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# Asymptotic behavior in phase-space scattering

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The phase-space formulation of quantum scattering is discussed and the asymptotic quantities describing potential scattering in one and three dimensions (transmittances, cross sections) are analyzed. It is found that under certain conditions the transmittance in time-dependent scattering only depends on the momentum distribution of the incident packet, being independent of its particular shape in coordinate space. For three-dimensional scattering, generalized cross sections are defined for momentum coherences and a physical interpretation of the generalized optical theorem is proposed.
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## I. INTRODUCTION

The phase-space description of collision processes has been considered in a variety of ways by several people. A review by Carruthers and Zachariasen [1] references much of the earlier work which was motivated by classical mechanical and/or Boltzmann-equation applications. Independently, one of the present authors has presented [2] a density-operator description of quantum scattering with the aim of organizing the structure of gas kinetic-theory cross sections [3]. In that work and that of Turner [4, 5] the object was to use exclusively quantum Liouville-space (equivalently phase-space) dynamics and methods to describe the collision process. From a study of the asymptotic (large-distance) behavior of the Wigner function [6], a phase-space representation [7] of the density operator, it was seen how the transition superoperator describes all aspects of gain and loss associated with the collision process. The advantage of this representation is that it is possible and meaningful to examine the large-distance behavior of the state of the system for a given (outgoing) momentum. To separate clearly the interaction region from the asymptotic behavior, our previous work [2] assumed that the phase-space representation of the transition superoperator matrix elements are short ranged, in analogy with the usual wave-function behavior. There followed an identification of a generalized cross section which takes into account the loss from the initial momentum state as well as the gain into other momentum states.

The motivation for the present paper is to examine the validity of the short-ranged behavior of the phase-space representation of the scattered state. What is found is that the short-ranged behavior assumed in Ref. [2] is not valid. There are in fact two types of terms in the scattered part of the density operator, namely, those terms which lead to a gain in probability into a final state and those terms that interfere with and deplete the incoming state. Neither part of the corresponding transition superoperator matrix elements is in fact short ranged, the former being found to decay with distance only as $r^{-2}$ while the latter oscillates without decay. In spite of this it is shown that the result of scattering in a density-operator formalism is still described by the generalized cross section. Thus the present work verifies the final result of Ref. [2], although the proof of this result is more elaborate than what was given at that time. As well, while the previous study was limited to stationary scattering (in particular incoming density matrices that are diagonal in momentum), the present treatment includes also the general time-dependent processes that involve momentum coherences.

In this work the state of the system is always described by a density operator or its equivalent Wigner function. In the momentum representation of the incoming density operator, there are diagonal elements which describe the probability that the system is in a given eigenstate of the free Hamiltonian and off-diagonal elements that are referred to here as coherences. Two types of coherences are distinguished in the following. First, if the two momenta associated with the coherence differ in magnitude, then the free-particle energies of the two states are different and the coherence oscillates in time with the frequency associated with this energy difference; these are energy coherences. Second, if the momenta have the same magnitude but differ in direction, referred to as directional (on-the-energy-shell) coherences, there is no time dependence and this merely describes the angular spreading of the incoming state.

This paper starts by extending the phase-space description of scattering to one dimension, both for time-dependent and stationary-state processes. There is nowadays a renewed interest in this subject because of the possibility of electronic-device applications of resonant tunneling properties [8]. It is shown how the relevant quantities (transmittance and reflectance) are related to the transition superoperator. The relations between the transmittance, the packet shape in coordinate space, and the initial momentum distribution are also spelled out. A similar analysis is then made in three-dimensional potential scattering. Connections between the asymptotic behavior of the particle flux, the differential cross section, and the generalized optical theorem are made. An Appendix has been included which contains some scattering-theory relations used in the text.

 

## II. SCATTERING IN ONE DIMENSION

In this section the relationship between the transition superoperator and the relevant quantities in one-dimensional scattering is described. In a general time-dependent collision the density operator $\rho(t)$ can be related to the incoming density operator $\wp(t)$ (state of the system in the absence of interaction) through the Møller superoperator

$$\rho(t) = \Omega_L \wp(t). \tag{1}$$

See the Appendix for the definition of the various scattering operators and superoperators. By using resolutions of the identity in terms of momentum states [normalized according to $< p''|p' >= \delta(p''-p')$], the incoming density operator is decomposed into its frequency components, which naturally display the time dependence of the density operator

$$\wp(t) = \int\!\!\int dp'dp'' e^{-i\omega_{p'p''}t}|p' > \wp_{p'p''}(0) < p''|. \tag{2}$$

Here the frequency $\omega_{p'p''} = (p'^2 - p''^2)/(2m\hbar)$ is that associated with the translational energy difference between $p'$ and $p''$. The time-dependent interacting density operator can then be given in terms of the parametrized Møller superoperator by

$$\rho(t) = \lim_{\eta\to 0} \int\!\!\int dp'dp'' e^{-i\omega_{p'p''}t}\Omega_L(\omega_{p'p''} + i\eta) \times |p' > \wp_{p'p''}(0) < p''|. \tag{3}$$

In order to discuss the asymptotic position dependence of the interacting density operator, it is convenient to consider the Weyl correspondence [7], the Wigner [6] equivalent representation, of this operator

$$W(x,p,t) \equiv \frac{1}{2\pi}\int e^{isx} < p + s\hbar/2|\rho(t)|p - s\hbar/2 > ds. \tag{4}$$

For scattering processes, it is the flux at time $t$ and position $x$ that is of interest, and this is given by the integral over the Wigner function

$$\begin{aligned} J(x,t) &= \int \frac{p}{m} W(x,p,t)dp \\ &= \int \frac{p}{m} dp \int\!\!\int dp'dp'' W_{p'p''}(x,p)\wp_{p'p''}(0)e^{-i\omega_{p'p''}t}. \end{aligned} \tag{5}$$

In the last line, this has been reexpressed in terms of the phase-space representative $W_{p'p''}(x,p)$ of a typical frequency component

$$\lim_{\eta\to 0} \rho_{\omega_{p'p''},\eta} \equiv \lim_{\eta\to 0} \Omega_L(\omega_{p'p''} + i\eta)|p' >< p''|. \tag{6}$$

Note that stationary (time-independent) scattering is completely described by the $\omega = 0$ components.

The frequency components of the density operator obey a Lippmann-Schwinger-type [9] equation [We use here a shorthand notation $\wp_{\omega_{p'p''}} \equiv |p' >< p''|$ for a free-motion frequency component. $\wp_{\omega_{p'p''}}$ is an *operator*, and should not be confused with the scalar amplitude $\wp_{p'p''}(0)$ of the initial state, see Eq.(3).]

$$\rho_{\omega,\eta} = \wp_\omega + (\omega + \mathcal{L}_0 + i\eta)^{-1}\mathcal{T}(\omega + i\eta)\wp_\omega. \tag{7}$$

The Weyl correspondence of the second term $W_\omega^{sc}$ (the scattered part) is given by

$$\begin{aligned} W_\omega^{sc}(x,p) &= (2\pi)^{-1}\int ds e^{isx} < p + s\hbar/2|(\omega - \mathcal{L}_0 + i\eta)^{-1}\mathcal{T}(\omega + i\eta)\wp_\omega|p - s\hbar/2 > \\ &= \frac{i}{2\pi}\int\!\!\int \frac{\exp[is(x-y)]}{\omega - ps/m + i\eta} M_\omega(y,p)dy\, ds, \end{aligned} \tag{8}$$

where

$$M_\omega(y,p) = (2\pi)^{-1}\int ds\, e^{isy} < p + s\hbar/2| - i\mathcal{T}(\omega + i\eta)\wp_\omega|p - s\hbar/2 > . \tag{9}$$

