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Reflection and transmission behaviour of a particle in a resonant tunnelling barrier

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Abstract
Stationary states are used to describe the transmission and the reflection of a wave packet through a resonant tunnelling barrier. The transmitted and the reflected spectra are studied and different links between numerical evaluations and the important characteristics of the resonant regime are underlined. The differences between the behaviours of wide and narrow near-resonant wave packets are delineated: two time scales appear in the case of quasi-bound states.

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1. Introduction

Resonant tunnelling is generally introduced as the last example that is tackled in theoretical studies on tunnelling, for instance about 'tunnelling time'. Usually, the interest is focused on the transmissivity (ultra-large scale integrated electronic devices) or, more generally, on the transmitted part of the wave.

However, when considering the crossing of a particle through a quantum barrier, the wave packet associated with the initial state of the particle is limited in the position space and its spectrum consequently has a non-null width. This induces the existence of a more or less important reflected part which is rarely considered. Of course, the behaviour of wave packets centred on mean wave vectors much below or much above the perfect transmissivity is similar to that observed in the usual pure tunnelling case. In contrast, the behaviour of wave packets around resonance shows spectacular characteristics which can be revealed on simple shaped barriers permitting analytical expressions of the complex transmission [1] and reflection coefficients. The spectra of the outgoing wave packet can be evaluated from their modulus and their phases furnish the phase delays which have been extensively considered in the traversal time ‘controversy’ [2–5].

On a more general level, the phase time has been considered for a long time in studies of asymptotic states in scattering events [6, 7]. In such cases, where the exact scattering potential is unknown, it is interesting to obtain a general treatment even for the one-dimensional problem (as it appears in the electronic domain), which cannot be directly found from particular analytical expressions. Thus, the presentation of these cases offers more generality.

In the present work, the case of a resonant quantum barrier is considered in that meaning. The Schrödinger equation is solved by using an iterative method based on the transfer matrix [8] currently used to study the transmissivity of barriers of any shape, appearing in resonant or non-resonant cases. The quality and the power of this method are well established and so we use it in order to obtain a sufficient basis of stationary states permitting a good description of wave packets. Thus, these stationary states give us direct solutions of the dynamical problem.

To offer links with the analytical expressions, we intentionally restrict the present numerical estimation to the simplest resonant barrier, that is the double rectangular barrier (let us however underline that our method has been tested for numerous more general examples).

Our paper is organized as follows. Section 2 briefly presents the wave packets and the principal characteristics that appear in the tunnelling passage, i.e. transmission and reflection coefficients, modification of the spectra and so on. Some of the more important aspects of the resonant tunnelling are recalled. A specific development is then attributed to the reflected wave packet. Section 3 presents numerical estimations of the reflection and of the transmission of a quantal particle. Section 3.1 considers the case of a perfect resonance: narrow wave packets (in the reciprocal space) reveal the particular behaviour of the reflected wave packet; large wave packets lead to the introduction of two time scales. The filling of the quasi-bound state, and its practically independent emptying, are clearly delineated. Afterwards, the case of an asymmetric barrier is analysed. It reveals the typical negative value of the reflected phase time.

2. Formalism

2.1. Fourier transform of the wave packet

Let a one-dimensional quantum barrier be described by the potential $V(x)$ and be limited by the points a and b, $0 < a < b$, on the Ox axis. Also assume that the potentials V_L and V_R in the left part $x < a$ and in the right part $x > b$ of the Ox axis are constant. Let us then consider a wave packet moving towards the barrier in the positive direction of the Ox axis.

The time-independent Schrödinger equation is solved in searching for quantum states associated with each eigenstate of the Hamiltonian. More precisely, each stationary state is constituted by a linear superposition of the incoming and of the outgoing parts of plane waves $\mathrm{e}^{\pm\mathrm{i}kx}$. Incoming waves are scattered by the barrier and give rise to the corresponding reflected and transmitted plane waves.

The incident wave packet is coming from the left. It is constructed so that, at time $t = 0$, it is non-zero between two given points in the left-hand space and zero elsewhere. Such a wave packet is described by a linear superposition of plane waves, with positive or negative k_L (the entering wave vector k_L is simply denoted by k, $k > 0$; the corresponding value, for the same energy, in the right space is k_R). In the case of a real potential, the corresponding modes permitting the complete description of the initial wave packet are, for a given energy E,

$$L(x,k) = \mathrm{e}^{\mathrm{i}kx} + r^{>}(k)\,\mathrm{e}^{-\mathrm{i}kx} \qquad A(x) \qquad t^{>}(k)\,\mathrm{e}^{\mathrm{i}k_R x} \tag{1}$$

$$L^{*}(x,k) = \mathrm{e}^{-\mathrm{i}kx} + r^{>*}(k)\,\mathrm{e}^{\mathrm{i}kx} \qquad A^{*}(x,k) \qquad t^{>*}(k)\,\mathrm{e}^{-\mathrm{i}k_R x} \tag{2}$$

In equation (1), $r^{>}(k)$ and $t^{>}(k)$ are the reflection and transmission coefficients for this left mode respectively; they are complex quantities and their phases contain the phase increment due to the propagation of the wave throughout the barrier. The functions $A(x, k)$ are the 'barrier parts' of the eigenfunctions; they can be complicated functions linked by continuity conditions with the corresponding left and right parts of the modes. But in the case of a simple shaped potential, they cannot be written analytically.

