Eur. Phys. J. C (2008) 56: 545–556
DOI 10.1140/epjc/s10052-008-0669-4

THE EUROPEAN PHYSICAL JOURNAL C

Regular Article - Theoretical Physics

Principle of stationary phase for propagating wave packets in the unidimensional scattering problem

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Received: 22 February 2007 / Published online: 5 August 2008

Abstract We point out some incompatibilities which appear when one applies the stationary phase method for deriving phase times to obtain the spatial localization of wave packets scattered by a unidimensional potential barrier. We concentrate on the above barrier diffusion problem where the wave packet collision implies the possibility of multiple reflected and transmitted wave packets, which, depending on the boundary conditions, can overlap or stand in relative separation in space. We demonstrate that the indiscriminate use of the method for such a particular configuration leads to paradoxical results for which the correct interpretation, confirmed by analytical/numerical calculations, imposes the necessity of the appearance of multiple peaks as a consequence of multiple reflections by the barrier steps.

PACS 02.30.Mv · 03.65.-w

1 Introduction

The analytical methods employed for describing the collision of a particle of mass m with a square (rectangular) potential barrier have been widely discussed in the context of (one dimensional) scattering phenomena [1–3]. In this extensively explored scenario, the stationary phase method (SPM) is the simplest and the most common approximation tool utilized for this aim. First introduced in physics by Stokes and Kelvin [4, 5], the principle of stationary phase to describe the spatial localization of a wave packet is well established, and it was employed by Sommerfeld and Brillouin in their early studies of wave propagation and group velocity [6]. The method has in time become a standard tool for several theoretical applications [7–10] adopted not only by physicists but also by biologists, economists etc. It can also be used in a statistical sense, such that the most likely events tend to be associated with slowly varying phase variation in the frequency domain, and unlikely events tend to be associated with a rapidly varying phase with frequency. The SPM basically provides an approximate value for the maximum of an integral by means of an analytical procedure which enables us to understand several subtleties of interesting quantum phenomena, such as tunneling [1, 11, 12], resonances [13], incidence–reflection and incidence–transmission interferences [2] as well as the Hartman effect [14–17] for tunneling phenomena. It is also commonly quoted in the context of testing the formalism of one-particle scattering for temporal quantities such as arrival, dwell and delay times [1, 3] and the asymptotic behavior at long times [17, 18].

In this manuscript we identify some limitations on the use of the SPM for obtaining the right position of a propagating wave packet subject to a very simple and common potential configuration. The limitations are not concerned with the domain of the method, i.e. with the mathematical basis and the analytical applicability of the method; they are focused on the indiscriminate application of the method to time-dependent scattering problems and, in particular, to deriving phase times. The time-dependent scattering of a wave packet by a potential barrier in the linear Schroedinger equation is interesting because it reconciles two types of wave theories. Those interested in linear theory often look at stationary (frequency-domain) solutions of a single frequency, whereas those interested in nonlinear theory usually look at time-dependent pulses. To implement an accurate analysis with the SPM, we work with the hypothesis of adding up the Fourier modes from the stationary solution to observe the evolution of a linear wave packet on collision with an obstacle.

Considering the conditions for the applicability of the SPM in the context of the problems here presented we concentrate in the investigation on the nonrelativistic scattering of an incoming single wave packet with energy spectrum

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localized totally above the potential barrier. We are particularly interested in obtaining an analytical description of the potential barrier scattering problem by pointing out some interpretive problems which inadequately exhibit the non-conservation of probability during the collision process. In this context, to clarify the analytical aspects which determine the choice of the methods applied to physical problems, in particular, by using the mathematical structure for constructing the *steepest descent* method (SDM), in Sect. 2 we discuss the general applicability of the SPM in the wave packet propagation problem. In Sect. 3 we introduce an analytical description of the above barrier diffusion problem where we recover the solution for the apparent physical inconsistency which is concerned with the non-conservation of probability during the collision process. By returning to a wave packet multiple peak decomposition [19], we can decompose the original colliding wave packet into *multiple* reflected and transmitted components by means of which the conservation of probabilities is recovered during the scattering process. The analytic expressions for all the reflected, transmitted, and intermediary components are obtained and the validity of them is discussed by means of an illustrative comparison between the analytic approximation and the exact numerical results. We draw our conclusions in Sect. 4, where we notice that an accurate quantification of some evident analytical incongruities can be extended to the study of a tunneling particle where, circumstantially depending on the scattering configuration, the use of the SPM deserves a careful analysis before being applied.

2 The stationary phase method

In analyzing mathematical problems in physics, one often finds it desirable to know the behavior of a function for large values of some parameter s, that is, the asymptotic behavior of the function. Specific examples are furnished by the well-known Gamma function and various Bessel functions [20]. All these analytic functions are defined by integrals:

$$I(s)=\int_C \mathrm{d}z\, H(z,s) \tag{1}$$

where H is analytic in z and depends on a real parameter s. In most cases of physical interest the integrals like $I(s)$ can be redefined in terms of

$$H(z,s)=h(z)\exp\bigl[sf(z)\bigr], \tag{2}$$

which leads to the explicit resolution of $I(s)$, for large values of s, by an asymptotic approximation procedure named the steepest descent method (SDM). The key idea in this method is that as s grows very large, the main contribution to the integral will come from values of z very close to the points at which $\mathrm{d}f(z)/\mathrm{d}z=0$. Irrespective of the nature of the particular function, for some paths of integration along which the imaginary part of $f(z)$ is constant, these points are called *saddle-points*, because they are the points where the real and imaginary parts of $f(z)$ are stationary with respect to the position in the complex plane (x,y) without being an absolute maximum or minimum. In fact, if we have $f(z)=u(x,y)+\mathrm{i}v(x,y)$, we can easily show from Cauchy–Riemann relations that along any path $v(x,y)=$ constant the rate of change of $u(x,y)$ can only vanish at a saddle-point [20]. From any point, the direction in which $u(x,y)$ decreases most rapidly is one along which $v(x,y)$ is constant, and in this sense such paths are paths of steepest descent. Perhaps the commonest situation where the SDM is applicable is that in which the path of integration $v(x,y)=$ constant runs from a saddle-point z_s to infinity, with $u(x,y)$ decreasing monotonically all the way. In a simplified analysis, the function $f(z)$ can be expanded around z_s into a Taylor expansion. If we replace $f(z)$ with the first two terms of this expansion in the exponential of (2),

$$f(z)\approx f(z_s)-\mu^2(z), \tag{3}$$

with

$$\mu(z)=\sqrt{-\frac{f''(z_s)}{2}}(z-z_s),$$

and extend the limits of integration from $-\infty$ to $+\infty$, we find

$$I(s)=-\sqrt{2}f''(z_s)\exp\bigl[sf(z_s)\bigr] \times\int_{-\infty}^{+\infty}\mathrm{d}\mu\, h\bigl(z(\mu)\bigr)\exp\bigl[-s\mu^2(z)\bigr]. \tag{4}$$

