Scattering theory, multiparticle detection, and time

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We consider the theory of multiple-particle fragmentation processes in the light of modern multihit position-sensitive detection. First, we give a formulation of time-independent many-body scattering theory as a direct generalization of standard textbook two-body potential scattering but in such a way as to emphasize position rather than momentum detection. Noteworthy is that *classical* asymptotic motion of fragments is shown to emerge from this quantum-mechanical time-independent theory and enables the definition of a classical time parameter. This in turn allows a transition to be made to a time-dependent scattering theory, even in the case where all Hamiltonians are time independent. Such a time-dependent description is the basis of the *imaging theorem*, which connects position detection to momentum detection.

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I. INTRODUCTION

The standard quantum-mechanical theory of scattering, leading to expressions for differential cross sections, was formulated in the 1950s and emphasizes detection of particle momenta in the final channel. Although these theories begin with the time-dependent Schrödinger equation (TDSE), the final quantities in which cross sections are expressed, scattering S, transition T, and Møller operators, are time independent and the theory is wholly quantum mechanical. Modern detector techniques rely more on position detection than energy or momentum detection and, despite the quantum nature of the theory, classical mechanics is used successfully to describe the extraction of charged particles and their passage from the microscopic reaction zone to the macroscopic detector. Also, the (quantum) momenta required by the theory are inferred from position measurements by defining classical velocities based on time and position detection. Our aim here is to reconcile the wholly quantum time-independent scattering theory with the introduction of a classical time and position-sensitive detection. We wish to confront the question as to how these time-dependent measurements can be interpreted and justified beginning with a quantum scattering theory which is time independent. This is an extension of considerations first discussed by Kemble for one particle [1].

From time-independent scattering theory we demonstrate how a classical time set by the preparation and detection process emerges naturally from a purely quantum theory. In this way, we see how a time-dependent theory is justified, how measured momenta are defined, and how the *imaging theorem* (IT) relating asymptotic position and momentum wave functions arises [2].

At the core of the analysis are three features which are not usually found in textbooks on scattering theory. The first is the derivation of a wholly time-independent scattering theory for many-particle many-channel fragmentation processes as a direct generalization of the standard textbook treatment of two-body single-channel potential scattering. This derivation is based upon an old but largely neglected work of Gerjuoy [3]. However, in contrast to Gerjuoy and to standard approaches, we derive the cross section directly in terms of a position measurement. Crucial to our argument is the demonstration that *classical* motion in the asymptotic region emerges naturally and allows a time variable to be defined from a time-independent theory.

The second important feature is to show that this time variable can be identified with the classical clock time of the detection apparatus, which leads to time-dependent expressions for quantum transition amplitudes. Time-dependent scattering theory, involving both time-independent and explicitly time-dependent interaction potentials, is shown to emerge from a time-independent theory in which the detector itself is treated first by quantum mechanics and then allowed to become macroscopically large and describable by time-dependent classical mechanics.

The third feature is to point out the importance of the IT which relates the asymptotic wave function in position space to the momentum-space wave function at the exit of the reaction zone, which wave function can be related to the quantum scattering amplitude [2]. Although proved by Kemble in 1937 [1] and rediscovered spasmodically since that time, the importance of the IT for the interpretation of scattering measurements has been appreciated only lately [4–6].

Once the detector time is defined from *time-independent* scattering theory and macroscopic position detection, the IT follows and shows that detection of fragments at different times and positions conforms to the classical Newton's equations *even when the particles still obey quantum mechanics*. A scattered fragment moves macroscopically according to Schrödinger's or Newton's equations since both give the same result for the fragment's motion. There is no need to invoke wave-function collapse or the creation of narrow wave packets.

The establishment of a time-dependent theory is crucial for the proof of the IT since this relies upon the notion of wave functions propagating in time from a collision region to a detector. Even though the collision Hamiltonian and that of subsequent propagation may be time independent, our derivation shows how this treatment is justified. The use of

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the IT in connection with modern multiparticle detection by electric and magnetic field extraction is discussed in detail in Ref. [7].

One must make a clear distinction between time-independent and time-dependent Hamiltonians. Only the former are relevant for standard quantum scattering theory, which does not involve time. Time-dependent Hamiltonians are approximate in the sense that the time arises only when some part of the scattering system is treated macroscopically and classically. One example is fast heavy-ion beams where the beam motion is not quantized but treated as obeying Newtonian mechanics. An even more common example is a strong laser beam where the electromagnetic field is not quantized but considered to be a time-dependent field obeying the classical Maxwell equations. Indeed, such an approximate description is central to the burgeoning field of femtosecond and attosecond spectroscopy. To account for the resulting time-dependent potentials, an explicitly time-dependent quantum scattering theory is employed. Time-dependent potentials appear naturally in our derivation of time-dependent scattering theory given below.

We begin by considering the quantum theory of scattering and the extraction from the theory of quantities which should allow direct comparison with experimentally detected physical quantities. Most textbooks introduce scattering theory with the example of so-called "potential" scattering, i.e., two-body scattering of structureless particles interacting via a position-dependent fixed potential. This is treated in time-independent quantum theory. That is, the scattering states are continuum eigenstates of a time-independent Hamiltonian. The measured quantity is derived as a cross section implying that incident and scattered beams of particles involve a constant time-independent flux of macroscopically many particles.

