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Tunnelling of narrow Gaussian packets through delta potentials

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Abstract
We consider transmission and reflection of narrow Gaussian wave packets by delta potentials in the cases of constant and specific (inverse linear) time-dependent strength. Both transmitted and reflected packets exhibit some 'squeezing' in the momentum probability distributions. Several different definitions of the transmission time are introduced and compared.

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1. Introduction

It is well known that the stationary Schrödinger equation with the potential

$$V(x) = \mathcal{Z}\delta(x) \tag{1}$$

admits a simple complete set of exact explicit solutions [1]. For this reason, it has been frequently used to model different phenomena in various fields of quantum physics, in the limit cases when the detailed form of a concrete potential is not essential and results depend on its integral characteristics, e.g., a product of effective height by effective width. In particular, such an approximation can be successfully applied to the analysis of various tunnelling devices in solid state physics [2], where the experimental technique of 'delta doping' has been used for creating different 'delta layers' for more than two decades [3]. Applications of three-dimensional delta potentials to the problems of atomic physics (photoionization, photodetachment) have been reviewed in [4]. Such potentials are also widely used in the theory of Bose–Einstein condensates [5, 6]. Exactly solvable models of many-body systems interacting via delta potentials were considered in [7, 8].

Various solutions of the *time-dependent* Schrödinger equation with potential (1) were also considered by many authors, beginning, perhaps, with the paper [9], where an original approach to the initial-value problem was proposed. In particular, many efforts have been directed towards finding the propagator $G(x, x'; t)$ [10–15], which enables us to calculate the evolution of any initial wavefunction $\psi(x, 0)$ according to the relation

$$\psi(x,t) = \int_{-\infty}^{\infty} G(x, x'; t)\psi(x', 0)\,\mathrm{d}x'. \tag{2}$$

Generalizations to the case of a time-dependent strength $\mathcal{Z}(t)$ were considered in [16–18]. Propagators for *moving* delta potentials were obtained in [17, 19–21]. For other studies and generalizations see, e.g., [22–36].

However, concrete calculations of the integral (2) and the analysis of evolution of different initial localized wave packets in the presence of delta-type potentials were performed only in a few studies [9, 13, 37]. The aim of our paper is to consider reflection and transmission by the potential (1) (with constant or specific time-dependent strength $\mathcal{Z}(t)$) of initial *narrow Gaussian* packets, with an emphasis on *slowly moving* packets. This special case could be realized in experiments with ultracold atoms. In particular, it is closely related to the phenomenon of *quantum deflection* of slow packets from reflecting and semitransparent mirrors [38–40]. For other recent publications devoted to propagation and reflection of quantum packets (matter waves) see, e.g., [41–48].

Our plan is as follows. In section 2 we derive analytical formulae describing reflection and transmission of initial narrow Gaussian packets through the stationary delta barrier. We discuss the effect of 'squeezing' the momentum and coordinate probability densities, the time-dependent and asymptotical transmission probabilities and the concept of conditional average values. In section 3 we compare different possible definitions of the 'transmission time'. In section 4 we consider a generalization to the case of a specific (inverse linear) time dependence of the delta-potential strength. Section 5 contains conclusions.

2. Evolution of packets in a stationary delta potential

The explicit form of the propagator for the delta potential was found in several papers [10, 12, 13]

$$\begin{aligned} G_{\mathcal{Z}}(x, x'; t) = {}& (2\pi \mathrm{i}t)^{-1/2} \exp\left[\frac{\mathrm{i}(x-x')^2}{2t}\right] \\ & - \frac{\mathcal{Z}}{2} \exp\left[\mathcal{Z}(|x| + |x'|) + \frac{\mathrm{i}\mathcal{Z}^2 t}{2}\right] \mathrm{erfc}\left[\frac{|x| + |x'| + \mathrm{i}\mathcal{Z}t}{\sqrt{2\mathrm{i}t}}\right] \end{aligned} \tag{3}$$

where

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} \exp(-y^2)\,\mathrm{d}y \equiv 1 - \mathrm{erf}(z) \tag{4}$$

is the complementary error function [49, 50]. To simplify formulae we assume formally that $\hbar = m = 1$. The return to the dimensional variables can be performed by means of the replacements

$$t \to \frac{\hbar t}{m} \qquad \mathcal{Z} \to \frac{m\mathcal{Z}}{\hbar^2}. \tag{5}$$

For imaginary time, i.e. for the equilibrium density matrix, a formula equivalent to (3) was obtained in [51], and the equilibrium Wigner function was calculated in [52]. The second term in the right-hand side of (3) is sometimes called the *Moshinsky function* [13, 53, 54], because a similar expression appeared in the paper [55] devoted to the 'diffraction in time' problem. Equation (3) holds for any sign of $\mathcal{Z}$ (although in some papers it was derived for attractive or repulsive potentials only). Other (integral) representations for the propagator were given in [11, 14, 15]. For $\mathcal{Z} \to \infty$ and fixed values of x, x' and t, the propagator (3) goes to the propagator in the half-space confined with an impenetrable wall (for $x, x' > 0$)

$$G_\infty(x, x'; t) = (2\mathrm{i}\pi t)^{-1/2}\left\{\exp\left[-\frac{(x'-x)^2}{2\mathrm{i}t}\right] - \exp\left[-\frac{(x'+x)^2}{2\mathrm{i}t}\right]\right\} \tag{6}$$

due to the asymptotical formula [49, 50]

$$\mathrm{erfc}(x) \approx \frac{\exp(-x^2)}{x\pi^{1/2}} \qquad |x| \to \infty \quad |\arg x| < \frac{3\pi}{4}. \tag{7}$$

Exact or quasi-classical propagators in the presence of additional potentials and for various boundary conditions on a half-line or in three-dimensional domains separated by screens and slits were obtained, e.g., in [56–63].

Putting expression (3) in the integral (2) one should remember that $G(x, x'; t)$ has different analytical forms for $x' > 0$ and $x' < 0$, so that the integration should be performed separately over the regions $x' > 0$ and $x' < 0$ (and the result is different for $x > 0$ and $x < 0$). However, if we suppose that the initial wavefunction is well localized far away to the right from the origin, being equal to zero for $x < 0$, then the integration in (2) should be performed over $x' > 0$ only, i.e. we may replace $|x'|$ by x' itself. We consider in this paper a Gaussian initial state[3]

$$\psi(x, 0) = (\pi s^2)^{-1/4} \exp\left[-\frac{(x-x_c)^2}{2s^2} + \mathrm{i}p_0 x\right] \qquad x_c \gg s. \tag{8}$$

