Effect of classically forbidden momenta in one dimensional quantum scattering

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The transmitted wave that results from a collision of a wave packet which is initially to the left of a potential barrier depends in general on the amplitudes of negative momenta of the initial state. The exact form of this dependence is shown and the importance of this classically forbidden effect is illustrated with numerical examples. Special care is taken to account properly for bound states.

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I. INTRODUCTION

Suppose that a classical ensemble of independent particles in one dimension is initially confined (at $t = 0$) in the spatial interval $a < x < b \leq 0$, and allowed to move freely after $t = 0$. Only particles with positive momenta may arrive at positive positions for $t > 0$. In contrast, the quantum wave function involves negative-momentum contributions as well,

$$\psi(x, t) = h^{-1/2} \int_{-\infty}^{\infty} dp e^{i p x / \hbar} \tilde{\psi}(p) e^{-i E_p t / \hbar},$$

where $E_p = p^2 / 2m$, and

$$\tilde{\psi}(p) = h^{-1/2} \int_{-\infty}^{\infty} dx e^{-i p x / \hbar} \psi(x, 0)$$

is the momentum representation of the initial state. The effect of negative momenta for $x, t > 0$ is however a transient one; the total final probability to find the particle at $x > 0$ is given only by positive momentum components,

$$P_T(\infty) \equiv \lim_{t \to \infty} \int_0^\infty dx |\psi(x, t)|^2 = \int_0^\infty dp |\tilde{\psi}(p)|^2,$$

see e.g. [1] or [2], since there are no bound states. This negative-momentum effect is also present in collisions, where it is combined with other classically forbidden effects. Consider the family of cut-off potentials of the form

$$V(x) = \begin{cases} 0 & \text{if } x < c, \\ U(x), & \text{if } c \leq x \leq d, \\ V_0, & \text{if } x > d, \end{cases}$$

where $V_0 \geq 0$ and $V(x)$ are real, as depicted in Fig. 1.

![FIG. 1. Scattering process in a “cut-off” potential: the support of the potential is compact; an incident wave with momentum $p$ produces a transmitted and a reflected wave.](image-url)
Let us suppose that the maximum value of the potential is $V_M$. For a classical ensemble confined between $a$ and $b$ (such that $a < b$ and $c \leq d \leq 0$) only particles with initial momentum above the “barrier momentum” $p_M \equiv (2mV_M)^{1/2}$ may pass to the right of the potential region. In the quantum case however, there are contributions from all the components of the initial wave packet: (a) $p > p_M \equiv (2mV_M)^{1/2}$ (above-the-barrier transmission); (b) $p_0 < p < p_M$ (“asymptotic” tunneling, these momenta contribute to the transmission probability $P_T(\infty)$); (c) $0 < p < p_0$ (“transient tunnelling”, these momenta do not contribute to $P_T(\infty)$); (d) $-\infty < p < 0$ (transient negative-momentum effect); (e) $p_j = i\gamma_j, \gamma_j > 0$ (tunnel effect associated with bound states, which do contribute to $P_T(\infty)$).

While the various tunnel effects have been well discussed in the literature, even though not as clearly distinguished as in the above classification, the negative momentum effect, actually the only one that survives for free motion, has been frequently overlooked, a clear exception being [3,4]. This paper is complementary to the more usual treatments of one dimensional scattering [5–8], and lies in the wake of [3,4], who did consider in a concise manner all these effects, with special emphasis on the inclusion of bound states. Our S-matrix treatment is more explicit than that of [3,4], and shows how the resolution of the identity in scattering eigenstates leads to compact expressions for the transmitted wave packet. We also illustrate the negative momentum effect with some numerical examples and work out in detail both the case when the state is confined initially to the lower level and when the initial confining is to the upper level (for which case the frequently overlooked contributions are those of positive momenta, including evanescent waves). The contribution of bound states is indicated explicitly, both formally and with some numerical examples.