The first term of the modes L^* corresponds to an incident plane wave e^{-ikx}, with amplitude 1, in the left x space. For the localization of the wave packet needing both of the two parts e^{ikx} and e^{-ikx}, these L^* modes do intervene in the Fourier transform of the incident packet. In the left and right semi-infinite spaces, the corresponding outgoing plane waves furnish the entire spectra of the reflected and the transmitted wave packets. However, it must be noted that in practice, with our incident wave packet having a significant averaged moment, it is possible in numerical calculations to limit its spectrum $\phi(k)$ to strictly positive values of k [9–11]. Moreover, one can choose the distribution $\phi(k)$ to be positive and having a simple shape.

With the above initial conditions, numerical calculations must show that, at time $t = 0$, the reflected and the transmitted wave packets have a null amplitude on their respective semi-infinite spaces. In the same way, at the beginning, the amplitude of the wavefunction inside the barrier must be zero. Numerically, this necessitates a sufficiently good description of the problem in the reciprocal space. For instance, this description ensures that an eventually great amplitude at the position x inside the barrier (for a specific E level in a resonant state) is cancelled by interferences with other near-resonant k states. In so doing, one does not have to consider another normalization condition than that of the incident packet in the left space.

So, let the incident wave packet be given at time $t = 0$; the time-dependent Schrödinger equation gives its behaviour for posterior times, along

$$\Psi(x,t) = \begin{cases} \dfrac{1}{\sqrt{2\pi}} \left\{ \displaystyle\int_{-\infty}^{\infty} \mathrm{d}k\, \phi(k)\, e^{i[kx - E(k)t/\hbar]} + \int_{-\infty}^{\infty} \mathrm{d}k\, \phi(k)\mathcal{R}_{ab}(k)\, e^{2ika}\, e^{-i[kx + E(k)t/\hbar]} \right\} \\ \qquad x \leqslant a \\ \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}k\, \phi(k) A(x,k)\, e^{-i[E(k)t/\hbar]} \qquad a \leqslant x \leqslant b \\ \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}k\, \phi(k)\mathcal{T}_{ab}(k)\, e^{ika - ik_R b}\, e^{i[k_R x - E(k)t/\hbar]} \qquad x \geqslant b. \end{cases} \tag{3}$$

It is important to note that in equation (3), as will be seen later, the total reflection and transmission coefficients $\mathcal{R}_{ab}$ and $\mathcal{T}_{ab}$ directly take into account the phase lag corresponding to the propagation through the barrier between a and b. So, once $\mathcal{R}_{ab}$ and $\mathcal{T}_{ab}$ are evaluated (this necessitates the calculation of the different $r^{>}$ and $t^{>}$, for each energy E) the problem is potentially solved.

There are many possibilities for obtaining a numerical estimation of the scattering of an entering wave with energy E. Apart from the simplest cases (rectangular or trapezoidal barriers, for example), the evaluation is possible only with approximated methods. In what follows, our results are obtained by using an iterative method based on a matrix treatment on stepwise discretization of the continuous potential $V(x)$. This gives in a few seconds the reflection and the transmission coefficients and the solution of the time-independent Schrödinger equation [12]. The solution of the time-dependent Schrödinger equation is then obtained with a simple discretization of the integral of equation (3).

2.2. Characteristics of resonant stationary states and of resonant packets

The behaviour of the wave packet around resonant states reveals spatial and temporal characteristics (the dynamics of the wave packet summit, for instance). The former can be obtained in analysing the spectrum of the reflected and the transmitted parts of the wave packet; the latter can be evaluated by using the stationary phase method. Both are compared with results obtained from direct numerical estimations.

Let us introduce

$$\mathcal{T}_{ab} = |\mathcal{T}_{ab}|\,\mathrm{e}^{\mathrm{i}\alpha} \qquad \mathcal{R}_{ab} = |\mathcal{R}_{ab}|\,\mathrm{e}^{\mathrm{i}\beta} \tag{4}$$

the modulus and the phases of the transmission and the reflection coefficients. In the more general case (we mean whatever may be the character, resonant or non-resonant, of the tunnelling) a sufficiently thin packet, in the k space, permits a limited development of the transmitted part around the peak k_0 of the packet as

$$\Psi_T(x,t) = \frac{1}{\sqrt{2\pi}}\mathcal{T}(k_0)\int_{-\infty}^{\infty}\mathrm{d}k\,\phi(k)\exp\left([k-k_0]\left(\frac{\mathrm{d}Ln|\mathcal{T}|}{\mathrm{d}k}\right)_{k_0}\right) \\ \times\exp\left(\mathrm{i}\left[k(a-b)+kx+(k-k_0)\left(\frac{\mathrm{d}\alpha}{\mathrm{d}k}\right)_{k_0} - Et/\hbar\right]\right). \tag{5}$$

The shape of the transmitted wave packet has two characteristics. Firstly, its spectrum is generally modified against the incident one which is centred on k_0. This can call for the introduction of a new wave vector k'_0 corresponding to the maximum of the transmitted spectrum. Secondly, for the wave vector k'_0, the stationary phase method permits us to determine the kinematics of the peak of the transmitted wave packet which goes out of the barrier (point b) at time t_b such that

$$t_b = \frac{m}{\hbar k'_0}\left[a + \left(\frac{\mathrm{d}\alpha}{\mathrm{d}k}\right)_{k'_0}\right]. \tag{6}$$

The transmitted phase delay $\Delta t_t^{\varphi}(a,b) = t_b - t_a$ is then obtained by considering the arrival time t_a of the peak of the incident packet at point a:

$$t_a = \frac{m}{\hbar k_0}a. \tag{7}$$

Let us emphasize that the phase delay $\Delta t_t^{\varphi}(a,b)$ contains one of the important subtleties presented at length in [13] concerning the variations of the mean value of the velocity $v(k)$ of the wave packet due to the transmission. Moreover, it is known [14] that these variations give sense to the imaginary part of the phase delay introduced by Pollack and Miller [15]. Actually, the stationary phase time appears to be a good candidate for defining transmission time in the case of a simple shaped wave packet [9, 10, 14]. However, as underlined in [2, 18], the phase times are not the only times that can be considered to express the traversal or the reflected times.

