}^{\alpha} dx\sqrt{\mathrm{E}-\frac{1}{2}\omega^2 x^2} = \sqrt{2}\sqrt{\frac{2}{\omega^2}}\frac{\mathrm{E}}{2}\sin^{-1}\frac{x}{\alpha}\Bigg|_{-\alpha}^{\alpha} = \frac{E\pi}{\omega}$, and then the quantization rule gives $\frac{\pi E_n}{\omega} = n\pi + \frac{\pi}{2} \Rightarrow E_n = (n+1/2)\omega$, which is the harmonic oscillator spectrum.

We may now investigate the effect of the previously revealed eigenvalues on the structure of the semiclassical Greens function.

$$C_{sym.}(E_n) = -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{(1+\rho)(0)}{(1+\rho)(0)+2\rho-2i\rho(-1)^n i} - \frac{(1+\rho)(0)}{(1+\rho)(0)+2\rho+2i\rho(-1)^n i}\right) \Rightarrow$$

$$C_{sym.}(E_n) = \begin{cases} -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{(1+\rho)}{(1+\rho)-2\rho+\rho} - \frac{0}{4\rho}\right) \cong -i(1+\rho) & \text{for n odd} \\ -ie^{\kappa} A^{I}_{\alpha\to\beta}\left(\frac{0}{4\rho} - \frac{(1+\rho)}{(1+\rho)-2\rho+\rho}\right) \cong i(1+\rho) & \text{for n even} \end{cases} \tag{23}$$

c) Next we can now investigate the case of maximum contribution which occurs by minimizing the denominators of $C_{sym.}$. We seek for a solution of the equation $(1+\rho)(1+\sigma)-2\rho\sigma \mp 2i\rho\sigma^{1/2}=0 \Rightarrow (1-\rho)\sigma \mp 2i\rho\sigma^{1/2}+(1+\rho)=0$ and we easily find $(\sigma_{1\sim 3,2\sim 4})^{1/2}=\pm\, i(1+\varepsilon),\ \mp\, i$, where we have defined $\varepsilon=\dfrac{2\rho}{1-\rho}>0$. In this way we can actually write

$$C_{sym.}=-ie^{\kappa}A^{I}_{\alpha\to\beta}\left(\frac{(1+\rho)(\sigma^{1/2}-i)(\sigma^{1/2}+i)}{(1-\rho)(\sigma^{1/2}-\sigma_1^{1/2})(\sigma^{1/2}-\sigma_2^{1/2})}-\frac{(1+\rho)(\sigma^{1/2}-i)(\sigma^{1/2}+i)}{(1-\rho)(\sigma^{1/2}-\sigma_3^{1/2})(\sigma^{1/2}-\sigma_4^{1/2})}\right)\Rightarrow$$
$$C_{sym.}=-ie^{\kappa}A^{I}_{\alpha\to\beta}(\varepsilon+1)\left(\frac{(\sigma^{1/2}-i)}{(\sigma^{1/2}-i-i\varepsilon)}-\frac{(\sigma^{1/2}+i)}{(\sigma^{1/2}+i+i\varepsilon)}\right) \quad (24)$$

It is obvious that each pole term corresponds to odd and even eigenvalue contribution. It is therefore desirable to develop the above expression around the eigenvalues of the unperturbed problem and call the expansion $C^{odd}_{sym.}$ and $C^{even}_{sym.}$ respectively. We can then write

$$C^{odd}_{sym.}\cong -ie^{\kappa}A^{I}_{\alpha\to\beta}\frac{\varepsilon+1}{\varepsilon/2+1}+ie^{\kappa}A^{I}_{\alpha\to\beta}(\varepsilon+1)\left(\frac{-i\varepsilon}{i\varepsilon+\frac{d\sigma^{1/2}}{dE}(E-E_n)+i\frac{d\varepsilon}{dE}(E-E_n)}\right)$$
$$=-i+\frac{1}{1-\rho}\left(\frac{\left(\frac{1}{\varepsilon}\frac{dk}{dE}+i\frac{d\ln\varepsilon}{dE}\right)^{-1}}{E-\left(E_n-\frac{\frac{d\ln\varepsilon}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2}-i\frac{\frac{1}{\varepsilon}\frac{dk}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2}\right)}\right) \quad (25)$$