II. "STATIONARY" EIGENSTATES OF THE HAMILTONIAN

The total Hamiltonian $H = H_0 + V$ may have a discrete set of bound states $\{ |E_j \rangle \}$, with energies $E_j < 0$ and (real) wavefunctions $\psi_j(x)$, and a continuum of “stationary scattering eigenstates” with $E_p > 0$. Only the former belong to the Hilbert space of square integrable functions. The latter however form a convenient basis normalized according to Dirac’s delta. For energies above $V_0$, the energy spectrum is doubly degenerate as corresponds physically to incidence from one side or the other. Below $V_0$ there is only one linearly independent solution. The resolution of the identity may be written in different ways, in particular as

$$1 = \sum_j |E_j\rangle \langle E_j| + \int_{-\infty}^{-p_0} dp |p^+\rangle \langle p^+| + \int_{p_0}^{\infty} dp |p^+\rangle \langle p^+| + \int_{p_0}^{-p_0} dp |p^-\rangle \langle p^-|,$$

(5)

where the states $|p^\pm\rangle$ have energy $E_p = p^2/(2m)$. Continuum and bound states are orthogonal. Moreover, $\langle p^\pm|p'^\pm\rangle = \delta(p-p')$, and $\langle E_j|E_k\rangle = \delta_{j,k}$. The first two integrals in Eq. (5) reflect the double degeneracy signalled above, whereas the last integral corresponds to the non-degenerate part of the continuous spectrum. The reason for the sign choice in front of the last integral is due to the unified notation we shall now introduce for the generalized eigenstates associated with the continuous part of the spectrum.

The states $|p^+\rangle$ with $p > 0$ are characterized by an incident plane wave of momentum $p$ from the left. The asymptotic behaviour of their wave-functions $\psi_{p^+}(x)$ is

$$\psi_{p^+}(x) = \frac{1}{h^{1/2}} \times \begin{cases} \exp(ipx/h) + R'(p)\exp(-ipx/h), & x < c \\ T'(p)\exp(ipx/h), & x > d, \end{cases}$$

(6)

where $q$ is the momentum with respect to the upper (right) level of the potential, $q = (p^2 - 2mV_0)^{1/2}$. For the evanescent regime, i.e. when $p^2 < 2mV_0$, the plane waves on the right become decaying exponentials so the positive imaginary square root is taken. $R'(p)$ and $T'(p)$ are reflection and transmission amplitudes for left incidence. They are obtained by solving the stationary Schrödinger equation subject to the boundary conditions specified in (6).

The states $|p^+\rangle$ for $p < -p_0$ are defined by having an incident plane wave from the right, oscillating with spatial frequency $|q|/h$, where now the negative square root is taken, $q = -(|p^2 - 2mV_0|)^{1/2}$. The asymptotic behaviour of the corresponding wave-functions is

$$\psi_{p^+}(x) = \frac{1}{h^{1/2}} \left( \frac{p}{q} \right)^{1/2} \times \begin{cases} T'(p)\exp(ipx/h), & x < c \\ \exp(ipx/h) + R'(p)\exp(-iqx/h), & x > d, \end{cases}$$

(7)

The factor $(p/q)^{1/2}$ is necessary for the proper delta normalization. $R'(p)$ and $T'(p)$ are reflection and transmission amplitudes for right incidence. Note that the arguments of transmission or reflection amplitudes are always positive for states $|p^+\rangle$, independently of the sign of $p$.

In both cases, (6) and (7), $q$ may be defined as the square root of $p^2 - 2mV_0$ with a branch cut that joins the branch points $p = \pm p_0$ going slightly below Im$(p) = 0$. In this way the sign of $q$ is the same as the sign of $p$ for $p^2 > p_0^2$. 