The reflected phase delay can be presented in the same way. However, its formulation is somehow more complicated. For the sake of simplicity, let us consider the case when the incident wave packet is centred on the resonant peak (wave vector K). Firstly, in the non-perfect resonance case (that of an asymmetric barrier) the spectrum of the reflected wave packet shows two maxima k' such that

$$k' \simeq K \pm \sqrt{\frac{\left(\frac{\partial^2|\mathcal{R}|}{\partial k^2}\right)_K\phi(K) + \left(\frac{\partial^2\phi}{\partial k^2}\right)_K|\mathcal{R}(K)|}{-\left(\frac{\partial^2|\mathcal{R}|}{\partial k^2}\right)_K\left(\frac{\partial^2\phi}{\partial k^2}\right)_K}} \tag{8}$$

which are real for sufficiently good resonance (which makes $|\mathcal{R}(K)|$ small and $(\frac{\partial^2|\mathcal{R}|}{\partial k^2})_K$ strong).

Secondly, in the case of a perfect resonance ($\mathcal{R}(K) = 0$), the most important characteristic concerns the phases; the variations of the coefficient around the value of the wave vector K are

$$\mathcal{R}(k) = |k - K| \left(\frac{\mathrm{d}|\mathcal{R}|}{\mathrm{d}k} \right)_K \exp\left(\mathrm{i} \left[\alpha + \mathrm{sign}(k - K) \frac{\pi}{2} \right] \right). \tag{9}$$

This last result leads to two specific characteristics of the reflected wave packet: first, a splitting of its spectrum into two parts and, second, a gap of π of its phase at resonance.

Apart from this particular behaviour around the perfect or nearly perfect resonance, the case of any reflected wave packet can be studied as done in the transmitted case (equation (5)). In the case of a very thin wave packet, it is possible to neglect the small difference between the reflected and the transmitted spectra versus the incident one. This leads to the usual phase delays,

$$\Delta t_t^{\varphi}(a, b) = \frac{1}{v(k)} \frac{\mathrm{d}\alpha}{\mathrm{d}k} = \hbar \frac{\mathrm{d}\alpha}{\mathrm{d}E} \qquad \Delta t_r^{\varphi}(a, a) = \frac{1}{v(k)} \frac{\mathrm{d}\beta}{\mathrm{d}k} = \hbar \frac{\mathrm{d}\beta}{\mathrm{d}E}. \tag{10}$$

In these expressions,

- the transmission delay $\Delta t_t^{\varphi}(a, b)$ is the difference between the instant of the exit of the peak of the transmitted wave packet at point b and that of the entrance of the incident one at point a.
- the reflection delay $\Delta t_r^{\varphi}(a, a)$ is the difference between the exit of the top of the reflected wave packet at the point a and the entrance of the incident one at point a (note that the reflected packet is then analysed as if the incident one were not present, in order to avoid interference effects between the incident and the reflected packets; in other words, as if interference effects in front of the barrier did not perturb the shape of the reflected packet [4]).

The time delays can be evaluated by calculating the phases $\alpha(E)$ and $\beta(E)$. Results can eventually be compared to other numerical results showing the behaviour of the peak. It is well known that for thin wave packets in the k space, numerical results agree with theoretical results, given by equations (10) [11, 16].

However, it was suggested [1, 9]—especially in the quantum electronics domain—that there are some cases when the stationary states introduce another natural time, namely the lifetime of quasi-bound states (QBS). Let us recall that such resonant states do not only appear in the cases of resonant tunnelling barriers. More generally, they also appear in the cases of simple barriers for states with energy corresponding to the ‘classical’ regime ($E > V$) (Ramsauer effect, for instance). Around these resonant states, the reflection and the transmission coefficients show rapid evolutions both of their modulus and of their phases. This implies a deformation of the initial shape of the packet and a rapid evolution of the phase time delays in relation to energy. Thus, an interesting problem is the links between the phase time delay and the lifetime of the QBS [1, 7–9]:

- In case of a thin resonance, the transmissivity curve $|\mathcal{T}_{ab}|^2$ appears to be locally Lorentzian; the half-height width of the curve then corresponds to the energy width, ΔE, of the QBS.
- The corresponding transmitted time delay curve $\Delta t_t^{\varphi}(b, a) = f(E)$ reveals the same characteristics.
- The calculated phase time, at resonance, is twice the lifetime of the QBS.
- At a perfect resonance, the reflection coefficient shows a gap of π. In the case of a symmetrical barrier, the phases of the reflection and the transmission coefficients differ by a $\pi/2$ term.