The form (8) implies that we consider the states without initial correlations between the coordinate and momentum (it was shown in [39, 40] that nonzero initial correlation coefficient does not change essentially the picture of reflection or transmission of narrow slow packets from barriers). Although function (8) has a nonzero ‘tail’ in the region $x < 0$, this tail is exponentially small (under the assumed condition $x_c \gg s$) and does not give any significant contribution. Therefore, the integration in (2) can be formally extended to the whole axis $-\infty < x' < \infty$. Using the integral [64]

$$\int_{-\infty}^{\infty} \mathrm{d}x \exp(-ax^2 + bx)\,\mathrm{erfc}(x) = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}\right) \mathrm{erfc}\left(\frac{b}{2\sqrt{a(1+a)}}\right) \tag{9}$$

and introducing new dimensionless variables and parameters

$$\tilde{x} = \frac{x}{x_c} \qquad \tilde{p} = \frac{ps}{\hbar\sqrt{2}} \qquad \tau = \frac{t\hbar\sqrt{2}}{msx_c} \qquad \mathcal{B} = \frac{ms\mathcal{Z}}{\hbar^2\sqrt{2}} \qquad \upsilon = 1 + \mathrm{i}\beta\tau \qquad \beta = \frac{x_c}{s\sqrt{2}} \tag{10}$$

we obtain

$$\begin{aligned}\psi(\tilde{x}, \tau) = \left(\frac{2\beta^2}{\pi\upsilon^2}\right)^{1/4} \Bigg\{ & \exp\left[-\frac{\beta^2}{\upsilon}(\tilde{x} - 1 - \tilde{p}_0\tau)^2 + \mathrm{i}\beta\tilde{p}_0(2\tilde{x} - \tilde{p}_0\tau)\right] \\ & - \mathcal{B}\sqrt{\pi\upsilon}\exp\left[\mathcal{B}^2\upsilon + 2\beta\mathcal{B}(|\tilde{x}| + 1) - \tilde{p}_0^2 + 2\mathrm{i}\tilde{p}_0(\beta + \mathcal{B})\right] \\ & \times \mathrm{erfc}\left[\frac{\beta}{\sqrt{\upsilon}}(|\tilde{x}| + 1) + \mathcal{B}\sqrt{\upsilon} + \frac{\mathrm{i}\tilde{p}_0}{\sqrt{\upsilon}}\right]\Bigg\}.\end{aligned} \tag{11}$$

[3] An exact formula describing the evolution of the initial packet of the form $\exp(-a|x - x_c|)$ was obtained and analysed in [13].

For $\mathcal{B} > 0$ (repulsive potential) and $\beta \gg 1$, the real part of the argument of the erfc-function on the right-hand side of equation (11) is large and positive for any value of τ, so we can simplify this expression using the asymptotical formula (7):

$$\psi(\tilde{x},\tau) \approx \left(\frac{2\beta^2}{\pi\upsilon^2}\right)^{1/4}\left\{\exp\left[-\frac{\beta^2}{\upsilon}(\tilde{x}-1-\tilde{p}_0\tau)^2 + \mathrm{i}\beta\tilde{p}_0(2\tilde{x}-\tilde{p}_0\tau)\right]\right.$$
$$\left. - \frac{\mathcal{B}\upsilon}{\beta(|\tilde{x}|+1)+\mathcal{B}\upsilon+\mathrm{i}\tilde{p}_0}\exp\left[-\frac{\beta^2}{\upsilon}(|\tilde{x}|+1+\tilde{p}_0\tau)^2 - \mathrm{i}\beta\tilde{p}_0(2|\tilde{x}|+\tilde{p}_0\tau)\right]\right\}. \quad (12)$$

2.1. Reflected packet

If $\mathcal{B} \to \infty$, the pre-exponential factor in the second line of equation (12) tends to 1 (for fixed $\tilde{x}$ and τ). In this limit, for $\tilde{x} > 0$ the right-hand side of (12) becomes a superposition of a freely expanding Gaussian packet (with zero mean initial momentum) and a packet reflected by an ideal boundary [38], whereas it goes to zero for $\tilde{x} < 0$. The probability density $|\psi(\tilde{x},\tau)|^2$ rapidly oscillates in the semispace $\tilde{x} > 0$ (if $\mathcal{B} \neq 0$) due to interference between the freely propagating part of the wave packet and the part reflected from the potential. The asymptotical (at $\tau \to \infty$) *momentum distribution* $|\varphi(\tilde{p})|^2$ does not depend on τ, but it contains rapidly oscillating terms containing sine or cosine functions of the big argument $\beta\tilde{p}$. After averaging over these oscillations (which do not really affect measurable quantities [39, 40]) we obtain a smooth distribution, which has different forms for positive and negative values of momentum

$$\overline{\mathcal{P}}^{(\pm)}_{\mathrm{as}}(\tilde{p}) = \begin{cases} |\varphi_0(\tilde{p})|^2 + |\varphi_0(-\tilde{p})|^2|\chi(\tilde{p})|^2 & \tilde{p} > 0 \\ |\varphi_0(\tilde{p})|^2(1-|\chi(\tilde{p})|^2) & \tilde{p} < 0 \end{cases} \quad (13)$$

where

$$|\chi(\tilde{p})|^2 = \frac{\mathcal{B}^2}{\mathcal{B}^2 + \tilde{p}^2} \quad (14)$$

is the well-known reflection coefficient from the delta barrier [1] and

$$|\varphi_0(\tilde{p})|^2 = (2/\pi)^{1/2}\exp[-2(\tilde{p}-\tilde{p}_0)^2] \quad (15)$$

is the initial momentum distribution corresponding to the state (8) (we confine ourselves to the case of *pure* initial Gaussian states; mixed initial states were discussed in [39, 40]). The asymptotical mean value of the momentum $\langle\tilde{p}_\infty\rangle$ is different from the initial value $\tilde{p}_0$. For example, if $\tilde{p}_0 < 0$ and $|\tilde{p}_0| \gg 1$ (this means that the absolute mean value of the momentum is much greater than the momentum spread in the initial state), then $\langle\tilde{p}_\infty\rangle = \tilde{p}_0 - 2\tilde{p}_0|\chi(\tilde{p}_0)|^2$. But the most interesting is the case of an almost perfectly reflecting potential (or $\mathcal{B} \gg 1$) and zero initial average momentum $\tilde{p}_0 = 0$, when the initial symmetrical momentum distribution (15) (with $\tilde{p}_0 = 0$) goes to a highly asymmetrical asymptotical averaged distribution with $\overline{\mathcal{P}}_{\mathrm{as}}(\tilde{p} > 0) \approx 2|\varphi_0(\tilde{p})|^2$ and $\overline{\mathcal{P}}_{\mathrm{as}}(\tilde{p} < 0) \approx 0$. As a consequence, the packet becomes narrower in the momentum space than it was initially, i.e. some kind of 'squeezing' of the momentum distribution can be observed. This effect of 'quantum deflection' (discussed in [38–40]) has a simple physical explanation, which is based on the wave–particle duality: partial plane waves with negative components of the momentum change the sign of the momentum after reflection from the potential, and this results in reducing the spread of the packet in the momentum space. It is worth noting that the effective width of the packet in the coordinate space (measured in terms of the coordinate variance σ_x) turns out to be also *less* in the case of almost perfectly reflecting potentials, compared to the case of free spreading of the packet [38, 39]. However, no violation of the uncertainty relations happens, because σ_x grows with time in all cases as t^2 (with a smaller coefficient for $|\mathcal{B}| \gg 1$ than for $\mathcal{B} = 0$), so that the product $\sigma_p\sigma_x$ also increases with time unlimitedly. On the other hand, the *invariant uncertainty product* $\sigma_p\sigma_x - \sigma_{px}^2$ asymptotically tends to some constant value (proportional to the parameter β^2, i.e. much greater than $\hbar^2/4$) [39, 40]. The asymptotical mean value of the momentum in the case discussed equals $\langle\tilde{p}_\infty\rangle = 1/\sqrt{2\pi}$ (note that the definition of the dimensionless momentum $\tilde{p}$ in equation (10) differs by the factor $\sqrt{2}$ from the definition adopted in [38–40]).