In extensions of this method complex analysis is used to find a contour of steepest descent for an equivalent integral expressed as a path integral. To get the first term in the asymptotic expansion of (4) the value of $\mu(z)h(z)/f'(z)$ at $z=z_s$ is required. Provided $f''(z_s)$ is not zero and $h(z_s)$ is not infinite, the integral $I(s)$ results:

$$I(s)=\sqrt{-\frac{2\pi}{sf''(z_s)}}h(z_s)\exp\bigl[sf(z_s)\bigr], \tag{5}$$

which, however, is *not* completely free of some particular supplementary conditions for its applicability [20]. An alternative, and very similar, method to the SDM is the stationary phase method (SPM). Though perhaps less general and less immediately convincing analytically, it often has the advantage of closer contact with the physical problem. The integral to be considered is more suitably written as

$$I(s)=\int_C \mathrm{d}z\, h(z)\exp\bigl[\mathrm{i}sf(z)\bigr], \tag{6}$$

where, in practice, the exponential commonly represents a traveling wave. The SPM was first introduced explicitly by Kelvin [4, 5]. A rigorous mathematical treatment, which would justify the statements made above, was subsequently given by Watson [21] and a complete discussion involving the asymptotic approximation was done given by Focke [22]. The deductions from the SPM follow much the same pattern as those from the SDM. The assumed paths of integration are $v(x, y) =$ constant, which means that the amplitude part of the exponential is constant along the path, while the phase part varies most rapidly, a reversal of the situation in the SDM. For asymptotic values of s the rapid oscillations of $sf(z)$ over most of the range of integration means that the integrand averages to almost zero. Exceptions to this cancellation rule occur only when the stationary phase condition is satisfied, i.e. the only significant contribution to the integral arises from portions of the path in the vicinity of the saddle-points or end-points, but the physical interpretation of the mechanism by which this comes about is now in terms of phase interference rather than amplitude decay. Thus, the approximation corresponding to (5) for the SDM is

$$I(s) = \sqrt{-\frac{2\pi}{sf''(z_s)}}h(z_s)\exp\left[-\frac{i\pi}{4}\right]\exp\left[isf(z_s)\right] \tag{7}$$

for the SPM. But one aspect in which there is some distinction between the methods should be noted. With a steepest descent path which starts at a saddle-point and does not go to infinity, the contribution of the point at the end of the path to the strict asymptotic expansion is zero in comparison with the saddle-point contribution by virtue of the extra exponential factor it contains. On the other hand, with a stationary phase path of the same type, the contribution of the point at the end of the path is, in general, of the order of that of the saddle-point merely divided by $\sqrt{s}$; it is excluded, therefore, from the asymptotic approximation only if the first term of the asymptotic expansion alone is retained. To sum up, the methods of steepest descent and stationary phase, stripped off of their mathematical expression, depend on choosing a path of integration in such a way that the integrand, due to its exponential factor, contributes irrelevantly to the integral except in the vicinity of certain saddle-points (or end-points).

To illustrate the applicability of the SPM to a physical problem it should be instructive to assume an equivalence between the complex variable, z, and a real one, k, so that the integral which represents a free quantum particle propagation can be identified by the wave packet solution of the unidimensional Schroedinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x,t), \tag{8}$$

with $V(x) = 0$, described in terms of the integral,

$$\psi(x,t) = \int_{-\infty}^{+\infty}\frac{dk}{\sqrt{2\pi}}G(k,k_0) \times \exp\left[-i\left(E(k)t + kx - kx_0\right)\right], \tag{9}$$

where we have set $\hbar = 1$, and the dispersion relation is $E(k) = k^2/(2m)$. The function $G(k, k_0)$ physically represents a narrow momentum distribution centered around the momentum k_0, and (9) can be identified as the integral of (6) by simply rewriting $G(k, k_0)$ as $\sqrt{2\pi}h(z)$ and $sf(z)$ as the phase $i(kx - kx_0 - Et)$ in an extension to the complex plane $(k \to z)$.

The integral (9) can therefore be estimated by finding the value for which the phase has a vanishing derivative, evaluating (approximately) the integral in the neighborhood of this point. The movement of the peak coordinate of the wave packet $\psi(x, t)$ can be obtained by imposing the stationary phase condition

$$\frac{d}{dk}\left[Et - k(x - x_0)\right]\bigg|_{k=k_s} = 0 \quad \Rightarrow \quad x_{\max} = x_0 + \frac{k_s}{m}t, \tag{10}$$

when $k_s = k_0$, the maximum of $G(k, k_0)$. This means that the peak of the wave packet propagates with a velocity $v = \frac{k_0}{m}$. In fact, we ratify this result when we explicitly calculate the integral of (9) by introducing a *Gaussian* momentum distribution given by

$$G(k,k_0) = g(k-k_0) = \left(\frac{a^2}{2\pi}\right)^{\frac{1}{4}}\exp\left[-\frac{a^2(k-k_0)^2}{4}\right]. \tag{11}$$

In this case, the result of the integration (9) gives

$$\psi(x,t) = \varphi[x - x_0, t], \tag{12}$$

where

$$\varphi[x,t] = \left[\frac{\pi a^2}{2}\left(1 + \frac{4t^2}{m^2a^4}\right)\right]^{-\frac{1}{4}} \times \exp\left[-\frac{(x - \frac{k_0}{m}t)^2}{a^2(1 + \frac{2it}{ma^2})} - \frac{i}{2}\arctan\left(\frac{2t}{ma^2}\right) + i(k_0x - E_0t)\right], \tag{13}$$

which evidently confirms the result of (10).

Meanwhile, the method leads to some new interpretive discussion when the momentum distribution becomes a complex function, i.e. when $G(k, k_0)$ can be written as $|G(k, k_0)|\exp[i\lambda(k)]$. In this case, the stationary phase condition for a free wave packet represented by (10) will be modified by the presence of an additional phase $\lambda(k)$. By assuming that $\lambda(k)$ can be expanded in the neighborhood of k_0, i.e.

$$\lambda(k) \approx \lambda(k_0) + (k-k_0)\left.\frac{\mathrm{d}\lambda(k)}{\mathrm{d}k}\right|_{k=k_0}, \tag{14}$$

the new stationary phase condition can hereby lead to

$$x_{\max} = x_0 - \left.\frac{\mathrm{d}\lambda(k)}{\mathrm{d}k}\right|_{k=k_0} + \frac{k_0}{m}t. \tag{15}$$

This can be interpreted as a space-time translation. As is commonly presented in textbooks on quantum mechanics [23], one may be convinced that one is justified to take the stationary phase condition as a necessary and *sufficient* statement for applying the method. Nevertheless, although it can be used to predict the most likely outcome of an experiment, even when it is related to the applicability of the stationary phase principle, it does not exclude the possibility of alternative outcomes. It is well known both SDM and SPM are applicable only if certain conditions apply. As we shall demonstrate in the following section, the results of the SPM, when applied to the unidimensional scattering problem, depend critically upon the manipulation of the generic amplitude $G(k,k_0)$ prior to the application of the method.