Another direct link can be noted between the transmissivity curve and the quasi-discrete levels contained in the barrier. Quasi-discrete levels reveal themselves by considering the complex energy domain [1, 8, 17]. It is well known that one can find discrete levels of a given bounded structure in looking for the poles of the reflection coefficient of an incoming plane wave (an infinite reflection coefficient being the sign of the presence of discrete levels [12]). In the present examples, there are no bounded states but quasi-discrete states which, if they are populated, can de-excitate by tunnelling, in the right or in the left space. A width ΔE of the quasi-discrete level [17] corresponds to such a de-excitation process. Its energy is

$$E = E_0 - \mathrm{i}\Delta E. \tag{11}$$

The components of the corresponding wave vector are complex: they are respectively $(k - \mathrm{i}k')$ in the right half-space and $(-k + \mathrm{i}k')$ in the left half-space (k and $k' > 0$). This corresponds to waves going out of the barrier in the two respective half-spaces [17] and equation (11) gives a decreasing presence probability in the barrier along

$$\mathrm{e}^{-2\Delta E t/\hbar}. \tag{12}$$

Let us add that there have only been a few comparisons between these theoretical times and the numerical results for a wave packet [9]. The conclusion that the phase time delay is the good one has sometimes been asserted. In contrast, the lifetime of the QBS has been considered for a long time as easily observable [7].

As for its temporal characteristics, the spatial shape of the outgoing packets can be analysed. In the case of a perfect resonance, the reflected part of the wave packet is often neglected and interest is thus focused on its transmitted part only. In the case of a well-defined QBS showing a thin transmissivity curve, the incident wave packet can spread sufficiently, in the energy space, to suffer the rapid variation of transmissivity. As seen above (equations (5) and (8)), this alters the transmitted spectrum (compared to the incident one). For some authors [3, 18], this fact has been the occasion of the rejection of the phase time delays as a pertinent quantity for defining the traversal time. However, as has often been underlined, the status of time in quantum mechanics can lead to different practical definitions associated with different experimental devices. In the present work, in which the behaviour of wave packets with simple shapes (with only one peak, for instance) is studied, the phase delay appears as a useful and measurable concept [14].

3. Applications

Let us consider the wave packet corresponding to a particle with a mass $m = 0.067$ electron mass [19], impinging on a resonant tunnelling double rectangular barrier constituted by a set of three potentials corresponding to an input and an output rectangular barrier, both having a width of 5 nm (for the symmetric case) and 0.230 eV height, separated by a homogeneous layer (width 5 nm) supposed to correspond to $V = V_L = V_R = 0$ eV (this set will be denoted simply by 5/5/5 nm). In this case, the scattering reveals the QBS associated with the quantum well. The variations of the width of the input or of the output barrier furnish an example of an asymmetric case.

The spectra of the packets are described with 200 values only; with our method, this small number in fact appears to be sufficient to get good results.

3.1. Symmetric barrier

3.1.1. Stationary aspects. For the double rectangular barrier, the analytical expression of the transmission coefficient (transmissivity and phase) is well known, and an easy analytical

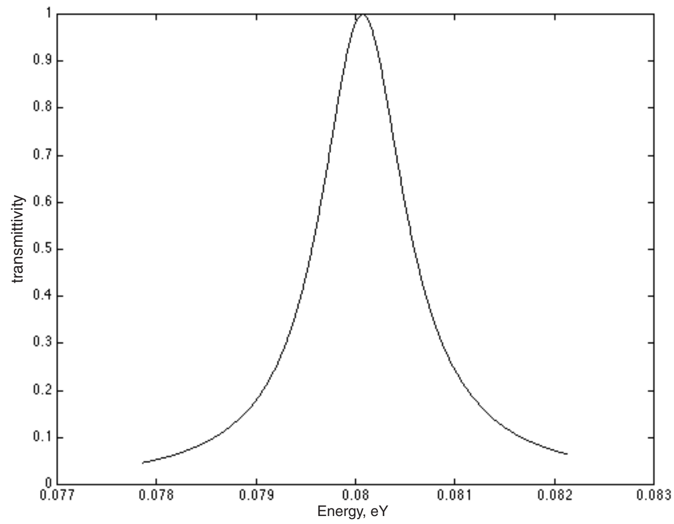

Figure 1. The transmissivity curve for the double barrier. It shows a thin peak at 0.080 64 eV associated with a QBS.

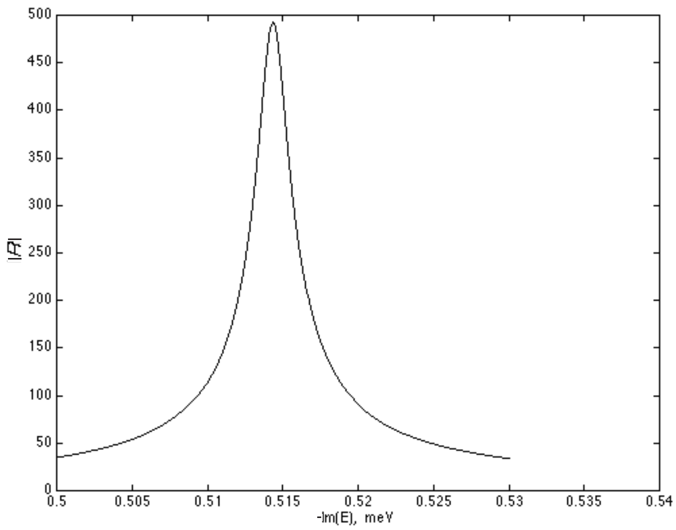

Figure 2. The generalized reflection coefficient curve for the complex energy value of the QBS.

calculus can reveal the Lorentzian response of the barrier (see, for instance, [9]). In the present case, this shape has been evaluated numerically from a scan on the height of the barrier (figure 1); for this barrier, there is only one tunnelling resonance, at 80.064 meV.