The $s$ integral in (8) can be carried out by contour integration, closing the $s$ contour above or below the real axis depending on whether $x - y$ is positive or negative. The position of the pole depends on the value of $p$ so the result is

$$\begin{aligned} I_s &\equiv \int \frac{\exp[is(x-y)]}{\omega - ps/m + i\eta} ds, \\ I_s\big|_{p<0} &= \frac{2im\pi}{p}\exp\left(\frac{im(x-y)}{p}(\omega + i\eta)\right)\Theta(y - x), \\ I_s\big|_{p>0} &= -\frac{2im\pi}{p}\exp\left(\frac{im(x-y)}{p}(\omega + i\eta)\right)\Theta(x - y), \end{aligned} \tag{10}$$

where $\Theta$ is the Heaviside function. For positive and negative $p$, the scattered Wigner function takes the form

$$\begin{aligned} W_\omega^{sc}(x,p)_{p>0} &= \frac{m}{p}\int_{-\infty}^{x} \exp\left(\frac{im(x-y)}{p}(\omega + i\eta)\right) M_\omega(y,p)dy, \\ W_\omega^{sc}(x,p)_{p<0} &= -\frac{m}{p}\int_{x}^{\infty} \exp\left(\frac{im(x-y)}{p}(\omega + i\eta)\right) M_\omega(y,p)dy. \end{aligned} \tag{11}$$

This is the starting point for the following discussion.

### A. Stationary scattering

The stationary case, with $\omega = 0$, is discussed first. Taking the $\eta \to 0$ limit gives the simple results

$$\lim_{x\to\infty} W_0^{sc}(x,p)_{p>0} = \frac{m}{p}\int M_0(y,p)dy, \quad \lim_{x\to-\infty} W_0^{sc}(x,p)_{p>0} = 0, \tag{12}$$

$$\lim_{x\to-\infty} W_0^{sc}(x,p)_{p<0} = -\frac{m}{p}\int M_0(y,p)dy, \quad \lim_{x\to\infty} W_0^{sc}(x,p)_{p<0} = 0.$$

The contribution to the flux at large positive $x$ from the zero-frequency term is given by

$$j^{sc}_{x\to\infty} = \int_0^\infty dp \int dy M_0(y,p) = \lim_{\eta\to 0}\int_0^\infty dp < p| - i\mathcal{T}(i\eta)\wp_0|p >, \tag{13}$$

where use has been made of the delta function $\delta(s) = (2\pi)^{-1}\int dy \exp(isy)$ arising from the $y$ integration. For the simplest possible initial state, a pure state with definite *positive* momentum $p'$, $\wp_0 = |p'>< p'|$, the scattered flux is (using Baranger's [10] notation for superoperator matrix elements)

$$j^{sc}_{x\to\infty} = \int_0^\infty dp << p,p| - i\mathcal{T}|p',p' >> \tag{14}$$

and $\mathcal{T}$ is the abstract transition superoperator. To calculate the total flux at large positive $x$ it is necessary to add the contribution from the incoming component of $\rho$:

$$j^{in} = \int_0^\infty \frac{p}{m} W^{in}_{p'p'}(x,p)dp = \frac{p'}{2\pi m\hbar}, \tag{15}$$

where

$$W^{in}_{p'p'}(x,p) = \frac{1}{2\pi}\int e^{isx} < p + s\hbar/2|p' >< p'|p - s\hbar/2 > ds = \frac{1}{\hbar}\delta(p-p'). \tag{16}$$

The expression (14) for the scattered flux is elaborated by separately considering the contributions from the terms containing one and two matrix elements of the transition operator $T$ [see Eq. (A10)]:

$$\begin{aligned} << p,p|\mathcal{T}|p',p' >> &= << p,p|\mathcal{T}_1|p',p' >> + << p,p|\mathcal{T}_2|p',p' >>, \\ << p,p|\hbar\mathcal{T}_1|p',p' >> &= < p|T|p' >< p'|p > - < p|p' >< p'|T^\dagger|p >, \\ << p,p|\hbar\mathcal{T}_2|p',p' >>, &= < p|T|p' >< p'|T^\dagger G_0^\dagger|p > - < p|G_0T|p' >< p'|T^\dagger|p > . \end{aligned} \tag{17}$$

The corresponding fluxes are

$$j^{sc}_{1,x\to\infty} = -\frac{i}{\hbar}\int_0^\infty dp\,\delta(p-p')(T_{pp'} - T^\dagger_{p'p}) = 2\,\mathrm{Im}\,T_{p'p'}/\hbar, \tag{18}$$

$$\begin{aligned} j^{sc}_{2,x\to\infty} &= -\frac{i}{\hbar}\int_0^\infty dp\,(2i\pi)\delta(E_p - E'_p)|T_{pp'}|^2 \\ &= \frac{2m\pi}{\hbar}\int dE_p \frac{1}{\sqrt{2mE_p}}\delta(E_p - E_{p'})|T_{pp'}|^2 \\ &= \frac{2\pi m}{p'\hbar}|T_{p'p'}|^2 \end{aligned}$$

by making use of the condition $p > 0$. Addition of these two contributions and use of the one-dimensional optical theorem (see Appendix) gives

$$j^{sc}_{x\to\infty} = \int_0^\infty dp << p,p| - i\mathcal{T}|p',p' >> = -\frac{2\pi m}{p'\hbar}|T_{-p'p'}|^2. \tag{19}$$

The flow at large negative $x$ is calculated by similar means. The important difference is that there is no contribution from $\mathcal{T}_1$, so that

$$j^{sc}_{x\to-\infty} = \int_{-\infty}^0 dp << p,p|i\mathcal{T}|p',p' >> = -\frac{2\pi m}{p'\hbar}|T_{-p'p'}|^2. \tag{20}$$

These scattering ($W^{sc}$) contributions to the flux at large positive and negative $x$ are equal. This is in agreement with flux conservation. The results are summarized in the following, where $j^{in}$ is the incoming flux, $j^R$ is the reflected flux, and $j^T$ is the transmitted flux:

$$\begin{aligned} j^{in} &= \frac{p'}{2\pi m\hbar}, \\ j^R &= -\frac{2\pi m}{p'\hbar}|T_{-p'p'}|^2, \\ j^T &= -\frac{2\pi m}{p'\hbar}|T_{-p'p'}|^2 + j^{in}. \end{aligned} \tag{21}$$

Note that $j^T = j^{in} + j^R$.

The reflectance coefficient $R_{p'}$ is defined as the ratio between the magnitude of the reflected flux and the incoming flux, while the transmittance coefficient $T_{p'}$ is the ratio between the transmitted and incident flux. It follows from the above definitions that

$$R_{p'} = \left(\frac{2\pi m}{p'}\right)^2 |T_{-p'p'}|^2 = \frac{2\pi m\hbar}{p'} \int_{-\infty}^{0} dp << p,p| - i\mathcal{T}|p',p' >> . \quad (22)$$

This means that $j^T = j^{\rm in}(1 - R_{p'})$ and therefore $T_{p'} = 1 - R_{p'}$, as it should for total-flux conservation. These are general results.