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The states $|p^-\rangle$ are obtained simply by considering $p < 0$ in expression (1) and $p > p_0$ in expression (7). In these states there appears an outgoing plane wave instead of an incident plane wave. Thus, the right hand side of Eq. (1), with $p < 0$, gives the corresponding states $|p^-\rangle$, as those with a left-outgoing plane wave of absolute momentum $|p|$, and can be read as $\psi_{p^-}(x)$, for $p < 0$. For $p < -p_0$, $q < 0$, whereas for $-p_0 < p < 0$, $q$ becomes as before a positive imaginary number. States $|p^-\rangle$ with a right-outgoing plane wave are defined by the right hand side of Eq. (7), with $p > p_0$, and $q > 0$. Note that the arguments of the amplitudes $R^{r,l}(p)$ and $T^{r,l}(p)$ are negative for $|p^-\rangle$ states. Since the formal boundary conditions that define the states $|p^\pm\rangle$ are in fact equal, the negative-argument amplitudes will be given by the same formal expressions valid for their positive-argument counterparts. For the same reason, we shall refer to $R^{r,l}(p)$ and $T^{r,l}(p)$ as “reflection” and “transmission” amplitudes independently of the sign of $p$, even though, on physical grounds, this terminology and notation would only be appropriate for the $p > 0$ case (only in that case does $T^{r,l}$ multiply a transmitted wave and $R^{r,l}$ a reflected wave).

Reflection and transmission amplitudes are not independent. The unitarity of the $S$ matrix imposes certain relations among them. The $S$ matrix elements are defined as the coefficients multiplying the outgoing plane waves when the incident plane wave is normalized to unit flux. When the two channels of the one dimensional scattering are open (this happens for $p > p_0$), they are given by

$$S(p) = \begin{pmatrix} \left(\frac{p}{q}\right)^{1/2} T^l(p) & R^l(p) \\ R^r(p) & \left(\frac{q}{p}\right)^{1/2} T^r(p) \end{pmatrix}$$

(8)

The unitarity of the $S$ matrix, $SS^\dagger = 1$, implies that

$$\frac{p}{q}|T^r(p)|^2 + |R^r(p)|^2 = 1,$$

(9)

$$|R^l(p)|^2 + \frac{q}{p}|T^l(p)| = 1,$$

(10)

$$\frac{p}{q} T^r(p) R^l(p)^* + R^r(p) T^l(p)^* = 0.$$  

(11)

For $0 < p < p_0$ only one channel is open, and the $S$ matrix reduces to a number, $R^l(p)$. Unitarity implies in this case

$$R^l(p) R^l(p)^* = 1, \quad 0 < p < p_0.$$  

(12)

All these equations, from (1) to (12), are also valid for negative momenta and relate the amplitudes associated with $|p^-\rangle$ states. They can also be derived by comparing various Wronskians of the stationary scattering states at different regions.

For the evanescent case, $0 < p < p_0$, one important relation follows by multiplying $|p^\pm\rangle$ by $R^l(p)^*$ and using (12). This gives the state $| - p^-\rangle$. Equating the coefficients for $x > d$,

$$T^l(-p) = T^l(p) R^l(p)^*, \quad 0 < p < p_0.$$  

(13)

Similarly, by taking the complex conjugate of the boundary conditions (3) and (5), it is found that $\psi_{-p^-}(x) = \psi_{p^+}(x)^*$, and comparing the coefficients that multiply the exponentials,

$$T^{r,l}(-p) = T^{r,l}(p)^*,$$

(14)

$$R^{r,l}(-p) = R^{r,l}(p)^*.$$  

(15)

Another important relation between $T^l(p)$ and $T^r(p)$ follows by equating the Wronskians of $\psi_{p\pm}(x)$ and $\psi_{-p\pm}(x)$ at $x < c$ and $x > d$,

$$T^r(p) p = T^l(p) q.$$  

(16)

As an illustration of the above, the reflection and transmission amplitudes for the simple step potential ($c = d = 0$, $U(x) = 0$) are given, for all $p$, by

$$T^l(p) = \frac{2p}{q + p}; \quad R^l(p) = \frac{p - q}{q + p};$$

$$T^r(p) = \frac{2q}{p + q}; \quad R^r(p) = \frac{q - p}{p + q}.$$  

(17)

The reader may easily check relations (14-16) for amplitudes that correspond to the step potential, Eq. (17), as a test of their validity.