This result has been verified by using the generalized reflection coefficient $\mathcal{R}$ for the double barrier, around the tunnelling peak of figure 1. By scanning the complex energy domain from $E = 80.064 - 0.500\text{i}$ meV to $E = 80.064 - 0.530\text{i}$ meV, we obtain a thin peak (figure 2) corresponding to the exact energy width of the level as deduced from the transmissivity curve (figure 1). Denoting by $2\Delta E$ the resonance width at half-height, the two approaches (figures 1 and 2) in fact give exactly the same result $\Delta E = 0.515$ meV leading to

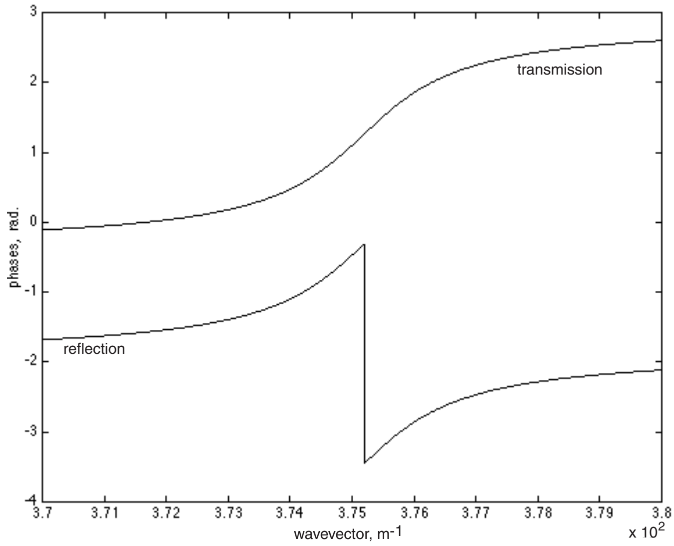

Figure 3. The phase curves of the reflection and transmission coefficients for the symmetrical double barrier: the phase delay can be obtained from the derivative with respect to the energy; the value of the level width can be verified by measuring the width of the corresponding Lorentzian curve at half its height.

the value $\tau = 6.34 \times 10^{-13}$ s for the lifetime. However, as underlined by several authors [1, 9], this time is not a tunnelling time but a time associated with the discrete level.

For a complete description of the characteristics of outgoing wave packets (amplitudes and phases), the phase curves (figure 3) for states subtending the packet are necessary. The phase delay at resonance is deduced from equation (10). We find 12.68×10^{-13} s; this value exactly corresponds to twice that of the lifetime [8, 9]. Let us underline here that, apart from the exact resonance wave vector analysed in the following section (cf equation (9)), the reflected and the transmitted phase times are equal, due to the symmetry of the barrier.

3.1.2. Dynamical aspects. As underlined earlier, two different kinds of behaviour are awaited according to the width Δk of the k-spectrum of the incident wave packet (which is supposed to include the energy resonance). Let us then consider two different Gaussian packets (corresponding to two different spatial widths Δx) defined according to equation (3), the peaks of which are at $x = 0$ at time $t = 0$. The first packet is a thin wave packet (in the k space); it is contained in the Lorentzian transmissivity peak of the barrier. In contrast, the second one is wide and contains the transmissivity peak (note that we consider the case of wave packets with spectra centred on the resonance only; also note that we use here a Gaussian wave packet for the sake of simplicity (cf equation (5)).

Figure 4 shows the probability density for finding the particle 33 ps after the top of the wave packet was at position 0, at time 0, in the case of a narrow wave packet ($\Delta k = 0.566 \times 10^6\ \mathrm{m}^{-1}$) centred at the resonance $k_0 = 3.752 \times 10^8\ \mathrm{m}^{-1}$. The non-perturbed incident wave packet is also shown in the figure in order to clearly illustrate the transmitted time (the direct evaluation of $\Delta t_t^{\varphi}(a, b)$ is not possible because of interferences in the front of the barrier destroying the peak of the impinging packet). According to the advance of the free packet on the actual top, an evaluation of the time delay gives, approximately, 11.2×10^{-13} s. That result can be compared with the value of the phase delay (12.68×10^{-13} s; actually, one can easily obtain this phase delay with a thinner packet).

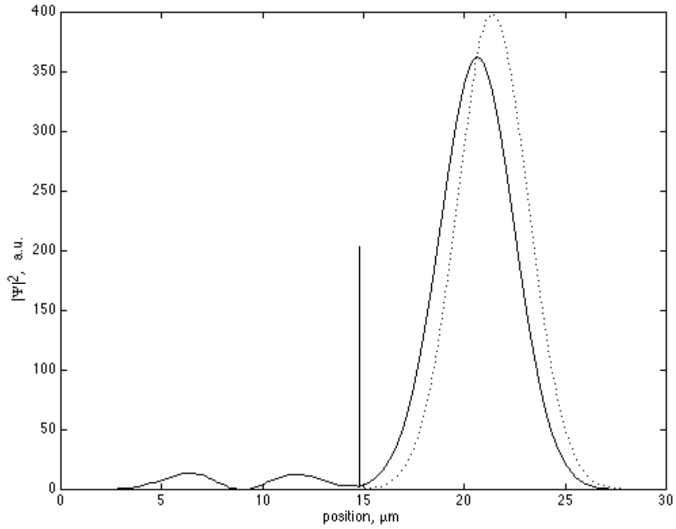

Figure 4. The probability density of finding the particle at some intermediate instant. Being thin in the k space, the wave packet is very large in x space: the double barrier is just in the centre of the window. The transmitted part, approximately Gaussian, has fallen behind the packet that would have gone in the absence of the barrier. The reflected part shows the double-hump shape which is characteristic of reflectivity curves at resonance.