Repeating the same procedure for the even eigenfunctions we similarly find

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$$C_{sym.}^{even} \cong ie^{\kappa} A^{I}_{\alpha\to\beta}\frac{\varepsilon+1}{\varepsilon/2+1} - ie^{\kappa}A^{I}_{\alpha\to\beta}\left(\varepsilon+1\right)\left(\frac{i\varepsilon}{-i\varepsilon+\frac{d\sigma^{1/2}}{dE}\left(E-E_n\right)-i\frac{d\varepsilon}{dE}(E-E_n)}\right)$$

$$= i-\frac{1}{1-\rho}\left(\frac{\left(\frac{1}{\varepsilon}\frac{dk}{dE}+i\frac{d\ln\varepsilon}{dE}\right)^{-1}}{E-\left(E_n-\frac{\frac{d\ln\varepsilon}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2}-i\frac{\frac{1}{\varepsilon}\frac{dk}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2}\right)}\right) \quad (26)$$

It is obvious that the form of the semiclassical Greens function is the same for both odd and even eigenfunctions. In addition the above expressions show that the Green's function is constituted by two terms, a non pole term that gives the general background of propagation and the pole term, which is the second term of the equation. The pole term reveals the complex energy eigenvalues, since now the initially prepared state of continuum 1, (particle in allowed region O), decays in the continuum 2, (particle in allowed region IV). The imaginary part of the energy pole expresses the rate with which continuum 1 decays into continuum 2 and for this it is interesting to notice that it is clearly negative as it should. This is true since k is an increasing function of energy and therefore the derivative dk/dE is a positive quantity. In addition there is a real energy shift also coming from the above interaction. Since the major contribution of the pole term can be written as a sum , we can actually write the Green's function in the following form

$$G_{sc}(E) \equiv G_{sc}^{n.p.}(E)+G_{sc}^{p.}(E)= i\frac{\exp[i\int_{z_1}^{\alpha}k^*(z)dz+i\int_{\delta}^{z_2}k^*(z)dz]}{\overline{p(z_1,z_2)}} - \sum_{n=0}^{n=n_{\max}}\frac{A_n}{E-Z_n} \quad (27)$$

where

$$A_n = \frac{\exp[i\int_{z_1}^{\alpha}k^*{}_n(z)dz+i\int_{\delta}^{z_2}k^*{}_n(z)dz]}{\overline{p_n(z_1,z_2)}\left\{\left(\rho+1\right)\left(\frac{1}{\varepsilon}\frac{dk}{dE}+i\frac{d\ln\varepsilon}{dE}\right)\right\}_{E\,=\,E_n}} \quad (28)$$

and

$$Z_n = E_n-\frac{\frac{d\ln\varepsilon}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2}-i\frac{\frac{1}{\varepsilon}\frac{dk}{dE}}{\frac{1}{\varepsilon^2}\left(\frac{dk}{dE}\right)^2+\left(\frac{d\ln\varepsilon}{dE}\right)^2} \quad (29)$$

and where $\overline{p_n(z_1,z_2)}$ and $k^*{}_n(z)$ are defined by $\overline{p(z_1,z_2)}$ and $k^*(z)$ respectively for $E=E_n$. We should note that the n_{max} corresponds to the maximum quantum number that the barriers can support. However a more accurate result should be produced by developing the $C_{sym.}$ in second order around the unperturbed eigenvalues, meaning

$$C_{sym.} \cong \left(\frac{(\rho+1)^{-1}}{i+\left(i\frac{d\ln\varepsilon}{dE}+\frac{1}{\varepsilon}\frac{dk}{dE}\right)(E-E_n)+i\left(\frac{-i}{2\varepsilon}\frac{d^2k}{dE^2}+\frac{1}{2\varepsilon}\left(\frac{dk}{dE}\right)^2+\frac{1}{2}\frac{d^2\ln\varepsilon}{dE^2}+\frac{1}{2}\left(\frac{d\ln\varepsilon}{dE}\right)^2\right)(E-E_n)^2} - i \right)$$