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III. A COMPACT EXPRESSION FOR THE TRANSMITTED WAVE FUNCTION

In this section we shall find, using the relations of the previous one, an expression for \( \psi(x, t) \), with \( t > 0 \) and \( x > d \), assuming that the initial wave function is restricted to \( a < x < b \leq c \). First we insert the resolution of the identity in terms of bound states and scattering states \( |p^+\rangle \),

\[
\psi(x, t) = \sum_j \phi_j(x) \langle E_j | \psi(0) \rangle e^{-iE_j t / \hbar} \\
+ \int_{-\infty}^{-p_0} dp \psi_{p^+}(x) \langle p^+ | \psi(0) \rangle e^{-iE_p t / \hbar} \\
+ \int_0^\infty dp \psi_{p^+}(x) \langle p^+ | \psi(0) \rangle e^{-iE_p t / \hbar}, \quad \forall x \text{ and } \forall t. \tag{18}
\]

Because of the initial restriction of the wave function, the matrix element \( \langle p^+ | \psi(0) \rangle \) may be evaluated with the aid of Eqs. (6) and (7),

\[
\langle p^+ | \psi(t = 0) \rangle = \begin{cases} \left( \frac{2}{\pi} \right)^{1/2} \tilde{\psi}(p) T^*(p), & p < -p_0, \\ \psi(p) + \tilde{\psi}(-p) R^i(p)^*, & p > 0. \end{cases} \tag{19}
\]

Now we use Eqs. (6-7) and (19) in (18), for \( x > d \),

\[
\psi(x, t) = \sum_j \phi_j(x) \langle E_j | \psi(t = 0) \rangle e^{-iE_j t / \hbar} \\
+ \hbar^{-1/2} \int_{-\infty}^{-p_0} dp \frac{p}{q} \left[ e^{iqx / \hbar} + R^r(-p) e^{-iqx / \hbar} \right] T^r(-p)^* \tilde{\psi}(p) e^{-iE_p t / \hbar} \\
+ \hbar^{-1/2} \int_0^\infty dp T^i(p) e^{iqx / \hbar} \left[ \tilde{\psi}(p) + R^i(p)^* \tilde{\psi}(-p) \right] e^{-iE_p t / \hbar}, \quad x > d, \tag{20}
\]

and reorganize the terms as follows,

\[
\psi(x, t) = \sum_j \phi_j(x) \langle E_j | \psi(t = 0) \rangle e^{-iE_j t / \hbar} \\
+ \hbar^{-1/2} \int_{-\infty}^{-p_0} dp \frac{p}{q} T^r(-p)^* \tilde{\psi}(p) e^{iqx / \hbar} e^{-iE_p t / \hbar} \\
+ \hbar^{-1/2} \int_{-\infty}^{-p_0} dp \left[ \frac{p}{q} R^r(-p) T^r(-p)^* + T^i(-p) R^i(-p)^* \right] \tilde{\psi}(p) e^{-iqx / \hbar} e^{-iE_p t / \hbar} \\
+ \hbar^{-1/2} \int_0^\infty dp T^i(-p) R^i(-p)^* \tilde{\psi}(p) e^{iqx / \hbar} e^{-iE_p t / \hbar} \\
+ \hbar^{-1/2} \int_0^\infty dp T^i(p) \tilde{\psi}(p) e^{iqx / \hbar} e^{-iE_p t / \hbar}, \quad x > d. \tag{21}
\]

Keep in mind that between \( -p_0 < p < p_0 \), \( q \) is a positive imaginary number, \( q = i(|p^2 - 2mV_0|)^{1/2} \). The second term in the third line and the fourth line come from a variable change \( p \to -p \).

Making use of Eqs. (11-16), there results the simple form

\[
\psi(x, t) = \sum_j \phi_j(x) \langle E_j | \psi(t = 0) \rangle e^{-iE_j t / \hbar} \\
+ \hbar^{-1/2} \int_{-\infty}^\infty dp T^i(p) \tilde{\psi}(p) e^{iqx / \hbar} e^{-iE_p t / \hbar}, \quad x > d. \tag{22}
\]

The equation can be put in an even more compact form as shown in the next section.
IV. BOUND STATES

None of the particles of the classical ensemble described in the introduction may be trapped by a potential well of the potential $U(x)$. In quantum mechanics though, a bound state wave function extends exponentially beyond the potential limits, and may overlap with the initial state $\psi(0)$, even when this state is localized outside the potential limits. The contribution of these bound states to the wave function at $t > 0$ is orthogonal to the scattering (continuum) part, and will remain spatially linked to the potential region at all times.