### B. The $\omega \neq 0$ components

For $\omega \neq 0$ the asymptotic Wigner function oscillates spatially according to

$$W_\omega^{\rm sc}(x,p)_{p>0} = \frac{m}{p}\int_{-\infty}^{x} \exp[i\kappa(x-y)]M_\omega(y,p)dy = \frac{m}{2\pi p}e^{i\kappa x}\int ds \int_{-\infty}^{x} dy e^{iy(s-\kappa)} < p + s\hbar/2| - i\mathcal{T}\wp_\omega|p - s\hbar/2 >, \quad (23)$$

where $\kappa = m(\omega + i\eta)/p$. As $x \to \infty$ the $y$ integration can be performed to give a $\delta$ function. On taking the limit $\eta \to 0$ this is simply $\delta(s-\kappa)$. After carrying out the $s$ integral

$$W_\omega^{\rm sc}(x,p)_{p>0} \underset{x\to\infty}{\sim} \frac{m}{p}e^{im\omega x/p} < p + m\omega\hbar/2p| - i\mathcal{T}\wp_\omega|p - m\omega\hbar/2p > . \quad (24)$$

Note that the contribution to the flux from the coherences oscillates both in time and space due to (5) and (24).

### C. Time-dependent scattering

The transmittance $< T >$ in the time-dependent case is discussed next. This is defined as the integral over all time of contributions of positive flux at asymptotically large $x$. In particular, there is the question of whether or not the nondiagonal coherences ($\omega \neq 0$ components of the density operator) contribute to the transmittance. However, since the only time-dependent factor in (3) is the exponential $e^{-i\omega t}$ and the definition of the transmittance involves an integration over time, this provides a delta function $\delta(\omega)$ which precludes any of the $\omega \neq 0$ components from contributing:

$$\begin{aligned} < T > &= \lim_{x\to\infty}\int_{-\infty}^{\infty} dt \int_0^\infty \frac{p}{m}W(x,p,t)dp \\ &= \lim_{x\to\infty}\int_{-\infty}^{\infty} dt \int_0^\infty dp\frac{p}{m}\iint W_{p'p''}(x,p)e^{-i\omega_{p'p''}t}\wp_{p'p''}(0)dp'dp'' \\ &= 2\pi \lim_{x\to\infty}\int_0^\infty dp\frac{p}{m}\iint W_{p'p''}(x,p)\delta(\omega_{p'p''})\wp_{p'p''}(0)dp'dp''. \end{aligned} \quad (25)$$

The reason for the notation $< T >$ will become clear later. It is convenient to divide this integral into incoming and scattered components $< T > = < T >^{\rm in} + < T >^{\rm sc}$ according to the decomposition $W_{p'p''}(x,p) = W_{p'p''}^{\rm in}(x,p) + W_{p'p''}^{\rm sc}(x,p)$. Writing $\delta(\omega_{p'p''}) = m\hbar\delta(|p'| - |p''|)/|p'|$, dividing the integrals into positive and negative integration intervals, interchanging the integration limits, and using the explicit expression for $W_{p'p''}^{\rm in}$, one obtains

$$< T >^{\rm in} = \int_0^\infty \wp_{p'p'}(0)dp', \quad (26)$$

as it should be. This equation states that in the absence of interaction, the positive part of the momentum distribution finds its way to the asymptotic region at large positive $x$. The scattered component becomes

$$< T >^{\rm sc} = 2\pi\int_0^\infty dp \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} << p,p| - i\mathcal{T}|p',p'' >> \wp_{p'p''}(0)\delta(\omega_{p'p''})dp'dp''. \quad (27)$$

It is clear that there are four ways to satisfy the frequency $\delta$ function, thus

$$\begin{aligned} < T >^{\rm sc} = -2\pi i\hbar\int_0^\infty dp \int_0^\infty dp'\frac{m}{p'}\big[ &<< p,p|\mathcal{T}|p',p' >> \wp_{p'p'}(0) \\ &+ << p,p|\mathcal{T}| - p',p' >> \wp_{-p'p'}(0) + << p,p|\mathcal{T}| - p',-p' >> \wp_{-p'-p'}(0) \\ &+ << p,p|\mathcal{T}|p',-p' >> \wp_{p'-p'}(0)\big]. \end{aligned} \quad (28)$$

The full expression for the transmittance is therefore the sum of (26) and (28). However it is expected on physical grounds that the contributions in the last equation from negative momenta $(-p')$ should be small or negligible in a standard wave-packet collision. If this is the case, only the first term in (28) remains. In this approximation, Eqs. (19), (22), and (28) imply that the scattered part of the transmitted packet takes the simple form

$$<T>^{\rm sc}= -\int_0^\infty R_{p'}\wp_{p'p'}(0)dp', \tag{29}$$

with the further consequence that

$$<T>= \int_0^\infty T_{p'}\wp_{p'p'}(0)dp'. \tag{30}$$

Thus if the whole initial packet is directed forward, the whole packet contributes to the "average" transmittance. On the contrary, if some of the packet is directed away from the scattering center, then there can be interference terms contributing to the transmittance. These are on-the-energy-shell terms including directional coherences. This effect can be particularly important at low average energies and/or with packets having a broad momentum distribution.

## III. THREE-DIMENSIONAL SCATTERING

In our [2] previous work on the phase-space representation of scattering processes the emphasis was on stationary scattering, where the initial density operator is assumed diagonal in momentum states but with possible nondiagonalities in internal states. That formalism is immediately applicable to potential scattering by dropping the internal-state labels. In the present work momentum off-diagonal components will also be dealt with. These arise naturally in time-dependent scattering as shown in the expansion of the density operator (2). In Ref. [2] it was assumed that the phase-space function $M(\mathbf{x},\mathbf{P})$, the three-dimensional analog of Eq. (9), is localized. This allowed a clear distinction to be made between the colliding motion and the asymptotic behavior of the scattered state. With the aid of this separation, a generalized collision cross section was identified. Here this assumption is examined and it is found that the localization of $M(\mathbf{x},\mathbf{P})$ is not strictly valid, in particular for the interference terms corresponding to the contributions that are linear in $T$ to $\mathcal{T}$, see Eq. (17). It is then one of the objectives of this section to show that the generalized cross section is still appropriate for the description of the collision process. A brief summary of the work reported in Ref. [2] is given first, then the problems and their resolution are addressed.

Except for the change from one to three dimensions, the basic formalism of this paper, namely, Eqs. (1) to (9), is still applicable. Thus the Wigner function for the scattered part of the frequency component of the density operator [analog of Eq. (8)] is

$$\begin{aligned} W^{\rm sc}(\mathbf{r},\mathbf{p}) &= (2\pi)^{-3}\int ds\, e^{i\mathbf{s}\cdot\mathbf{r}} < \mathbf{p}+\mathbf{s}\hbar/2|(\omega-\mathcal{L}_0+i\eta)^{-1}\mathcal{T}(\omega+i\eta)\wp_\omega|\mathbf{p}-\mathbf{s}\hbar/2> \\ &= \frac{i}{(2\pi)^3}\int\int \frac{\exp[i\mathbf{s}\cdot(\mathbf{r}-\mathbf{x})]}{\omega-\mathbf{p}\cdot\mathbf{s}/m+i\eta}M(\mathbf{x},\mathbf{p})d\mathbf{x}\,d\mathbf{s} \\ &= \frac{m}{p}\int \frac{\exp(i\kappa|\mathbf{r}-\mathbf{x}|)}{|\mathbf{r}-\mathbf{x}|^2}M(\mathbf{x},\mathbf{p})\delta\left(\hat{\mathbf{p}}-\frac{\mathbf{r}-\mathbf{x}}{|\mathbf{r}-\mathbf{x}|}\right)d\mathbf{x}, \end{aligned} \tag{31}$$

