Universal Journal of Physics and Application 2(3): 193-199, 2014
DOI: 10.13189/ujpa.2014.020308 http://www.hrpub.org

Dynamics of Wave Packets Generated at a Finite Distance from a Scattering Step

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Abstract The scattering process of wave packets is often described recovering the simple monochromatic scheme supposing that the particle comes from $-\infty$ with a sharp momentum distribution, thus allowing for approximations usually used in common calculations of physical quantities involved in the process. In this work, we study the scattering process of a Gaussian wave packet impinging on the step potential, finding out that its dynamics depends on the initial conditions of the incident particle, and in particular on the wave packet origin x_0. We propose a semi-classical approximated model to describe the dynamics of the scattering wave packet, also defining a characteristic time interval t_{f} as the time required for the formation of transmitted packet beyond the step. Through a comparison with the numerical solution of the Schrödinger equation, our model explains the t_{f} as a function of the origin x_0 and spread of the incident wave packet in coordinate space, giving rise to such a dependence for a finite distance scattering processes.

Keywords Scattering, Tunneling Time, Wave Packet Dynamics, Step Potential

1 Introduction

The recent developments of nanotechnology and the advent of modern high-speed high-density MOS devices, have revived the technological and theoretical interest of the scientific community in the tunneling problem, since they require extremely short channel lengths for improving performance and decreasing size. The development of ultrascaled nanometric CMOS compatible single electron transistors (SETs) and single atom trasistors [1, 2] has lead, together with sequential tunneling of single/few electrons regime, the emergence of density of states graining and fluctuations in the contacts [3, 4]. Confinement effects in the contacts may determine discretization of energy levels, charge localization at intradopant length scale, valley orbital splitting [5], and selection rules on quantum states in tunnelling. Consequently, the understanding of dependence of tunneling across a barrier from the position constitutes a relevant aspect in view of Beyond CMOS and More Moore technology developments.

The large relevance of such quantum effects on micro devices has also revived the theoretic interest in the well known problem of the tunneling time, i.e. the time spent by the particle to tunnel through the barrier [6, 7, 8, 9, 10, 11, 12, 13, 14, 15], insomuch as numerous works were published on this subject over the last ten years [16, 17, 18, 19]. Surprisingly, no answer to such a question has been definitively accepted yet despite the fact that a variety of definitions of tunneling time have been proposed. We emphasise that, in most of these approaches, while the particle is described as a wave packet, its energy is assumed to be an assigned value so that its dispersion, which may play a fundamental role in several dynamical situations, is completely ignored.

In this work we point out that, in real cases, only a wave packet approach can adequately describe the dynamics of a particle. In fact, the stationary plane wave picture, usually adopted as an approximated scheme for standard analysis of such problems, intrinsically neglects the initial conditions of the wave packet in terms of its origin $x(0)$ and spread $\sigma_x(0)$, which conversely play, as we will show, an important role in such an analysis. First, we concentrate our attention on the dynamics of a Gaussian wave packet (GWP) scattering on a step potential. Through a numerical solution of the Schrödinger equation we analyse the evolution of the system calculating the transmission of the scattering GWP as a function of the initial $\sigma_x(0)$ and $x(0)$ conditions, and comparing simulated data with theoretical results.

Further important issue about scattering emerges by the numerical analysis on the probability of the system to cross the barrier as a function of time t, which seems to be neglected by literature to the best of our knowledge. Namely, how much time after the scattering event the wave packet spends to reach the asymptotic regime, in which the particle has achieved its asymptotic probability to be observed beyond the barrier. Of course, since the support of a Gaussian is not compact, the interactions with the potential are ever-present and, in principle, this time is not finite. However, for all practical purposes, we define a finite time which accounts, within the confident limits, for a fixed amount (namely 0.99) of the normalized probability of the transmitted wave

packet. We name this time interval the *formation time* t_f. Numerical results show that t_f strongly depends on x_0. To analytically express such a dependence, we propose a semi-classical approximated model in which t_f is described as the time spent by a finite support (accounting for the 0.99 of the probability) of the incident wave packet to cross the barrier, namely the time required to locate, in coordinate space, the greatest amount of the GWP's probability distribution beyond the barrier interface. This could be a relevant aspect, mainly in solid state physics, in those phenomena, of large conceptual and practical interest, which are characterized by incoming particles generated by scattering centres at a finite and randomly distributed distance from surface.