(30)

Proceeding the algebra by first defining the following quantities,

$$\delta = \frac{d\ln\varepsilon}{dE}, \gamma = \frac{1}{\varepsilon}\frac{dk}{dE}, \beta = \frac{\varepsilon}{2}\gamma^2 + \frac{1}{2}\frac{d\delta}{dE} + \frac{1}{2}\delta^2, \alpha = \frac{1}{2\varepsilon}\frac{d(\gamma\varepsilon)}{dE}$$
$$\rho = \sqrt{\left(\gamma^2-\delta^2+4\beta\right)^2+\left(2\gamma\delta-4\alpha\right)^2}, \varphi = \tan^{-1}\frac{2\gamma\delta-4\alpha}{\gamma^2-\delta^2+4\beta} \quad (31)$$

we find for the perturbed eigenvalues, the following result

$$Z_n^* \cong E_n + \frac{-\alpha\gamma-\beta\delta}{2\left(\alpha^2+\beta^2\right)} \pm \sqrt{\rho}\,\frac{\alpha\cos{}^{\varphi}\!/_2+\beta\sin{}^{\varphi}\!/_2}{2\left(\alpha^2+\beta^2\right)} - \frac{i}{2}\left(\frac{\alpha\delta-\beta\gamma}{\left(\alpha^2+\beta^2\right)} \pm \sqrt{\rho}\,\frac{\beta\cos{}^{\varphi}\!/_2-\alpha\sin{}^{\varphi}\!/_2}{2\left(\alpha^2+\beta^2\right)}\right) \quad (32)$$

Not symmetric barriers case:

In the case of not symmetric potential barriers neither the $A^{III}_{\gamma\to\gamma} = A^{I}_{\beta\to\beta}$ nor the $A^{I}_{\alpha\to\beta} = A^{III}_{\gamma\to\delta}$ relation holds. The total path contribution from α to δ can be simply written as

$$C_{not\ sym} = \frac{A^{I}_{\alpha\to\beta}A^{II}_{\beta\to\gamma}A^{III}_{\gamma\to\delta}}{\left(1-A^{III}_{\gamma\to\gamma}A^{II}_{\beta\to\beta}\right)\left(1-A^{I}_{\beta\to\beta}A^{II}_{\beta\to\beta}\right)-A^{III}_{\gamma\to\gamma}\left(A^{II}_{\beta\to\gamma}\right)^2 A^{I}_{\beta\to\beta}} \quad (33)$$

The numerator of the above fraction expresses direct propagation from α to δ without interchanging the regions of motion while the denominator equals unity when the barriers strongly confine the inner quantum well. Looking the above relation in a more accurate way and since it is true that $A^{II}_{\beta\to\gamma} = ie^{-ik_o}A^{II}_{\beta\to\beta}$, the denominator becomes a second order polynomial of the amplitude $A^{II}_{\beta\to\beta}$. Since the amplitude $A^{II}_{\beta\to\beta} = A^{II}_{\gamma\to\gamma}$ is defined according to (18c) as $A^{II}_{\beta\to\beta} = -i\frac{\sigma}{\sigma+1}$ and $A^{II}_{\beta\to\gamma}$ according to (18b) as $A^{II}_{\beta\to\gamma} = \frac{\sqrt{\sigma}}{\sigma+1}$ we can actually write equation (30) in the following form