where

$$M(\mathbf{x},\mathbf{p}) = (2\pi)^{-3}\int ds\, e^{i\mathbf{s}\cdot\mathbf{x}} < \mathbf{p}+\mathbf{s}\hbar/2|-i\mathcal{T}(\omega+i\eta)\wp_\omega|\mathbf{p}-\mathbf{s}\hbar/2> \tag{32}$$

and the integration over the free motion resolvent and the method of writing the result is discussed in Ref. [2]. $\kappa \equiv m(\omega+i\eta)/p$ and $\hat{\mathbf{p}}$ is the unit vector in the direction of $\mathbf{p}$. In the earlier work [2] the asymptotic behavior of the scattered state was obtained by letting $|\mathbf{r}|\to\infty$ and resulted in the identification of the generalized (both gain and loss contributions are included) cross section

$$\sigma_{\mathbf{p}'\to\hat{\mathbf{p}}} = (j^{\rm in})^{-1} << \hat{\mathbf{p}},\hat{\mathbf{p}}|-i\mathcal{T}|\mathbf{p}',\mathbf{p}'>>, \tag{33}$$

where $j^{\rm in} = |\mathbf{j}^{\rm in}| = p'/mh^3$ is the magnitude of the incoming planar flux. The validity of this result is to be discussed.

### A. Terms linear in $T$

The contributions to $M(\mathbf{x},\mathbf{p})$ that are linear in $T$ are studied first by taking a typical frequency component $\wp_{\omega_{p'p''}} = |\mathbf{p}'><\mathbf{p}''|$ of the incoming state. From Eqs.(17) and (32), this contribution is

$$M_1(\mathbf{x},\mathbf{p}) = \frac{-8i}{h^3\hbar}\Big(e^{2i\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}'')/\hbar} < 2\mathbf{p}-\mathbf{p}''|T|\mathbf{p}'> \\ -e^{2i\mathbf{x}\cdot(\mathbf{p}'-\mathbf{p})/\hbar} < \mathbf{p}''|T^\dagger|2\mathbf{p}-\mathbf{p}'>\Big). \tag{34}$$

Clearly, as a function of $\mathbf{x}$, this oscillates and is *not* short ranged. But because of its simple structure, it is possible to exactly compute its contribution to the scattered part of the Wigner function via Eq. (31):

$$W_1^{sc}(\mathbf{r},\mathbf{p}) = \frac{16m}{h^3}\left(\frac{e^{2i(\mathbf{p}-\mathbf{p}'')\cdot\mathbf{r}/\hbar}}{p'^2-(2\mathbf{p}-\mathbf{p}'')^2+i\eta} < 2\mathbf{p}-\mathbf{p}''|T|\mathbf{p}' > -\frac{e^{2i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{r}/\hbar}}{(2\mathbf{p}-\mathbf{p}')^2-p''^2+i\eta} < \mathbf{p}''|T^\dagger|2\mathbf{p}-\mathbf{p}' >\right). \tag{35}$$

An understanding of the properties of this contribution to the Wigner function is made difficult by the presence of the oscillatory exponentials. It is easier to evaluate first its contribution to the particle flux before looking at the behavior at large distances. The particle flux contribution is found by the three-dimensional analog of Eq. (5), neglecting the initial weighting factor $\wp_{\mathbf{p}'\mathbf{p}''}(0)$,

$$\begin{aligned}\mathbf{j}_1^{sc}(\mathbf{r},t) &\equiv \int \frac{\mathbf{p}}{m} W_1^{sc}(\mathbf{p},\mathbf{r}) e^{-i\omega_{p'p''}t} d\mathbf{p} \\ &= \frac{1}{h^3} e^{-i\omega_{p'p''}t}\int\left(\frac{(\mathbf{P}+\mathbf{p}'')e^{i(\mathbf{P}-\mathbf{p}'')\cdot\mathbf{r}/\hbar}}{p'^2-P^2+i\eta} < \mathbf{P}|T|\mathbf{p}' > -\frac{(\mathbf{P}+\mathbf{p}')e^{i(\mathbf{p}'-\mathbf{P})\cdot\mathbf{r}/\hbar}}{P^2-p''^2+i\eta} < \mathbf{p}''|T^\dagger|\mathbf{P} >\right) d\mathbf{P},\end{aligned} \tag{36}$$

where the changes of variable, $\mathbf{P} = 2\mathbf{p} - \mathbf{p}''$ in the first term and $\mathbf{P} = 2\mathbf{p} - \mathbf{p}'$ in the second, have been made in order to simplify the integrals, and the time-dependent exponential factor has been explicitly included in accordance with the density-operator decomposition (2). In order to carry out the $\mathbf{P}$ integration, it is convenient to express the $T$ matrices in a representation that is half position, half momentum, for example,

$$< \mathbf{P}|T|\mathbf{p}' >= h^{-3/2}\int d\mathbf{r}' e^{-i\mathbf{P}\cdot\mathbf{r}'/\hbar} < \mathbf{r}'|T|\mathbf{p}' > . \tag{37}$$

Introducing cylindrical coordinates ($P_r$, $u$, $\theta$) for $\mathbf{P}$ with the direction $\hat{\mathbf{R}} \equiv (\mathbf{r}-\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$ being the symmetry axis, the $\mathbf{P}$ integral in the first term then becomes

$$\begin{aligned}\int \frac{(\mathbf{P}+\mathbf{p}'')e^{i\mathbf{P}\cdot(\mathbf{r}-\mathbf{r}')/\hbar}}{p'^2-P^2+i\eta} d\mathbf{P} &= 2\pi\int_0^\infty u\,du\int_{-\infty}^\infty \frac{[P_r\hat{\mathbf{R}}+\mathbf{p}'']e^{iP_r|\mathbf{r}-\mathbf{r}'|/\hbar}}{p'^2-P_r^2-u^2+i\eta} dP_r \\ &= -2\pi^2 i\int_0^\infty \frac{[w\hat{\mathbf{R}}+\mathbf{p}'']e^{iw|\mathbf{r}-\mathbf{r}'|/\hbar}}{w} u\,du.\end{aligned} \tag{38}$$

Cylindrical symmetry of the integral has been used in the first step to eliminate all but the $P_r\hat{\mathbf{R}}$ contribution to the vector $\mathbf{P}$ in the numerator. Contour integration with closure in the upper half plane has allowed the $P_r$ integral to be carried out, with only the pole at $w \equiv (\sqrt{p'^2-u^2+i\eta})_+$ contributing [$(\sqrt{\ })_+$ designates that square root having positive imaginary part]. A further change in variable, from $u$ to $w$ ($u\,du = -w\,dw$) allows the final integration to be done and completes the analytical evaluation of the $\mathbf{P}$ integral of Eq. (38). Note that the $w$ contour goes from $p'$ on the positive real axis to $+i\infty$, as $\eta \to 0$, so that the integral becomes

$$-\frac{2\pi^2\hbar}{|\mathbf{r}-\mathbf{r}'|}\left[\hat{\mathbf{R}}\left(p'+\frac{i\hbar}{|\mathbf{r}-\mathbf{r}'|}\right)+\mathbf{p}''\right] e^{ip'|\mathbf{r}-\mathbf{r}'|/\hbar}. \tag{39}$$