2 Materials and Methods

2.1 Quantum Scattering

Without loss in generality, we limit for simplicity a one dimensional (1D) step potential, located in x_B in coordinate space and with an height V_B. The interaction of a particle in a box with a potential barrier is generally achieved by describing the particle in terms of monochromatic waves [20, 21, 22, 23, 24, 25]. However, we note that there are a variety of phenomena, mainly in solid state physics, in which the incoming particles are generated by scattering centres at a *finite* distance from the potential barrier. We refer, for example, to the following scenarios: the passage of hot electrons from the channel to the floating gate, in non-volatile memories, during the writing cycle; the Fowler–Nordheim tunneling of trapped electrons during the erase of the information stored in floating gate; the filtering of hot electrons by defects, in thermoelectricity. In the above contexts, it is especially interesting to observe that the entire treatment of the problem of scattering at the surface, in terms of energy eigenstate, is manifestly difficult and any description of such phenomena in terms of stationary plane waves is inadequate. On the other hand, they are easily framed in the wave packet description, simply assuming that the scattering centers generating the wave packet are localized. If these centres are of atomic nature, the maximum information one can provide on the origin of the particle is a distribution of atomic size (say 0.2–0.4 nm), whereas if they are attributed to lattice imperfections the particle is localized with an uncertainty typically of the order of 5 nm. For the above phenomena, the spread resulting from the localization condition is not negligible with respect to the mean free path (for electrons in solids $\lambda \approx 10$ nm)—that renders especially difficult the disentanglement of phenomena due to the initial wave packet spread and mean free path.

More generally, the description of a particle in a non-stationary state as a wave packet (usually a GWP) has striking advantages. *First* of all, the wave packet description provides a detailed knowledge of the wave function evolution approaching the step potential, and it is able to provide a measure of the time required to form the escaping and backscattered wave functions as a function of particle dynamical properties (mean kinetic energy, energy dispersion) and of its original position and space dispersion. *Second*, while the description in terms of stationary waves can be applied to physically interesting problems only for potentials subject to very restrictive conditions, the use of GWP can be applied to potentials which vary even in a non-monotonic way with x. In the last case, the major difficulties come from the fact that a wave packet, initially Gaussian, remains so only for quadratic, linear, or constant potentials and that, in general, a non-Gaussian packet does not preserve the norm [26]. *Third*, the use of GWP allows an easy interpretation in semi-classical terms. Just like the free motion of a classical particle with momentum p is frictionless occurring with velocity v, given by $v = p/m$, the free motion of the GWP with mean wave number $\langle k \rangle$ is frictionless and occurs with a group velocity v_g given by $v_g = \hbar\langle k \rangle/m$ (the classical velocity). In extreme synthesis, the above behaviours can be summarized as follows:

$$\begin{aligned} \langle x(t) \rangle &= x_0 + \hbar k_0 t/m \\ \sigma_x^2(t) &= \sigma_x^2(0) + \frac{\hbar^2 t^2}{4m^2\sigma_x^2(0)} \\ \langle k(t) \rangle &= k_0 \\ \sigma_k(t) &= \hbar/2\sigma_x(0) \end{aligned} \tag{1}$$

where $\langle x(t) \rangle$ and $\langle k(t) \rangle$ are the expectation values of position and momentum, x_0 and k_0 are their values at initial time ($x_0 = \langle x(0) \rangle$ and $k_0 = \langle k(0) \rangle$), and $\sigma_x(t)$ and $\sigma_k(t)$ denote the space and momentum dispersion of the GWP.