3 Scattering problem with energy above potential barrier

To elucidate some of the questions on the ambiguities which appear when we utilize the SPM, let us study the scattering of an incoming wave packet by a potential barrier for propagating energies larger than the barrier upper limit V_0. The stationary wave solution of the Schroedinger equation (8)[1] obtained when we consider the potential barrier described by

$$\begin{aligned} &0 \quad \text{if } x<0 \quad \text{region I},\\ &V_0 \quad \text{if } 0<x<L \quad \text{region II},\\ &0 \quad \text{if } x>L \quad \text{region III} \end{aligned} \tag{16}$$

can be decomposed into different wave functions for each interval of x, i.e.

$$\Phi(k,x) = \underbrace{\phi_{\mathrm{I}}(k,x)}_{\phi_{\mathrm{Inc}}(k,x)+\phi_R(k,x)} + \underbrace{\phi_{\mathrm{II}}(k,x)}_{\phi_\alpha(k,x)+\phi_\beta(k,x)} + \underbrace{\phi_{\mathrm{III}}(k,x)}_{\phi_T(k,x)}, \tag{17}$$

where

$$\begin{aligned} \phi_{\mathrm{Inc}}(k,x) &= \exp[\mathrm{i}kx],\\ \phi_R(k,x) &= R(k)\exp[-\mathrm{i}kx],\\ \phi_\alpha(k,x) &= \alpha(k)\exp[\mathrm{i}qx],\\ \phi_\beta(k,x) &= \beta(k)\exp[-\mathrm{i}qx],\\ \phi_T(k,x) &= T(k)\exp[\mathrm{i}kx], \end{aligned} \tag{18}$$

with $q=(k^2-w^2)^{\frac{1}{2}}$ and $w=\sqrt{2mV_0}$. By solving the constraint equations [23] which set the continuity conditions at $x=0$ and $x=L$, we obtain

$$\begin{aligned} \alpha(k) &= \left[\frac{k(k+q)}{\mathcal{F}(k)}\right]\exp\bigl[\mathrm{i}\Theta(k)-\mathrm{i}qL\bigr],\\ \beta(k) &= -\left[\frac{k(k-q)}{\mathcal{F}(k)}\right]\exp\bigl[\mathrm{i}\Theta(k)+\mathrm{i}qL\bigr],\\ R(k) &= -\mathrm{i}\left[\frac{k^2-q^2}{\mathcal{F}(k)}\right]\sin[qL]\exp\bigl[\mathrm{i}\Theta(k)\bigr],\\ T(k) &= \left[\frac{2kq}{\mathcal{F}(k)}\right]\exp\bigl[\mathrm{i}\Theta(k)-\mathrm{i}kL\bigr], \end{aligned} \tag{19}$$

where

$$\mathcal{F}(k) = \left\{4k^2q^2\cos^2[qL] + \left(k^2+q^2\right)^2\sin^2[qL]\right\}^{\frac{1}{2}} \tag{20}$$

and

$$\Theta(k) = \arctan\left\{\frac{k^2+q^2}{2kq}\tan[qL]\right\}. \tag{21}$$

The explicit expression for the corresponding propagating wave packets can be obtained by solving integrals like

$$\psi_f(x,t) = \int_w^{+\infty}\frac{\mathrm{d}k}{\sqrt{2\pi}}g(k-k_0)\phi_f(k,x)\exp[-\mathrm{i}Et], \tag{22}$$

with $f\equiv\alpha,\beta,R,T$. As a first approximation, which is commonly used in quantum mechanics textbooks [23], we obtain the analytical formulas to these integrals by assuming that the momentum distribution $g(k-k_0)$ is sufficiently sharply peaked around the maximum point k_0, with $k_0>w$. In this case, the integration can be extended from $[w,\infty]$ to $[-\infty,\infty]$ without modifying the final result. However, a careful investigation of $\Theta(k)$ in (21) would clearly indicate that the above integral is not dominated by the exponential for certain values of k_0/w (see Fig. 1, where we describe the derivative of $\Theta(k)$ as a function of k_0/w). In the sense we are investigating, as we shall demonstrate in the following, it is *erroneously* assumed that the k-dependent phase terms $\Theta(k)$ and $q\equiv q(k)$ can be approximated by a

[1] The same analysis can be applied to relativistic wave equations, for instance, to the Klein–Gordon and Maxwell equations.

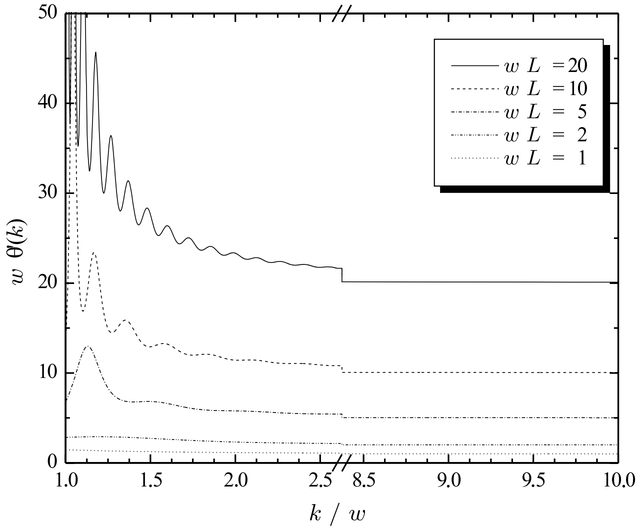

Fig. 1 The phase derivative $\Theta'(k)$ dependence on k/w. $\Theta'(k)$ does not present adequate analytical behavior (smoothness) for the applicability of the SPM when k approximates w since the phase derivative oscillates too rapidly (the phase is not stationary). The method can be accurately applied for larger values of k/w when the phase is really stationary

series expansion around $k = k_0$ up to the first order term, i.e.

$$\Theta(k) \approx \Theta(k_0) + (k-k_0)\Theta'(k_0) \quad \text{and}$$
$$q \approx q_0 + (k-k_0)\left.\frac{\mathrm{d}q}{\mathrm{d}k}\right|_{k=k_0}, \tag{23}$$

where

$$\Theta'(k) = \frac{2m}{q}\left[\frac{(k^2+q^2)k^2qL - (k^2-q^2)^2\sin[qL]\cos[qL]}{4k^2q^2 + (k^2-q^2)^2\sin^2[qL]}\right]$$

and

$$\left.\frac{\mathrm{d}q}{\mathrm{d}k}\right|_{k=k_0} = \frac{k_0}{q_0}.$$

At the same time, when k is approximated by k_0, it is assumed that the modulating amplitude $|\phi_f(k_0,x)|$ can be put out of the integral, giving the following results:

$$\psi_{\mathrm{Inc}}(x,t) \approx \varphi[x - x_0, t],$$
$$\psi_R(x,t) \approx R(k_0)\int_{-\infty}^{+\infty}\frac{\mathrm{d}k}{\sqrt{2\pi}}g(k-k_0) \times \exp\bigl[-\mathrm{i}Et - \mathrm{i}k(x+x_0) + \mathrm{i}(k-k_0)\Theta'(k_0)\bigr]$$
$$= R(k_0)\exp\bigl[-\mathrm{i}k_0\Theta'(k_0)\bigr] \times \varphi\bigl[-x - x_0 + \Theta'(k_0), t\bigr],$$
$$\psi_\alpha(x,t) \approx \alpha(k_0)\int_{-\infty}^{+\infty}\frac{\mathrm{d}k}{\sqrt{2\pi}}g(k-k_0) \times \exp\left[-\mathrm{i}(Et + kx_0 - q_0x) + \mathrm{i}(k-k_0)\left(\frac{k_0}{q_0}(x-L) + \Theta'(k_0)\right)\right]$$
$$= \alpha(k_0)\exp\left[\mathrm{i}q_0x - \mathrm{i}\frac{k_0^2}{q_0}(x-L) - \mathrm{i}k_0\Theta'(k_0)\right] \times \varphi\left[\frac{k_0}{q_0}(x-L) - x_0 + \Theta'(k_0), t\right],$$
$$\psi_\beta(x,t) \approx \beta(k_0)\int_{-\infty}^{+\infty}\frac{\mathrm{d}k}{\sqrt{2\pi}}g(k-k_0) \times \exp\left[-\mathrm{i}(Et + kx_0 + q_0x) - \mathrm{i}(k-k_0)\left(\frac{k_0}{q_0}(x-L) - \Theta'(k_0)\right)\right]$$
$$= \beta(k_0)\exp\left[-\mathrm{i}q_0x + i\frac{k_0^2}{q_0}(x-L) - \mathrm{i}k_0\Theta'(k_0)\right] \times \varphi\left[-\frac{k_0}{q_0}(x-L) - x_0 + \Theta'(k_0), t\right],$$
$$\psi_T(x,t) \approx T(k_0)\int_{-\infty}^{+\infty}\frac{\mathrm{d}k}{\sqrt{2\pi}}g(k-k_0) \times \exp\bigl[-\mathrm{i}Et + \mathrm{i}k(x-x_0) + \mathrm{i}(k-k_0)\bigl(\Theta'(k_0) - L\bigr)\bigr]$$
$$= T(k_0)\exp\bigl[-\mathrm{i}k_0\Theta'(k_0)\bigr] \times \varphi\bigl[x - x_0 - L + \Theta'(k_0), t\bigr]. \tag{24}$$

By observing the *Gaussian* shape of $\varphi[x,t]$ given by (13), one could easily (but wrongly!) identify the position of the peak of the wave packets. The times corresponding to the position x of the incident and reflected wave packet peaks would be respectively given by

$$t_{\mathrm{Inc}}(x) = \left.\left[\frac{x-x_0}{v_k}\right]\right|_{k=k_0} \quad \text{and}$$
$$t_R(x) = \left.\left[-\frac{x+x_0-\Theta'(k)}{v_k}\right]\right|_{k=k_0}, \tag{25}$$

where $v_k = \frac{\mathrm{d}E}{\mathrm{d}k} = \frac{k}{m}$. Only $x < 0$ is physical in this result, since these waves, by definition, lie in region I. Since the phase of the incoming wave contains only the plane wave factors, i.e. it is devoid of $\Theta(k)$, the incoming peak reaches the barrier at $x = 0$ at time $t_{\mathrm{Inc}}(0) = -(x_0/v_{k_0})$ (neglecting interference effects). The presence of the phase term $\Theta'(k_0) = (\mathrm{d}\Theta(k)/\mathrm{d}k)|_{k=k_0}$ for $t_R(x)$ *would* imply a time delay, or a time advance, which depends on the sign of

$\Theta'(k_0)$, for the reflected wave with respect to the incident one, i.e.

$$t_R(0) = t_{\mathrm{Inc}}(0) - \left.\frac{\Theta'(k)}{v_k}\right|_{k=k_0}. \tag{26}$$

It is analogous to what happens for the step potential tunneling penetration when $E < V_0$ [23]. When $0 < x < L$ in region II, the times for the "intermediary" α and β wave packet peaks would be given by

$$\begin{aligned} t_\alpha(x) &= \left.\left[\frac{(x-L)}{v_q} - \frac{(x_0 - \Theta'(k))}{v_k}\right]\right|_{k=k_0} \quad \text{and} \\ t_\beta(x) &= \left.\left[-\frac{(x-L)}{v_q} - \frac{(x_0 - \Theta'(k))}{v_k}\right]\right|_{k=k_0}. \end{aligned} \tag{27}$$

And finally, when $x > L$ in region III, the peak of the transmitted wave packet would be written as

$$t_T(x) = \left.\left[\frac{x - x_0 - L + \Theta'(k)}{v_k}\right]\right|_{k=k_0}. \tag{28}$$

The above results (25)–(28) could be directly obtained by applying the SPM to the wave functions $\psi_f(x,t)$ expressed in (22), where the stationary phases for each decomposed wave component f would be given by

$$\begin{aligned} \vartheta_{\mathrm{Inc}}(x,t,k) &= -Et + k(x - x_0), \\ \vartheta_R(x,t,k) &= -Et - k(x + x_0) + \Theta(k), \\ \vartheta_\alpha(x,t,k) &= -Et - kx_0 + q(x-L) + \Theta(k), \\ \vartheta_\beta(x,t,k) &= -Et - kx_0 - q(x-L) + \Theta(k), \\ \vartheta_T(x,t,k) &= -Et + k(x - x_0 - L) + \Theta(k). \end{aligned} \tag{29}$$

Meanwhile, these time-dependencies must be carefully interpreted. In Fig. 2, we illustrate the wave packet diffusion analytically described by the results of (24). The "pictures" display the wave function in the *proximity* of the barrier for suitably chosen times. By taking separately the right (α) and left (β) moving components in region II, independent of the value of $\Theta(k)$, we may observe that

$$\begin{aligned} \Delta t_\alpha &= t_\alpha(L) - t_\alpha(0) = \Delta t_\beta = t_\beta(0) - t_\beta(L) \\ &= \left.\frac{L}{v_q}\right|_{k=k_0}, \end{aligned} \tag{30}$$

which correspond to the transit time values "classically" expected. However, by considering the information carried by the wave packet peaks, we would have a complete time discontinuity at $x = 0$ represented by (26) and by the fact that

$$t_\alpha(0) = -\left.\left[\frac{x_0}{v_k} + \frac{L}{v_q} - \frac{\Theta'(k)}{v_k}\right]\right|_{k=k_0} \neq t_{\mathrm{Inc}}(0), \tag{31}$$

i.e. the α wave could appear in region II at a time $t_\alpha(0)$ before (or after) the incident wave arrives at $x = 0$. The results expressed by (26) and (31) which are illustrated in Fig. 2 immediately imply the nonconservation of probabilities, since they lead to discontinuity points ($x = 0$ and/or $x = L$) for the wave functions, which are Schroedinger equation solutions, and for the spatial derivatives. The normalized squared modulus of these wave functions represents the spatial probability distribution of finding the corresponding propagating particle. At $x = 0$ (and/or $x = L$) the incoming flux of probabilities is different from the outgoing flux, which, from the basic definitions of the quantum mechanical continuity equation [23], leads to the non-conservation of probabilities. It is, in principle, unacceptable.