The second $\mathbf{P}$ integral is of the same form, being the complex conjugate of the first, together with an interchange of $\mathbf{p}'$ and $\mathbf{p}''$. Thus $\mathbf{j}_1^{sc}$ can be exactly expressed as

$$\begin{aligned}\mathbf{j}_1^{sc}(\mathbf{r},t) = &\frac{-\pi}{h^{7/2}} e^{-i\omega_{p'p''}t}\int d\mathbf{r}'\frac{e^{ip'|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|}\left[\hat{\mathbf{R}}\left(p'+\frac{i\hbar}{|\mathbf{r}-\mathbf{r}'|}\right)+\mathbf{p}''\right] < \mathbf{r}'|T|\mathbf{p}' > e^{-i\mathbf{p}''\cdot\mathbf{r}/\hbar} \\ &-\frac{\pi}{h^{7/2}} e^{-i\omega_{p'p''}t}\int d\mathbf{r}'\frac{e^{-ip''|\mathbf{r}-\mathbf{r}'|/\hbar}}{|\mathbf{r}-\mathbf{r}'|}\left[\hat{\mathbf{R}}\left(p''-\frac{i\hbar}{|\mathbf{r}-\mathbf{r}'|}\right)+\mathbf{p}'\right] < \mathbf{p}''|T^\dagger|\mathbf{r}' > e^{i\mathbf{p}'\cdot\mathbf{r}/\hbar}.\end{aligned} \tag{40}$$

It is well known [11–13] that for large $r$, the exponential $\exp(i\mathbf{p}\cdot\mathbf{r}/\hbar)$ can be approximated according to

$$\exp(i\mathbf{p}\cdot\mathbf{r}/\hbar) \sim ih(pr)^{-1}[\delta(\hat{\mathbf{r}}+\hat{\mathbf{p}})e^{-ipr/\hbar} - \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}})e^{ipr/\hbar}], \tag{41}$$

while $|\mathbf{r}-\mathbf{r}'| \sim r - \hat{\mathbf{r}}\cdot\mathbf{r}'$. With the use of these asymptotic formulas and recognizing that the $\mathbf{r}'$ integrals can be performed after taking the asymptotic limit, the one-particle scattered flux is given by (neglecting terms depending on $r^{-3}$)

$$
\begin{aligned}
\mathbf{j}_1^{\rm sc} \sim e^{-i\omega_{p'p''}t}\Bigg( & \frac{-i\pi}{p''hr^2}(\hat{\mathbf{r}}p'+\mathbf{p}'') < p'\hat{\mathbf{r}}|T|\mathbf{p}' > \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}'')e^{i(p'-p'')r/\hbar} \\
& +\frac{i\pi}{p'hr^2}(\hat{\mathbf{r}}p''+\mathbf{p}') < \mathbf{p}''|T^\dagger|p''\hat{\mathbf{r}} > \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}')e^{i(p'-p'')r/\hbar} \\
& \times\frac{i\pi}{p''hr^2}(\hat{\mathbf{r}}p'+\mathbf{p}'') < p'\hat{\mathbf{r}}|T|\mathbf{p}' > \delta(\hat{\mathbf{r}}+\hat{\mathbf{p}}'')e^{i(p'+p'')r/\hbar} \\
& +\frac{-i\pi}{p'hr^2}(\hat{\mathbf{r}}p''+\mathbf{p}') < \mathbf{p}''|T^\dagger|p''\hat{\mathbf{r}} > \delta(\hat{\mathbf{r}}+\hat{\mathbf{p}}')e^{-i(p'+p'')r/\hbar}\Bigg) .
\end{aligned}
\tag{42}
$$

If an integral over time is to be performed, as is the case when computing the total number of scattered particles for a given direction, only zero-frequency components contribute (see the discussion in Sec. III C). But for zero frequency, $|\mathbf{p}'| = |\mathbf{p}''|$, the last two terms in the former expression vanish, and the time dependence disappears. The contribution to the scattered spherical flux (number of particles per steradian per second, per momentum cubed of the incoming beam) is then

$$
\begin{aligned}
j_1^{\rm sph}(\hat{r}) &\equiv \lim_{r\to\infty} r^2\hat{\mathbf{r}}\cdot\mathbf{j}_1^{\rm sc} \\
&= \frac{-2\pi i}{h}[< p'\hat{\mathbf{r}}|T|\mathbf{p}' > \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}'') \\
&\quad - < p'\hat{\mathbf{p}}''|T^\dagger|p'\hat{\mathbf{r}} > \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}')].
\end{aligned}
\tag{43}
$$

Note the "double-interference" effect associated with the two directions in the incoming angular coherence. The linear (in $T$) contribution to the total flux, irrespective of the angle and time, from a given on-the-energy-shell component, is then obtained by integrating this scattered spherical flux over all angles

$$
\begin{aligned}
j_1^{\rm tot} &= \int d\hat{\mathbf{r}} j_1^{\rm sph}(\hat{\mathbf{r}}) = \frac{i}{\hbar} < p'\hat{\mathbf{p}}''|T^\dagger - T|\mathbf{p}' > \\
&= -\frac{2\pi}{\hbar}\int d\mathbf{p} < \mathbf{p}|T|\mathbf{p}' > \delta(E_p - E_{p'}) < p'\hat{\mathbf{p}}''|T^\dagger|\mathbf{p} > \\
&= -\frac{2\pi m p'}{\hbar}\int d\hat{\mathbf{p}} < p'\hat{\mathbf{p}}|T|\mathbf{p}' >< p'\hat{\mathbf{p}}''|T^\dagger|p'\hat{\mathbf{p}} > .
\end{aligned}
\tag{44}
$$

Note that both $j_1^{\rm sph}$ and $j_1^{\rm tot}$ are scalar quantities. The generalized optical theorem has been applied to express the linear (in $T$) result as a quadratic (in $T$) integral. It will be seen later that this integral exactly compensates the total flux from the quadratic (in $T$) term of the transition superoperator. In other words, the total scattered flux through a spherical surface for a given coherence vanishes, $j^{\rm tot} = j_1^{\rm tot} + j_2^{\rm tot} = 0$, and this implies particle conservation (the total flux from the incoming part of the density operator is also zero). While the generalized optical theorem is usually given as an abstract relation [15], the present formalism gives it a physical content, which can be formulated in the following way. "The total flux due to any on-the-energy-shell coherence vanishes." This statement is well known for the particular case $\mathbf{p}' = \mathbf{p}''$, which corresponds to standard stationary scattering [13], but to our knowledge, had not been spelled out for a general zero-frequency coherence. That these coherences contribute to the scattered differential flux (*integral over time of the spherical flux in a given direction*) is an interesting result. In practice, this means that density operators whose incoming parts have the same diagonal elements in momentum representation but different coherences do not necessarily give the same differential flux. Thus, for the theoretical modeling of a scattering experiment in which only the average energy and energy resolution, typically the two first moments of a Gaussian distribution, are specified *it is not equivalent* to compute the differential fluxes from the time evolution of a Gaussian packet (retaining nonzero coherences), or from a stationary density operator having identical incoming diagonal elements to the Gaussian packet. For the special case where the incoming state is diagonal in momentum (direction as well as magnitude), the standard "forward interference"

$$
\begin{aligned}
j_1^{\rm sph} &= \frac{2i\pi}{h} < \mathbf{p}'|T^\dagger - T|\mathbf{p}' > \delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}') \\
&= \frac{-2\pi}{\hbar}\delta(\hat{\mathbf{r}}-\hat{\mathbf{p}}')\int d\mathbf{p}|< \mathbf{p}'|T|\mathbf{p} >|^2\delta\left(\frac{p'^2-p^2}{2m}\right)
\end{aligned}
\tag{45}
$$

is obtained.