Despite the fact that wave packet approach offers the above advantages, some of the aspects connected with the wave packet dynamics remain controversial. We refers, for example, to the dependence of the phase and delay time on the distance between the wave packet origin x_0 and the barrier , or the acceleration of the transmitted wave packet by an opaque potential barrier [6, 12]. Moreover, within the context of the non-stationary scheme, two problems seem physically interesting. First of all, the description of the evolution of the original GWP into two non-overlapping wave packets, as a function of the initial position, and in particular the characteristic time spent by the system to reach the above condition. As we will see in the next session, we define it, within some approximations, as the *formation time* t_f. Second, the relation between such a time and the underlying energetics (energy and energy dispersion) of the impinging particle and of the newly formed particles. For these kind of problems, literature is mainly focused on the potential barrier (rather than on the step) looking at estimating the *tunneling time*, i.e. the time spent by the particle to tunnel through the barrier [16, 17, 18, 19]. We stress that in most of these approaches while the particle is imagined as a wave packet, it is assumed to be in an assigned energy value so that its dispersion is totally ignored.

In the next sections, we will concentrate our attention on the above two problems, proposing a semi-classical model, to study the dynamics of the wave packet impinging a potential step and comparing it with numerical results. As we will see, our approach picks out the relevance of the energy spread and of the initial condition x_0 on the behaviour of the system. Manifestly, these quantities are not considered in any treatment of

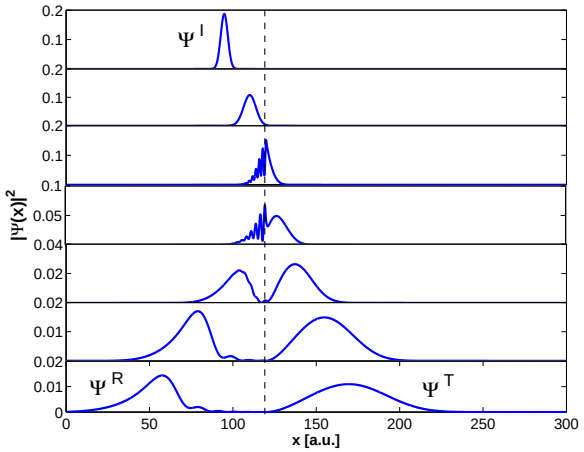

Figure 1. Picture of the scattering of a GWP provided by our code, with: $k_0 = 1.54$ a.u., $x_{\rm B} = 120$ a.u. and $V_{\rm B} = 1$ a.u.

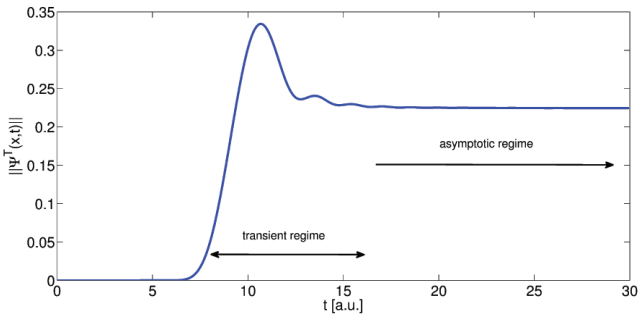

Figure 2. The norm $||\Psi^{\rm T}(x,t)||$ of a transmitted GWP as a function of time, and with the following initial conditions: $\Delta x = 70$ a.u. ($\Delta x = x_{\rm B} - x_0$), $k_0 = 1.28$ a.u., $\sigma_x(0) = 2$ a.u., $V_{\rm B} = 1$ a.u. The transient regime and the asymptotic one are showed

the problem where the particle is initially in an energy eigenstate.

2.2 The Formation time

On the basis of the axioms of quantum mechanics, for assigned mean energy, the asymptotic value of the transmission and reflection probability of a particle (described by the wave function $\Psi(x,t)$) are provided by the following equations:

$$\begin{array}{rcl} \overline{T} & = & \lim_{t\to+\infty} \int_{x>x_{\rm B}} |\Psi(x,t)|^2 {\rm d}x. \\ \overline{R} & = & \lim_{t\to-\infty} \int_{x<x_{\rm B}} |\Psi(x,t)|^2 {\rm d}x. \end{array} \quad (2)$$