2.2. *Transmitted packet*

Now let us discuss the properties of the *transmitted* packet. For $\tilde{x} < 0$ the arguments of both exponential functions in formula (12) are the same, so that it reads

$$\psi(\tilde{x},\tau) \approx \left(\frac{2\beta^2}{\pi\upsilon^2}\right)^{1/4} \frac{\beta(1-\tilde{x}) + \mathrm{i}\tilde{p}_0}{\beta(1-\tilde{x}) + \mathcal{B}\upsilon + \mathrm{i}\tilde{p}_0} \exp\left[-\frac{\beta^2}{\upsilon}(\tilde{x} - 1 - \tilde{p}_0\tau)^2 + \mathrm{i}\beta\tilde{p}_0(2\tilde{x} - \tilde{p}_0\tau)\right]. \tag{16}$$

Taking β large enough, one can neglect $\tilde{p}_0$ in the pre-exponential factor, as well as the parameter $\mathcal{B}$ in the real part of its denominator (remember that $\upsilon = 1 + \mathrm{i}\beta t$ and $\tilde{x} < 0$). Therefore, the probability distribution to the left of the barrier does not depend on β under the conditions

$$\beta \gg 1 \qquad \beta \gg |\tilde{p}_0| \qquad \beta \gg \mathcal{B} \qquad \beta\tau \gg 1 \tag{17}$$

(which imply that $\mathcal{B}$ is finite, i.e. the barrier is not totally reflecting):

$$\mathcal{P}^{(-)}(\tilde{x},\tau) \equiv |\psi(\tilde{x},\tau)|^2 \approx \left(\frac{2}{\pi\tau^2}\right)^{1/2} \frac{(1-\tilde{x})^2}{(1-\tilde{x})^2 + \tau^2\mathcal{B}^2} \exp\left[-\frac{2}{\tau^2}(\tilde{x} - 1 - \tilde{p}_0\tau)^2\right]. \tag{18}$$

It is clear that for $\tilde{p}_0 < 0$ and $|\tilde{p}_0|\tau \gg 1$, the maximum of the distribution (18) is attained at $\tilde{x} - 1 = \tilde{p}_0\tau$. In this case one can replace the term $\tilde{x} - 1$ in the pre-exponential factor by $\tilde{p}_0\tau$ at the points near the maximum. Consequently, the transmitted packet (in the sense of its probability density) asymptotically is close to the freely expanding initial Gaussian packet, multiplied by the transmission coefficient

$$T(\tilde{p}) = 1 - |\chi(\tilde{p})|^2 = \frac{\tilde{p}^2}{\mathcal{B}^2 + \tilde{p}^2} \tag{19}$$

corresponding to the initial momentum $\tilde{p}_0$. This was noticed (without explicit proof) as far back as in [9].

However, this simple result holds only if $|\tilde{p}_0|$ is not very small. If $|\tilde{p}_0| \ll 1$, the situation is different, and we consider here the extreme case of $\tilde{p}_0 = 0$. In this case the main part of the freely expanding initial packet reaches the barrier at $\tau \sim 1$, therefore, the most interesting regime is $\tau > 1$. In contrast to a freely expanding packet, whose maximum is fixed at the point $\tilde{x} = 1$, the position of the maximum of the transmitted packet (18) with $\tilde{p}_0 = 0$ is gradually shifted to the left according to the formula

$$(1 - \tilde{x}_m)^2/\tau^2 = \tfrac{1}{2}\left(\mathcal{B}\sqrt{2 + \mathcal{B}^2} - \mathcal{B}^2\right). \tag{20}$$

In particular, $|1 - \tilde{x}_m| \approx 2^{-1/4}\tau\sqrt{\mathcal{B}}$ for an almost transparent barrier ($\mathcal{B} \ll 1$). On the other hand, the velocity of the maximum of the packet *does not depend* on $\mathcal{B}$ for an almost perfectly

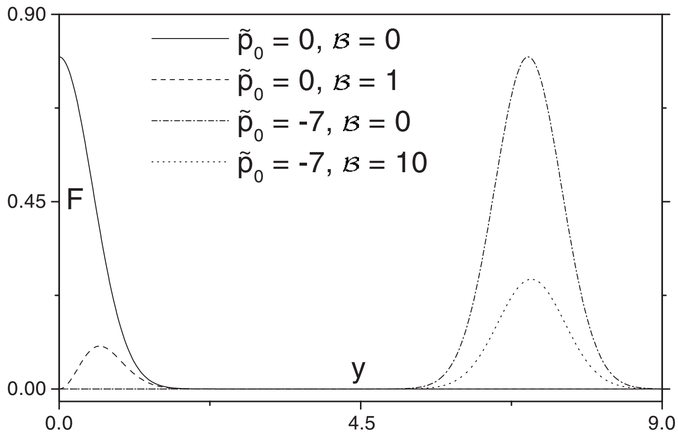

Figure 1. The function $F(y)$ (23) for $\tilde{p}_0 = 0, \mathcal{B} = 0$ (upper left curve), $\tilde{p}_0 = 0, \mathcal{B} = 1$ (lower left curve), $\tilde{p}_0 = -7, \mathcal{B} = 0$ (upper right curve), $\tilde{p}_0 = -7, \mathcal{B} = 10$ (lower right curve).

reflecting barrier ($\mathcal{B} \gg 1$):

$$(1 - \tilde{x}_m)^2/\tau^2 \to 1/2 \qquad |\mathrm{d}\tilde{x}_m/\mathrm{d}\tau| \to 1/\sqrt{2} \tag{21}$$

(although the height of the maximum becomes very small). In the latter case

$$\mathcal{P}^{(-)}(\tilde{x}) \approx \left(\frac{2}{\pi}\right)^{1/2} \frac{(1-\tilde{x})^2}{\tau^3\mathcal{B}^2} \exp\left[-\frac{2}{\tau^2}(1-\tilde{x})^2\right]. \tag{22}$$

Using the approximation $\mathcal{P}^{(-)}(\tilde{x}) \approx \mathcal{P}(\tilde{x}_m) \exp[-4(\tilde{x}-\tilde{x}_m)^2/\tau^2]$ in the vicinity of maximum, one can check that the ratio of the width of the packet $\Delta\tilde{x} = \tau/(2\sqrt{2})$ to the coordinate of its maximum $\tilde{x}_m$ does not depend on time: $\Delta\tilde{x}/\tilde{x}_m \approx 1/2$.