### B. Terms quadratic in $T$

The quadratic (in $T$) contribution to $M(\mathbf{x},\mathbf{p})$ is found in an analogous manner. From Eqs. (17) and (32) the formal expression is

$$
\begin{aligned}
M_2(\mathbf{x},\mathbf{p}) = \frac{-2mi}{(2\pi)^3\hbar}\int d\mathbf{s}\, e^{i\mathbf{x}\cdot\mathbf{s}} & < \mathbf{p}+\mathbf{s}\hbar/2|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{p}-\mathbf{s}\hbar/2 > \\
& \times\left(\frac{1}{p''^2-(\mathbf{p}-\mathbf{s}\hbar/2)^2-i\eta} - \frac{1}{p'^2-(\mathbf{p}+\mathbf{s}\hbar/2)^2+i\eta}\right) .
\end{aligned}
\tag{46}
$$

It is desirable to show that this is local in $x$, i.e., that it falls off fairly rapidly with $x$ so that the asymptotic properties of the scattered Wigner function as discussed in Ref. [2] would be valid. For this purpose, the asymptotic behavior of $M_2(\mathbf{x},\mathbf{p})$ is now examined. It is found to decrease but not as rapidly as was expected.

In order to carry out the s integration, it is again useful to introduce the mixed representation (37) of the transition operator so that $M_2(\mathbf{x},\mathbf{p})$ can be written

$$M_2(\mathbf{x},\mathbf{p}) = \frac{-2mi}{(2\pi)^3 h^3 \hbar} \int\int d\mathbf{r}' d\mathbf{r}'' < \mathbf{r}'|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{r}'' >$$
$$\times \int d\mathbf{s}\, e^{i\mathbf{x}\cdot\mathbf{s}} e^{-i\mathbf{r}'\cdot(\mathbf{p}+\mathbf{s}\hbar/2)/\hbar} e^{i\mathbf{r}''\cdot(\mathbf{p}-\mathbf{s}\hbar/2)/\hbar}$$
$$\times \left( \frac{1}{p''^2 - (\mathbf{p}-\mathbf{s}\hbar/2)^2 - i\eta} - \frac{1}{p'^2 - (\mathbf{p}+\mathbf{s}\hbar/2)^2 + i\eta} \right). \quad (47)$$

The s integration can now be explicitly carried out. Each resolvent needs to be treated separately and if the transformation from s to $\mathbf{P} = \mathbf{p} + \mathbf{s}\hbar/2$ is made for the second resolvent, then the $\mathbf{P}$ integral can be read off of the result, Eqs. (38) and (39). The first resolvent is integrated in an analogous manner so that

$$M_2(\mathbf{x},\mathbf{p}) = \frac{4mi}{\pi \hbar^3 h^3} \int\int d\mathbf{r}' d\mathbf{r}'' \frac{< \mathbf{r}'|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{r}'' >}{|2\mathbf{x} - \mathbf{r}' - \mathbf{r}''|}$$
$$\times \left( e^{2i(\mathbf{x}-\mathbf{r}')\cdot\mathbf{p}/\hbar} e^{-ip''|2\mathbf{x}-\mathbf{r}'-\mathbf{r}''|/\hbar} - e^{2i\mathbf{p}\cdot(\mathbf{r}''-\mathbf{x})/\hbar} e^{ip'|2\mathbf{x}-\mathbf{r}'-\mathbf{r}''|/\hbar} \right). \quad (48)$$

It is now appropriate to consider the behavior as $x \to \infty$. On the basis that the potential $V$ is short ranged, the vector magnitude can be expanded as $|2\mathbf{x} - \mathbf{r}' - \mathbf{r}''| \sim 2x - \hat{\mathbf{x}}\cdot(\mathbf{r}' + \mathbf{r}'')$ while the exponential involving $\mathbf{x}$ can be expanded using Eq. (41). Of the two terms in Eq. (41), only one can at least partially compensate the spatial oscillations arising from the exponential involving the absolute value. For each term in Eq. (48), only the partially compensating exponential term has been retained, to give

$$M_2(\mathbf{x},\mathbf{p}) \sim \delta(\hat{\mathbf{x}} - \hat{\mathbf{p}}) \frac{2m}{\hbar^2 h^3 p x^2} \int\int d\mathbf{r}' d\mathbf{r}'' < \mathbf{r}'|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{r}'' >$$
$$\times \left( e^{2i(p-p'')x/\hbar} e^{i[(p''-2p)\hat{\mathbf{p}}\cdot\mathbf{r}' + p''\hat{\mathbf{p}}\cdot\mathbf{r}'']/\hbar} + e^{2i(p'-p)x/\hbar} e^{[2i\mathbf{p}\cdot\mathbf{r}'' - p'\hat{\mathbf{p}}\cdot(\mathbf{r}'+\mathbf{r}'')]/\hbar} \right)$$
$$\sim \delta(\hat{\mathbf{x}} - \hat{\mathbf{p}}) \frac{2m}{\hbar^2 p x^2} [e^{2i(p-p'')x/\hbar} < (2p - p'')\hat{\mathbf{p}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|p''\hat{\mathbf{p}} >$$
$$+ e^{2i(p'-p)x/\hbar} < p'\hat{\mathbf{p}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|(2p - p')\hat{\mathbf{p}} >]. \quad (49)$$

For the special case of on-the-energy-shell collisions, so that $p = p'' = p'$, this reduces to

$$M_2(\mathbf{x},\mathbf{p}) \sim \delta(\hat{\mathbf{x}} - \hat{\mathbf{p}}) \frac{4m}{\hbar^2 p' x^2} < p'\hat{\mathbf{p}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|p'\hat{\mathbf{p}} > . \quad (50)$$

In all cases this shows that $M(\mathbf{x},\mathbf{p})$ falls off as $x^{-2}$. It was expected that this would decay with $x$ somewhat as rapidly as does $V(\mathbf{x})$, but this is not the case. The resolvents limit the decay rate. However this is still sufficient to warrant the use of the asymptotic methods of Ref. [2].

The asymptotic behavior of $W_2^{\rm sc}(\mathbf{r},\mathbf{p})$ has been discussed in Ref. [2]. Alternatively, the properties of the corresponding scattered flux $\mathbf{j}_2^{\rm sc}$ can be examined. It follows directly from Eq. (31) and the form for $\mathcal{T}_2$, Eq. (47), that

$$\mathbf{j}_2^{\rm sc}(\mathbf{r},t) \equiv \int \frac{\mathbf{p}}{m} W_2^{\rm sc}(\mathbf{r},\mathbf{p}) e^{-i\omega_{p'p''}t} d\mathbf{p}$$
$$= \frac{4me^{-i\omega_{p'p''}t}}{(2\pi)^3 h^3} \int\int d\mathbf{r}' d\mathbf{r}'' < \mathbf{r}'|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{r}'' >$$
$$\times \int\int d\mathbf{p}\, d\mathbf{s} \frac{\mathbf{p} e^{-i(\mathbf{r}'-\mathbf{r})\cdot(\mathbf{p}+\mathbf{s}\hbar/2)/\hbar} e^{i(\mathbf{r}''-\mathbf{r})\,(\mathbf{p}-\mathbf{s}\hbar/2)/\hbar}}{[p''^2 - (\mathbf{p}-\mathbf{s}\hbar/2)^2 - i\eta][p'^2 - (\mathbf{p}+\mathbf{s}\hbar/2)^2 + i\eta]}. \quad (51)$$