In the case of a GWP, to recover from the equations (2) the usual definitions of T and R (see the analogous treatment for square barrier case in [6, 8]), in terms of transmission and reflection coefficient as functions of initial momentum, it is sufficient to rewrite the whole wave function $\Psi(x,t)$ in the Fourier space as a linear combination of the appropriate normalized energy eigenfunctions $\psi_k(x)$ for the step potential, parametrized by momentum k. Let's consider, for $\psi_k(x)$, the following expression in terms of *incident*, *reflected* and *transmitted* components:

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} \left(\psi_k^{\rm I} + r\psi_k^{\rm R} + t\psi_k^{\rm T}\right) \quad (3)$$

with:

$$\begin{array}{rcll} \psi_k^{\rm I}(x) & = & e^{ikx}\Theta(x_{\rm B}-x) & \textit{incident w.f.} \\ \psi_k^{\rm R}(x) & = & e^{-ikx}\Theta(x_{\rm B}-x) & \textit{reflected w.f.} \\ \psi_k^{\rm T}(x) & = & e^{ik'x}\Theta(x-x_{\rm B}) & \textit{transmitted w.f.} \end{array} \quad (4)$$

where $k'^2 = k^2 - 2mV_{\rm B}/\hbar^2$, r and t represents respectively the the plane wave reflection and transmission coefficients for step potential and are given by the following equations:

$$\begin{array}{rcl} t & = & \frac{2\sqrt{k}\sqrt{k'}}{k+k'} \\ r & = & \frac{k-k'}{k+k'} \end{array} \quad (5)$$

Here, we are assuming that only eigenstates with energy eigenvalues $E > V_{\rm B}$ will be present in the Fourier decomposition of the incident packet and hence we exclude those $\psi_k(x)$ with imaginary k'. Now the GWP $\Psi(x,t)$ can be expanded as:

$$\Psi(x,t) = \int \psi_k(x)\phi(k,t){\rm d}k \quad (6)$$

where $\phi(k,t)$ is the Fourier transform of the GWP in the momentum space, which has the following analytic form:

$$\phi(k,t) = (\sigma_0^2/\pi)^{1/4} e^{-(k-k_0)^2\sigma_0^2/2} e^{kx_0} e^{-iE(k)t/\hbar} \quad (7)$$

Substituting eq.(3) and eq.(7) in eq.(6), the wave function $\Psi(x,t)$ can be represented as the following expansion:

$$\begin{array}{rcl} \Psi(x,t) & = & (\sigma_0^2/4\pi^3)^{1/4} \int e^{-(k-k_0)^2\sigma_0^2/2} e^{kx_0} e^{-iE(k)t/\hbar} \times \\ & \times & (\psi_k^{\rm I}(x) + r\psi_k^{\rm R}(x) + t\psi_k^{\rm T}(x)){\rm d}k \end{array} \quad (8)$$

Aside from the square modulus of eq.(8), the application of eq.(2) requires the limit for t approaching $+\infty$. In such a limit the incident term vanishes and, after some algebra, the usual relations for T and R are recovered:

$$\begin{array}{rcl} \overline{T} & = & \int t^2 |\phi(k,0)|^2 {\rm d}k. \\ \overline{R} & = & \int r^2 |\phi(k,0)|^2 {\rm d}k. \end{array} \quad (9)$$

As a consequence of eq.(9), the above T and R quantities are independent of the initial position x_0 of the incident GWP and they depend only on the initial GWP momentum distribution, whose modulus is constant on time. Rather, an inspection of Figure 3 shows immediately that, within the confidence limits, the time spent to reach the asymptotic value $\overline{T}$ increases with the separation of the initial position from the step. The same result can be showed for the reflected probability $\overline{R}$.

Here, we will just define the time interval spent by the system to reach $\overline{T}$, which we call *formation time* $t_{\rm f}$, relating it to the dynamical variables of the incident GWP.

Due to the non-compactness of the Gaussian functions, strictly, the scattering process of a GWP through a barrier starts once the GWP is present and ends in the limit of time t approaching infinity. However, the evolution of the system can be characterized by two different dynamical regimes (see Fig.2) introducing the approximations, clarified in the following paragraph.