Another striking characteristic appears if one considers the reflected wave packet. In the nearly perfect resonance, the reflected wave packet presents two humps which can be understood taking into account the phase gap of π occurring at resonance. The reflected wave packet is obtained from the reflection of the two symmetrical parts of its spectrum (that above and that below the resonance). Because of their phase gap, these two parts of the spectrum give nearly totally destructive interference. So, although it could appear that the reflection gives two different reflected packets [9], there is actually only one, the 'peak' of which has been destructed leading thus to a minimum. It can be noted that the kinematics of this 'peak' is perfectly symmetrical to that of the summit of the transmitted wave packet.

Figure 5 shows the evolution of the probability density of finding the particle in the central part of the resonant barrier versus time, as revealed in the previous figure. In the case corresponding to that of a wave packet narrower than the energy level of the QBS, this level is progressively filled and emptied by the Gaussian incident wave packet, the sign of which appears in the parabolic shape of the logarithm of the probability density. In practice, the wave packet sustains a global delay. At very great times, one can observe a modification towards linear behaviour; in this semi-logarithmic representation, this reveals the free emptying of the QBS, lightly populated with the thin packet—this is the principal characteristic of the case of a wide packet.

Let us now consider the case of a wide incident wave packet (in the k space), $\Delta k = 0.566 \times 10^7\,\mathrm{m}^{-1}$ centred on the resonance $k_0 = 3.752 \times 10^8\,\mathrm{m}^{-1}$, and wider than the Lorentzian transmissivity peak of the barrier. The study of this new case follows that of the previous one, some of its characteristics being similar. However, the kinematics of the peak of the transmitted wave packet and that of the reflected one shows typical behaviour. Comparison with the kinematics of the free wave packet gives approximately 5.1×10^{-13} s for the transmission or for the reflection time (figure 6). This value can be compared with that of the theoretical phase time: in the present case, the transmitted wave packet is characterized

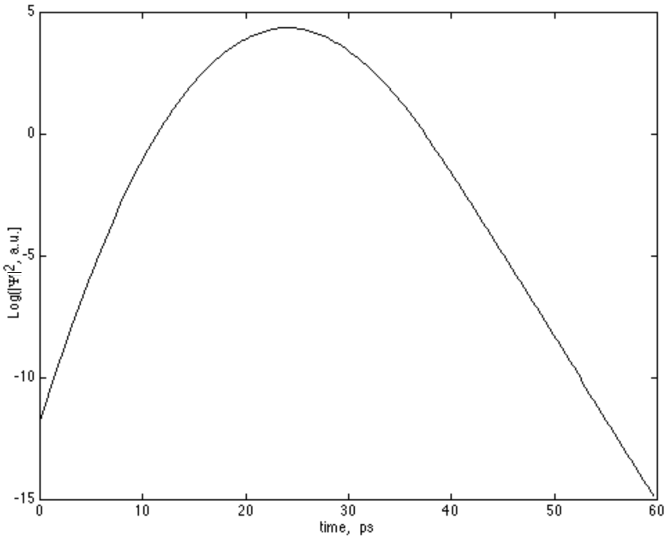

Figure 5. The probability density for finding the particle inside the barrier, versus time. The parabolic shape (in this logarithmic representation) reflects the Gaussian shape of the incident wave packet: at the beginning, the quantum well empties itself at the same time as it fills up; after that, the QBS reveals itself by the exponential decreasing.

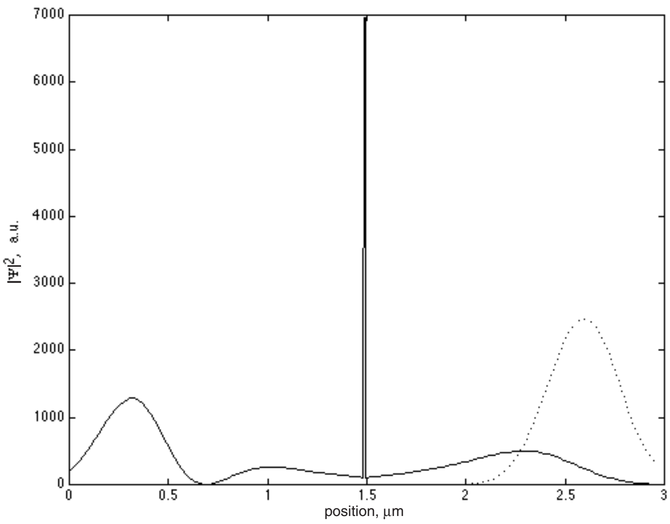

Figure 6. The probability density for finding the particle during emptying of the QBS. The peak of the transmitted packet is out of the barrier, the interference node of the reflected packet is in a symmetrical position to the transmitted peak. The long exponential (right and left) tails are characteristic of the QBS alone, the incident wave packet is rapidly forgotten.

by a Lorentzian spectrum centred on the resonant wave vector for which the phase delay is maximum. However, the transmitted spectrum includes wave vectors for which the phase delay is well below the resonance one. The delay for the summit of the wave packet must rather be compared to the phase time corresponding to half of the transmissivity curve, that is 6.4×10^{-13} s.