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$$C_{not\ sym}=\frac{A^{I}_{\alpha\to\beta}A^{III}_{\gamma\to\delta}\sqrt{\sigma}}{-\sigma A^{III}_{\gamma\to\gamma}A^{I}_{\beta\to\beta}+i\sigma\left(A^{I}_{\beta\to\beta}+A^{III}_{\gamma\to\gamma}\right)+\sigma+1}\equiv\frac{A^{I}_{\alpha\to\beta}A^{III}_{\gamma\to\delta}\sqrt{\sigma}}{\sigma(1-\rho^{*})+1} \tag{34}$$

where we have defined the real barrier factor $\rho^{*}>0$ as

$$\rho^{*}=-4\frac{e^{-(\kappa_1+\kappa_2)}}{\left(4+e^{-2\kappa_1}\right)\left(4+e^{-2\kappa_2}\right)}+2\left(\frac{e^{-2\kappa_1}}{4+e^{-2\kappa_1}}+\frac{e^{-2\kappa_2}}{4+e^{-2\kappa_2}}\right) \tag{35}$$

As in the symmetric case direct remarks can be expressed concerning the structure of the above formula:

a) It is obvious that when $A^{I}_{\alpha\to\beta}, A^{III}_{\gamma\to\delta}, \rho^{*}<<1$ which is the case of strong barrier confinement of the inner classically allowed region, practically no interaction with the continuum appears, we get

$$C_{not\ sym}\cong\frac{0\cdot\sqrt{\sigma}}{\sigma+1}=0 \tag{36}$$

b) Again as was shown in remark b) of the symmetric barriers case the condition $1+\sigma=0$ determines the eigenvalues of the classically allowed region of motion.

c) We can now investigate the case of maximum contribution which occurs when we minimize the denominator of the $C_{not\ sym}$. This is equivalent to finding the solution of the equation $\sigma(1-\rho^{*})+1=0$ which is $\sigma_o=-\frac{1}{1-\rho^{*}}$. Since ρ^{*} is a small real quanti-ty σ becomes also a real quantity close but not equal to -1 which contradicts to its form of $\sigma\equiv e^{2ik}$. For this we develop the denominator around $\sigma=-1$, or equivalently around the eigenvalues of the inner quantum well, and substitute to the numerator the value $\sigma_o=-\frac{1}{1-\rho^{*}}$.

$$C_{not\ sym}\cong\frac{A^{I}_{\alpha\to\beta}A^{III}_{\gamma\to\delta}\sqrt{-\frac{1}{1-\rho^{*}}}}{\rho^{*}-\frac{d\sigma}{dE}(\rho^{*}-1)\left(E-E_n\right)-\sigma\frac{d\rho^{*}}{dE}\left(E-E_n\right)}$$

$$=\frac{A^{I}_{\alpha\to\beta}A^{III}_{\gamma\to\delta}\sqrt{-\frac{1}{1-\rho^{*}}}\left[\left(\frac{d\rho^{*}}{dE}+2i(\rho^{*}-1)\frac{dk}{dE}\right)_{E=E_n}\right]^{-1}}{\left\{E-E_n+\left.\frac{\rho^{*}\frac{d\rho^{*}}{dE}}{\left(\frac{d\rho^{*}}{dE}\right)^2+\left(2(\rho^{*}-1)\frac{dk}{dE}\right)^2}\right|_{E=E_n}-i\left.\frac{2\rho^{*}(\rho^{*}-1)\frac{dk}{dE}}{\left(\frac{d\rho^{*}}{dE}\right)^2+\left(2(\rho^{*}-1)\frac{dk}{dE}\right)^2}\right|_{E=E_n}\right\}} \tag{37}$$

In this way the perturbed eigenvalues, for the not symmetric case, take the following form

$$Z_n \cong E_n - \frac{\rho^* \dfrac{d\rho^*}{dE}}{\left(\dfrac{d\rho^*}{dE}\right)^2 + \left(2(\rho^*-1)\dfrac{dk}{dE}\right)^2}\Bigg|_{E=E_n} - i\frac{2\rho^*(1-\rho^*)\dfrac{dk}{dE}}{\left(\dfrac{d\rho^*}{dE}\right)^2 + \left(2(\rho^*-1)\dfrac{dk}{dE}\right)^2}\Bigg|_{E=E_n} \tag{38}$$