Far from the potential, the front of the incident GWP weakly interacts with the barrier. For all practical purpose, the GWP moves towards the barrier as a free

packet. Once the interaction between the front of the GWP and the potential become relevant, the system starts to bifurcate in opposite directions, forming transmitted and reflected wave packets (see Fig.1), with one or multiple peaks, as suggested in [27]. We call this time instant $t_{\rm in}$. For $t > t_{\rm in}$, the system enters in a transient regime dominated by the superposition of the incoming and reflected waves, in the $x < x_{\rm B}$ zone, and by the oscillating distribution probability in the $x > x_{\rm B}$ zone. On the other hand, after the tail of the incident GWP has arrived to the barrier, oscillations decrease with increasing time and, after a sufficient long time, the transmitted and reflected probability distributions approach a limit value, corresponding to the theoretical values expressed by eqs.(2) (see Fig.2). Strictly, the demixing process is complete only in the limit of time t approaching infinity, where the system could be considered decoupled in transmitted and reflected free packets with non-overlapping supports. However, also in this case, we can consider a finite time limit $t_{\rm out}$ such that, for $t > t_{\rm out}$, the system enters into an asymptotic regime, characterized by the two resulting GWPs escaping as free packets from the barrier and assuming definitively their constant distributions and probabilities in momentum space. Finally, we define the characteristic formation time as the interval $t_{\rm f} = t_{\rm out} - t_{\rm in}$. Let's concentrate our attention on the GWP of the transmitted particle. Determining the interval $t_{\rm f}$ requires finding the two time limits $(t_{\rm in}, t_{\rm out})$ of the scattering region. Within the confident limits, they respectively represent the time step in which the front of the incident GWP impinges the potential step, yielding a non zero transmitted probability, and the time step in which the transmitted GWP approaches the $\overline{T}$ value. Thus, $t_{\rm in}$ and $t_{\rm out}$ can be operatively determined assigning a confidence accuracy $\epsilon_{\rm r}$ (hereafter we use a value $\epsilon = 10^{-2}$) while $t_{\rm f}$ can be deduced calculating the time interval spent by the norm $||\Psi^{\rm T}(x,t)||$ to pass from $\epsilon_{\rm r}$ to the value $||\Psi^{\rm T}_{\rm out}||$ - $\epsilon_{\rm r}$ (Fig. 2). By definitions, it follows that:

$$\begin{aligned} ||\Psi^{\rm T}(x,t_{\rm in})|| &= \epsilon_{\rm r} \\ ||\Psi^{\rm T}(x,t_{\rm out})|| &= T - \epsilon_{\rm r} \\ t_{\rm f} &= t_{\rm out} - t_{\rm in} \end{aligned} \tag{10}$$

In such a way we have defined the characteristic time $t_{\rm f}$ as the time required to a fixed amount (namely 0.99) of the normalized probability of the transmitted wave packet to be observed beyond the step barrier. Moreover, the $t_{\rm f}$ values are directly accessible by our simulations. From now on, we concentrate our attention on the description of the formation time in terms of the dynamical parameters of the system.

2.3 The model

In this section, we propose a model to analytically describe the formation time $t_{\rm f}$ as a function of initial conditions x_0 and $\sigma_x(0)$. First we note that $t_{\rm f}$, should be not shorter then the time required to the system to demix in two different reflected and transmitted components, even though having overlapping support. On the basis of the definitions from the previous section, this demixing process starts when the front of the incident GWP impinges the step interface and it terminates once

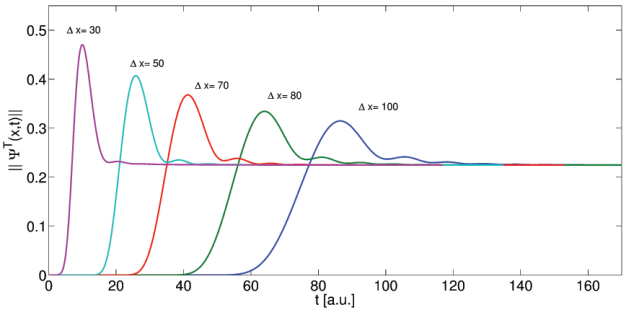

Figure 3. The norm $||\Psi^{\rm T}(x,t)||$, with $k_0 = 1.28$ a.u., $\sigma_x(0) = 2$ a.u., and $V_{\rm B} = 1$ a.u. for different initial wave packet centers ($\Delta x = 30, 50, 70, 100$ a.u.)