A bound state with energy $E_j$ corresponds to a simple pole of $T^l(p)$, or a zero of $1/T^l(p)$ on the positive imaginary axis, at $p_j = i\gamma_j$, $\gamma_j > 0$. In this section we shall see that the bound state terms may be written as a residue

$$\phi_j(x)e^{-iE_j t/\hbar}\langle E_j|\psi(0)\rangle = -2\pi i \hbar^{-1/2} \text{Res} \left[ T^l(p)\tilde{\psi}(p)e^{ip_j x/\hbar} e^{-iE_j t/\hbar}\right]_{p=p_j}, \quad x > d$$

where $q_j = i\sqrt{\gamma_j^2 + p_j^2}$. The function $\tilde{\psi}(p)$ is defined on the complex plane by the integral

$$\tilde{\psi}(p) = \frac{1}{\hbar^{1/2}} \int_a^b dx e^{-ip x/\hbar}\psi(x,0),$$

as has been used all along.

For the formal treatment of bound states it is convenient to introduce Jost solutions $f_1(p,x)$ and $f_2(p,x)$ of the Schrödinger equation. They are defined by the boundary conditions

$$f_1(p,x) \to e^{ip x/\hbar}, \quad as \quad x > d, \quad and$$

$$f_2(p,x) \to e^{-ip x/\hbar}, \quad x < c.$$  \hspace{1cm} (25)

We generalize here the treatment of ref. [5] for $V_0 = 0$ to the case $V_0 \geq 0$. It is easy from (6) and (7) to obtain the explicit expressions of $f_1$ and $f_2$ at $x < c$ and $x > d$ respectively,

$$f_1(p,x) = \begin{cases} e^{ip x/\hbar}, & x > d \\ e^{ip x/\hbar} \frac{1}{T^l(p)} + e^{-ip x/\hbar} \frac{R^l(p)}{T^l(p)}, & x < c \end{cases}$$

(26)

$$f_2(p,x) = \begin{cases} e^{ip x/\hbar} \frac{R^l(p)}{T^l(p)} + e^{-ip x/\hbar} \frac{1}{T^l(p)}, & x > d \\ e^{-ip x/\hbar}, & x < c \end{cases}$$

(27)

In particular, if for some value $p_j$, $1/T^l(p_j) = 0$, then $f_2$ and $f_1$ become real, proportional to each other,

$$f_2 = C f_1,$$  \hspace{1cm} (28)

and decay exponentially for $x < c$ and $x > d$. Defining the normalization constant $N$ by

$$N^2 = \int_{-\infty}^{\infty} dx f_1^2,$$  \hspace{1cm} (29)

we may write the wave-function of the bound state $|E_j\rangle$ as

$$\phi_j(x) = \frac{1}{N} f_1(p_j,x) = \frac{1}{CN} f_2(p_j,x).$$  \hspace{1cm} (30)

The overlap between the bound state $|E_j\rangle$ and the initial state, which has support only on the interval $[a, b] \leq c$, is as usual

$$\langle E_j|\psi(0)\rangle = \int_a^b dx \phi_j(x)\psi(x,0).$$  \hspace{1cm} (31)

