Transmittance for wave-packet scattering

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Different expressions for the transmittance in wave-packet scattering in one dimension are examined. Special attention is paid to the difficulties when the initial packet $\rho(0)$ has negative momentum components. A general formula is provided for this case, and the domain of applicability of a simple approximate expression is indicated. A model calculation illustrates the results.

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The question "What is the probability of overcoming a potential barrier $V(x)$ for a given wave packet?" arises in many different contexts. Recently, resonant tunneling in electronic devices and the tunneling time problem have been important examples [1–3]. Here we are interested in the answer from a fundamental point of view rather than for particular applications. It might appear that such a simple question should have a simple answer within standard scattering theory, in terms of the initial state and scattering theory matrices or operators. And indeed this is the case, at least formally. However, there are some subtleties that are easy to miss, especially when the packet is not fully directed against the potential barrier, i.e., when the initial momentum distribution has negative components. There are also different expressions in the literature and therefore a need to clarify their relations and/or validity.

The original motivation of the present paper was to check numerically the importance of various terms in an expression found in a previous work [4] on phase-space scattering. This work will be referred to as I in the following. The formula [(I.26)+(I.28)] for the transmittance $<T>$, defined as the *integral over all times of the positive flux* [5] *at asymptotic distances on the right*, was written in terms of tetradic matrix elements of the transition superoperator $\mathcal{T}$ and the free incoming density operator $\wp^{\rm in}(0)$. The incoming free density operator $\wp^{\rm in}$ (without superscript in I) is *equal* [6] to the full density operator in the infinite past, but evolves in the absence of the potential. The full density operator $\rho(0)$ is related to the incoming density operator by $\rho(t)=\Omega^{(+)}\wp^{\rm in}(t)\Omega^{(+)\dagger}$, where $\Omega^{(+)}$ is the Möller operator relating the free incoming wave and the full wave, (while $\Omega^{(-)}$ relates the free outgoing wave with the full wave. See e.g. [7]). In a more familiar language

$$<T>=\int_0^\infty dp\, <p|S\wp^{\rm in}(0)S^\dagger|p> = \int_0^\infty dp\, <p|\wp^{\rm out}|p>, \qquad (1)$$

$S=\Omega^{(-)\dagger}\Omega^{(+)}$ being the scattering operator, and $\wp^{\rm out}$ the outgoing free density operator to which the full density operator ρ tends after the collision. Since both $\wp^{\rm in}$ and $\wp^{\rm out}$ are free-particle states, their diagonal in momentum matrix elements $\wp^{\rm in}_{pp}$ and $\wp^{\rm out}_{pp}$ are independent of time. That (1) and our previous result in I are equal can be demonstrated by writing the matrix elements of $\mathcal{T}$ and of S in terms of matrix elements of the transition operator $T=V\Omega^{(+)}$. An alternative route making use of the Liouville–von Neumann equation may be found in [8].

In a real physical situation a density operator $\rho(0)$ is created at some instant of time (taken here as time 0) by some preparative procedure. For instance, one can create a packet in a higher potential surface by laser excitation from a lower one. The time $t=0$ corresponds to the moment when the laser ceases pumping. The question then to be considered is what transmittance is to be associated with $\rho(0)$. It is tempting to equate $\rho(0)$ with $\wp^{\rm in}(0)$ and apply Eq. (1). However $\wp^{\rm in}$ is an ideal state that in the infinite past tends to the full ρ but evolves without the potential action. In order to make the identification between these two operators at time $t=0$ they should be equal at all times $t<0$; in other words, the real packet ρ should not be affected by the potential at $t<0$. Moreover, even if the state $\rho(0)$ is located (in coordinate representation) asymptotically far from the potential center, this location does not automatically makes it a *free* state in the scattering theory sense that would allow $\rho(0)$ and $\wp^{\rm in}(0)$ to be equated. In particular, if $\rho(0)$ has a negative momentum component, this implies that in the past the packet was not free since the full ρ has collided in the past with the potential. In general, when one refers to the *past*, it must be understood as *the past that would occur if the present (time $t=0$) Hamiltonian were the only one to consider at all times.* Summarizing, the seemingly paradoxical conclusion is that a packet at an asymptotic position on the left with non-negligible negative and positive momentum components is in a sense in the midst of a collision, and is to be described by the full density operator $\rho(0)$. Specifically, it cannot be equated to the free state $\wp^{\rm in}(0)$.