Although one can generalize potential scattering to the case of composite particles, again in standard texts this is restricted to two particles in the final channel [8]. Somewhat paradoxically, when the generalization is made to a formal scattering theory encompassing *many-particle* fragmentation of composite particles, even in the case of time-independent Hamiltonians, the derivation usually proceeds by beginning with the *time-dependent* Schrödinger equation (TDSE). However, this "time" is eliminated subsequently by defining the relevant time-independent scattering operators (e.g., S,T or Møller operators) through some infinite-time limiting process. In this way, a fully time-independent formulation is achieved [9,10]. Hence, in these standard derivations the time must be redundant and has no physical meaning but serves only to satisfy certain mathematical limits. Nevertheless, since the 1950s this is the approach adopted by standard textbooks such as Goldberger and Watson [11], Newton [12], and Gottfried and Yan [13].

However, it was shown by Gerjuoy [3], shortly after the presentation of the now-standard theories, that indeed the introduction of a time is unnecessary and one can derive a wholly time-independent theory for collisions involving many composite particles. Unfortunately, perhaps because Gerjuoy's formulation is rather forbidding in its notation, since it applies to any number of composite particles in incident and final channels, his approach has not found its way into the general literature of scattering theory. As far as we can ascertain, the only book in which it is used is Friedrich's treatment of a three-body fragmentation problem [14]. Apart from being a natural extension of textbook time-independent two-body scattering theory, such a many-particle theory, formulated in coordinate space, is well suited to one aim of this paper which is to concentrate on the detection of particles at given positions. Hence, in this paper first we give a simple reformulation of Gerjuoy's theory designed specifically to show the close parallel to the usual textbook treatment of two-body potential scattering. Then, we give a simpler, alternative derivation of cross sections based on a position measurement. In this way, we circumvent the complicated outgoing flux calculations required in Gerjuoy's derivation of cross sections.

One very important result is to see how quantities to be identified with final measured momenta are defined in the asymptotic region. This aspect is hardly given attention in the two-body case, which reduces to an effective one-body problem. However, we show that it is precisely the asymptotic relationship amongst the *spatial* coordinates of the scattered fragments that leads naturally to the introduction of a classical time variable. Correspondingly, the relation between time and position allows a classical velocity and momentum to be identified.

From the time-independent approach, by considering initially that the detector is quantized and then allowing the detector to become macroscopically large, we demonstrate the emergence of the time variable which leads to a TDSE for the scattering complex. Again, we relate the time-dependent scattering amplitude to a position measurement. The recognition that time is classical is in line with Wigner's demonstration [15] that a clock must be macroscopic and follows from a general proof of how the TDSE is derivable from the time-independent Schrödinger equation (TISE) [16–18].

The time-dependent approach is essential to the stationary-phase argument, first given by Kemble [1], used to prove the IT. All these results indicate how the information in the quantum wave function can be made compatible with the assumed classical interpretation of the particle movement to the detector. Of course, ultimately this is due to the happy accident of nature that the *exact* free quantum propagator can be derived from the action along a single trajectory for classical motion [19,20].

The logical development of the paper is as follows. In Sec. II, we present many-particle scattering theory as a direct generalization of simple two-body potential scattering. In particular, we define a many-particle scattering amplitude and a measurement probability as a function of detector position. This theory is completely quantum mechanical and time independent. In Sec. III, we show how the asymptotic behavior of the time-independent wave function leads naturally to the definition of classical velocity and thereby a time parameter. This allows further a definition of fixed asymptotic momenta to be made in terms of asymptotic *quantum spatial* coordinates. In turn, this leads to the concept of particle flux in terms of velocity and the formulation of a differential cross section.

Having identified a classical time parameter, in Sec. IV we consider the transition to a time-dependent scattering theory by deriving time from the interaction of the quantum scattering complex with a classical detector. Then, the ensuing time-dependent form of the scattering wave function is used to

prove the many-particle form of the IT, relating the spatial wave function to its momentum-space Fourier transform. The conclusions are summarized in Sec. V.

II. TIME-INDEPENDENT SCATTERING THEORY

A. Two-particle case

Since we wish to generalize the simplest two-particle potential scattering theory, first of all we remind ourselves of the salient points of its derivation presented in many textbooks. Specific equations can then be related to their n-body counterparts. We consider the elastic collision of two particles of reduced mass μ. For a total Hamiltonian which is the sum of kinetic energy operator H_0 and potential energy operator V, i.e., $H = H_0 + V$ the full Green operator at total energy E is defined by $G^+ = (E - H + i\epsilon)^{-1}$, where ϵ is a positive infinitesimal, and satisfies the equations

$$G^+ = G_0^+ + G_0^+ V G^+ = G_0^+ + G^+ V G_0^+, \tag{1}$$

where $G_0^+ = (E - H_0 + i\epsilon)^{-1}$ is the free-particle Green operator.