On substituting the second equality of Eq. (30) in Eq. (31), and taking into account definition (24) and Eq. (27), we obtain

$$\langle E_j|\psi(0)\rangle = \frac{1}{CN} \int_a^b dx f_2(p_j,x)\psi(x,0) = \frac{1}{CN} \int_a^b dx e^{-ip_j x/\hbar}\psi(x,0) = \frac{\hbar^{1/2}}{CN} \tilde{\psi}(p_j).$$  \hspace{1cm} (32)
Therefore, for $x > d$, we have

$$
\phi_j(x)\langle E_j | \psi(0) \rangle = \left( \frac{1}{N} f_1(p_j, x) \right) \langle E_j | \psi(0) \rangle = \left( \frac{1}{N} e^{iq_j x/h} \right) \langle E_j | \psi(0) \rangle
$$

$$
= \frac{h^{1/2}}{CN^2} e^{iq_j x/h} \tilde{\psi}(p_j) = -2\pi i h^{-1/2} e^{iq_j x/h} \tilde{\psi}(p_j) \text{Res} T^I(p=p_j),
$$

so that (33) is obtained. In the last line of (33) we have used (3). A relation that may be obtained by differentiating the Schrödinger equation for $f_1$ with respect to $p$, integrating $f_1 f_2$ between $-R$ and $R$ as $R \to \infty$, and comparing with the derivative of the Wronskian of $f_1$ and $f_2$ with respect to $p$ for $p = p_j$, see also (34). Finally, combining (22) and (23) we can write the transmitted wave packet very compactly as

$$
\psi(x, t) = h^{-1/2} \int_\Omega dp T^I(p) \tilde{\psi}(p) e^{iqx/h} e^{-iE_pt/h}, \quad x > d,
$$

where the contour $\Omega$ goes from $-\infty$ to $\infty$ passing above the bound state poles, as shown in Fig. 2.

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**V. INITIAL STATE IN THE UPPER LEVEL**

Imagine now that the initial state has support only to the right, where the potential is $V_0$; that is, assume that the initial support of the state is the interval $[a, b]$, such that $d \leq a < b$. In this case, instead of Eq. (19), we have

$$
\langle p^+ | \psi(t = 0) \rangle = \begin{cases} 
T^I(p)^* \tilde{\psi}(q), & p > p_0, \\
T^I(p)^* \tilde{\psi}(-q), & 0 < p < p_0, \\
\left( \frac{q}{\tilde{\psi}(q)} \right)^{1/2} \left( \tilde{\psi}(q) + R^c(-p)^* \tilde{\psi}(-q) \right), & p < -p_0,
\end{cases}
$$

where, as before, $q = (p^2 - p_0^2)^{1/2}$, with the branch cut going slightly below $\text{Im}(p) = 0$, and $\tilde{\psi}(q)$ is defined by Eq. (24). Expression (18), as such, is also valid for $x < c$. Let us then substitute Eq. (36) in Eq. (18), and use Eqs. (6) and (7). The result analogous to Eq. (21) reads then, for $x < c$ when the initial state is restricted at $x > d$,

$$
\psi(x, t) = \sum_j \phi_j(x) \langle E_j | \psi(t = 0) \rangle e^{-iE_j t/h}
$$
where the asymptotic expressions for the scattering states are accurate.

These expressions have been obtained for cut-off potentials, the may be easily generalized for potentials that decay

the transmitted wave packet in terms of the initial momentum distrib ution and bound state contributions. Whereas

for \( x < c \)

from which we can conclude that when the initial state is restricted t o the interval \([-\infty, a] \) immediately below the branch cut. Notice that for \( p = -i\gamma \),

with real positive \( \gamma \), \( q \) becomes \( -i\sqrt{\gamma^2 + p_0^2} \), which accounts for the minus sign in front of \( q \) in the third and fifth integrals of Eq. (37).

In order to include the bound states in a more compact expression, let us substitute the first equality of Eq. (30)
in Eq. (31). Thus, using definition (24) and Eq. (26), we obtain

\[
\langle E_j | \psi(0) \rangle = \sum_j \phi_j(x) (E_j | \psi(t = 0) \rangle e^{-iE_j t/\hbar} + h^{-1/2} \int_{\Gamma} dp T^l(-p) \tilde{\psi}(q) e^{ipx/\hbar} e^{-iE_p t/\hbar},
\]

where the path of integration \( \Gamma \) goes from \(-\infty\) to \(+\infty\) immediately below the branch cut. Notice that for \( p = -i\gamma \),

with real positive \( \gamma \), \( q \) becomes \( -i\sqrt{\gamma^2 + p_0^2} \). Therefore, for \( x < c \), we have in this situation, using Eqs. (27) and (30),

\[
\phi_j(x) (E_j | \psi(0) \rangle = \left( \frac{1}{CN} f_2(p_j, x) \right) \langle E_j | \psi(0) \rangle = \left( \frac{1}{CN} e^{-ip_j x/\hbar} \right) \langle E_j | \psi(0) \rangle
\]

\[
= \frac{h^{1/2}}{CN^2} e^{-ip_j x/\hbar} \tilde{\psi}(-q_j).
\]