It is convenient to rewrite the probability density (18) as a function of the scaled variable $y = (1-\tilde{x})/\tau$ (whose range varies from τ^{-1} to ∞) multiplied by the normalization factor τ^{-1}:

$$\mathcal{P}^{(-)}(\tilde{x}, \tau) = \frac{F(y)}{\tau} \qquad F(y) = \sqrt{\frac{2}{\pi}} \frac{y^2}{y^2 + \mathcal{B}^2} \exp[-2(y+\tilde{p}_0)^2] \qquad y = \frac{1-\tilde{x}}{\tau}. \tag{23}$$

Comparing (23) with (13), (15) and (19), one can see that the function $F(y)$ with $y = -\tilde{p}$ is exactly the asymptotical momentum distribution $\overline{\mathcal{P}}_{\mathrm{as}}^{(-)}(-\tilde{p})$. Consequently, the asymptotical coordinate probability density in the transmitted packet $\mathcal{P}^{(-)}(\tilde{x}, \tau)$ reproduces (after some rescaling) the asymptotical momentum probability density. The plots of function $F(y)$ for different values of $\tilde{p}_0$ and $\mathcal{B}$ are given in figure 1. One can see that for $|\tilde{p}_0| \gg 1$, the function $F(y; \mathcal{B})$ behaves as a scaled function $F(y; 0)$, while the functions $F(y; \mathcal{B})$ and $F(y; 0)$ are completely different in the case of $\tilde{p}_0 = 0$.

2.3. Time-dependent transmission probability and conditional average values

The time-dependent transmission probability can be defined as the probability of discovering the particle to the left of the barrier:

$$\mathcal{L}(\tau) = \int_{-\infty}^{0} \mathcal{P}^{(-)}(\tilde{x}, \tau)\,\mathrm{d}\tilde{x}. \tag{24}$$

Taking the limit $\tau \to \infty$ in equation (24), we obtain the asymptotical transmission probability for the packet [40]

$$\mathcal{L}_\infty = \lim_{\tau\to\infty} \int_{-\infty}^{0} \mathcal{P}^{(-)}(\tilde{x}, \tau)\, \mathrm{d}\tilde{x} = \int_{-\infty}^{0} |\varphi_0(\tilde{p})|^2 (1 - |\chi(\tilde{p})|^2)\, \mathrm{d}\tilde{p}. \tag{25}$$

The 'conditional' asymptotical average value of some function of momentum can be defined as [40, 65]

$$\langle\langle f(\tilde{p})\rangle\rangle_\infty = \mathcal{L}_\infty^{-1} \int_{-\infty}^{0} f(\tilde{p}) |\varphi_0(\tilde{p})|^2 (1 - |\chi(\tilde{p})|^2) \mathrm{d}\tilde{p}. \tag{26}$$

The physical meaning of this definition seems to be clear: it corresponds to the statistics of only those events which are related to the detection of a particle *behind the barrier*. For large negative values of $\tilde{p}_0$, $\mathcal{L}_\infty = T(\tilde{p}_0)$, moreover, one can replace a slowly varying reflection coefficient $|\chi(\tilde{p})|^2$ by its value at $p = p_0$ (keeping in mind that the main contribution to the integral in (26) is from a small region near the point p_0, due to the exponential form of the initial momentum distribution). Consequently, in this asymptotical case we have $\langle\langle f(\tilde{p})\rangle\rangle_\infty \approx \langle f(\tilde{p})\rangle_{t=0}$. In particular, $\langle\langle \tilde{p}\rangle\rangle_\infty \approx \tilde{p}_0$.

The situation is different if $|\tilde{p}_0| < 1$. We consider the case of $\tilde{p}_0 = 0$, when the effect is maximal. The calculations are simplified in the case of an almost perfectly reflecting barrier with $\mathcal{B} \gg 1$, when the plane wave transmission coefficient can be simplified as $1 - |\chi(\tilde{p})|^2 \approx \tilde{p}^2/\mathcal{B}^2$. Then equations (15) and (25) yield $\mathcal{L}_\infty = (8\mathcal{B}^2)^{-1}$. Moreover, the conditional asymptotical value of the average momentum in the transmitted packet does not depend on $\mathcal{B}$ in this limiting case: $|\langle\langle \tilde{p}\rangle\rangle| = \sqrt{2/\pi}$. Note that this value is twice as high as the mean momentum of reflected particles and the conditional mean value of the momentum of particles moving to the left in the absence of any barrier (for the Gaussian packet). Also, the value $|\langle\langle \tilde{p}\rangle\rangle|$ is slightly ($2/\sqrt{\pi}$ times) greater than the momentum corresponding to the velocity (21) of the peak of the transmitted packet, due to the finite width of the transmitted packet in the momentum space, which equals

$$\overline{\Delta_p} \equiv \sqrt{\langle\langle \tilde{p}^2\rangle\rangle - \langle\langle \tilde{p}\rangle\rangle^2} = \sqrt{(3\pi - 8)/(4\pi)} \approx 1/3.$$

We see that $\overline{\Delta_p}$ is less than the width of the initial momentum distribution (15) (which equals $1/2$ for the dimensionless variable $\tilde{p}$). Consequently, the transmitted packet also exhibits some 'squeezing' in the momentum distribution. It becomes narrower than the initial one, because the low energy plane wave components of the initial packet are transmitted through the barrier with much smaller probabilities than the high energy ones, so that the low energy components are 'lost' in the transmitted packet. This also explains why the conditional average value of the momentum in the transmitted packet is greater than that in the reflected packet. The product of conditional uncertainties $\overline{\Delta_p}\,\overline{\Delta_x}$ linearly increases with time (in the asymptotical regime), although its value is less than that in the case of a free packet.

3. Transmission times

There is a vast literature on the problem of 'tunnelling time' [66–68] or 'arrival time' [69] of quantum particles moving in various potentials or passing through potential barriers. However, the case of tunnelling through the *delta barrier* seems to have been missed (the 'delay time' for delta barriers was considered recently using the Floquet formalism [70] or initial cut-off plane waves [71]). Explicit expressions for the time-dependent packets give us a rare possibility of studying the problem in detail in this special case.