In the standard textbook approach, one considers the scattering state $\Psi_i^+(\boldsymbol{r})$, where $\boldsymbol{r}$ is the coordinate of relative motion, as a continuum eigenstate of H at fixed energy E and so defined as

$$\begin{aligned}\Psi_i^+(\boldsymbol{r}) &\equiv \psi_i(\boldsymbol{r}) + \Psi_{sc}(\boldsymbol{r}) \\ &= \psi_i(\boldsymbol{r}) + \int G_0^+(\boldsymbol{r},\boldsymbol{r}')V(\boldsymbol{r}')\Psi_i^+(\boldsymbol{r}')\,d\boldsymbol{r}',\end{aligned} \tag{2}$$

where $\psi_i(\boldsymbol{r})$ is taken to be a plane-wave eigenstate with momentum $\boldsymbol{k}_i$ of the operator H_0 only. In coordinate representation one has

$$G_0^+(\boldsymbol{r},\boldsymbol{r}') = -\frac{\mu}{\hbar^2}\frac{1}{2\pi}\frac{e^{ik_i|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{3}$$

where the initial conserved energy is $E = \hbar^2 k_i^2/2\mu$. The asymptotic $r \to \infty$ form of the Green function is

$$G_0^+ \sim -\sqrt{2\pi}\,\frac{\mu}{\hbar^2}\frac{e^{ik_i r}}{r}\frac{e^{-ik_i\hat{\boldsymbol{r}}\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}}. \tag{4}$$

It is usual to define the "momentum" $\hbar\boldsymbol{k} \equiv \hbar k_i \hat{\boldsymbol{r}}$, where $\hat{\boldsymbol{r}}$ is the direction of $\boldsymbol{r}$. Hence, $k = k_i$. We emphasize that $\hbar\boldsymbol{k}$, although in standard texts assumed tacitly to represent final measured momentum, is introduced here as a mathematical construct and it is not clear yet that it can be associated with a classical momentum. Indeed it is defined in terms of $\boldsymbol{r}$, a quantum variable which has little to do with a time measurement defining a classical velocity and hence a momentum.

To comply with our many-particle coordinates to be introduced later, we can also assume that the scattering center is infinitely massive so that $\boldsymbol{r}$ is the laboratory-fixed coordinate and μ the mass of a single scattered particle. In the following, we will refer to this as "the one-body case." However, simply replacing μ by a two-body reduced mass and interpreting $\boldsymbol{r}$ as a relative coordinate gives the two-body scattering case usually considered.

B. Scattering amplitude and detection probability in the one-body case

The asymptotic form of the full scattering wave function is, with $k_i = k$,

$$\lim_{r\to\infty}\Psi_i^+(\boldsymbol{r}) = \psi_i(\boldsymbol{r}) - \frac{\mu}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\Psi_i^+(\boldsymbol{r}')\,d\boldsymbol{r}'. \tag{5}$$

Comparison with the asymptotic form of an incident wave plus scattered outgoing spherical wave multiplied by a scattering amplitude, i.e.,

$$\lim_{r\to\infty}\Psi_i^+(\boldsymbol{r}) = \psi_i(\boldsymbol{r}) + f(\boldsymbol{k})\frac{e^{ikr}}{r}, \tag{6}$$

gives the scattering amplitude in the form

$$\begin{aligned}f(\boldsymbol{k}) &= -\sqrt{2\pi}\,\frac{\mu}{\hbar^2}\int\frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}}\,V(\boldsymbol{r}')\,\Psi_i^{(+)}(\boldsymbol{r}')\,d\boldsymbol{r}' \\ &= -\sqrt{2\pi}\,\frac{\mu}{\hbar^2}\langle\boldsymbol{k}|V|\Psi_i^{(+)}\rangle,\end{aligned} \tag{7}$$

where we use the notation $\langle\boldsymbol{k}|$ for the bra-vector of the plane-wave state. The asymptotic scattered wave can now be written

$$\lim_{r\to\infty}\Psi_{sc}(\boldsymbol{r}) = f(\boldsymbol{k})\frac{e^{ikr}}{r}. \tag{8}$$

The probability amplitude of a particular outcome of a measurement is given as the projection of the final state on the total scattered state. If we consider an ideal position detector (infinite position resolution) placed at position $\boldsymbol{R}$, then detection implies projection on the wave function $\delta(\boldsymbol{r} - \boldsymbol{R})$. Hence, the probability amplitude for detection is given by $\langle\boldsymbol{R}|\Psi_{sc}\rangle = \Psi_{sc}(\boldsymbol{R})$ for asymptotically large R, that is,

$$\Psi_{sc}(\boldsymbol{R}) = f(\boldsymbol{k})\frac{e^{ikR}}{R}, \tag{9}$$

where now $\boldsymbol{k} \equiv k\hat{\boldsymbol{R}}$. Then, the detection probability P of particles scattered into a small volume $d\boldsymbol{R} = R^2 dR\,d\Omega$ at the face of a distant detector plate is given by

$$dP = |\Psi_{sc}(\boldsymbol{R})|^2 d\boldsymbol{R} \tag{10}$$

or

$$\frac{dP}{d\Omega\,dR} = |f(\boldsymbol{k})|^2 \tag{11}$$

for the differential probability of scattering [21]. Here, $d\Omega$ is the solid angle subtended by $d\boldsymbol{R}$ at the origin defined by the scattering center. We note that this is still fully time independent. Further we remark, although historically not viewed in this way, a theory in which this differential expression is calculated can be confronted directly with experiment. In elastic scattering, it is sufficient to measure the *position* of the outgoing particle. Thereby, one measures the modulus squared of $f(\boldsymbol{k}) = f(k\hat{\boldsymbol{R}})$, that is, a function dependent on position. This quantity is provided by the theory through the transition-matrix element $\langle\boldsymbol{k}|V|\Psi_i^+\rangle$.