the tail of the GWP arrives on the step. We call this time interval the *crossing time* $t_\times$. It can be seen simply as the time required to the incident GWP support to cross the coordinate $x_{\rm B}$ at the step interface. Of course, since the support of a Gaussian is not compact we must define it via some operative criterion, summarized in a parameter γ, defining the number of dispersions putatively forming the support of the GWP. To compute $t_{\rm f}$, we first consider a semi-classical model for the evolution of a free expanding GWP in the absence of the step potential $V(x)$. First, by the use of eqs.(1), we deduce an expression for $t_\times$ in terms of initial conditions x_0, k_0 and $\sigma_x(0)$. Then to account for the corrections, due to the interaction with the potential, we compare $t_\times$ with the real values of $t_{\rm f}$ obtained by simulations of the system in the presence of the potential $V(x)$. In this way we obtain an analytical expression explaining real $t_{\rm f}$ data, as a function of initial conditions and fitting parameters.

Consider a free GWP originated in x_0 and with momentum k_0, moving towards the coordinate position $x_{\rm B}$, first in absence of the potential $V_{\rm B}$. To calculate the time spent by the GWP to completely cross the $x_{\rm B}$ we must take into account that its motion is the combination of both the motion of its center of mass and the motion of the two fronts of the packet. Let us define $t_{\rm a}$ and $t_{\rm b}$ respectively as the maximum time value for which the support, in coordinate space, is still totally included in the region $x < x_{\rm B}$, and at the minimum time step for which the finite support is already totally located in in the $x > x_{\rm B}$ zone, (Fig.4). Consistently with the definition given for $t_\times$, we obtain:

$$\begin{aligned} \langle x(t_{\rm a})\rangle &= x_{\rm B} + \gamma\sigma(t_{\rm a})/2 \\ \langle x(t_{\rm b})\rangle &= x_{\rm B} - \gamma\sigma(t_{\rm b})/2 \end{aligned} \tag{11}$$

Hence, $t_\times = t_{\rm b} - t_{\rm a}$. In the case of a free wave packet the relations (1) still hold. On the other hand, in the range of parameters in which we run, the following condition is satisfied:

$$k_0 \ll \frac{(\langle x(t)\rangle - x_0)}{2\sigma_x^2(0)} \tag{12}$$

which, by the use of the first of (1), reads:

$$\sigma_x^2(0) \ll \frac{\hbar^2 t^2}{4m^2\sigma_x^2(0)} \tag{13}$$

In such a regime, we can approximate the second of the equations (1) with the following:

$$\sigma_x(t) = \frac{\hbar t}{2m\sigma_x(0)} \tag{14}$$

Actually we can write an equation for $t_\times$ only in terms of initial parameters, by resolving the system composed by the first of (1) and (14) calculated in $t \equiv t_a$, and the first of (11). As a solution we obtain:

$$t_{\rm a} = \frac{4m\sigma_x(0)}{\hbar(4k_0\sigma_x(0) - \gamma)}(x_{\rm B} - x_0) \qquad (15)$$

In a likely manner, by simultaneously solving the first of (1) and (14) calculated in $t \equiv t_b$, and the second of (11):

$$t_{\rm b} = \frac{4m\sigma_x(0)}{\hbar(4k_0\sigma_x(0) + \gamma)}(x_{\rm B} - x_0) \qquad (16)$$

Subtracting (15) from (16), we obtain the crossing time $t_\times$ as a function of initial position x_0:

$$t_\times = \frac{8m\gamma\sigma_x(0)}{\hbar(16k_0^2\sigma_x^2(0)_0 - \gamma^2)}(x_{\rm B} - x_0) \qquad (17)$$

Figure 5 compares $t_{\rm f}$ and $t_\times$ as a function of x_0 for different values of k_0. Both quantities show a linear dependence increasing with the separation of the origin of the incident GWP from the step.