To be more accurate in such an analysis and to clear up some dubious points, it should be more convenient to verify two simple particular cases. In order to simplify the calculations, we set $x_0 = 0$ and we choose $q_0 L = n\pi$ ($n = 1, 2, 3, \ldots$), so that we can write

$$\begin{aligned} &\mathcal{F}(k_0) = 2k_0 q_0, \qquad \Theta(k_0) = 0, \\ &R(k_0) = 0, \qquad T(k_0) = 1 \end{aligned} \tag{32}$$

and

$$\Theta'(k) = \frac{mL}{q_0}\frac{k_0^2 + q_0^2}{2k_0 q_0} > \frac{mL}{q_0}, \tag{33}$$

so that

$$t_\alpha(0) = \frac{mL}{q_0}\frac{(k_0 - q_0)^2}{2k_0 q_0} > 0. \tag{34}$$

Otherwise, if we choose $q_0 L = (n + \frac{1}{2})\pi$, we shall obtain

$$\begin{aligned} &\mathcal{F}(k_0) = k_0^2 + q_0^2, \qquad \Theta(k) = \frac{\pi}{2}, \qquad R(k_0) = \frac{k_0^2 - q_0^2}{k_0^2 + q_0^2}, \\ &T(k_0) = \frac{2k_0 q_0}{k_0^2 + q_0^2}\exp\left[\mathrm{i}\left(\frac{\pi}{2} - k_0 L\right)\right] \end{aligned} \tag{35}$$

and

$$\Theta'(k) = \frac{mL}{q_0}\frac{2k_0 q_0}{k_0^2 + q_0^2} < \frac{mL}{q_0}, \tag{36}$$

which gives

$$t_\alpha(0) = -\frac{mL}{q_0}\frac{(k_0 - q_0)^2}{k_0^2 + q_0^2} < 0. \tag{37}$$

The latter *negative* value illustratively corroborates with the absurd possibility of the appearance of a peak associated with the α wave occurring before the arrival of the peak of the incident wave packet at $x = 0$, a clear representation of

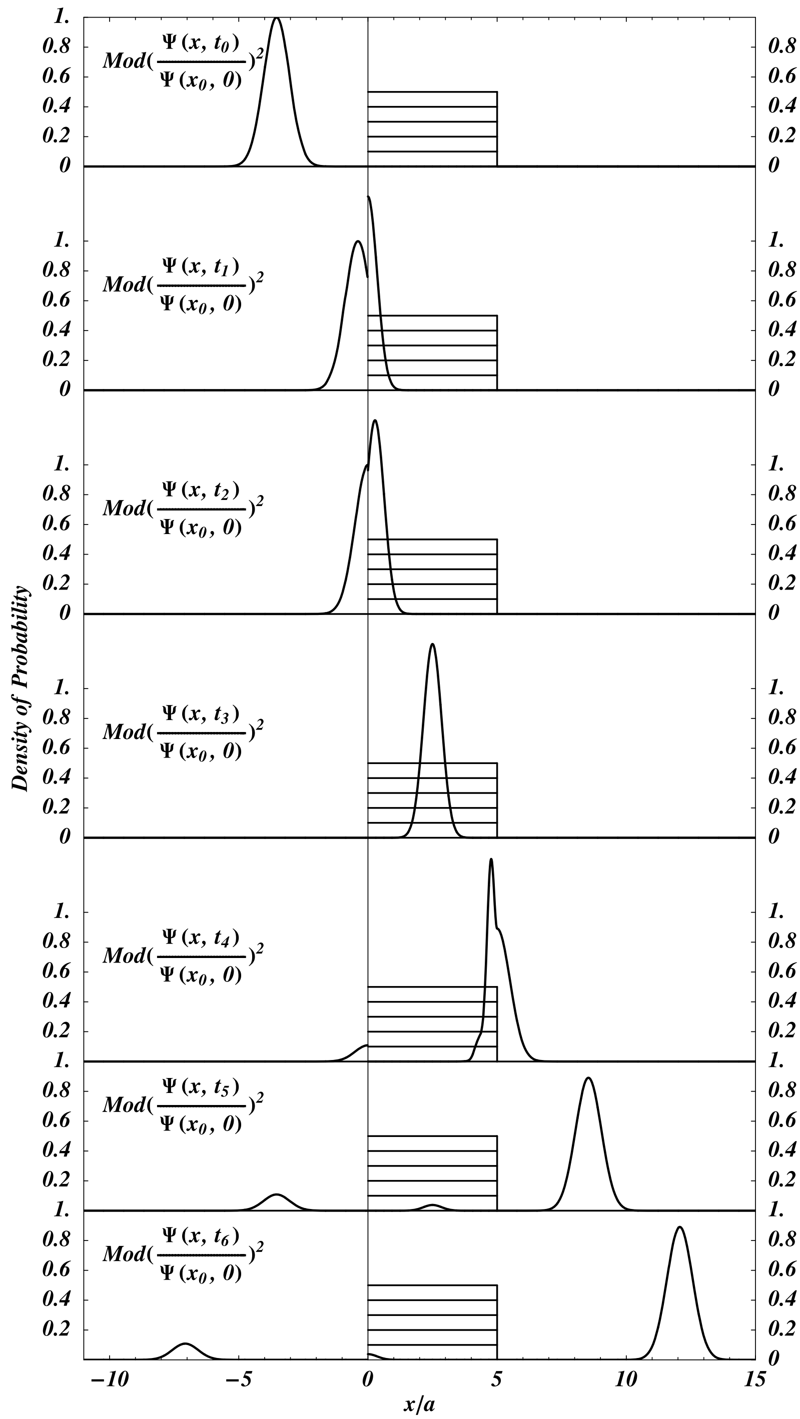

Fig. 2 Erroneous interpretation of the scattering of an incoming wave packet by a unidimensional potential barrier of height V_0 and width L. It has the purpose of illustrating the deficiencies inherent to the *wrong* applicability of the SPM. We have plotted the propagating wave packets at the corresponding times $t_n = (ma^2)[n\,(L/a)]/(a\,q_0)$ (with $n = 0, 1, \ldots, 5$ and with the normalization constraint $ma^2 = 1$) by assuming the incoming wave packet starts at $x = -(k_0 L)/(2q_0)$. From the *false* behavior of the density of probabilities it becomes obvious that the total probability is not conserved, as was expected. The square of the amplitude modulus would supposedly represent a collision of a wave packet of average width a with a potential barrier V_0 of width $L = 5a$ where, for illustration reasons, we have adopted $k_0 = \sqrt{2}w$ and $wa = 10{,}000$. Only a fixed region in x close to the barrier is shown

the discontinuity at $x = 0$. As we have stated before, the phase derivative $\Theta'(k)$ illustrated in Fig. 1 does not present the adequate behavior for applying the SPM accurately. In spite of this, it is currently ignored in the literature.