In standard treatments, next one proceeds to define a scattering cross section in terms of the scattering amplitude. This is done by comparing incident and outgoing probability currents

in terms of particle velocities. These classical elements are simply inferred from the *time-independent* wave function $\Psi_i^+(\boldsymbol{r})$ via a construct involving $\mathrm{Re}(\Psi_i^{+*}\boldsymbol{\nabla}\Psi_i^+)$. This step, although yielding the correct cross section, we find logically unjustified and therefore we defer derivation of a cross section until after we have defined classical velocity and time through the asymptotic $r \to \infty$ limit.

C. General *n*-body case

In the above, we have considered the case of potential scattering of two structureless particles. Now, we wish to consider the general case of the scattering of many particles possessing internal structure leading possibly to a different number of composite particles in the final channel. Unfortunately, then of necessity the notation becomes excessively complicated. To make the analysis more transparent and in particular to connect to the two-body case, we will introduce simplifications, however, such as not to impinge seriously on the generality of the theory. To this end, we make two restrictions. First, we limit discussion to only two composite particles in the initial channel. Almost all directly observable collisions in the laboratory are of this type. Three-body collisions are important, for example in plasmas, but their effect is usually incorporated in numerical simulations rather than the collision itself being studied in an experiment.

Second, we will treat the collisions as those of structureless particles in both initial and final channels. This simplifies the notation. The correct inclusion of internal structure is discussed in Appendix A and requires only multiplying the continuum wave function of the particle by its internal wave function and concomitant suitable modification of the energy of the particle. In addition, for rearrangement collisions the potentials operating in initial and final channels must be modified.

In the two-body elastic scattering case of the preceding section, it is simpler to split off the center-of-mass motion and discuss in terms of the three-dimensional relative coordinate $\boldsymbol{r}$. Then, one has an effective one-body problem. For three or more particles, however, the definition of internal coordinates is not unique. For this reason, the general case will be analyzed in terms of laboratory coordinates and the transformation to a particular choice of internal coordinates deferred to Appendix A.

We consider then a collision of two composite particles which fragment into n structureless particles in the final scattering state. In the following, it is important to distinguish three $3n$-dimensional vectors. In the laboratory frame, we denote the coordinates of the n particles with masses m_j by the $3n$-dimensional position vector $\mathsf{R} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n)$ and *hyperradius* $\mathsf{R} = (r_1^2 + r_2^2 + \cdots + r_n^2)^{1/2}$. Later, we use $\boldsymbol{R} = (\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots, \boldsymbol{R}_n)$ to denote the collective position coordinates of n detectors. We define also mass-weighted position coordinates $\boldsymbol{\mathcal{R}}_j \equiv \sqrt{m_j/m}\,\boldsymbol{r}_j$ and a corresponding $3n$-dimensional vector $\boldsymbol{\mathcal{R}} = (\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \ldots, \boldsymbol{\mathcal{R}}_n)$ that defines a mass-weighted hyperradius $\mathcal{R}$ according to

$$m\mathcal{R}^2 = \sum_j m_j r_j^2, \tag{12}$$

where m is an arbitrary scaling mass and can be chosen to define appropriate units.

As in Sec. II A, the key element in calculating the scattering amplitude is the free Green function. This Green function relates the probability amplitude in the coordinate representation of locating the scattered particles in the configuration $\boldsymbol{\mathcal{R}}$ given they started out at $\boldsymbol{\mathcal{R}}'$ just outside the reaction volume. For n particles of mass m_j and total kinetic energy $E_\mathcal{K} \equiv E_f - \mathcal{E}_f$, where E_f is the total energy and $\mathcal{E}_f$ the total binding energy of the n fragments, the free Green function is given as [14]

$$G_0^+(\boldsymbol{\mathcal{R}}, \boldsymbol{\mathcal{R}}'; E_\mathcal{K}) = -i\,\frac{m}{2\hbar^2}\left(\frac{\mathcal{K}}{2\pi}\right)^\alpha \frac{H_\alpha^{(1)}(\mathcal{K}|\boldsymbol{\mathcal{R}} - \boldsymbol{\mathcal{R}}'|)}{|\boldsymbol{\mathcal{R}} - \boldsymbol{\mathcal{R}}'|^\alpha}, \tag{13}$$

where $\alpha = (3n-2)/2$, $H_\alpha^{(1)} = J_\alpha + iN_\alpha$ is a Hankel function. The effective wave number $\mathcal{K}$ is defined as $\mathcal{K} \equiv \sqrt{2mE_\mathcal{K}}/\hbar$.

Now, we consider the limit $\mathcal{R} \gg \mathcal{R}'$, which for detection of all particles at asymptotically large distance from the reaction center specifically requires $\mathcal{R}_j \gg \mathcal{R}'_j$ for all j. In this limit, the asymptotic behavior of G_0^+ is given by

$$G_0^+(E_\mathcal{K}) \sim -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,(-i\mathcal{K})^{(3n-3)/2}\,\frac{e^{i\mathcal{K}\mathcal{R}}}{\mathcal{R}^{(3n-1)/2}}\,\frac{e^{-i\mathcal{K}\hat{\boldsymbol{\mathcal{R}}}\cdot\boldsymbol{\mathcal{R}}'}}{(2\pi)^{3n/2}}. \tag{14}$$

Equation (14) is the generalization of Eq. (4) for the one-particle case and reduces to it for $n = 1$ with $\boldsymbol{\mathcal{R}} \to \boldsymbol{r}$ and $m \to \mu$. Exactly as in the one-particle case, in Eq. (14) we define a generalized "momentum" $\hbar\boldsymbol{\mathcal{K}} \equiv \hbar\mathcal{K}\hat{\boldsymbol{\mathcal{R}}}$.