Here the free Liouville resolvent has been cancelled by the numerator arising from combining the two Hamiltonian resolvents (technically there is a difference of $i\eta$ and $2i\eta$, but as $\eta \to 0$ this difference vanishes). Now it is noticed that the combinations $\mathbf{p} \pm \mathbf{s}\hbar/2$ are the natural variables for the last integrand. Thus changing variables from $\mathbf{p}$ and $\mathbf{s}$ to these combinations, the latter integrals can be performed using Eqs. (38) and (39). It follows that

$$\mathbf{j}_2^{\rm sc}(\mathbf{r},t) = \frac{\pi m e^{-i\omega_{p'p''}t}}{\hbar h^3} \int\int \frac{d\mathbf{r}' d\mathbf{r}''}{|\mathbf{r}-\mathbf{r}'||\mathbf{r}-\mathbf{r}''|} \left[ \hat{\mathbf{R}} \left( p' + \frac{i\hbar}{|\mathbf{r}-\mathbf{r}'|} \right) + \hat{\mathbf{R}}' \left( p'' - \frac{i\hbar}{|\mathbf{r}-\mathbf{r}''|} \right) \right]$$
$$\times e^{ip'|\mathbf{r}-\mathbf{r}'|/\hbar} < \mathbf{r}'|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{r}'' > e^{-ip''|\mathbf{r}-\mathbf{r}''|/\hbar}$$
$$\sim \frac{2\pi m}{\hbar r^2} \hat{\mathbf{r}} \left( \frac{p' + p''}{2} \right) e^{i(p'-p'')r/\hbar} e^{-i\omega_{p'p''}t} < p'\hat{\mathbf{r}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|p''\hat{\mathbf{r}} >, \quad (52)$$

where $\hat{\mathbf{R}}' \equiv (\mathbf{r}-\mathbf{r}'')/|\mathbf{r}-\mathbf{r}''|$. This flux is in the radial direction and decays with $r^{-2}$ as appropriate for the radiation condition. But it also oscillates in time and space due to the energy nondiagonality of the incoming state. In the particular case where $p''=p'$ both these oscillations vanish but there can still be a coherence between different directions. The scattered spherical flux in the radial direction is then

$$j_2^{\rm sph}(\hat{\mathbf{p}}) \equiv \lim_{r\to\infty} r^2\hat{\mathbf{p}}\cdot\mathbf{j}_2^{\rm sc} = \frac{2\pi m p'}{\hbar} < p'\hat{\mathbf{p}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|p'\hat{\mathbf{p}} >, \quad (53)$$

where $\hat{\mathbf{p}}=\hat{\mathbf{r}}$. This completes the comment on the total scattered flux made following Eq. (44). In Ref. [2] the generalized scattering cross section was given by Eq.(33). Generalizing this to the case where there is a coherence in the initial-momentum direction defines

$$\sigma_{(\mathbf{p}',\mathbf{p}'')\to\hat{\mathbf{p}}} \equiv j^{\rm sph}(\hat{p})/j^{\rm in} = \frac{mh^3}{p'} << \hat{\mathbf{p}},\hat{\mathbf{p}}| -iT|\mathbf{p}',\mathbf{p}'' >>, \quad (54)$$

with the implicit assumption that the momentum magnitudes $p''$ and $p'$ are equal and using $j^{\rm sph}(\hat{\mathbf{p}}) = j_1^{\rm sph}(\hat{\mathbf{p}}) + j_2^{\rm sph}(\hat{\mathbf{p}})$ for the spherical flux due to the $|\mathbf{p}'><\mathbf{p}''|$ coherence. The validity of the second equality is now shown in detail:

$$\begin{aligned}\frac{mh^3}{p'}&\int p^2dp << \mathbf{p},\mathbf{p}| -iT|\mathbf{p}',\mathbf{p}'' >>\\ &= \frac{-imh^3}{\hbar p'}\int p^2dp\Big[< \mathbf{p}|T|\mathbf{p}' > \delta(\mathbf{p}-\mathbf{p}'') - \delta(\mathbf{p}-\mathbf{p}') < \mathbf{p}''|T^\dagger|\mathbf{p} >\\ &\qquad +2m < \mathbf{p}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|\mathbf{p} > \left(\frac{1}{p''^2-p^2-i\eta} - \frac{1}{p'^2-p^2+i\eta}\right)\Big]\\ &= \frac{-imh^3}{\hbar p'}[< \mathbf{p}''|T|\mathbf{p}' > \delta(\hat{\mathbf{p}}-\hat{\mathbf{p}}'') - \delta(\hat{\mathbf{p}}-\hat{\mathbf{p}}') < \mathbf{p}''|T^\dagger|\mathbf{p}' >]\\ &\quad +(2\pi m h)^2 < p'\hat{\mathbf{p}}|T|\mathbf{p}' >< \mathbf{p}''|T^\dagger|p'\hat{\mathbf{p}} > . \end{aligned} \quad (55)$$

Use has been made of the restriction that $p''=p'$ in order to convert the difference of resolvents into a $\delta$ function. After taking into account the factor $mh^3/p'$ which converts the spherical flux into a cross section, it is seen that the last expression is precisely the ratio $j^{\rm sph}/j^{\rm in}$.

### C. Time-dependent scattering

So far, the stress has been on particular components of the incoming density operator, and more specifically on zero-frequency components (diagonal elements and directional coherences). Nevertheless, the physical flux in a time-dependent collision is given by an integral over all components of the incoming state, and this usually involves energy coherences as well as the zero-frequency components. In this subsection the various integrated physical fluxes include the coherence contributions, and the special relevance of the zero-frequency components is justified by resorting to time integration.

Different fluxes associated with coherences have been previously represented as functions of position and time. However they also depend parametrically on the coherence momenta. Here it is useful to indicate this dependence explicitly in their arguments. Thus $\mathbf{j}^{\rm sc} = \mathbf{j}^{\rm sc}(\mathbf{r},t;\mathbf{p}',\mathbf{p}'')$ and $j^{\rm sph} = j^{\rm sph}(\hat{\mathbf{p}},r,t;\mathbf{p}',\mathbf{p}'')$, where $\hat{\mathbf{p}} = \hat{\mathbf{r}}$. While for directional coherences the $r$ and $t$ dependence of $j^{\rm sph}$ vanishes, for an energy coherence this flux does oscillate with time and distance from the origin, see (42) and (52).

With this notational convention, the total scattered flux at given position and time becomes, using the three-dimensional analog of (5):

$$\mathbf{J}^{\rm sc}(\mathbf{r},t) = \iint d\mathbf{p}'d\mathbf{p}''\,\mathbf{j}^{\rm sc}(\mathbf{r},t;\mathbf{p}',\mathbf{p}'')\wp_{\mathbf{p}'\mathbf{p}''}(0) \quad (56)$$

and the corresponding spherical flux is

$$J^{\rm sph}(\hat{\mathbf{p}},r,t) = \iint d\mathbf{p}'d\mathbf{p}''\, j^{\rm sph}(\hat{\mathbf{p}},r,t;\mathbf{p}',\mathbf{p}'')\,\wp_{\mathbf{p}'\mathbf{p}''}(0). \quad (57)$$

From the explicit form for the time dependence, the integral over time of this quantity gives

$$\begin{aligned}N^{\rm sph}(\hat{\mathbf{p}}) &\equiv \int dt\, J^{\rm sph}(\hat{\mathbf{p}},r,t)\\ &= h\iint d\mathbf{p}'d\mathbf{p}''j^{\rm sph}(\hat{\mathbf{p}},r,0;\mathbf{p}'\mathbf{p}''),\\ &\qquad \times\,\delta((p'^2-p''^2)/2m)\,\wp_{\mathbf{p}'\mathbf{p}''}(0). \end{aligned}\quad (58)$$

This is independent of $r$ because the $\delta$ function requires the magnitudes $p'$ and $p''$ to be equal. Assuming that the flux due to the incoming part of the density operator is negligible at this angle $N^{\rm sph}$ represents the fraction of particles that arrive asymptotically in a given unit solid angle. It can be written in terms of the generalized cross section as

$$\begin{aligned}N^{\rm sph}(\hat{\mathbf{p}}) = \iint & d\mathbf{p}'d\mathbf{p}''\,\frac{p'}{mh^2}\,\sigma_{(\mathbf{p}'\mathbf{p}'')\to\hat{\mathbf{p}}}\\ &\times\delta\left(\frac{p'^2-p''^2}{2m}\right)\wp_{\mathbf{p}'\mathbf{p}''}(0). \end{aligned}\quad (59)$$

Clearly only directional coherences contribute to the time-averaged spherical flux.

