Dwell and phase time singularities in electron tunneling through double complex barrier

Nikola Opačak, Vitomir Milanović and Jelena Radovanović

Abstract—**An investigation about tunneling times in complex potentials is reported. Analyzed potential structure consists out of complex double Dirac delta potential barriers and analytical expressions for dwell time, self-interference time and group delay are obtained. It is stated that appropriate values for the set of parameters of the potential can be acquired in order for the tunneling times to achieve very large values and even approach infinity for the case of resonance. The conditions for the occurrence of tunneling times singularities, which will be given, are satisfied for only one particular positive value of the imaginary part of the potential, if all other parameters are known.**

Index Terms—**infinite tunneling times, double potential barrier, complex potentials, transmission.**

I. Introduction

Let us consider a case where a free particle impinges a potential barrier, with value of the potential higher than the energy of the particle. A finite, non-vanishing probability for the particle to overcome the barrier is implied by the quantum mechanics (i.e. the tunneling effect). Electron tunneling through double barrier structure has been the subject of intensive theoretical and experimental study over the years due to its application in high speed electronic devices. Possibly the most important feature of the tunneling effect is the time which electrons take to go through the barrier, i.e. the traversal time. Throughout the past, there have been presented many definitions and solutions to the question of tunneling times [1-9] and none have gained general approval yet. However, among many formulations of relevant times, the two most commonly used are [10]: the dwell time, which is the time a particle spends in the barrier, independent on whether it is transmitted or reflected; and the phase time or group delay which considers the propagation of a wave packet. Until some insight was given in [11-12], it was not clear whether the dwell time and group delay are connected with each other under the quantum tunneling conditions, other than they have the same asymptotic value in classical domain. In [13] it was shown that sum of the dwell time and the self-interference time is equal to the group delay, which led to the explanation of the paradox of the Hartmann effect [14] in quantum tunneling and alleged violation of causality.

Nikola Opačak is with the School of Electrical Engineering, University of Belgrade, 73 Bulevar kralja Aleksandra, 11020 Belgrade, Serbia (e-mail: opacaknn@gmail.com).

Vitomir Milanović is with the School of Electrical Engineering, University of Belgrade, 73 Bulevar kralja Aleksandra, 11020 Belgrade, Serbia (e-mail: milanovic@etf.bg.ac.rs).

Jelena Radovanović is with the School of Electrical Engineering, University of Belgrade, 73 Bulevar kralja Aleksandra, 11020 Belgrade, Serbia (e-mail: radovanovic@etf.bg.ac.rs).

In quantum mechanics, a change of the incident probability flux during the wave propagation is modeled with potentials which have a non-vanishing imaginary part. The case of absorptive medium where we have reduction of the incident flux, corresponds to the potential with negative imaginary part, and conversely, the case where the absorption is negative and we have gain of the incident flux corresponds to the potential with positive imaginary part. Numerous effects are analyzed in this manner [15-18] and extensive review on complex potentials and absorption is given in [19-20]. The global tunneling time, which is equal to the sum of the semi-classical traversal and group delay time, was analytically calculated for the first time in [21] for a complex square barrier.

A study of the tunneling times in the case of two successive delta barriers with complex potential is reported in this paper. Analysis will primarily be focused on the group delay, also covering the case of resonant tunneling, which occurs when the energy of the metastable state which exists in the well region between the delta barriers coincides with the incident electron energy. The relation between group, dwell and self-interference time, accounting one additional term originating from the non-vanishing imaginary part of the potential, which is valid for arbitrary complex potential, is obtained in [22]. The aim is to acquire analytical expressions for the relevant tunneling times in the case of double delta complex barrier. In our recent paper [23] we have shown that if the parameters of the potential structure are selected precisely, the resonant transmission approaches infinity when the incident electron energy is equal to the resonant metastable state. This phenomenon is possible only for positive values of the imaginary part of the potential. We will show that the tunneling times diverge for the same set of parameters and for the same energy. In [23] we have studied both double rectangular and delta barriers, but in this paper the analysis will be conducted only for the delta potentials, because it is impossible to obtain analytical expressions in the case of rectangular barriers, and at the same time identical conclusions can be made. The occurrence of infinite tunneling times will be the main subject of investigation in this paper. We will further show that this phenomenon also occurs for potentials with negative real part (i.e. potential wells) as long as the imaginary part is positive.