D. Scattering amplitude and detection probability in the *n*-body case

In the general case where rearrangement of the collision partners or fragmentation takes place we have to distinguish interactions in initial and final channels. The scattering state derived from the initial state $|\psi_i\rangle$ is written

$$|\Psi_i^+\rangle = |\psi_i\rangle + G^+V_i|\psi_i\rangle \equiv |\psi_i\rangle + |\Psi_{sc}\rangle, \tag{15}$$

where G^+ is the full Green function defined by the total Hamiltonian which is decomposed according to the channel, i.e.,

$$H = H_i + V_i = H_f + V_f, \tag{16}$$

such that $|\psi_i\rangle$ and $|\psi_f\rangle$ are eigenstates of H_i and H_f, respectively.

We require the asymptotic behavior of $\Psi_{sc}(\boldsymbol{\mathcal{R}}) = \langle\boldsymbol{\mathcal{R}}|G^+V_i|\psi_i\rangle$ on a large sphere of radius $\mathcal{R}$ in $\boldsymbol{\mathcal{R}}$ space. We use the formal expansion

$$G^+ = G_f^+ + G_f^+V_fG^+ \tag{17}$$

and identify $G_f^+ \equiv G_0^+$ the Green operator for n free particles in the final channel. Then, with Eq. (14) we can calculate the scattered wave as

$$\begin{aligned}
&\lim_{\mathcal{R}\to\infty} \Psi_{sc}(\boldsymbol{\mathcal{R}}) \\
&= \lim_{\mathcal{R}\to\infty} \langle\boldsymbol{\mathcal{R}}|G^+V_i|\psi_i\rangle \\
&= \lim_{\mathcal{R}\to\infty} \int \langle\boldsymbol{\mathcal{R}}|G_0^+|\boldsymbol{\mathcal{R}}'\rangle\langle\boldsymbol{\mathcal{R}}'|(1 + V_fG^+)V_i|\psi_i\rangle\, d\boldsymbol{\mathcal{R}}' \\
&= -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,(-i\mathcal{K})^{(3n-3)/2}\,\frac{e^{i\mathcal{K}\mathcal{R}}}{\mathcal{R}^{(3n-1)/2}}\,\langle\Psi_f^-|V_i|\psi_i\rangle,
\end{aligned} \tag{18}$$

where we have defined the incoming-wave exact scattering state as

$$\langle \Psi_f^- | = \langle \boldsymbol{\mathcal{K}} | (1 + G^- V_f) \tag{19}$$

with $\langle \boldsymbol{\mathcal{K}}|$ the plane-wave state defined by

$$\langle \boldsymbol{\mathcal{K}} | \boldsymbol{\mathcal{R}}' \rangle \equiv \frac{e^{-i\boldsymbol{\mathcal{K}}\cdot\boldsymbol{\mathcal{R}}'}}{(2\pi)^{3n/2}}. \tag{20}$$

The matrix element $\langle \Psi_f^- | V_i | \psi_i \rangle$ in Eq. (18) is referred to as the post form of the transition-matrix element. This can be replaced by the equivalent prior form $\langle \boldsymbol{\mathcal{K}} | V_f | \Psi_i^+ \rangle$, as we show in Appendix B. Then, defining the n-particle scattering amplitude

$$f(\boldsymbol{\mathcal{K}}) = -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,(-i\mathcal{K})^{(3n-3)/2}\,\langle \boldsymbol{\mathcal{K}} | V_f | \Psi_i^+ \rangle, \tag{21}$$

we rewrite Eq. (18) as

$$\lim_{\mathcal{R}\to\infty} \Psi_{sc}(\boldsymbol{\mathcal{R}}) = f(\boldsymbol{\mathcal{K}}) \frac{e^{i\mathcal{K}\mathcal{R}}}{\mathcal{R}^{(3n-1)/2}}. \tag{22}$$

Equations (21) and (22) are the general n-body forms corresponding to Eq. (9) for the effective one-particle case.

The probability of detection at the $3n$-dimensional position $\mathcal{R}$ is given as

$$dP = |\Psi_{sc}(\boldsymbol{\mathcal{R}})|^2 d\boldsymbol{\mathcal{R}}. \tag{23}$$

Transforming to the volume element in hyperspherical coordinates $d\boldsymbol{\mathcal{R}} = \mathcal{R}^{3n-1} d\mathcal{R}\, d\Omega_{\mathcal{R}}$ (given below explicitly for the laboratory coordinates $\mathbf{R}$) and substituting Eq. (22), one has

$$\frac{dP}{d\Omega_{\mathcal{R}} d\mathcal{R}} = |f(\boldsymbol{\mathcal{K}})|^2. \tag{24}$$

This is form-identical with the one-particle expression (11). As in the one-particle case, since $\boldsymbol{\mathcal{K}} \equiv \mathcal{K}\boldsymbol{\mathcal{R}}/\mathcal{R} = (\mathcal{K}/\mathcal{R})(\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \ldots, \boldsymbol{\mathcal{R}}_n)$, this expression describes the probability that a fragmentation event leads to particle detection at the given positions. However, note that in hyperspherical coordinates, the $d\Omega_{\mathcal{R}}$ must include not only the product of n angular elements $d\hat{\boldsymbol{r}}_j$, but also n additional *hyperangles*, which we will define following Gerjuoy [3] in terms of coordinate length ratios (see Sec. III B).