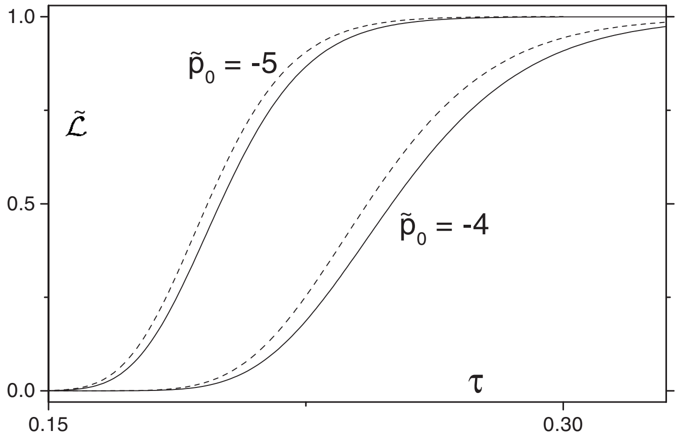

Figure 2. Normalized transmission probability $\tilde{\mathcal{L}}(\tau) = \mathcal{L}(\tau)/\mathcal{L}_\infty$ for initial packets with negative mean values of the momentum $\tilde{p}_0 = -4$ (right curves) and $\tilde{p}_0 = -5$ (left curves), for different values of the delta-potential strength $\mathcal{B} = 0$ (solid curves) and $\mathcal{B} = 20$ (dashed curves).

There are several possible ways of defining the 'transmission time'. For example, introducing the normalized transmission probability $\tilde{\mathcal{L}}(\tau) = \mathcal{L}(\tau)/\mathcal{L}_\infty$, one may assume that the transmission is practically finished when the difference $1 - \tilde{\mathcal{L}}(\tau)$ reaches some small given number ϵ, defining the 'conventional transmission time' τ_ϵ by means of the equation $1 - \tilde{\mathcal{L}}(\tau_\epsilon) = \epsilon$. Using equations (23) and (24) we obtain

$$\mathcal{L}(\tau) = \sqrt{\frac{2}{\pi}} \int_{1/\tau}^{\infty} \frac{y^2}{y^2 + \mathcal{B}^2} \exp(-2(y + \tilde{p}_0)^2)\, \mathrm{d}y. \tag{27}$$

An approximate analytical formula for the integral (27) can be easily found for large negative initial momenta: $\tilde{p}_0 < 0, |\tilde{p}_0| \gg 1$. Indeed, it is clear that the transmission probability is exponentially small until $|\tilde{p}_0|\tau < 1$, and it practically coincides with $T(|\tilde{p}_0|)$ when $|\tilde{p}_0|\tau \gg 1$. A rapid increase of $\mathcal{L}(\tau)$ from zero to the asymptotical value $\mathcal{L}_\infty = T(|\tilde{p}_0|)$ occurs during a rather short interval of time, when $|\tilde{p}_0|\tau \approx 1$. Writing $|\tilde{p}_0|\tau = 1 + \delta$ with $|\delta| \ll 1$, we can replace y by $|\tilde{p}_0|$ in the pre-exponential factor. Then the integral is reduced to the complementary error function (4), and we obtain an approximate analytical formula

$$\tilde{\mathcal{L}}(\tau) \approx \tfrac{1}{2}\,\mathrm{erfc}(\xi) \qquad \xi = \sqrt{2}|\tilde{p}_0|(1 - |\tilde{p}_0|\tau) \qquad |\tilde{p}_0| \gg 1. \tag{28}$$

Typical dependences $\tilde{\mathcal{L}}(\tau)$ for $|\tilde{p}_0|\tau \gg 1$, following from numerical integration of (27), are shown in figure 2. One can see that with increasing absolute value of the initial momentum $|\tilde{p}_0|$, the transition region moves to shorter times and becomes narrower. The same behaviour is observed if one increases the strength of the delta potential $\mathcal{B}$ for a fixed value of p_0. However, this effect is rather weak, and it is neglected in the approximate formula (28). Taking into account formula (7), we obtain asymptotical expressions for $|\xi| \gg 1$:

$$\tilde{\mathcal{L}}(\tau) \approx \begin{cases} \dfrac{\exp(-\xi^2)}{2\sqrt{\pi}|\xi|} & \xi > 0 \\[2ex] 1 - \dfrac{\exp(-\xi^2)}{2\sqrt{\pi}|\xi|} & \xi < 0. \end{cases} \tag{29}$$

As a matter of fact, deviations from the asymptotical values are already less than 1% for $|\xi| = 2$. Thus, the transmission time $\tau_{0.01}$ equals approximately the difference between two

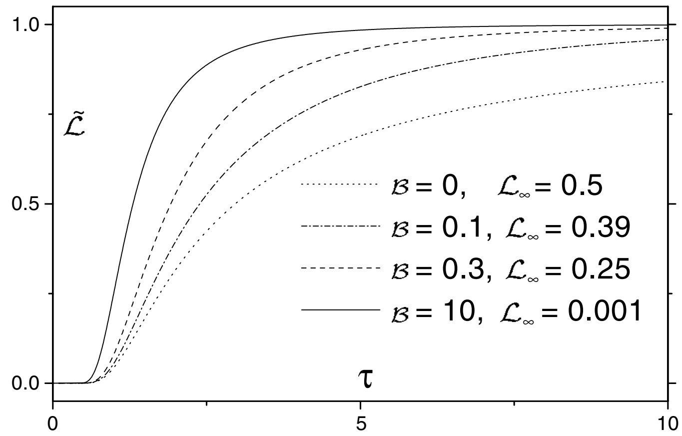

Figure 3. Normalized transmission probability $\tilde{\mathcal{L}}(\tau) = \mathcal{L}(\tau)/\mathcal{L}_\infty$ for the initial packet with zero mean value of the momentum $\tilde{p}_0 = 0$, for different values of the dimensionless strength of delta potential $\mathcal{B}$ (from bottom to top): 0; 0.1; 0.3; 10.

values of variable τ which give $\xi = \pm 2$. Therefore, $\tau_{0.01} \approx 2\sqrt{2}\big/\tilde{p}_0^2$ (or $4m\hbar x_c\big/\left(p_0^2 s\right)$ in the dimension variables). This value does not depend on the strength of the delta potential (remember that we consider the limit of packets with large initial momentum p_0, exceeding the width of the initial momentum distribution, which has an order of $\hbar/s$), being determined completely by the difference between the instants of time when the plane wave components of the initial packet, corresponding to the 'effective borders' $p = p_0 \pm 2\hbar/s$ of the momentum distribution (15), reach the position of the barrier $x = 0$ from the initial point x_c.