II. General consideration

Consider a one-dimensional arbitral complex potential $U(\mathrm{x})$ which occupies $0 < x < L$ part of the x axis, and $U(x) = 0$ for all other values of x. Let $T = |T|e^{i\phi_t}$ and $R = |R|e^{i\phi_r}$ stand for transmission and reflection amplitudes respectively. Definitions of group delay, self-interference-time and dwell time, can be found in [22].

The dwell time, i.e. the average total time the particle spends in the barrier, regardless of transmission or reflection, is given by following relation:

$$\tau_d = \frac{m}{\hbar k}\int_0^L |\psi(x)|^2\, dx, \tag{1}$$

where m is the effective mass of the particle, $k = \sqrt{\frac{2m}{\hbar^2}E}$ is the wave number and $\psi(x)$ is the wave function.

Total group delay is the measure of the delay in appearance of the wave function at the front and the end of the potential barrier and it is calculated as the weighted sum of group delays in transmission τ_{gt} and reflection τ_{gr}, which are defined as:

$$\tau_{gt} = \hbar\frac{d\phi_0}{dE},\ \tau_{gr} = \hbar\frac{d\phi_r}{dE}, \tag{2}$$

where $\phi_0 = \phi_t + kL$.

The group delays in transmission and reflection are only equal for a symmetric real barrier. The bidirectional delay is then given by:

$$\tau_g = |T|^2\tau_{gt} + |R|^2\tau_{gr} \tag{3}$$

When the wave packet impinges the barrier, the total incident probability current is divided into transmitted and reflected current. As a consequence, the reflected wave packet overlaps with the incident in the area just before the barrier and they interfere with one another, hence we have self-interference time [13], which is defined as:

$$\tau_i = -\frac{\hbar}{k} Im\{R\}\frac{\partial k}{\partial E} \tag{4}$$

where $Im\{R\}$ is the imaginary part of the reflection amplitude.

Now we can finally arrive to the final relationship between the mentioned tunneling times [22]:

$$\tau_g = \tau_d + \tau_i - \frac{2m}{\hbar k}\int_0^L U_I Im\left\{\psi^*\frac{d\psi}{dE}\right\}dx = \tau_d + \tau_i - \tau_a. \tag{5}$$

The last term τ_a comes from a non-vanishing value of the imaginary part of the potential U_i. If the potential is strictly real, we arrive to the well-known relation [13]: $\tau_g = \tau_d + \tau_i$.

III. Double delta potential

We will further analyze double delta potential structure:

$$U(x) = V_0\left(\delta\left(x + \frac{w}{2}\right) + \delta\left(x - \frac{w}{2}\right)\right), \tag{6}$$

which is a centralized symmetrical structure, and with complex potential in general case $V_0 = V_{0R} + iV_{0I}$.

Let us investigate a free particle impinging the barrier from the left hand side. A wave function of the particle can be obtained after solving the Schrödinger's equation:

$$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx},\ x < -\frac{w}{2} \\ C_1e^{ikx} + C_2e^{-ikx},\ -\frac{w}{2} < x < \frac{w}{2} \\ Te^{ikx},\ x > \frac{w}{2} \end{cases}. \tag{7}$$

Expressions for reflection and transmission amplitudes, R and T respectively, can be acquired in many ways, e.g. transfer matrix method. After some calculations, we arrive to:

$$T = \frac{{t_0}^2}{1 - {r_0}^2e^{i2kw}}, \tag{8}$$

$$R = r_0e^{-ikw} + \frac{{t_0}^2 r_0 e^{ikw}}{1 - {r_0}^2e^{i2kw}}. \tag{9}$$

In the last two relations (8) and (9), r_0 and t_0 are reflection and transmission amplitudes respectively corresponding to just one delta potential barrier defined as $U(x) = V_0\delta(x)$. We have taken into account that the barriers are identical and separated by the distance w. The expressions are acquired after some simple calculations:

$$r_0 = -\frac{\chi}{1+\chi} \text{ and } t_0 = \frac{1}{1+\chi}, \tag{10}$$

where $\chi = \sqrt{m{V_0}^2/2\hbar^2 E}$.