Since $t_\times$ is the crossing time in the case of free GWP, as expected, it is settled below $t_{\rm f}$ at a fixed k_0 and the difference between $t_\times$ and $t_{\rm f}$ seems to be constant, within the confidence, also on varying k_0. Now, to get a model for $t_{\rm f}$ including the effects of the interaction, we describe the difference between the two quantities introducing a term t^*. This term takes into account the deviations from the free GWP due to the presence of the potential and we relate it to an additional dependence of the demixing process on the initial conditions x_0, k_0 and $\sigma_x(0)$, namely

$$t_{\rm f} \quad = \quad t_\times + t^* \qquad (18)$$

A fitting procedure is required to evaluate the free parameters γ and t^*. Recalling that we supposed the origin x_0 was the leading parameters in determining $t_{\rm f}$, through the spread $\sigma_x(t)$ in the scattering region, here we assume a linear fitting functions both for γ and t^* on x_0, with α and β as fitting parameters.

$$\begin{aligned} t^* &= t^*(x_0, \alpha, \beta) \\ \gamma &= \gamma(x_0, \alpha', \beta') \end{aligned} \qquad (19)$$

Equations (18) and (19) define the semi-classical linear model only in terms of initial parameters and the fitting parameters α, β and α', β':

$$t_{\rm f} = t_\times(x_0, k_0, \sigma_x(0), \gamma(x_0, \alpha', \beta')) + t^*(x_0, \alpha, \beta) \qquad (20)$$

After performing a set of simulations to evaluate $t_{\rm f}$, through the definition (10), we compare the results with data provided by the model (20). For initial values x_0, k_0 and $\sigma_x(0)$ in the range considered, we obtain the values $\alpha = -2.422$, $\beta = 411.632$ and $\alpha' = -0.004$, $\beta' = 19.895$, as fitting parameters. Figure 6 plots both simulated and expected $t_{\rm f}$ values, as a function on x_0 and at different k_0 and with fixed $\sigma_x(0) = 2$ a.u. Actually, the formation time given in eq.(20) results to be different from $t_{\rm f}$ in eq.(10): this could be ascribed to the influence of the initial conditions on wave packets with large momentum spread [30] The value of γ seems to depend slightly on

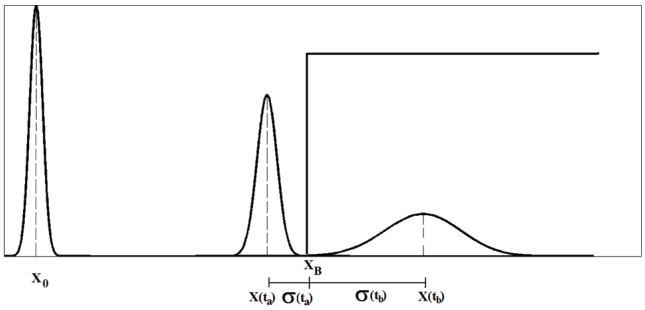

Figure 4. Evolution of a GWP, originally centered in x_0, passing from incoming time $t_{\rm a}$ to outgoing time $t_{\rm b}$

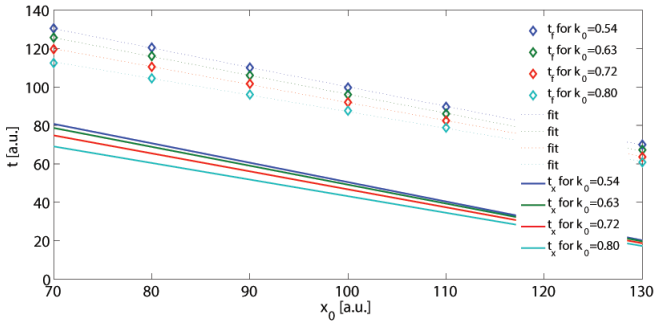

Figure 5. Comparison between $t_{\rm f}$ and $t_\times$ as a function of x_0 for initial values $k_0 = 0.54, 0.63, 0.72, 0.80$ a.u.,$V_{\rm B} = 0.2$ a.u. and $x_{\rm B} = 150$ a.u. is The family of diamonds are the data from simulations by the use of (10); dotted lines are the correspondent regression curves; the full lines are the data obtained by (17).

x_0, and it is appreciably different from the free values ($\gamma = 6\sigma_x(0)$). This is due to the variations caused by the presence of the potential.