For the special case that $\rho(0)$ has a negligible negative momentum component (and is asymptotically far to the left of the scattering center) the expression for the transmittance reduces [4] to

$$<T>\approx \int_0^\infty dp\, T_p\, \rho(0)_{pp}. \tag{2}$$

Thus $\rho(0)$ and $\wp^{\rm in}(0)$ can be equated. Here T_p is the transmission coefficient for incident momentum p [not to be confused with the transition operator T (without subscripts), the transition matrix $T_{p'p''}$ (two momentum subscripts), or the transmittance $<T>$. According to I, $T_p = 1 - (2\pi m/p)^2 |T_{-pp}|^2]$. As a function of p, $\rho(0)_{pp}$ is the initial momentum distribution. The above integral has been termed [9] the "effective transmission probability." It is a very useful expression because there are efficient methods [10] to calculate the coefficients T_p. It is also the formula one would assume [11] to be based on classical intuition. Nevertheless, in the general case, there are additional terms, depending on the coherences $\wp^{\rm in}(0)_{-pp}$, $\wp^{\rm in}(0)_{p-p}$, and on $\wp^{\rm in}(0)_{-p-p}$ $(p > 0)$. By using the formalism in I or (1), and if the identification $\wp^{\rm in}(0) = \rho(0)$ were valid, the term depending on $\wp^{\rm in}(0)_{-p-p}$ would be

$$\int_0^\infty (1 - T_{-p})\, \rho(0)_{-p-p}\, dp. \tag{3}$$

But if the whole packet $\rho(0)$, located at $t = 0$ on the left side of the barrier, is directed leftwards, then the only nonvanishing term appears to be (3), which is clearly an absurd result. The problem is that such a state was not free in the past, as we discussed above, and therefore the identification $\rho(0)$ with $\wp^{\rm in}(0)$ is incorrect, in spite of the fact that the packet is not affected by the potential at time $t = 0$. As a consequence the first form of (1) is not useful in practice, since what we actually have is $\rho(0)$ and not $\wp^{\rm in}(0)$. This is an important distinction, which is worth emphasizing since, to our knowledge, it has not been previously spelled out.

A different perspective needs to be taken and the following is proposed. The packet at $t = 0$ cannot be considered a free packet but may be related to the outgoing free packet by means of

$$\begin{aligned}\wp^{\rm out}(t) &= \Omega^{(-)\dagger}\rho(t)\Omega^{(-)}\\ &= \int\!\!\int |p'><p'^{(-)}|\rho(t)|p''^{(-)}><p''|\, dp'\, dp'',\end{aligned} \tag{4}$$

where $|p'^{(-)}>= \Omega^{(-)}|p'>$. Using (1) and the above relation between ρ and $\wp^{\rm out}$ the transmittance may be written as

$$<T>= \int_0^\infty <p^{(-)}|\rho(0)|p^{(-)}>\, dp. \tag{5}$$

The last integral may be taken as well as the definition of the transmittance. Note that (5) is in agreement with (1) and with our previous result in I. The important difference is that now the expression in (5) for $<T>$ contains the actual $\rho(0)$, which is the originally given data. This equation considers in principle diagonal and nondiagonal elements of $\rho(0)$, as well as positive and negative momentum contributions. The question then is whether the simple formula (2) is a good approximation to (5) and in what circumstances. Clearly, if the initial negative momentum components of $\rho(0)$ are negligible [and $\rho(0)$ is asymptotically far from the scattering center], (2) becomes exact. In this case $\rho(0) = \wp^{\rm in}(0)$. To examine the validity of (2) with initial negative momentum components we have performed a calculation with a delta potential $<x|V|x'>= V_0\delta(x - x')\delta(x)$ that allows an analytical treatment. The chosen initial state is in coordinate representation,