3.1 Analytic solution for the multiple peak decomposition

Other incongruities in the naive application of the SPM presented above have been pointed out [19]. Differently from the analytical analysis presented above, the numerical simulations of wave packet diffusion by a potential barrier shows the appearance of multiple peaks due to the two reflection points at $x = 0$ and $x = L$ (see the figures). In fact, numerical calculations automatically conserve probabilities, at least within the numerical errors. This observation suggests a new analysis and subsequent interpretation/quantification of the ambiguities presented in the previous section. In order to correctly apply the SPM and accurately obtain the position of the peak of the propagating wave packet with an accurate time dependence, we are to solve the continuity constraints of the Schroedinger equation at each potential discontinuity point $x=0$ and $x=L$ by considering multiple successive reflections and transmissions. The phenomenon was already described in [19] and consists of an incoming wave of unitary amplitude with momentum distribution centered at k_0 which reaches the interface $x=0$, where, at an instant $t=t_0$, it is decomposed into a reflected wave component of amplitude (see the diagram) R_1 and a transmitted wave component of amplitude α_1. The transmitted wave continues propagating until it reaches $x=L$, where, at $t=t_1$, it is now decomposed into a reflected wave component of amplitude β_1 and a transmitted wave component of amplitude T_1. This new reflected wave component comes back to $x=0$ where, at $t=t_2$, it is again decomposed into another reflected wave component of amplitude α_2 and a transmitted wave component of amplitude R_2 which will be added to R_1. This iterative process continues for an infinity of times as we can see in the following diagram:

$$
\begin{array}{r|l}
\exp[\mathrm{i}kx]+R_1\exp[-\mathrm{i}kx] & \alpha_1\exp[\mathrm{i}qx] \\
R_2\exp[-\mathrm{i}kx] & \alpha_2\exp[\mathrm{i}qx]+\beta_1\exp[-\mathrm{i}qx] \\
\vdots & \quad\vdots \quad + \quad \vdots \\
R_n\exp[-\mathrm{i}kx] & \alpha_n\exp[\mathrm{i}qx]+\beta_{n-1}\exp[-\mathrm{i}qx] \\
\multicolumn{2}{c}{x=0}
\end{array}
\qquad
\begin{array}{r|l}
\alpha_1\exp[\mathrm{i}qx]+\beta_1\exp[-\mathrm{i}qx] & T_1\exp[\mathrm{i}kx] \\
\alpha_2\exp[\mathrm{i}qx]+\beta_2\exp[-\mathrm{i}qx] & T_2\exp[\mathrm{i}kx] \\
\vdots \quad + \quad \vdots & \quad\vdots \\
\alpha_n\exp[\mathrm{i}qx]+\beta_n\exp[-\mathrm{i}qx] & T_n\exp[\mathrm{i}kx] \\
\multicolumn{2}{c}{x=L.}
\end{array}
$$

The continuity constraints over $\psi(x,t)$ for each potential step at $x=0$ and $x=L$ determine the coefficients

$$
\begin{aligned}
R_1 &= \frac{k-q}{k+q}, \qquad \alpha_1=\frac{2k}{k+q}, \\
\beta_1 &= \frac{2k(q-k)}{(k+q)^2}\exp[2\mathrm{i}qL], \\
T_1 &= \frac{4kq}{(k+q)^2}\exp\big[\mathrm{i}(q-k)L\big], \qquad R_2=\frac{q}{k}\alpha_1\beta_1,
\end{aligned}
\tag{38}
$$

and thus we establish the recurrence relations

$$
\frac{R_{n+2}}{R_{n+1}}=\frac{\alpha_{n+1}}{\alpha_n}=\frac{\beta_{n+1}}{\beta_n}=\frac{T_{n+1}}{T_n}=\left(\frac{k-q}{k+q}\right)^2\exp[2\mathrm{i}qL], \quad n=1,2,\ldots, \tag{39}
$$

which allow us to write the sum of the coefficients R_n, α_n, β_n, and T_n as

$$
\begin{aligned}
R &= \sum_{n=1}^{\infty}R_n = R_1+R_2\left[1-\left(\frac{k-q}{k+q}\right)^2\exp[2\mathrm{i}qL]\right]^{-1}, \\
\alpha &= \sum_{n=1}^{\infty}\alpha_n = \alpha_1\left[1-\left(\frac{k-q}{k+q}\right)^2\exp[2\mathrm{i}qL]\right]^{-1}, \\
\beta &= \sum_{n=1}^{\infty}\beta_n = \beta_1\left[1-\left(\frac{k-q}{k+q}\right)^2\exp[2\mathrm{i}qL]\right]^{-1}, \\
T &= \sum_{n=1}^{\infty}T_n = T_1\left[1-\left(\frac{k-q}{k+q}\right)^2\exp[2\mathrm{i}qL]\right]^{-1}.
\end{aligned}
\tag{40}
$$

The above summations exactly reproduce the expressions in (19). In this form the interpretation is easy. R_1 represents the first reflected wave (it has no time delay since it is real). R_2 represents the second reflected wave and, as a consequence of the continuity condition at $x=0$, it is the sum, in region II, of the first left-going wave (β_1) and the second right-going amplitude (α_2), i.e.

$$
R_2=\alpha_2+\beta_1\equiv\frac{q}{k}\alpha_1\beta_1.
$$

This structure is the same as that given by considering two "step functions" back-to-back. Thus at each interface the "reflected" and "transmitted" waves are instantaneous i.e. without any delay time.

Now we can calculate the time at which each transmitted and/or reflected wave appears by applying the SPM for each component of the total transmitted T or reflected R coefficients. It will give us the recurrence relation

$$
t_n=t_{n-1}+\frac{m(x-L)}{q_0}, \tag{41}
$$

which coincides with the "classically" predicted value for the velocity of the particle above the barrier. Indeed the SPM *applied separately* to each term in the above series expansion for R yields delay multiples of $2\,(\mathrm{d}q/\mathrm{d}E)|_{q=q_0}L=2(m/q_0)L$. This agrees perfectly with the fact that, since the peak momentum in region II is q_0, the α and β waves have group velocities of q_0/m and hence transit times (one way) of $(m/q_0)L$. The first transmitted peak appears (according to this version of the SPM) after a time $(m/q_0)L$, in perfect agreement with the above interpretation.

Is this compatible with probability conservation? It is, because of the following identity:

$$\sum_{n=1}^{\infty}\left(|R_n|^2+|T_n|^2\right)=1. \tag{42}$$

This result is by no means obvious, since it coexists with the well-known result from a plane wave analysis that

$$|R|^2+|T|^2=\left|\sum_{n=1}^{\infty}R_n\right|^2+\left|\sum_{n=1}^{\infty}T_n\right|^2=1. \tag{43}$$

To conclude, we can state that the conditions for applying the SPM in scattering problems of such a type depend upon the correct manipulation of the amplitude. A posteriori this seems obvious, but the point is that unless we know the number of separate peaks the SPM is inaccurate. There is, however, a converse to this question. If the modulating function is such that two or more wave packets overlap, then we cannot treat them separately without considering all the interference effects. The above barrier analysis is simply a particular example of this ambiguity.