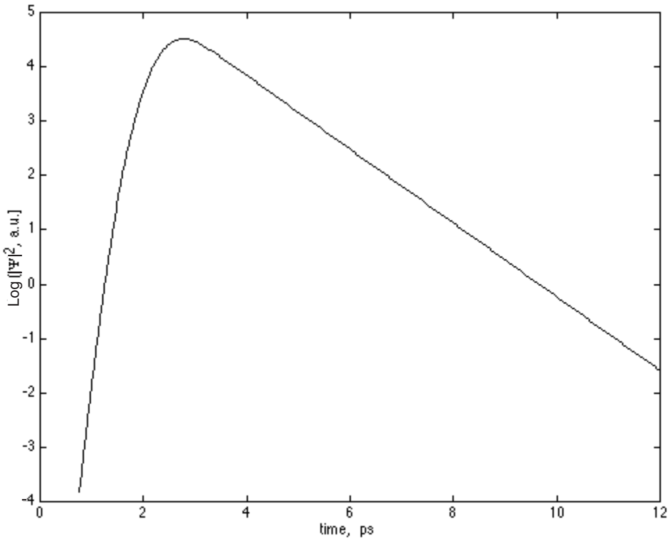

Figure 7. The probability density for finding the particle in the barrier reveals the filling and the emptying of the QBS. In this logarithmic representation, the linear part leads to a direct evaluation of the lifetime of the level.

Figure 6 illustrates the packet at the instant 40×10^{-13} s (the incident wave packet is supposed to be at point $x = 0$ at time $t = 0$). Let us underline that the wider, in the k space, the incident packet, the more important the reflected one, the smaller the two-hump phenomenon. More exactly, the important upper and lower parts of the spectrum correspond to stationary states with high reflectivity and small phase delays so that one can say that the *front* of the reflected wave packet is principally constituted from these wave vectors. Let us note, however, that there is only one reflected packet with a complicated spectrum. A last characteristic observed in that case (wide packet) appears while studying the filling of the QBS. Figure 7 shows a curve mixing the parabolic behaviour of the filling with a linear behaviour (see equation (12)) corresponding to the emptying of the QBS. After approximately 35×10^{-13} s, the incident wave packet which has filled the QBS has gone; the QBS then empties itself, giving the left (reflected) and right (transmitted) exponential waves appearing in figure 6, equation (11). On this linear part, one rediscovers the lifetime of the QBS. This corresponds to the long tails of the reflected and the transmitted packets, the shapes of which are independent of that of the incident wave packet.

3.2. Asymmetric barrier

Asymmetry is obtained by choosing the input rectangular barrier wider (or thinner) than the output one. For instance, figures 8 and 9 correspond to the 4.5/5/5 nm and 5/5/4.5 nm sets for the double rectangular barrier. The reflection and the transmission coefficients are calculated for values of the k-spectrum giving a fine description of the non-perfect transmissivity peak. A thin wave packet is then built so as to underline the principal characteristics of the response; as above, we consider the case of a wave packet ($k_0 = 3.7513 \times 10^8\ \mathrm{m}^{-1}$, $\Delta k = 0.566 \times 10^6\ \mathrm{m}^{-1}$) centred on the resonance (the small lowering of the resonance compared to the previous case is due to the more important coupling of the QBS with the left or right space).

Figure 8 gives the phase delays as obtained from equation (10). Around the resonance, the asymmetric barrier reveals the different behaviour of the reflection and the transmission for

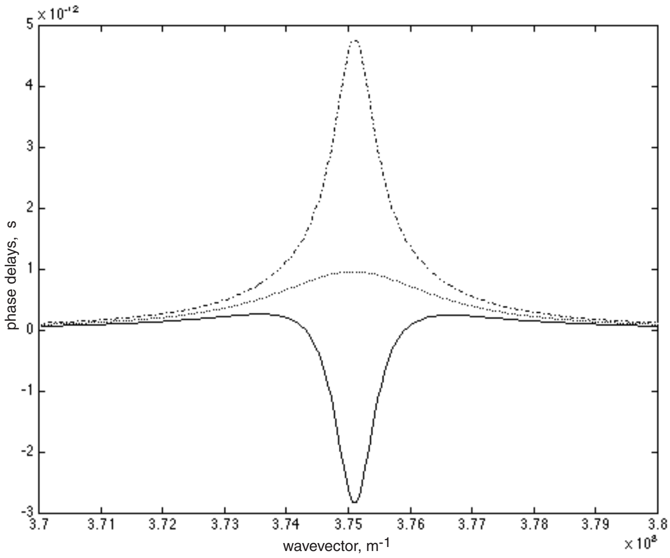

Figure 8. The phase delays for the asymmetric barrier. A 5 nm width for the input barrier and a 4.5 nm width for the output barrier give a negative reflected phase delay (plain curve) at the resonance. In the reversal case (dashed-dotted lines), one obtains a positive value. The dotted curve gives the transmitted phase delay which is identical in the two cases. At the perfect resonance limit, the three curves are identical, apart from an infinite value $\pm\infty$ for the resonant wave vector.