It is not difficult to calculate the expressions for C_1 and C_2 from relation (7) after using the condition of continuity of the wave function and appropriate condition for the first derivative of the wave function (as a consequence of considering delta potentials) in $x = \pm w/2$:

$$C_1 = \frac{Te^{ik3w/2} - e^{-ikw/2} - Re^{ikw/2}}{e^{ik3w/2} - e^{-ikw/2}},$$

$$C_2 = \frac{Re^{ik3w/2} + e^{ikw/2} - Te^{ikw/2}}{e^{ik3w/2} - e^{-ikw/2}}. \tag{11}$$

We hope to calculate the group delay. An exact definition is given by (3) and the best approach would be to obtain τ_{gt} and τ_{gr}. For the studied potential, this method would produce complex expressions that would be hard to analyze. Smarter approach would be to obtain analytical relations for dwell time, self-interference time and the additional term (τ_a) and combine them with relation (5).This can be done with relative ease.

First, let us write the definition of self-interference time in a more suitable form, which we can use directly:

$$\tau_i = -\frac{\hbar}{2E} Im\{R\}. \tag{12}$$

Next, we can derive the expression for the dwell time using (1) and changing the domain of the integration to $\left(-\frac{w}{2},\frac{w}{2}\right)$:

$$\tau_d=\frac{m}{\hbar k}\int_{-\frac{w}{2}}^{\frac{w}{2}}\left|C_1e^{ikx}+C_2e^{-ikx}\right|^2dx=\frac{m}{\hbar k}\int_{-\frac{w}{2}}^{\frac{w}{2}}\left||C_1|^2+|C_2|^2+2Re\{C_1{C_2}^{*}e^{i2kx}\}\right|^2dx.$$

After some calculations we arrive to:

$$\tau_d=\frac{mw}{\hbar k}\left[|C_1|^2+|C_2|^2+2Re\{C_1{C_2}^{*}\}\frac{\sin(kw)}{kw}\right]. \quad (13)$$

Ultimately, we obtain the expression for the additional term τ_a. Having in mind that $U_i=V_{0I}\left(\delta\left(x+\frac{w}{2}\right)+\delta\left(x-\frac{w}{2}\right)\right)$ the integral in relation (5) transforms to the sum of two addends:

$$\tau_a=\frac{2mV_{0I}}{\hbar k}\left[Im\left(\psi^{*}\frac{d\psi}{dE}\right)\bigg|_{x=w/2}+Im\left(\psi^{*}\frac{d\psi}{dE}\right)\bigg|_{x=-w/2}\right]. \quad (14)$$

It is possible to derive exact form of τ_a, but we will stop at (14) in this paper because, otherwise, expressions would be very complicated while at the same time not improving the insight into the problem very much.

We can now finally show the values of the tunneling times depending on the values of incident energy E and imaginary part of the potential V_{0I}as is shown in Figs. 1., 2. and 3. We have focused on positive values of V_{0I} to show the tunneling times singularities with more detail. Later in the paper we will investigate the case with negative V_{0I}, i.e. an absorptive medium. We used the following parameters: The distance between two delta barriers is $w=4$nm, effective mass $m=0.067\,m_0$ (m_0 electron rest mass) and real part of V_0 is $V_{0R}=2\ \mathrm{nm}\cdot\mathrm{eV}$.

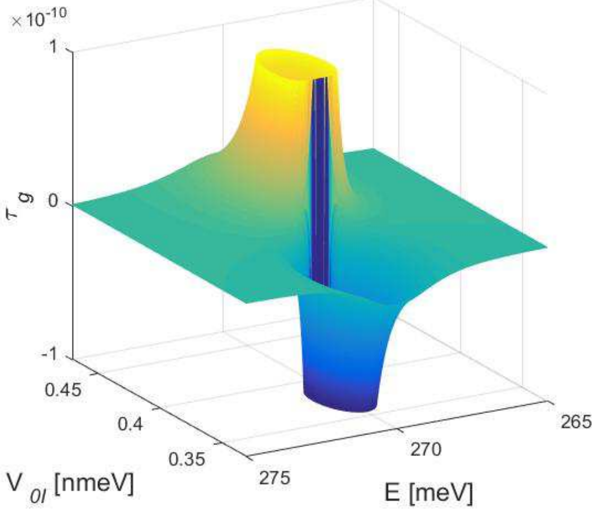

Fig.1. Group delay τ_g (in units of s) as a function of the imaginary part of the potential V_{0I} (in units of nm · eV) and incident energy E (in units of meV). Singularity occurs for $V_{0Iinf}=0.3921\ \mathrm{nm}\cdot\mathrm{eV}$ and for energy $E_{inf}=270$ meV.