III. PARTICLE MOMENTA

A. Definition of time

To reiterate the development so far, we have presented a fully time-independent scattering theory for multiparticle fragmentation, where the scattering wave function is an energy eigenfunction and occupies the whole of space. The probability of detecting particles at a set of detector positions is proportional to the modulus squared of this wave function.

At this stage, to connect directly to measured quantities, we will introduce one-particle momenta $\hbar\boldsymbol{k}_j$ but which are defined in terms of the laboratory position coordinates of *all* particles. To this end, one notes that the plane-wave state $e^{-i\boldsymbol{\mathcal{K}}\cdot\boldsymbol{\mathcal{R}}'}$ of Eq. (20), which derives from the asymptotic form of the Green function (14), defines an asymptotic wave vector $\boldsymbol{k}_j$ of the jth scattered particle according to

$$\boldsymbol{\mathcal{K}}\cdot\boldsymbol{\mathcal{R}}' = \sum_j \boldsymbol{\mathcal{K}}_j \cdot \boldsymbol{\mathcal{R}}_j{}' = \sum_j \frac{\mathcal{K}}{\mathcal{R}} \frac{m_j}{m} \boldsymbol{r}_j \cdot \boldsymbol{r}_j' \equiv \sum_j \boldsymbol{k}_j \cdot \boldsymbol{r}_j' \tag{25}$$

since $\boldsymbol{\mathcal{R}}_j \equiv \sqrt{m_j/m}\,\boldsymbol{r}_j$, so that the plane-wave factor in Eq. (14) can be expressed as

$$\langle \boldsymbol{\mathcal{K}} | \boldsymbol{\mathcal{R}}' \rangle \equiv \frac{e^{-i\boldsymbol{\mathcal{K}}\cdot\boldsymbol{\mathcal{R}}'}}{(2\pi)^{3n/2}} = \prod_{j=1}^{n} \frac{e^{-i\boldsymbol{k}_j\cdot\boldsymbol{r}_j'}}{(2\pi)^{3/2}} \equiv \langle \boldsymbol{K} | \mathbf{R}' \rangle, \tag{26}$$

introducing the $3n$-dimensional wave vector $\boldsymbol{K} = (\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_n)$. Then, $\boldsymbol{\mathcal{K}}$ is the corresponding $3n$-dimensional vector with (reciprocal) mass-weighted elements $\boldsymbol{\mathcal{K}}_j \equiv \sqrt{m/m_j}\,\boldsymbol{k}_j$.

That is, in terms of the spatial direction $\hat{\boldsymbol{r}}_j$ of the jth particle and its relative distance $r_j/\mathcal{R}$ from the reaction volume, we have defined, from Eq. (25), the one-particle wave vectors

$$\boldsymbol{k}_j \equiv \frac{m_j}{m}\frac{r_j}{\mathcal{R}}\,\mathcal{K}\hat{\boldsymbol{r}}_j \tag{27}$$

which correspond to the effective wave vector $\boldsymbol{k} = k_i\hat{\boldsymbol{r}}$ of the $n = 1$ case. These wave vectors can also be written

$$\hbar\boldsymbol{k}_j = \left(\frac{2E_{\mathcal{K}}}{\sum_i m_i r_i^2}\right)^{1/2} m_j \boldsymbol{r}_j \tag{28}$$

since $\mathcal{R} = \sqrt{\sum_i m_i r_i^2/m}$ and $\mathcal{K} = \sqrt{2mE_{\mathcal{K}}}/\hbar$. Evidently,

$$\sum_j \frac{\hbar^2 k_j^2}{2m_j} = \frac{\hbar^2\mathcal{K}^2}{2m} = E_{\mathcal{K}}. \tag{29}$$

Nevertheless, these one-particle "momenta" $\hbar\boldsymbol{k}_j$ are a mathematical construct defined in terms of *all* the quantum position variables. That is, the k_j being functions of $(r_j/\mathcal{R})$ cannot be taken as constants so that the condition in Eq. (29) appears at the moment as a sum rule.

To emphasize once again, we have considered strictly a position detection of all particles so any and all actual momenta from the full spectrum defined by the scattering amplitude (21) will be detected and counted. There are no issues with the uncertainty principle. However, the question arises as to how well-defined constant momenta can be inferred. Remarkably, as intimated by Gerjuoy [3] and Friedrich [14], the fully quantum time-independent treatment of asymptotic free motion does lead to well-defined momenta independent of the position of their measurement. Furthermore, it also leads to the definition of a variable with the dimensions of time that can be associated with a classical clock.