The pole of \( T^l(p) \) at \( p_j = i\gamma_j \) becomes a pole of \( T^l(-p) \) at \(-p_j\). Thus,

\[
T^l(-p) = \frac{-i\hbar}{CN^2} \frac{1}{p + p_j} + \cdots,
\]

and it follows that

\[
\phi_j(x) (E_j | \psi(t = 0) \rangle e^{-iE_j t/\hbar} = 2\pi i\hbar^{-1/2} \text{Res} \left[ T^l(-p) e^{ipx/\hbar} \tilde{\psi}(q) e^{-iE_p t/\hbar} \right]_{p = -p_j},
\]

from which we can conclude that when the initial state is restricted to the interval \([a, b] \), with \( d < a < b \),

\[
\psi(x, t) = \frac{h^{-1/2}}{\Omega} \int_{\Omega} dp T^l(-p) \tilde{\psi}(q) e^{ipx/\hbar} e^{-iE_p t/\hbar},
\]

for \( x < c \), where \( \Omega' \) is a path of integration that goes from \(-\infty\) to \(+\infty\) below the branch cut and the poles \(-p_j\).

VI. DISCUSSION

The main results of this paper are Eqs. (33) and (43), that provide simple, compact, and exact expressions for the transmitted wave packet in terms of the initial momentum distribution and bound state contributions. Whereas these expressions have been obtained for cut-off potentials, they may be easily generalized for potentials that decay fast enough, so that the initial wave packet does not overlap significantly with the potential region, and for \( x \) values where the asymptotic expressions for the scattering states are accurate.
These two equations make clear the need to include different contributions for the transmitted wave-packet. Even though tunnelling terms are of course included in theoretical analysis of wave packet collisions, the contribution of negative momenta is frequently overlooked in integral expressions of the wave function. Similarly, the contribution of the evanescent momentum region when the wave packet is initially on the potential upper level has been also disregarded. We have applied these equations in [10] to establish the relation between source boundary conditions, in which the wave function is specified at a point and for all times, with standard initial-value-problem boundary conditions where the wave function is specified in all space at \( t = 0 \). One further intended application is the study of arrival-time measurement models where a clock dial is coupled to the particle’s motion in such a way that the particle’s crossing stops the dial’s motion [11,12]. These models are described by step potentials of the form considered in section V.

Let us now illustrate the formal results obtained above with some simple explicit computations. In all of them, the initial wave packet is taken as the ground state of an infinite well; it is located between \( a \) and \( b \),

\[
\psi(x, 0) = \left( \frac{2}{b - a} \right)^{1/2} \sin[(x - a)k_w]H(a, b),
\]

where \( k_w = \pi/(b - a) \), and

\[
H(a, b) = \begin{cases} 
1 & a < x < b, \\
0 & \text{otherwise.}
\end{cases}
\]

See [10] for details of the analytical time dependence of \( \psi(x, t) \). Here we shall evaluate the norm for \( x > 0 \),

\[
PT(t) = \int_0^\infty dx |\psi(x, t)|^2,
\]

as well as the contributions from positive and negative momenta, the interference terms, and, whenever required, the contribution of bound states and evanescent waves.