## IV. DISCUSSION

Special attention has been paid to the asymptotic behavior of the particle flux. This has allowed the generalized differential cross section (in three dimensions) or the transmittance (in one dimension) to be expressed in terms of the transition superoperator. In a previous work, the expression for the differential cross section was obtained by assuming that the Weyl transform of the transition superoperator decays as rapidly as the interaction potential. It has here been shown that this expected behavior is not correct. But using a proper derivation, the original result, namely identifying a generalized cross section and relating it to the transition superoperator, remains valid.

The present treatment extends the scope of the former phase-space descriptions since time-dependent scattering is considered. This involves momentum coherences, or nondiagonal elements of the incoming density operator. An expression obtained for the one-dimensional transmittance in time-dependent scattering contains nondiagonal contributions. However, only on-the-energy-shell coherences are present in it. If the initial average energy is not too low and the momentum distribution is not too broad, this coherence effect can be neglected and the transmittance becomes the average of the stationary transmittances, the weighting function being the initial momentum distribution. It is then interesting to see that, under these suitable conditions and provided that the momentum distribution remains the same, the shape of the initial state, pure or mixed, in coordinate space does not affect the transmittance. This is in agreement with classical reasoning and numerical evidence [14].

In three dimensions, a precise and physically transparent expression for on-the-energy-shell matrix elements of the generalized optical theorem has been found, namely: "The total flux through a spherical surface due to any on-the-energy-shell coherence vanishes." These on-shell coherences are also privileged in three-dimensional scattering in the sense that they are the only ones contributing after time integration, and the only ones whose flux is free from time and spatial oscillations. The flux contribution from a particular on-shell coherence $|\mathbf{p}'> \wp_{\mathbf{p}'\mathbf{p}''} <\mathbf{p}''|$ is in general a complex quantity. The real flux contribution is obtained by addition of the effects of the conjugate coherence $|\mathbf{p}''> \wp_{\mathbf{p}''\mathbf{p}'} <\mathbf{p}'|$. The Hermiticity of the density operator assures that cancellation of the imaginary part always occurs. Generalized cross sections are defined for directional coherences. In general, these coherences contribute to the total flux in a given direction together with the standard differential (populational or diagonal in momentum) cross section, and cannot be disregarded unless the experimental conditions justify doing so. In particular, for an incoherent beam of sharply peaked packets (in momentum) directed along a homogeneously distributed set of impact parameters there is no significant coherence contribution [5, 16]. Mixed incoming states diagonal in momentum are also free from such contributions and give strictly stationary scattering. Pure-state wave packets, on the other hand, have an asymptotic total flux contribution due to initial on-shell coherences. Pure wave packets are also characterized by time-dependent nonstationary behavior due to the off-the-energy-shell coherences.

The recent development of efficient numerical methods for propagating time dependent wave packets is frequently considered a practical alternative to stationary computations. However, care should be exercised in analyzing the results, in the light of the present discussion. A study of the quantitative importance of the coherence contributions is in preparation.

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## APPENDIX: SCATTERING-THEORY RELATIONS

Operator relations are discussed first, then superoperator relations. The abstract Møller and transition operators are defined as

$$\Omega = \lim_{t\to-\infty} e^{iHt/\hbar} e^{-iH_0t/\hbar}, \quad T = V\Omega. \tag{A1}$$

They are related to the parametrized operators by

$$\Omega\phi = \int \lim_{\varepsilon\to 0} \Omega(E_p + i\varepsilon)|p><p|\phi> dp, \tag{A2}$$

$$T|p>= \lim_{\varepsilon\to 0} T(E_p + i\varepsilon)|p>, \tag{A3}$$

where

$$\Omega(z) = 1 + \frac{1}{z - H_0} T(z), \quad T(z) = V + V\frac{1}{z - H} V. \tag{A4}$$

Some useful relations between resolvents and parametrized operators are

$$\frac{1}{z-H} = \frac{1}{z-H_0} + \frac{1}{z-H_0} T(z) \frac{1}{z-H_0},$$
$$T(z)\frac{1}{z-H_0} = V\frac{1}{z-H}. \tag{A5}$$

The *generalized optical theorem* in abstract operator form can be written as

$$T - T^\dagger = -2\pi i T\delta(E - H_0)T^\dagger$$
$$= -2\pi i T^\dagger \delta(E - H_0)T \tag{A6}$$

with the understanding that the free-particle states on which this operator relation acts (both ket and bra) have energy $E$. The corresponding expression for the matrix elements diagonal in momentum is the *optical theorem* [15]. In one dimension it reads

$$\text{Im}T_{pp} = -\frac{m\pi}{p}(|T_{pp}|^2 + |T_{-pp}|^2). \quad \text{(A7)}$$

The abstract Møller and transition superoperators are defined as

$$\Omega_L = \lim_{t\to-\infty} e^{i\mathcal{L}t}e^{-i\mathcal{L}_0 t}, \quad \mathcal{T} = \mathcal{V}\Omega_L, \quad \text{(A8)}$$

where the Liouville superoperator $\mathcal{L} = \hbar^{-1}[H, \ ]$ is decomposed into its free and potential parts, $\mathcal{L} = \mathcal{L}_0 + \mathcal{V}$,

$$\mathcal{L}_0 = \hbar^{-1}[H_0, \ ], \quad \mathcal{V} = \hbar^{-1}[V, \ ]. \quad \text{(A9)}$$

The abstract $\Omega_L$ and $\mathcal{T}$ can also be expressed in terms of $\Omega$ and $T$ as

$$\Omega_L A = \Omega A \Omega^\dagger, \qquad \hbar\mathcal{T}A = TA\Omega^\dagger - \Omega A T^\dagger. \quad \text{(A10)}$$

They are also related to the parametrized superoperators by

$$\Omega_L A = \int \lim_{\eta\to 0} \Omega_L(\omega_{pp'}+i\eta)|p,p'>><<pp'|A>> \, dp\, dp' \quad \text{(A11)}$$

and

$$\mathcal{T}|p,p'>> = \lim_{\eta\to 0} \mathcal{T}(\omega_{pp'}+i\eta)|p,p'>>, \quad \text{(A12)}$$

where

$$\Omega_L(z) = 1 + \frac{1}{z-\mathcal{L}_0}\mathcal{T}(z), \quad \mathcal{T}(z) = \mathcal{V} + \mathcal{V}\frac{1}{z-\mathcal{L}}\mathcal{V}. \quad \text{(A13)}$$

The one-dimensional expressions [(A2), (A3), (A11), and (A12)] can readily be generalized to three dimensions by changing from scalar to vector momenta.

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