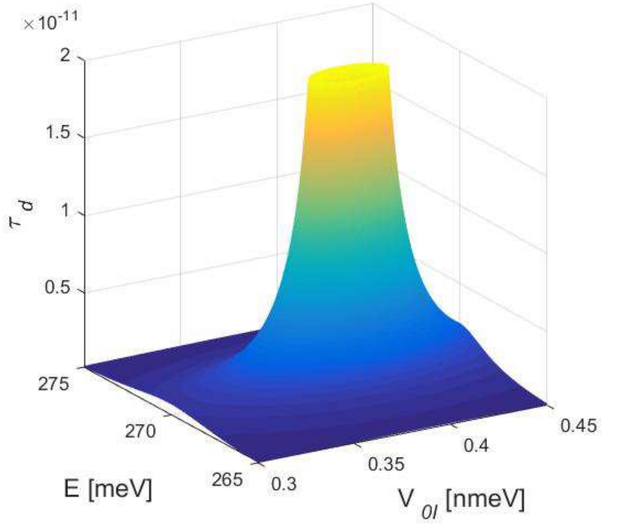

Fig.2. Dwell time τ_d (in units of s) as a function of the imaginary part of the potential V_{0I} (in units of nm · eV) and incident energy E (in units of meV). Singularity occurs for $V_{0Iinf}=0.3921\ \mathrm{nm}\cdot\mathrm{eV}$ and for energy $E_{inf}=270$ meV.

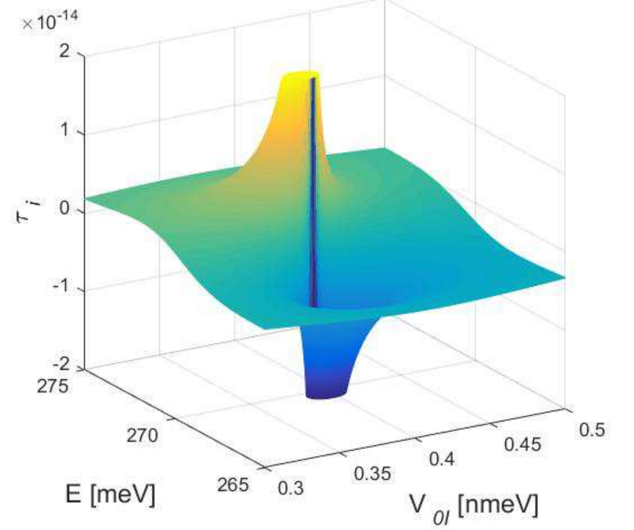

Fig.3. Self-interference time τ_i (in units of s) as a function of the imaginary part of the potential V_{0I} (in units of nm · eV) and incident energy E (in units of meV). Singularity occurs for $V_{0Iinf}=0.3921\ \mathrm{nm}\cdot\mathrm{eV}$ and for energy $E_{inf}=270$ meV.

In figs.1.-3. we can see that the tunneling times exhibit very intriguing behavior around the $V_{0I}=V_{0Iinf}$, which is the same value of V_{0I} where we have infinite transmission [23], which will be shown later. Resonant energy for the case $V_{0I}=V_{0Iinf}$ equals E_{inf}. Fig.1. depicts group delay as a function of V_{0I} and E. We can see that around E_{inf} and for values of V_{0I}slightly larger than V_{0Iinf}, the group delay reaches very high values, and even approaches infinity for $V_{0I}=V_{0Iinf}+\varepsilon,\varepsilon\to0^{+}$ and for $E=E_{inf}$. These high values were not shown on the picture deliberately, as they would obscure more subtle changes in values of τ_g. Conversely, when V_{0I} is slightly lower than V_{0Iinf}, we have very large negative value of group delay, and they approach negative infinity when

$V_{0I} = V_{0Iinf} - \varepsilon, \varepsilon \to 0^+$ and $E = E_{inf}$. Fig.2. shows the dwell time as a function of V_{0I} and E. From the definition of dwell time, it can be expected to observe only positive values of τ_d, and we can see that on fig.2. It can also be observed that for values of V_{0I} in the vicinity of V_{0Iinf}, τ_d has very large values, and approaches infinity for $V_{0I} = V_{0Iinf}$ and for $E = E_{inf}$. Fig.3. depicts self-interference time as a function of the same variables as the previous two graphs. It too possesses singularities and exhibits similar behavior as the group delay depicted in fig.1.