One sees readily how this comes about. From Eq. (27), one has

$$\frac{r_j}{\hbar k_j/m_j} = \frac{\mathcal{R}}{\hbar\mathcal{K}/m} = \left(\frac{\sum_i m_i r_i^2}{2E_{\mathcal{K}}}\right)^{1/2}. \tag{30}$$

Now, we introduce "velocities" $\boldsymbol{v}_j \equiv \hbar\boldsymbol{k}_j/m_j$ and $\boldsymbol{\mathcal{V}} \equiv \hbar\boldsymbol{\mathcal{K}}/m$ with $\mathcal{V} = \sqrt{2E_{\mathcal{K}}/m}$ to give the identity

$$\frac{r_j}{v_j} = \frac{\mathcal{R}}{\mathcal{V}} = \left(\frac{\sum_i m_i r_i^2}{2E_{\mathcal{K}}}\right)^{1/2} \tag{31}$$

for *each and every* $j = 1, \ldots, n$. Clearly, this can only be true in general, as the r_j and therefore $\mathcal{R}$ vary, if each side of the equation is equal to a constant. This constant has the physical dimensions of time and so we introduce a time variable

$$t \equiv \left(\frac{\sum_i m_i r_i^2}{2E_{\mathcal{K}}}\right)^{1/2} = \frac{\mathcal{R}}{\mathcal{V}} = \frac{m\mathcal{R}}{\hbar\mathcal{K}}. \tag{32}$$

Then, the validity of Eq. (31) is assured at all times by the conditions $\boldsymbol{r}_j = \boldsymbol{v}_j t$ where the $\boldsymbol{v}_j$ are constants. Hence, each time value defines a different set of positions $\{\boldsymbol{r}_j(t)\}$ but such that all ratios $r_j/r_i = v_j/v_i$ are constants in time. Now, the sum rule of Eq. (29) corresponds to conservation of energy. Since we have shown that each quantum coordinate obeys a linear classical time dependence, a general measurement would involve a set of detectors at positions $\{\boldsymbol{R}_j\} = \{\boldsymbol{v}_j t_j\}$ registering particles of different velocities at different times. In short, to determine velocities the position "hits" on the detector have to be accompanied by measurement of the time of flight from the interaction zone to the detector. We elaborate in Sec. IV.

We stress that the standard approach is simply to associate, without proof, the particle quantum momenta, defined in terms of position coordinates, with classical momenta and hence with measured classical velocities. Our demonstration that the quantum position variables defining the quantum momenta asymptotically vary linearly with a parameter of the dimensions of time provides the proof for this association.

Here, we are using laboratory coordinates for each emitted particle. In Appendix A, we show that the cross section is transformed readily to the more usual center-of-mass and relative coordinates. It is interesting that, in the two-body case presented in most textbooks, the implicit dependence of defined momenta on particle distances is not evident and the necessity to introduce a time via $\boldsymbol{r} = \boldsymbol{v}t$ is not apparent. This is because for two bodies only the effective one-body motion in relative coordinate $\boldsymbol{r} \equiv \boldsymbol{r}_a - \boldsymbol{r}_b$ with reduced mass μ is relevant. Then, for the final momentum $\hbar\boldsymbol{k}$, Eq. (28) with $m_j = \mu$, $E_{\mathcal{K}} = E$, and $\mathcal{R} = r_j = r$ becomes simply

$$\hbar\boldsymbol{k} = \sqrt{2\mu E}\,\hat{\boldsymbol{r}} = \hbar k_i \hat{\boldsymbol{r}}, \tag{33}$$

which expresses $\boldsymbol{k}$ in terms of the constant k_i and a direction only, i.e., independent of particle distance.

However, in the laboratory coordinates (and also in internal coordinates for many bodies) one sees explicitly the necessity to introduce linear behavior of distance with time. In laboratory coordinates one has the momenta $\hbar\boldsymbol{k}_j$ from Eq. (28), from which follows the sum rule of Eq. (29). Thus, one sees that the classical relations established above, i.e., $\hbar\boldsymbol{k}_j = m_j\boldsymbol{v}_j$ with $\boldsymbol{r}_j = \boldsymbol{v}_j t$ are consistent since one obtains from Eq. (28), with $t = (2E_{\mathcal{K}}/\sum_i m_i r_i^2)^{-1/2}$ from Eq. (32),

$$\hbar\boldsymbol{k}_j = m_j\frac{\boldsymbol{r}_j}{t} = m_j\boldsymbol{v}_j \tag{34}$$

and $\hbar\mathcal{K} \equiv m\mathcal{R}/t = m\mathcal{V}$.

The classical momenta also appear when we transform to internal coordinates. For example, for two particles a and b we use center-of-mass and relative coordinates

$$\boldsymbol{R}_{cm} \equiv \frac{m_a\boldsymbol{r}_a + m_b\boldsymbol{r}_b}{m_a + m_b}, \quad \boldsymbol{r} \equiv \boldsymbol{r}_a - \boldsymbol{r}_b. \tag{35}$$

The conjugate momenta then are, from Eq. (28), the center-of-mass momentum $\hbar\boldsymbol{\kappa}$,

$$\begin{aligned}\hbar\boldsymbol{\kappa} \equiv \hbar(\boldsymbol{k}_a + \boldsymbol{k}_b) &= \left(\frac{2E}{m_a r_a^2 + m_b r_b^2}\right)^{1/2}(m_a\boldsymbol{r}_a + m_b\boldsymbol{r}_b)\\ &= M\frac{\boldsymbol{R}_{cm}}{t} \equiv M\boldsymbol{V}_{cm},\end{aligned} \tag{36}$$

where total mass $M = m_a + m_b$, and the relative momentum

$$\begin{aligned}\hbar\boldsymbol{k} &\equiv \hbar(m_b\boldsymbol{k}_a - m_a\boldsymbol{k}_b)/M\\ &= \left(\frac{2E}{m_a r_a^2 + m_b r_b^2}\right)^{1/2}(m_b m_a\boldsymbol{r}_a - m_a m_b\boldsymbol{r}_b)/M\\ &= \mu\frac{\boldsymbol{r}}{t} \equiv \mu\boldsymbol{v},\end{aligned} \tag{37}$$

where μ is the reduced mass. Here, although obscured in the standard derivation, one sees even in the two-body case the necessity to assume classical free motion, distance proportional to time, in order that changes in distance are associated with measured momenta.