In the case of zero initial momentum $p_0 = 0$, the integral (27) can be calculated exactly if $\mathcal{B} = 0$ and approximately if $|\mathcal{B}| \gg 1$ (when one can neglect the term y^2 in the denominator of the integrand):

$$\tilde{\mathcal{L}}(\tau) = \operatorname{erfc}(\sqrt{2}/\tau) \qquad \mathcal{B} = 0 \tag{30}$$

$$\tilde{\mathcal{L}}(\tau) = \operatorname{erfc}\left(\frac{\sqrt{2}}{\tau}\right) + \frac{\sqrt{8}}{\sqrt{\pi}\,\tau}\exp\left(-\frac{2}{\tau^2}\right) \qquad \mathcal{B} \gg 1. \tag{31}$$

Thus, we obtain the following asymptotical behaviour of the normalized transmission probability at $\tau \gg 1$ in these two opposite limit cases:

$$\tilde{\mathcal{L}}(\tau) = \begin{cases} 1 - \dfrac{8\sqrt{2}}{3\sqrt{\pi}\,\tau^3} + \mathrm{O}(\tau^{-5}) & \mathcal{B} \gg 1 \\[2ex] 1 - \dfrac{2\sqrt{2}}{\sqrt{\pi}\,\tau} + \mathrm{O}(\tau^{-3}) & \mathcal{B} \ll 1. \end{cases} \tag{32}$$

Results of numerical calculations of the function $\tilde{\mathcal{L}}(\tau)$ for different values of $\mathcal{B}$ are shown in figure 3. We see that the time of transmission of the packet to the left half-space in the presence of a delta barrier is shorter than for a freely expanding packet with zero initial momentum, and it goes to some finite asymptotical value for $\mathcal{B} \gg 1$. Equation (32) shows that for $p_0 = 0$, roughly speaking, $\tau_\epsilon \sim \epsilon^{-1}$ for $\mathcal{B} \ll 1$ and $\tau_\epsilon \sim \epsilon^{-1/3}$ for $\mathcal{B} \gg 1$.

An obvious disadvantage of the parameter τ_ϵ is an arbitrariness in the choice of ϵ. This ambiguity can be removed if one notes that the function $\tilde{\mathcal{L}}(\tau)$ is *monotonic*: see figures 2

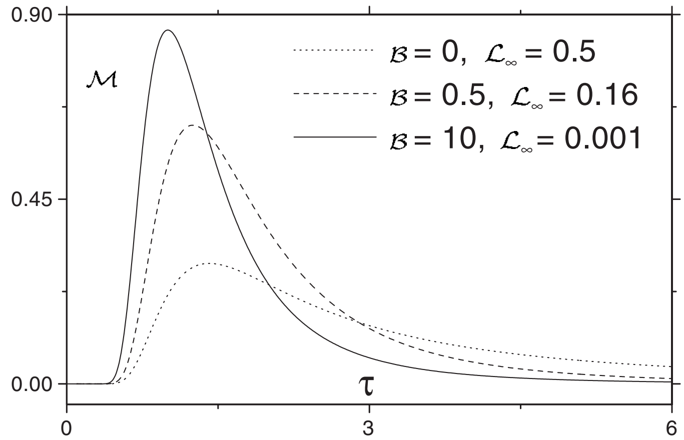

Figure 4. The 'transmission time probability density' function (34) for $\tilde{p}_0 = 0$ and different values of $\mathcal{B}$ (from bottom to top for τ small and in the inverse order for τ big): 0; 0.5; 10.

and 3. Consequently, the derivative $\mathcal{M}(\tau) \equiv \mathrm{d}\tilde{\mathcal{L}}(\tau)/\mathrm{d}\tau$ is nonnegative, and it can be considered as the probability density of particle transmission through the barrier in the interval between τ and $\tau + \mathrm{d}\tau$, because $\int_0^\infty [\mathrm{d}\tilde{\mathcal{L}}(\tau)/\mathrm{d}\tau]\,\mathrm{d}\tau = 1$. Thus, we can define the *mean transmission time* as (cf [72])

$$\bar{\tau} = \int_0^\infty \tau \mathcal{M}(\tau)\,\mathrm{d}\tau. \tag{33}$$

In view of equation (27) we have

$$\mathcal{M}(\tau) = \sqrt{\frac{2}{\pi}} \frac{\exp[-2(1+\tilde{p}_0\tau)^2/\tau^2]}{\mathcal{L}_\infty \tau^2(1+\mathcal{B}^2\tau^2)}. \tag{34}$$

In the special case of $\tilde{p}_0 = 0$, the integral (33) with the function (34) can be reduced to the integral exponential function

$$E_1(x) \equiv \int_x^\infty \frac{\mathrm{d}t}{t}\,\mathrm{e}^{-t} \tag{35}$$

by means of the substitution $t = 2\mathcal{B}^2 + 2/\tau^2$, and we find

$$\bar{\tau} = \frac{\mathcal{L}_\infty^{-1}}{\sqrt{2\pi}} E_1(2\mathcal{B}^2)\,\mathrm{e}^{2\mathcal{B}^2}. \tag{36}$$

For $\mathcal{B} \gg 1$ one can use the asymptotics of $E_1(x)$ for $x \gg 1$ or calculate the integral (33) directly, neglecting 1 with respect to $\mathcal{B}^2\tau^2$ in the denominator of (34) and making the substitution $t = \tau^{-2}$ in the integral. Both ways lead to the same result: since $\mathcal{L}_\infty \sim \mathcal{B}^{-2}$, the mean transmission time goes to the constant asymptotical value $\bar{\tau}_\infty = \sqrt{8/\pi}$ for $\mathcal{B} \gg 1$ and $\tilde{p}_0 = 0$. However, the integral (33) with the function (34) diverges as $\mathcal{B} \to 0$, so that $\bar{\tau} = \infty$ for the free packet with any value of $\tilde{p}_0$. Although one could try to find some explanation for such behaviour in the case of $\tilde{p}_0 = 0$, where the function $\mathcal{M}(\tau)$ behaves more or less differently for $\mathcal{B} = 0$ and $\mathcal{B} \gg 1$ (see figure 4), there are no reasonable physical explanations for the divergence of transmission time at $\mathcal{B} \to 0$ for $|\tilde{p}_0| \gg 1$, where the plots of $\mathcal{M}(\tau)$ practically do not depend on $\mathcal{B}$: see figure 5. This divergence seems, therefore, to be a mathematical artefact, indicating that the integral (33) is not, in fact, a good measure of the transmission time.

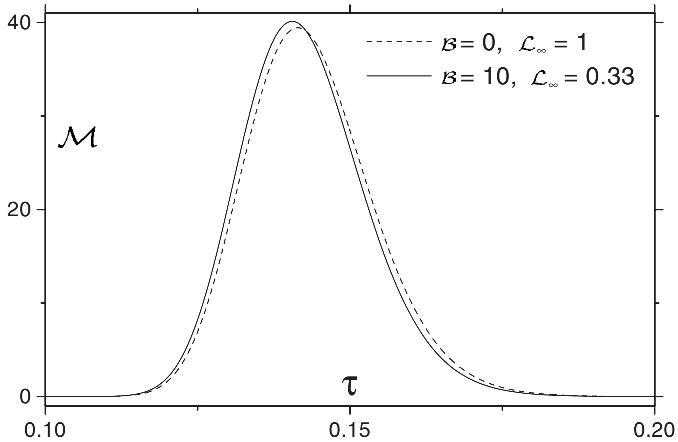

Figure 5. The 'transmission time probability density' function (34) for $\tilde{p}_0 = -7$ and different values of the dimensionless strength of delta potential $\mathcal{B} = 0$ (dashed curve) and $\mathcal{B} = 10$ (solid curve).