![FIG. 3. The contributions of positive and negative momentum to the probability of finding the particle in the half line \( x > 0 \) for time \( t \) in the free case are shown with a dotted and a dashed line, respectively. The interference term is depicted with a dash-dotted line, and the total probability of finding the particle in the half line \( x > 0 \) for time \( t \) is portrayed as a thick continuous line. The initial state is given by expression (44), with \( a = -2.01 \), \( b = -0.01 \). The mass \( m \) equals 1. Atomic units are used throughout.](image)

For instance, in the case of free motion, by defining the projectors

\[
P = \int_0^\infty dp |p\rangle\langle p| \quad \text{and} \quad Q = 1 - P,
\]

\( PT \) is decomposed into three terms, \( PT = PT_+ + PT_- + PT_{int} \):
\begin{align}
Pt_+(t) &= \int_0^\infty dx \vert \langle x \vert P\psi(t) \rangle \vert^2, \\
Pt_-(t) &= \int_0^\infty dx \vert \langle x \vert Q\psi(t) \rangle \vert^2, \\
P_{T,int}(t) &= \int_0^\infty dx \, 2\text{Re}\langle \langle x \vert P\psi(t) \rangle \langle Q\psi(t) \vert x \rangle \rangle.
\end{align}

These quantities are shown as functions of \( t \) for free motion in Fig. 3. The interference term is important only for early times, and the limit \( Pt(\infty) = Pt_+(\infty) \) is clearly checked visually, although the decay of \( Pt_- \) is rather slow.

In Fig. 4 we show how the addition of an attractive delta potential, that creates a bound state, modifies the analogous contributions, since the bound state component has to be detracted from them. \( Pt_{\text{bound}} \) is constant in time, since there is only one bound state, and it is no longer true that the total final probability equals \( Pt_+(\infty) \); actually, we have \( Pt(\infty) = Pt_{\text{bound}} + Pt_+(\infty) \). In the picture we have only shown the interference term between positive and negative momenta, which is the most relevant one in this case.

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{fig4.png}
\caption{The initial state is as in Eq. (44), but multiplied by \( \exp(ipx) \), where \( p = 0.5 \) (all quantities in atomic units). Again we have \( a = -2.01 \) and \( b = -0.01 \). The motion of the particle is free everywhere, except for an attractive delta potential, \( U(x) = -U_0\delta(x) \), with \( U_0 = 1/8 \). The contribution of the bound state to the total probability of finding the particle in the half line \( x > 0 \) is shown with a thin continuous line; the contributions of positive and negative momenta with a dotted and a dashed line, respectively. The interference term between positive and negative momenta is depicted with a dash-dotted line, and the total probability as a thick continuous line.}
\end{figure}

In order to show the applicability of expression (35), we portray in Fig. 3 and Fig. 4 the squared moduli of the total amplitude and of different components of the amplitude for a step potential with an attractive delta potential; that is, the potential is \( V(x) = -U_0\delta(x) + V_0\theta(x) \). In this situation, additional to the positive and negative momenta components, we have evanescent waves and the contribution of the bound state. At the time of both pictures, \( t = 5 \) in atomic units), the evanescent waves are the major contributor to the wavefunction in the vicinity of the origin. It should be noticed though that interference terms are relevant in that region and elsewhere.

The magnitude of the component of negative momenta, as well as that corresponding to the bound state, is rather small relative to the positive momenta component of the amplitude modulus squared, but it is nonetheless very important even for large distances because of the interference between components, as is clearly reflected in Fig. 3. Fig. 4 is added to show more clearly the relative importance of the negative momenta and bound state components.
FIG. 5. The particle of mass $m = 1$ moves in the potential $V(x) = -U_0 \delta(x) + V_0 \theta(x)$, where $U_0 = 1/8$ and $V_0 = 1$ (in atomic units). The initial state is as in Eq. (44), with $a = -2.01$ and $b = -0.01$, but multiplied by $\exp(ipx)$, where $p = 0.5$. Time $t = 5$ has elapsed since the initial state was released. The moduli squares of different contributions to the amplitude are depicted: continuous thick line, total amplitude modulus squared; dotted line (resp. dashed line), square modulus of the contribution to the amplitude of positive (resp. negative) momenta; dot-dashed line, evanescent waves; continuous thin line, bound state contribution.

FIG. 6. Close-up of Fig. 5 in the lower left corner.

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