3.2 The analytical formula

In order to obtain an analytical formula for the wave packet propagation, we consider the *Gaussian* momentum distribution given by (11). Using the linear approximation for the momentum q given by (23) and considering the expressions in (40) resulting from the multiple peak decomposition in (22), again, with the same pertinent approximations used for obtaining (24), we can analytically construct the following simplified expressions:

$$\begin{aligned}
\psi_I(x,t)&=\varphi[x-x_0,t],\\
\psi_R(x,t)&=\frac{k_0-q_0}{k_0+q_0}\varphi[-x-x_0,t]\\
&\quad+\frac{4k_0q_0(q_0-k_0)}{(k_0+q_0)^3}\exp\left[-\mathrm{i}\frac{2w^2}{q_0}L\right]\\
&\quad\times\sum_{n=0}^{\infty}\left(\frac{k_0-q_0}{k_0+q_0}\exp\left[-\mathrm{i}\frac{w^2}{q_0}L\right]\right)^{2n}\\
&\quad\times\varphi\left[-x-x_0+2(n+1)\frac{k_0}{q_0}L,t\right],\\
\psi_\alpha(x,t)&=\frac{2k_0}{k_0+q_0}\exp\left[-\mathrm{i}\frac{w^2}{q_0}x\right]\\
&\quad\times\sum_{n=0}^{\infty}\left(\frac{k_0-q_0}{k_0+q_0}\exp\left[-\mathrm{i}\frac{w^2}{q_0}L\right]\right)^{2n}\\
&\quad\times\varphi\left[(x+2nL)\frac{k_0}{q_0}-x_0,t\right],\\
\psi_\beta(x,t)&=\frac{2k_0(q_0-k_0)}{(k_0+q_0)^2}\exp\left[\mathrm{i}\frac{w^2}{q_0}(x-2L)\right]\\
&\quad\times\sum_{n=0}^{\infty}\left(\frac{k_0-q_0}{k_0+q_0}\exp\left[-\mathrm{i}\frac{w^2}{q_0}L\right]\right)^{2n}\\
&\quad\times\varphi\left[(2nL+2L-x)\frac{k_0}{q_0}-x_0,t\right],\\
\psi_T(x,t)&=\frac{4k_0q_0}{(k_0+q_0)^2}\exp\left[-\mathrm{i}\frac{w^2}{q_0}L\right]\\
&\quad\times\sum_{n=0}^{\infty}\left(\frac{k_0-q_0}{k_0+q_0}\exp\left[-\mathrm{i}\frac{w^2}{q_0}L\right]\right)^{2n}\\
&\quad\times\varphi\left[x-x_0-L+(2n+1)\frac{k_0}{q_0}L,t\right],
\end{aligned}\tag{44}$$

which allow us to visualize the multiple peak decomposition illustrated in Fig. 3. By comparing with the exact numerical results, the analytic approximations expressed in (44) will be valid only under certain restrictive conditions. To explain such a statement, when we analytically solve the integrals like (22), the exponential $\exp[2\mathrm{i}qL]$, which appears in the recurrence relations (39), is approximated by

$$\exp\left[2\mathrm{i}q_0L+2\mathrm{i}(k-k_0)\frac{k_0}{q_0}\right]. \tag{45}$$

In this case, the above analytical expressions can be obtained only when the exponential function does not oscillate in the interval of relevance of the envelope *Gaussian* function $g(k-k_0)$, i.e. when $\Delta qL<\pi$, which can be expressed in terms of the wave packet width as

$$\Delta qL\approx\left.\frac{\mathrm{d}q}{\mathrm{d}k}\right|_{k=k_0}\Delta kL\approx\frac{k_0}{q_0}\frac{L}{a}<\pi. \tag{46}$$

Here we have used $\Delta k\approx 1/a$. The above constraint is implicitly of a very peculiar character: the multiple peak decomposition can also be given evidence for when the wave packet width a is larger than the potential barrier width L, i.e. when we assume that the relation k_0/q_0 is in the interval $1<k_0/q_0<\pi$ we may have propagating wave packets with $a>L$ satisfying the requirements for the multiple peak resolution (44). To illustrate this possibility, in Fig. 4 we plot the density of probabilities representing the collision of a wave packet of average width a with a potential barrier V_0 of width $L=0.8a$. We compare the analytical (line) with the numerical (star symbols) results from which we can evidently observe the accurate equivalence between them, since we are respecting the condition (46). Both the figures (3) and (4) display the square of the wave function in the *proximity* of the barrier for suitably chosen times. One clearly sees the appearance of multiple peaks due to the two reflection points at $x=0$ and $x=L$.