For these reasons, it seems more natural to define the transmission time as

$$T_{\mathrm{tr}} = [\max_{0<\tau<\infty} \mathcal{M}(\tau)]^{-1} \tag{37}$$

(a similar definition of the *spatial* extension of packets was used in [48]), because it agrees with the usual estimation of the width of the normalized distribution $\mathcal{M}(\tau)$ by means of the relation $T_{\mathrm{tr}} \cdot \max \mathcal{M} = 1$. For $\tilde{p}_0$ negative and $|\tilde{p}_0| \gg 1$, the maximum of function (34) is attained for $\tau_m \approx |\tilde{p}_0|^{-1}$ (when the argument of the exponential function is close to zero), and we find $T_{\mathrm{tr}} \approx \sqrt{\pi/2}\tilde{p}_0^{-2}$, independently of $\mathcal{B}$, i.e. the same dependence (up to a numerical coefficient) as for $\tau_{0.01}$. For $\tilde{p}_0 = 0$, changing $\mathcal{B}$ from 0 to ∞ shifts the position of maximum of function $\mathcal{M}(\tau)$ from $\tau = \sqrt{2}$ to $\tau = 1$ and diminishes the transmission time $T_{\mathrm{tr}}(\mathcal{B}, \tilde{p}_0)$ from $T_{\mathrm{tr}}(0, 0) = e\sqrt{\pi/2}$ to $T_{\mathrm{tr}}(\infty, 0) = e^2\sqrt{\pi/128}$ (about three times).

4. Time-dependent delta potential

It was shown in [18] (following the ideas of [73]) that the propagator (3) can be easily generalized to the case of a specific time dependence of the delta-potential strength

$$V(x,t) = \frac{\mathcal{Z}\delta(x)}{\zeta(t)} \qquad \zeta(t) = 1 + \alpha t. \tag{38}$$

The generalized propagator in the dimensionless variables is (to return to dimensional values one should use transformations (5) and the substitution $\alpha \to m\alpha/\hbar$)

$$G_{\mathcal{Z}}^{(\alpha)}(x,x';t) = G_0(x,x';t) - \frac{\mathcal{Z}}{2\sqrt{\zeta}} \operatorname{erfc}\left[\frac{|x| + |x'|\zeta + \mathcal{Z}\mathrm{i}t}{\sqrt{2\mathrm{i}t\zeta}}\right] \times \exp\left[\frac{\mathrm{i}\alpha}{2\zeta}(x^2 - x'^2\zeta) + \frac{\mathcal{Z}}{\zeta}\left(|x| + |x'|\zeta + \frac{\mathrm{i}\mathcal{Z}t}{2}\right)\right] \tag{39}$$

where $G_0(x,x';t)$ is the free-space propagator given by the first term on the right-hand side of equation (3). Formula (39) holds for $0 < t < \infty$ if α is positive and for $0 < t \leqslant t_* = |\alpha|^{-1}$ if α is negative, because in the last case, the strength of the delta potential becomes infinite at the instant of time t_*, when $\zeta(t_*) = 0$, and there is no unambiguous way to continue the solutions for $t > t_*$. At the critical instant t_*, one can use the asymptotical formula (7) to obtain the expression resembling (6), but with some modifications:

$$G_*(x, x'; t_*) = (2\mathrm{i}\pi t_*)^{-1/2} \left\{ \exp\left[\frac{\mathrm{i}(x'-x)^2}{2t_*}\right] - \left(1 - \frac{\mathrm{i}|x|}{\mathcal{Z} t_*}\right)^{-1} \exp\left[\frac{\mathrm{i}(|x'|+|x|)^2}{2t_*}\right] \right\}. \quad (40)$$

Note that the modifying pre-exponential factor does not depend on the second argument x' of the propagator (over which the integration in formula (2) is performed).

Applying the propagator (39) to the initial state (8), we obtain the generalization of formula (11)

$$\begin{aligned} \psi(\tilde{x}, \tau) = {} & \left(\frac{2\beta^2}{\pi \upsilon^2}\right)^{1/4} \exp\left[-\frac{\beta^2}{\upsilon}(\tilde{x} - 1 - \tilde{p}_0\tau)^2 + \mathrm{i}\beta\tilde{p}_0(2\tilde{x} - \tilde{p}_0\tau)\right] \\ & - \frac{\mathcal{B}\left(2\pi\beta^2\right)^{1/4}}{[\zeta(1+\mathrm{i}A)]^{1/2}} \operatorname{erfc}\left[\frac{\beta(1+\mathrm{i}A)|\tilde{x}| + \mathcal{B}\upsilon + \zeta(\beta + \mathrm{i}\tilde{p}_0)}{[\zeta(1+\mathrm{i}A)\upsilon]^{1/2}}\right] \\ & \times \exp\left[\frac{\beta|\tilde{x}|}{\zeta}(2\mathcal{B} + \mathrm{i}A\beta|\tilde{x}|) + \frac{\mathcal{B}^2\upsilon}{\zeta(1+\mathrm{i}A)} + \frac{2\mathrm{i}\tilde{p}_0(\beta+\mathcal{B}) + \beta(2\mathcal{B} - \mathrm{i}A) - \tilde{p}_0^2}{1+\mathrm{i}A}\right] \end{aligned} \quad (41)$$

where

$$\zeta(\tau) = 1 + A\beta\tau \qquad A = \alpha m s^2/\hbar \quad (42)$$

and other variables and parameters were defined in (10). Obviously, the parameter α^{-1} has the meaning of time of existence of the barrier (for $\alpha > 0$), whereas the quantity $ms^2/\hbar$ characterizes the time of spreading of the initial packet. Therefore, we confine ourselves to the analysis of the case $|A| \ll 1$ (otherwise the delta potential practically disappears long before the main part of the packet reaches the point $x = 0$). On the other hand, the product $A\beta \sim \alpha m s x_c/\hbar$ has the meaning of the ratio of the time necessary to reach the position of the barrier (x_c/v_s, where the spreading velocity has the order $\hbar/ms$) to the time of existence of the barrier, so that it is reasonable to suppose that $|A|\beta$ can be of the order of unity or bigger (otherwise we have the case of practically stationary delta potential). We shall also assume that

$$\beta \gg 1 \qquad \beta\tau \gg 1 \qquad \beta \gg |\tilde{p}_0| \qquad \beta \gg |\mathcal{B}|. \quad (43)$$

Let us consider first the case of α positive. Replacing again the complementary error function in (41) by its asymptotical form (7) and taking into account the restrictions (43), one can verify that the probability density of the transmitted part of the packet (for $\tilde{x} < 0$) can be expressed in almost the same form as in equation (18), with the only difference that the terms $1 - \tilde{x}$ should be replaced by $\zeta(\tau) - \tilde{x}$ *in the pre-exponential factor* (but not in the argument of the exponential):

$$\mathcal{P}^{(-)}(\tilde{x}, \tau) \approx \left(\frac{2}{\pi\tau^2}\right)^{1/2} \frac{(\zeta - \tilde{x})^2}{(\zeta - \tilde{x})^2 + \tau^2\mathcal{B}^2} \exp\left[-\frac{2}{\tau^2}(\tilde{x} - 1 - \tilde{p}_0\tau)^2\right]. \quad (44)$$