$$<x|\psi(0)>= \sqrt{\alpha}\, e^{-\alpha|x-x_0|} e^{ip_0(x-x_0)/\hbar}, \tag{6}$$

where the cusp at x_0 is the price that is paid for the analyticity [12] of the propagated wave $\psi(t)$. For $p > 0$ the $<x|p^{(-)}>$ eigenstate takes the form

$$<x|p^{(-)}>= \frac{1}{h^{1/2}}\left[e^{ixp/\hbar} - \frac{c\, e^{-i|x|p/\hbar}}{c + ip}\right], \tag{7}$$

where $c = mV_0/\hbar$, and (if $x_0 < 0$)

$$\begin{aligned}&<p^{(-)}|\psi(0)>\\ &= \frac{2\, ip\hbar\sqrt{\alpha/h}}{(ip - c)}\\ &\quad\times\left[\frac{e^{-ix_0p/\hbar}\,\hbar\,\alpha}{(p - p_0)^2 + (\hbar\alpha)^2} + \frac{c\, e^{x_0(\alpha - ip_0/\hbar)}}{p^2 - (p_0 + i\hbar\alpha)^2}\right].\end{aligned} \tag{8}$$

The exact transmittance is then given by (5) with $\rho(0) = |\psi(0)><\psi(0)|$. One may also evaluate the approximate expression (2) explicitly. The stationary transmission coefficient and $\rho(0)_{pp}$ are, respectively,

$$T_p = \frac{p^2}{(p^2 + c^2)}, \qquad \rho(0)_{pp} = \frac{2\alpha^3\hbar^3/\pi}{[(p - p_0)^2 + (\hbar\alpha)^2]^2}, \tag{9}$$

giving

$$\begin{aligned}&\int_0^\infty T_p\, \rho(0)_{pp}\, dp\\ &= \int_0^\infty dp \frac{p^2 2\alpha^3\hbar^3/\pi}{(p^2 + c^2)[(p - p_0)^2 + (\hbar\alpha)^2]^2}.\end{aligned} \tag{10}$$

This integral can be done by decomposition into partial fractions after a lengthy but relatively straightforward calculation. However, the result is not particularly enlightening and is not reported here. For our purposes it is enough to point out that for this model (10) is recovered from (5) when the center of the packet at $t = 0$, x_0, is sufficiently far from the potential. More precisely, neglecting the exponentially decaying term in (8), one obtains Eq. (10) by using the exact expression (5). Clearly for $x_0 < 0$ and sufficiently large, no negative momentum components of $\rho(0)$ contribute to the transmittance, even the interference terms having decayed sufficiently (with distance) so that they give no contribution. Actually the validity of (2) when the packet is initially far from the potential is a general, model-independent result. To show this, $<p^{(-)}|\rho(0)|p^{(-)}>$ in (5) is decomposed into three terms having zero, one, and two matrix elements of the transition operator $T^{(-)} = V\Omega^{(-)}$, by using the Lippmann-Schwinger equation $\Omega^{(-)}|p>=|p> +(E_p - i0 - H_0)^{-1}T^{(-)}|p>$. Inserting resolutions of the identity in coordinate representation in the second and third terms, assuming that the potential is far from the packet initial location, considering that T decays essentially as V does in coordinate space, and using the coordinate space representation of the resolvents, the one-dimensional optical theorem [4] and the relation $T^{(-)}_{pp} = T^*_{pp}$, one obtains (2). The described steps are now illustrated more explicitly for the second, single-T, term:

$$2\,\mathrm{Re}\int_0^\infty dp\int dx\int dx' <p|\rho(0)|x><x|\frac{1}{E_p - i0 - H_0}|x'><x'|T^{(-)}|p>$$

$$\approx 2\,\mathrm{Re}\int_0^\infty dp\int dx\int dx' <p|\rho(0)|x>\frac{ime^{ip(x-x')/\hbar}}{p\hbar}<x'|T^{(-)}|p>$$
$$= -\int_0^\infty dp\,\rho(0)_{pp}\frac{4m\pi}{p}\,\mathrm{Im}\,T^{(-)}_{pp} = -\int_0^\infty dp\left(\frac{2\pi m}{p}\right)^2\rho(0)_{pp}\,|T_{pp}|^2 - \int_0^\infty dp\,\rho(0)_{pp}\,(1-T_p). \quad (11)$$

The approximation is due to the approximate form for the Green's function in position representation, associated with the restriction that $x << x'$, since $\rho(0)$ is far away from the scattering center (at negative positions). In the final form, the first integral exactly cancels the third (two-T) term while the last integral plus the first (no-T) term gives the desired result (2).

For making further connections among different transmittance expressions it is useful to write (1) or (5) in phase-space language. Within this framework the integral of the positive flux at a large positive position y takes the form

$$<T>=\int_{-\infty}^\infty dt\int_0^\infty dp\frac{p}{m}W^{\mathrm{out}}(y,p,t), \quad (12)$$

where W^{out} is the phase-space representative of $\wp^{\mathrm{out}}$

$$W^{\mathrm{out}}(x,p,t) = \frac{1}{2\pi}\int e^{is(x-pt/m)} \times <(p+s\hbar/2)^{(-)}|\rho(0)|(p-s\hbar/2)^{(-)}>ds. \quad (13)$$

Substituting (13) into (12) one immediately recovers (5) by integration of the resulting δ function. An additional formula for $<T>$ as a double integral in coordinate space, involving the wave function at asymptotic positive times, was derived from (12) by Turner and Snider.[8]

Another common definition for the transmittance is *the probability to find the particle at $x > y >> 0$ at a time τ large enough so as to make this probability independent of time.* Thus $\rho(t)$ has become equal to $\wp^{\mathrm{out}}(t)$ for $t \geq \tau$. This may be written in different ways:

$$<T>=\int_y^\infty dx\rho(\tau)_{xx} = \int_{-\infty}^\infty dp\int_y^\infty dxW^{\mathrm{out}}(x,p,\tau)$$
$$=\int_0^\infty dt\int_{-\infty}^\infty dp\frac{p}{m}W^{\mathrm{out}}(y,p,t), \quad (14)$$

where the last equality follows from integrating the quantum continuity equation twice, once over position and once over time, with the understanding that $W^{\mathrm{out}}(x,p,t)$ vanishes at $x=\infty$; and moreover, at $t=0$, $W^{\mathrm{out}}(y,p,0)$ vanishes (or is negligibly small), since none of the packet has yet reached position y. Finally the upper time integration limit has been shifted to ∞. These expressions are useful when the numerical propagation of the wave packet is feasible. Connection with the previous definition (12) and Eq. (5) is made by noticing that, due to the rapidly oscillating exponential factor in (13), the lower integration limits for t and p in (14) may be changed to $-\infty$ and 0, respectively. We have numerically checked the full agreement between (14) and (5) for the δ potential.

Different exact and approximate transmittance formulae have been deduced, reviewed, and related. Prepared initial states may have a combination of negative and positive momenta. A laser-induced transition between different bands in a semiconductor device will create such states. In this case some of the transmittance expressions cannot be directly used because, even though the state is far from the collision region, it is not a free state, due to its interaction in the past with the potential. The correct procedure and formalism have been indicated and exemplified with a model. The precise limits of validity of the simple formula (2) have been indicated.

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