Again the imaginary part is clearly negative since quantity ρ^* is normally much less than unity and the derivative *dk/dE* is a positive quantity. Again we can write the Green's function as a sum of poles meaning

$$G_{sc}(E) \equiv \sum_{n=0}^{n=n_{\max}} \frac{B_n}{E-Z_n} \tag{39}$$

where

$$B_n = \left\{ A^{I}_{\alpha\to\beta} A^{III}_{\gamma\to\delta} \sqrt{-\frac{1}{1-\rho^*}} \left[\left(\frac{d\rho^*}{dE} + 2i(\rho^*-1)\frac{dk}{dE}\right)\right]^{-1} \right\}_{E=E_n} \tag{40}$$

In each case of symmetry, equation (29,32) or (38), the complex energy poles take the general form, $Z_n = E_n + \Delta_n - i\dfrac{\Gamma_n}{2}$ and the width of the decaying state is analytically given as follows:

$$\Gamma_{n,sym.} = \frac{\dfrac{2}{\varepsilon}\dfrac{dk}{dE}}{\dfrac{1}{\varepsilon^2}\left(\dfrac{dk}{dE}\right)^2 + \left(\dfrac{d\ln\varepsilon}{dE}\right)^2}\Bigg|_{E=E_n} \tag{41a}$$

and

$$\Gamma_{n,not\ sym.} = \frac{4\rho^*(1-\rho^*)\dfrac{dk}{dE}}{\left(\dfrac{d\rho^*}{dE}\right)^2 + \left(2(\rho^*-1)\dfrac{dk}{dE}\right)^2}\Bigg|_{E=E_n} \tag{41b}$$

The fundamental time associated with the tunneling process if the exponential law is assumed for its evolution , is often taken as the lifetime of the quasi – bound state and is related to the width via the $\tau = \dfrac{\hbar}{\Gamma}$. In this way we can write for the transport time, for the symmetric and the not symmetric case respectively, the following relations

$$\tau_{n,sym.} = \hbar \frac{\dfrac{1}{\varepsilon^2}\left(\dfrac{dk}{dE}\right)^2 + \left(\dfrac{d\ln\varepsilon}{dE}\right)^2}{\dfrac{2}{\varepsilon}\dfrac{dk}{dE}}\Bigg|_{E=E_n} \tag{42a}$$

and

$$\tau_{n,not\ sym.} = \hbar \frac{\left(\frac{d\rho^*}{dE}\right)^2 + \left(2(\rho^* - 1)\frac{dk}{dE}\right)^2}{4\rho^*(1-\rho^*)\frac{dk}{dE}}\Bigg|_{E=E_n} \tag{42b}$$

For once again we should emphasize that the above expressions describe the transport time as long as the other time constants are significantly minimized.

5. CONCLUDING REMARKS

In this work we studied quantum transmission in a double barrier structure via the semi-classical path integral method. This kind of potential covers a large area of interest and applications from different branches of physical sciences, from quantum chemistry up to nanoelectronics. As such we demonstrated the model of a quantum tunneling diode. We produced analytic relations for the transmission amplitude, which is the Green's function for single charge transport between the two metals of the diode, due to resonant tunneling. The Green's function, as was expected, appears to have a pole structure which reveals the complex energy spectrum of the structure. The later is described via analytic relations. The imaginary part of each complex pole is related to the time needed for transport, under certain circumstances where the barrier penetration strongly dominates all the other mechanisms generating an intrinsic time constant. The above study was done for both the symmetric and the not symmetric barrier case, concerning the absence or the application respectively of an external electric field, on the diode's band profile.

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