As a consequence, we have the following generalization of formula (34) for the transmission time probability density:

$$\mathcal{M}(\tau) = \mathcal{L}_\infty^{-1} \left(\frac{2}{\pi}\right)^{1/2} \frac{\zeta^2}{\tau^2(\zeta^2 + \mathcal{B}^2\tau^2)} \exp\left[-\frac{2}{\tau^2}(1 + \tilde{p}_0\tau)^2\right] \quad (45)$$

where

$$\mathcal{L}_\infty = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \mathrm{d}y \frac{(y + A\beta)^2}{(y + A\beta)^2 + \mathcal{B}^2} \exp[-2(y + \tilde{p}_0)^2]. \quad (46)$$

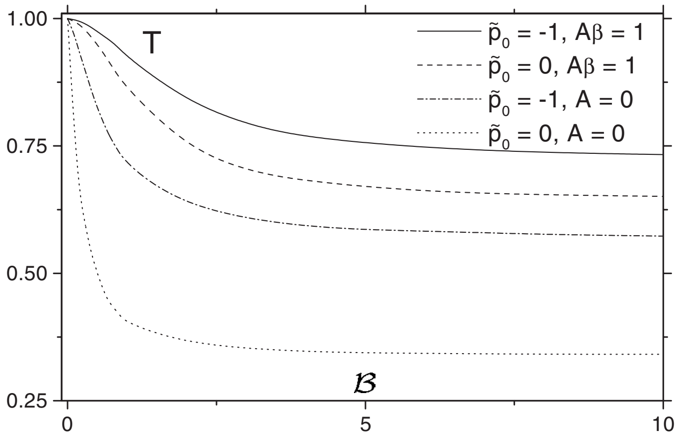

Figure 6. The ratio $T(\mathcal{B}) \equiv T_{\rm tr}(\mathcal{B})/T_{\rm tr}(0)$ as a function of $\mathcal{B}$ for fixed values of the mean initial momentum $\tilde{p}_0$ and the parameter $A\beta$, characterizing the rate of decay of the barrier.

If $A\beta \gg 1$ and $\tilde{p}_0 = 0$, then $\mathcal{L}_\infty \approx \frac{1}{2}[1 + (\mathcal{B}/A\beta)^2]^{-1}$. In figure 6 we show the dependence of the ratio $T_{\rm tr}(\mathcal{B})/T_{\rm tr}(0)$ on $\mathcal{B}$ for some fixed values of parameters $\tilde{p}_0$ and $A\beta$. We see that in all the cases, this ratio decreases with increase of the delta-potential strength $\mathcal{B}$, going to nonzero asymptotical values. In turn, these asymptotical values increase with increase of $|\tilde{p}_0|$ and $A\beta$, approaching the unit value when either of these parameters becomes large enough.

For α negative, it is interesting to analyse what happens at the critical instant of the dimensionless time $\tau_* = (\beta|A|)^{-1}$, when 'the tunnel to behind the mirror closes up'. Under the conditions (43), the coordinate probability density behind the mirror ($\tilde{x} < 0$) is given by

$$\mathcal{P}^{(-)}(\tilde{x}, \tau_*) = \beta|A| \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{\tilde{x}^2}{\tilde{x}^2 + \mathcal{B}^2\tau_*^2}\right) \exp[-2(\beta|A|)^2(\tilde{x} - 1 - \tilde{p}_0\tau_*)^2]. \tag{47}$$

The coordinate dependent pre-exponential factor can be replaced by unity if $\beta|A| \gg \mathcal{B}$. In this case, the ultimate transmission probability equals

$$\mathcal{L}(\tau_*) = \tfrac{1}{2}\,\mathrm{erfc}[(\beta|A| + \tilde{p}_0)\sqrt{2}]. \tag{48}$$

For the reflected part of the packet, it is interesting to know the asymptotical value (when $\tau \to \infty$, i.e. for $A > 0$) of the average momentum for $\tilde{p}_0 = 0$. Under the conditions (43), it can be reduced to the integral

$$\langle \tilde{p}_\infty \rangle \approx \frac{4\mathcal{B}}{(2\pi)^{1/2}} \int_0^\infty \frac{\mathrm{d}y(\mathcal{B}y + Ay^2)\,\exp(-2y^2)}{(A\beta + y)^2 + (Ay + \mathcal{B})^2}. \tag{49}$$

Due to the presence of the exponential factor in the integrand, the main contribution to the integral (49) is from the domain $y < 2$. If $\mathcal{B} \gg 1$ (almost perfectly reflecting initial barrier) and $A \ll \mathcal{B}$, then one can neglect the variable y in the denominator of the integrand (retaining the factor $A\beta$, which can be large) and the term Ay^2 in the numerator. After this, the integral becomes trivial, and we obtain the expression

$$\langle \tilde{p}_\infty \rangle \approx \{(2\pi)^{1/2}[1 + (A\beta/\mathcal{B})^2]\}^{-1} \tag{50}$$

containing again the characteristic combination $(A\beta/\mathcal{B})^2$. We see that increasing the product $A\beta$ makes the same effect as decreasing the initial strength of the delta potential $\mathcal{B}$. This is quite clear, because the value of $A\beta$ characterizes the time necessary for the expanding packet to reach the barrier. But at this moment in the nonstationary case the packet will 'meet' not the initial barrier, but a barrier whose strength became $A\beta$ times weaker, due to the specific time dependence (38).

5. Conclusion

We have analysed the problem of transmission and reflection of initially narrow Gaussian packets by the delta potentials of constant and special time-dependent strengths. We have obtained approximate analytical expressions for the coordinate and momentum probability densities behind the barrier. These expressions demonstrate some 'squeezing' both in the momentum and coordinate distributions (as soon as these distributions reproduce each other in the asymptotical regime after some scaling of variables), compared with the case of free expansion in the absence of a barrier. Nonetheless, the uncertainty relations are not violated, because the coordinate variance unlimitedly grows with time (although slower than in the case of a free packet).

Also, we have introduced two functions, which can be interpreted as a transmission time probability density and a total time-dependent transmission probability. Using these functions, we have considered several possible definitions of the transmission time and analysed their dependence on the parameters of the initial packet and the potential. Qualitatively, all the definitions lead to the conclusion that the transmission time diminishes with increase of the strength of the delta potential. However, this effect is significant only for slow initial packets, being practically unobservable in the case of packets with large negative initial average momenta. Moreover, the transmission times do not reduce unlimitedly, but they tend to some finite asymptotical values as the strength of the delta potential goes to infinity (when the total transmission probability tends to zero). The best definition of the transmission time in the case under study seems to be the inverse height of the maximum of the transmission time probability density.

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