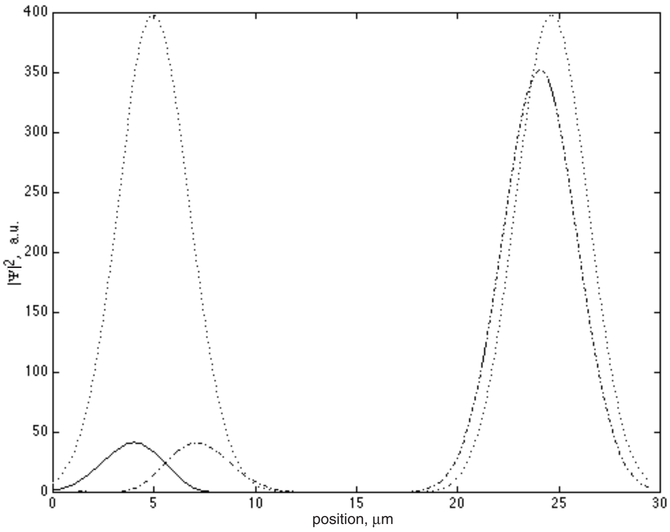

Figure 9. The reflected and the transmitted wave packets in the case of an asymmetric barrier. The wider the input barrier, the more in advance the reflected packet (compare the plain curve obtained in the case of a wider barrier to the dashed-dotted curve obtained in the case of a thinner barrier); the dotted curves show the 'perfectly' reflected packet (on the left) and the perfectly transmitted packet (on the right).

the reversal of the barrier geometry. It is well known that the transmission is insensitive to the reversal, in contrast to the reflection which then offers a negative (for the 5/5/4.5 geometry) or a positive (4.5/5/5) phase delay. This result is given in figure 9 (showing the probability densities for finding the particle) in the two cases at time 38×10^{-12} s.

It must be underlined that, even when the spectrum, equation (8), shows two maxima, in the first instants after scattering, the wave packet shows one prominent maximum in the position space.

The principal characteristic of this case (corresponding to a negative time delay) is obviously the advance of the reflected packet versus the reflected one that would be associated with a perfect reflection (for instance a reflection on an infinite high potential step) such that $\Delta t^{\varphi}_{r\infty}(a, a) = 0$. One could say that the wave packet is reflecting before its arrival on the barrier. This is in some way similar to the well-known Hartman effect leading to the *appearance* of a supraluminal velocity associated with the passage of the peak of the transmitted wave packet through a wide purely tunnelling barrier [16].

When the difference of the two barrier widths (that of the incoming and that of the outgoing barriers) is made smaller and smaller in order to tend towards the perfect symmetrical case, we find both a thinner and thinner width for the negative and the positive peaks of the reflected phase delays, and a consolidation of the remaining parts of the curves with that of the transmitted one. At the limit of perfect resonance, the resonant-reflected component is an infinitely advanced, or retarded, component with zero amplitude.

4. Discussion and conclusion

Let us begin with some remarks about our numerical estimations. Our iterative method is based on a discretization of the potential $V(x)$ as a stepwise homogeneous multilayer. In the limit of the calculating power of the software, the calculation is exact in what concerns stationary states. In particular, in the frame of the potential discretization, the choice of the points x where the wavefunction is evaluated does not matter. In the present study, we are principally interested in the behaviour of wave packets outside the barrier, so we have only considered one point in each layer constituting the double rectangular barrier. The transfer matrix method is known to be numerically stable; the only problem in the calculations would appear when the energy of a stationary state is equal to the height of the barrier.

For stationary states, some of our results have been compared with direct results associated with analytically simple expressions corresponding to the double rectangular barrier. Some others, concerning the behaviour of the wave packet, have been compared with the results that can be obtained with the finite difference methods [9]; they are in perfect agreement with them at this stage. So, although some of our results are known, our presentation, which does not use finite difference methods, presents the advantage of permitting us to discuss all the different aspects of tunnelling through potential barriers in the same mathematical language. On the other hand, the iterative method that we use gives access to the study of potential barriers of any shape.

The time-dependent solutions are obtained from a discretized basis of different stationary states. This permits rapid calculations for different packet shapes. When studying resonant states, one must consider a careful description of the transmissivity peak, ensuring that the probability of finding the particle is zero inside the barrier for the initial wave packet. In our examples, that probability density at time $t = 0$ in the barrier is about 10^{-6}, in the arbitrary units of figures 4, 6 and 9, for a 200 basis.

The case of the negative reflected delays does not offer any problem at this stage of the interpretation. As for the Hartman effect, one can show that the amplitude of the reflected wavefunction is always smaller, at any *advanced* position, than that corresponding to the packet which would be perfectly reflected at point a.

On the other hand, the 'camel form' of the reflected wave packet appearing in the case of perfect tunnelling (that has been noted in [9]) can be clearly understood from our presentation. Because of the phase shift of π at resonance (figure 3), the lower and the higher momentum parts of the wave packet interfere destructively and so induce a hollow between the two humps. It is interesting to note that the dynamics of that hollow is quite symmetrical to that of the summit of the transmitted part of the wave packet. This is the sign of the identity of the transmitted and the reflected phase delay for a symmetrical barrier. Let us underline that, in the first instants after scattering, the splitting of the spectrum into two parts is not the reason for the appearance of two tops on the wave packet shape; actually, the splitting will introduce separated packets, in the position space, only at very great times.

Another interesting result of that work deals with the filling and the emptying of quasi-bound states (QBS). As expected, for incident wave packets with tightened spectrum, compared with that of the QBS, the transmitted packet keeps its initial shape globally and the QBS only appears via the great phase delay and via the transmissivity. In contrast, for wide (in the k-space) packets the QBS is totally filled giving rise to an exponential decrease in its occupation; the shape of the transmitted packet is then characteristic of the QBS, rather than of the incident wave packet.

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