As stated before, for the same values of parameters for which the tunneling times exhibit singularities, the resonant transmission probability approaches infinity. The condition for resonance can be defined as [23]:

$$\sin(2kw) = -\frac{M}{\sqrt{M^2+N^2}}, \ \cos(2kw) = -\frac{N}{\sqrt{M^2+N^2}}, \tag{15}$$

where:

$$M = 2a^2 V_{0R} V_{0I}\left({V_{0R}}^2 - {V_{0I}}^2\right) - 2aV_{0R}V_{0I} + 4a^{3/2} V_{0R} {V_{0I}}^2 - 2a^2 V_{0R} V_{0I}\left({V_{0R}}^2 - {V_{0I}}^2\right) + 2a^{3/2} V_{0R}({V_{0R}}^2 - {V_{0I}}^2),$$

$$N = 4a^{3/2} V_{0I} {V_{0R}}^2 + a\left({V_{0R}}^2 - {V_{0I}}^2\right) - a^2({V_{0R}}^2 - {V_{0I}}^2)^2 - 2a^{3/2} V_{0I}\left({V_{0R}}^2 - {V_{0I}}^2\right) - 4(aV_{0R}V_{0I})^2. \tag{16}$$

In the last eq. (16) $a = \sqrt{m/2\hbar^2 E}$. Combining eqs. (8) and (15), it is possible to calculate transmission in the case of resonance for different values of the imaginary part of the potential. We have done so in fig.4. and it can clearly be observed that for $V_{0I} = V_{0Iinf}$ the resonant transmission approaches infinity, thus showing that transmission and tunneling times singularities occur simultaneously.

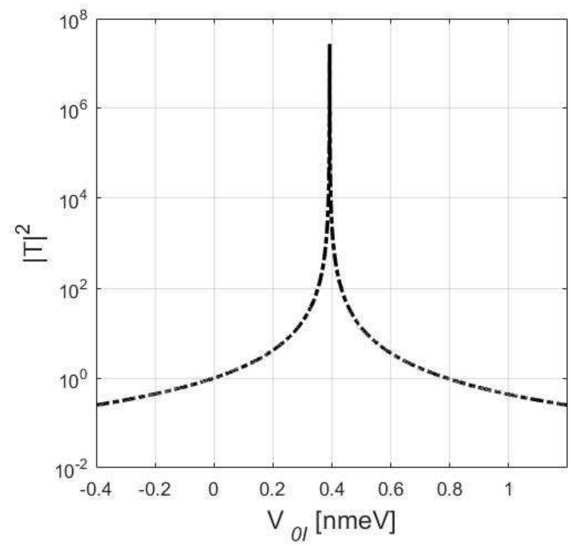

Fig.4. Resonant transmission probability as a function of the imaginary part of the potential V_{0I} (in units of $\mathrm{nm} \cdot \mathrm{eV}$. $V_{0Iinf} = 0.3921\ \mathrm{nm} \cdot \mathrm{eV}$ and for energy $E_{inf} = 270$ meV.

Our next goal is to show that the phenomenon of infinite tunneling times also exists in the case of potential wells, when V_{0R} is negative. In [23] we have derived the equation which shows the relationship between V_{0R}, V_{0I} and E at the point of singularity (when $V_{0I} = V_{0Iinf}$ and $E = E_{inf}$):

$$V_{0R} = \begin{cases} V_{0I} tg\left(\frac{mw}{\hbar^2} V_{0I}\right), & \frac{mw}{\hbar^2} V_{0I} \in \left(n\pi, n\pi + \frac{\pi}{2}\right) \\ -V_{0I} ctg\left(\frac{mw}{\hbar^2} V_{0I}\right), & \frac{mw}{\hbar^2} V_{0I} \in \left(n\pi + \frac{\pi}{2}, n\pi + \pi\right) \end{cases}, \tag{17}$$

where $n = 0,1,2$ ... for positive values of V_{0I}.