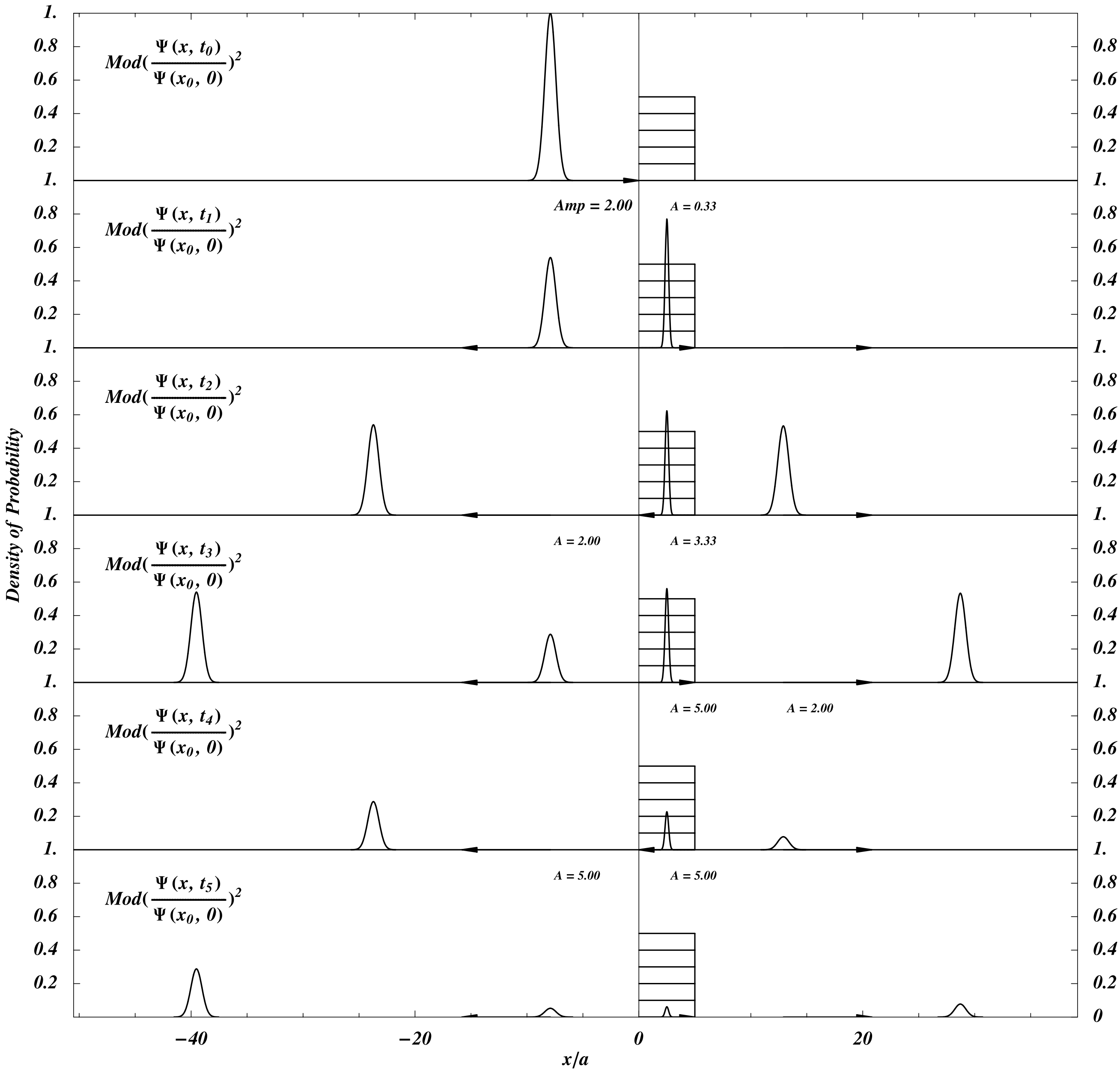

Fig. 3 Multiple peak decomposition of a propagating wave packet in the above potential barrier scattering problem. We have plotted the first few reflected and transmitted waves for times $t_n = (ma^2)[n(L/a)]/(aq_0)$ (with $n = 0, 1, \ldots, 5$ and $ma^2 = 1$) in correspondence with (41), by assuming that the incoming wave packet starts at $x = -(k_0 L)/(2q_0)$. The density of probabilities represents the collision of a wave packet of average width a with a potential barrier V_0 of width $L = 5a$. Just for illustration reasons, we have adopted $k_0 = (\sqrt{10w})/3$ ($wa = 10{,}000$) and we have printed the wave packet amplification multiplying factor (A) (individually adopted for visual convenience for each wave packet) when necessary

4 Conclusions

We have studied wave packet scattering by a unidimensional rectangular potential barrier. In particular, we have employed the SPM, for which some inherent ambiguities were noticed and correctly interpreted. The main point we have elaborated upon shows that the results of the SPM depend critically on the manipulation of the amplitude prior to the application of the method. Essentially, what we have demonstrated is that the barrier results can be obtained by treating the barrier as a two-step process. This procedure involves multiple reflections at each step and predicts the existence of multiple (infinite) outgoing peaks. Unless we know, by some other means, at least the number of separate peaks involved in the scattering problem, the immediate use of the

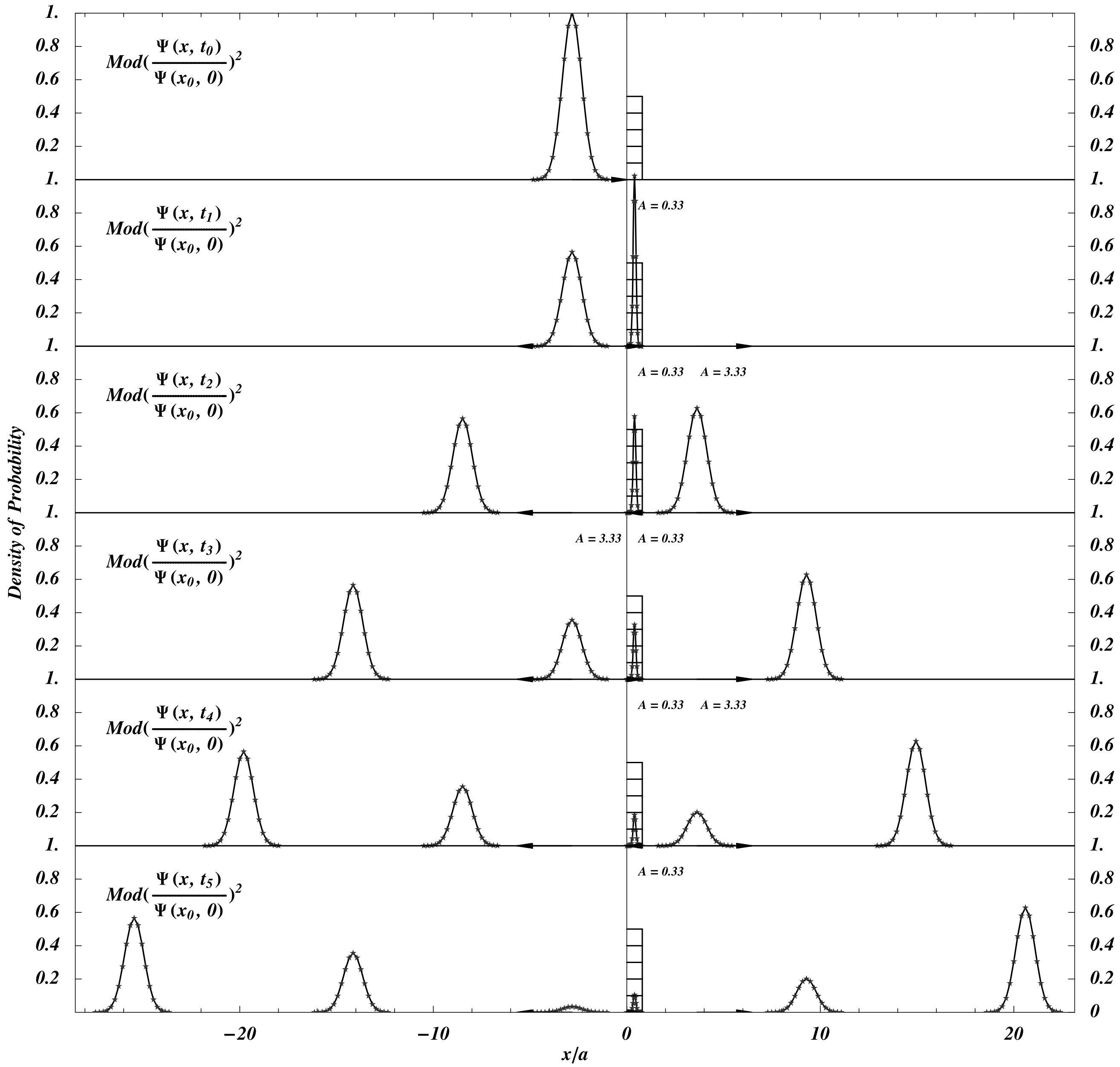

Fig. 4 The illustrative confrontation of the analytical (*line*) and the numerical (*star symbols*) results for reflected and transmitted waves when the condition $1 < k_0/q_0 < \pi$ is satisfied and, consequently, the analytical and the numerical results have to be equivalent. The stars are from the numerical convolution of the plane wave solution and the curves are from the analytical expressions for the first three R_n and T_n. The density of probabilities represents the collision of a wave packet of average width a with a potential barrier V_0 of width $L = 0.8\,a$. Again for illustration reasons, we have adopted $k_0 = (5\sqrt{2}\,w)/7$ and we have printed the wave packet amplification multiplying factor (A) when necessary. The reason for choosing a so large value for the parameter wa ($wa = 10{,}000$) in all these figures is to guarantee the convergence between the analytical and the numerical results for all the decomposed peaks

SPM by itself cannot lead to a convincing resolution. In this scenario, some extensions of which we have discussed here, can be used for analyzing some particular configurations of tunneling of a particle [24–30]. Some of the barrier transposing time definitions based on the SPM lead, in tunneling time conditions, to very short times, which can even become negative. This seems to contradict the most obvious concepts of causality. To partially overcome these incompatibilities, we suppose that we may utilize the multiple peak decomposition analysis in order to, at least partially, recover the conditions for the SPM applicability.

Acknowledgement This work was supported by FAPESP (grant No. 2004/13770-0).

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