The above equations establish a connection between $t_{\rm f}$ and initial parameters of the system. Results show a relevant dependence of the dynamics of the wave packet on the origin x_0. In particular $t_{\rm f}$, i.e. the interval time needed to make accessible the outgoing wave packets for experimental measurements, is strongly dependent on the origin and increases with the separation from the barrier ($\Delta x = x_{\rm B} - x_0$). At the same time, due to the norm conservation, the maximum value of the probability density, as a function on time, decreases with x_0.

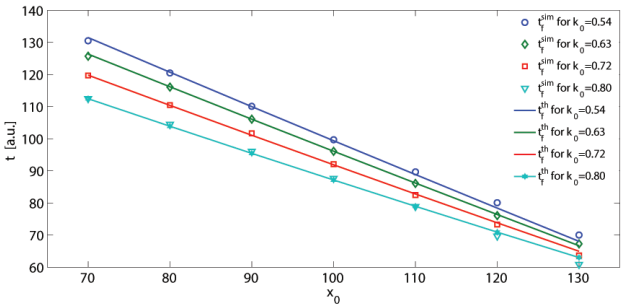

Figure 6. Comparison between $t_{\rm f}$, as a function of x_0 for initial values $k_0 = 0.54, 0.63, 0.72, 0.80$ a.u., $V_{\rm B} = 0.2$ a.u. and $x_{\rm B} = 150$ a.u, obtained by the use of (10) (diamonds) and by (19) (full lines).

3 Conclusions

Usually, mainly for practical purposes, the description of the scattering event is provided in terms of monochromatic waves instead of a wave packet, relaxing the description assuming that the particle energy E is well defined around its mean value. There are however a number of situations that are characterized by the fact that the incoming particles are generated at a finite distance from randomly distributed scattering centres and with an energy spread that is comparable to the potential height, so they cannot be reduced to a monochromatic waves scheme. In this scenario, the initial conditions x_0 and $\sigma_x(0)$ can assume a relevant role in the description of the dynamics of the system. However describing the system in terms of Gaussian wave packet requires resolving numerically the Schrödinger equation. Hence, through the numerical solution, we analyse the evolution of the Gaussian wave packet, calculating the transmission of the scattering Gaussian wave packet as a function of x_0, $\sigma_x(0)$ and k_0,and comparing simulated data with theoretical results. We introduce a time interval, which we call formation time t_{f}, as the time required to a fixed amount (0.99) of the normalized probability of the transmitted wave packet to reach the asymptotic regime after scattering. A numerical analysis of the probability of the system to cross the barrier as a function of t shows that the the formation time t_{f} strongly depends on the GWP x_0 and increases with the separation from the barrier. At the same time, due to the norm conservation, the charge density decreases with x_0. In the range of parameters studied, data suggest a linear behaviour of t_{f} on x_0, supporting the comparison with the model (17) proposed for a free Gaussian. To study such dependence we propose a semi-analytical model for t_{f} decomposing it in two terms, linearly dependent on x_0: one describing the transit of a free GWP across the discontinuity point at the step, and the other one, describing the residual dependence both on x_0 and k_0 and explaining the deviation from linearity due to the interaction with the barrier. Results show a good match between simulations and data coming from the model, confirming it could be considered a useful tool to obtain informations on the time required to observe the particle beyond the step, at least in the range of initial parameters typically adopted in condensed matter. Such a dependence of the charge density on the coordinate x_0 could be an important issue in those system in which scattering event occur within the nanoscopic scale and the conduction mechanism of the scattered particles involves charge interactions with instabilities usually lying at the barrier interface.

Acknowledgements

The first author (F. Carone Fabiani) is most grateful to Guido Montagna, Oreste Nicrosini and Lucio Andreani for very helpful comments in the final stages of this work, and Enrico Prati for useful discussions about technological aspects.

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