Furthermore, if we know the value of V_{0I} we can calculate the resonant energy using the following equation, which also shows that infinite tunneling times occur only for positive values of the imaginary part of the potential:

$$E = \frac{2m}{\hbar^2} {V_{0I}}^2. \tag{18}$$

If we choose the potential with negative values of V_{0R}, we have potential wells instead of barriers and obtain the same relation as (17) only with ranges of values of $\frac{mw}{\hbar^2} V_{0I}$ switched places with one another. In other words, for every value of V_{0R} we can find a corresponding value of V_{0I} so that for resonant energy transmission approaches infinity, and we have singularities in the tunneling times. For instance, if we choose $V_{0R} = -2\ \mathrm{nm} \cdot \mathrm{eV}$, from $V_{0R} = V_{0I} tg\left(\frac{mw}{\hbar^2} V_{0I}\right)$ we get that corresponding value of imaginary part of the potential is $V_{0I} = 0.5195\ nm \cdot eV$. We kept the initial distance between the wells $w = 4\ nm$ and will do so for all calculations in this paper. This situation corresponds to the particle meeting a double delta potential well and the behavior of τ_g is qualitatively identical to the one depicted on fig.1.

At last, we will plot the group delay as a function of E and only negative values of V_{0I}, i.e. we will be considering absorptive medium. We will study the case of particle meeting a double delta potential barrier (fig.5.). The case of double delta potential well is analogous and won't be shown in this paper.

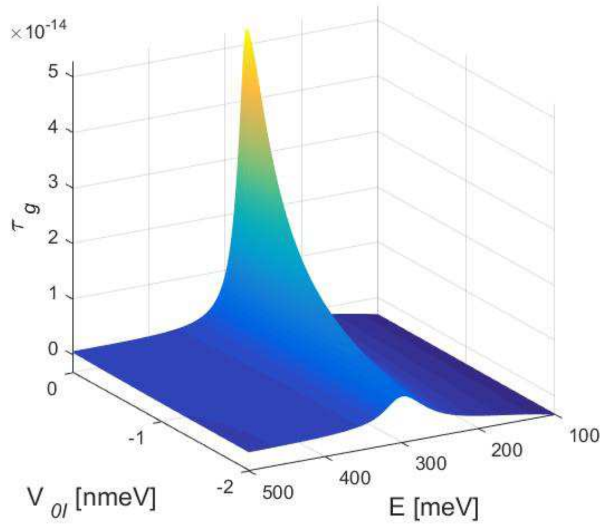

Fig.5. Group delay τ_g (in units of s) as a function of the imaginary part of the potential V_{0I} (in units of $\mathrm{nm} \cdot \mathrm{eV}$) and incident energy E (in units of meV). Real part of V_0 is $V_{0R} = 2\ \mathrm{nm} \cdot \mathrm{eV}$.

It can be seen on fig.5. that for absorptive media group delay has a finite maximum value for resonant energy and its value decreases as the energy moves away from the value of the resonant energy. It can also be observed that the maximum value of τ_g is obtained for strictly real barriers.

A few closing remarks will be given. Complex potentials are often used in calculations in quantum mechanics and have proven to be very useful. Potentials with negative imaginary part have found application in numerous problems, which is not the case for potentials with positive imaginary part which increase the probability current and represent a source. It is not wanted for an arbitrary state to be injected, so the analysis of the source potentials is more harder. Sources in electron transport devices such as quantum dots, nanoscale transistors and multi terminal devices are modeled in the mentioned way. We have analysed a double rectangular complex potential structure and its simplification in the form of double delta potential. This potential structure is based on electron transport devices e.g. resonant tunnel diode and hence has potential application. Transmission singularities have been reported earlier but only in PT-symmetric potentials [24]. However, the phenomenon of infinite transmission has not been reported for structures such as one analysed here, which are not PT-symmetric. Object of future research could be possible realisation of the potential structure. Such research would find application in high speed electronic devices.

IV. Conclusion

In this paper we considered a free particle meeting double complex delta potential. The analysis was directed at the case of positive imaginary part of the potential and at the investigation of the behavior of the tunneling times. We obtained the analytical expressions of the dwell time, self-interference time and group time using the extended relationship between the mentioned times, which accounts the additional term originating from the imaginary part of the potential in general case. It has been demonstrated that for both the cases of potential barriers and potential wells, if the real part of the potential and distance between the barriers have fixed known values, we can always find a corresponding value of the imaginary part of the potential so that the tunneling times achieve very large values and diverge at the point of singularity, when energy of the particle is equal to the resonant energy. The conditions for the occurrence of this peculiar phenomenon are satisfied only for the positive values of the imaginary part of the potential. At the end, the behavior of the group delay as a function of the energy and imaginary part of the potential is briefly studied for the case of absorptive medium, where the imaginary part of the potential is negative, and it is shown that there are no conditions for the previously mentioned phenomenon to exist.

Acknowledgment

This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia under Project No. III 45010.

References

[1] D. Bohm, Quantum Theory, New York, USA: Prentice Hall, 1951.
[2] E.P. Wigner, “Lower Limit for the Energy Derivative of the Scattering Phase Shift,” Phys. Rev. 98, pp.145-147, April 1955.
[3] M. Büttiker, “Larmor precession and the traversal time for tunneling,” Phys. Rev. B 27, pp. 6178-6188, May 1983.
[4] J.G. Muga, S. Brouard, R. Sala, “Transmission and reflection tunneling times,” Phys. Lett. A 167, pp. 24-28, July 1992.
[5] W. Li, Y. Guo, “Dresselhaus spin-orbit coupling effect on dwell time of electrons tunneling through double-barrier structures, ” Phys. Rev. B 73, 205311, May 2006.
[6] H.G. Winful, M. Ngom, N.M. Litchinitser, “Relation between quantum tunneling times for relativistic particles,” Phys. Rev. A 70, 052112, 2004.
[7] H.M. Nussenzveig, “Average dwell time and tunneling,” Phys. Rev. A 62, 042107, Sept. 2000.
[8] P. Thanikasalam, R. Venkatasubramanian, M. Cahay, “Analytical Expressions for Tunneling Time Through Single and Double Barrier Structures,” IEEE J. Quantum Electron. 29, pp. 2451-2458, Sept. 1993.
[9] G. Privitera, G. Salesi, V. S. Olkhovsky, E. Recami, “Tunneling times: An elementary introduction,” Riv. Nuovo Cimento, 26 4, pp. 1-55, Jan. 2003.
[10] E.H. Hauge, J.A. Støvneng, “Tunneling times: a critical review,” Rev. Mod. Phys. 61, pp. 917-936, Oct. 1989.
[11] C.R. Leavens, G.C. Aers, “Dwell time and phase time for transmission and reflection,” Phys. Rev. B 39, pp.1202-1206, Jan. 1989.
[12] S. Brouard, R. Sala, J.G. Muga, “Systematic approach to define and classify quantum transmission and reflection times,” Phys. Rev. A 49, pp. 4312-4325, June 1994.
[13] H.G. Winful, “Delay time and the Hartman effect in quantum tunneling,” Phys. Rev. Lett. 91, 260401. Dec. 2003.
[14] T. E. Hartman, Tunneling of a wave packet,” J. Appl. Phys. 33, pp. 3427-3433, Dec. 1962.
[15] P. Mollinas-Mata, P. Molinas-Mata, “Electron absorption by complex potentials: One-dimensional case,” Phys. Rev. A 54, pp. 2060-2065, Sept 1996.
[16] B. Sahu, L. Satpathy, C.S. Shastry, “Identification of resonances in scattering theory with a test imaginary potential,” Phys. Lett. A 303 pp. 105-234, Oct. 2002
[17] J.M. Cervero, A. Rodriguez, “Absorption in atomic wires,” Phys. Rev. A 70, 052705, Sept. 2004.
[18] B. Sahu, I. Jamir, E.F.P. Lyngdoh, C.S. Shastry, Phys. Rev. C 57, 1853, Apr. 1998.
[19] J.G. Muga, J.P. Palao, B. Navarro, I.L. Egusquiza, “Complex absorbing potentitals,” Phys. Rep. Volume 395 6, pp. 357-426, Jul. 2004.
[20] Z. Ahmed, “Coherent perfect absorption with and without lasing in complex potentials,” Phys. A: Math. Theor. 47, 385303, Sept. 2014.
[21] F. Raciti, G. Salesi, “Complex barrier tunneling times,” J. Phys. I France 4, pp. 1783-1789, Dec. 1994.
[22] S. Lj. S. Kočinac, V. Milanović, “Tunneling times in complex potentials,” Phys. Lett. A 372, pp. 191-196, Jan. 2008.
[23] N. Opacak, V. Milanovic, J. Radovanovic, “Transmission singularities in resonant electron tunneling through double complex potential barrier, ” arXiv:1704.08890, May 2017.
[24] A. Mostafazadeh, “Spectral singularities of complex scattering potentials and infinite reflection and transmission coeffcients at real energies,” Phys. Rev. Let. 102, 220402, Jun 2010.