We stress that we are still fully quantum mechanical and time independent in our approach and yet a classical time dependence has emerged from the free asymptotic behavior of the wave function. This allows a sharp classical momentum to be associated with a sharp quantum position variable via $\boldsymbol{r} = \boldsymbol{v}t$. At no stage do we need to invoke wave-function collapse or narrow wave packets as Kemble [1] surmised. Our scattering wave function occupies all space and we need only interpret detection probability as given by the modulus squared of this wave function. We have shown that we are justified in associating the mathematically defined momenta with final measured classical momenta. Also, since now we have a classical time variable, we can use these quantum momenta to define classical velocities. In this way, we show next how standard expressions for cross sections are obtained from the quantum probabilities without the necessity to infer a particle flux in terms of time-independent wave functions.

B. Differential cross section

Again, first we consider the effective one-body case, where the differential scattering probability is given by Eq. (10), i.e.,

$$dP = |f(\boldsymbol{k})|^2 dR\, d\Omega. \tag{38}$$

We define the scattering cross section as the effective area $d\sigma$ the exit channel defined by $d\Omega$ presents to a steady incident beam with speed $v_i \equiv \hbar k_i/\mu$. Then, we have that $v_i dt\, d\sigma \equiv dP$, assuming one particle in the incident beam per unit volume [21]. At asymptotically large distances we put $dR = (\hbar k/\mu)dt = v\,dt$ and obtain for the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{v}{v_i}|f(\boldsymbol{k})|^2 = |f(\boldsymbol{k})|^2. \tag{39}$$

It is standard practice to define a differential cross section with respect to measured momenta $\boldsymbol{k}$. This expression is readily obtained. To express the cross-section differential in momentum, one must integrate the above equation over an energy (or momentum) acceptance but recognizing energy

conservation. Then one has, reverting to momenta rather than velocity,

$$\frac{d\sigma}{d\Omega} = \frac{k}{k_i}|f(\boldsymbol{k})|^2\delta(E_k - E_{k_i})\,dE_k. \tag{40}$$

With $E_k = \hbar^2k^2/(2\mu)$ one obtains

$$\frac{d\sigma}{d\boldsymbol{k}} = \frac{\hbar^2}{\mu k_i}|f(\boldsymbol{k})|^2\,\delta\big(E_k - E_{k_i}\big)\,dE_k \tag{41}$$

or, putting again $v_i \equiv \hbar k_i/\mu$ and substituting for $f(\boldsymbol{k})$ from Eq. (7), we obtain the final expression

$$\frac{d\sigma}{d\boldsymbol{k}} = \frac{2\pi}{\hbar v_i}|\langle\boldsymbol{k}|V|\Psi_i^+\rangle|^2\,\delta\big(E_k - E_{k_i}\big), \tag{42}$$

which is the standard result for the differential scattering cross section. However, here it was derived from the point of view of a position measurement without the need to calculate an outgoing flux. Note that we have identified the solid angle element $d\Omega$ of the spatial coordinate $\boldsymbol{r}$ with that of the final momentum which is justified precisely by the definition of $\boldsymbol{k} = k\hat{\boldsymbol{r}}$.

In the general case we have also given a derivation of the detection counting probability, exactly following Eqs. (9) and (10) for potential scattering, in terms of a position measurement by the detectors. This assumes the simple form of Eq. (24) in mass-weighted coordinates. In laboratory coordinates, the detectors for particles j placed at positions $\boldsymbol{r}_j = \boldsymbol{R}_j$ effect a projection of the scattered wave onto a wave function $\prod_j \delta(\boldsymbol{r}_j - \boldsymbol{R}_j)$. Denoting the $3n$-dimensional detector position vector by $\boldsymbol{R} = (\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n)$, the detection probability amplitude is given by $\Psi_{sc}(\boldsymbol{R})$.

The volume element in $\mathbf{R}$ space is given by

$$d\mathbf{R} = r_1^2 dr_1 d\hat{\boldsymbol{r}}_1\, r_2^2 dr_2 d\hat{\boldsymbol{r}}_2 \ldots r_n^2 dr_n d\hat{\boldsymbol{r}}_n. \tag{43}$$

We will write this as

$$d\mathbf{R} \equiv \mathsf{R}^{3n-1} d\mathsf{R}\, d\Omega, \tag{44}$$

where following Gerjuoy [3] we define

$$d\Omega \equiv d\hat{\mathbf{R}} = \frac{q_2^2\, q_3^2 \ldots q_n^2}{\big(1 + q_2^2 + q_3^2 + \ldots q_n^2\big)^{3n/2}} \times dq_2\, dq_3 \ldots dq_n\, d\Omega_1 d\Omega_2 \ldots d\Omega_n \tag{45}$$

with $d\Omega_j \equiv d\hat{\boldsymbol{r}}_j$. The $n-1$ ratios are defined with respect to an arbitrary coordinate denoted r_1, i.e., $q_j = r_j/r_1$ for $j = 2, \ldots, n$. The directions $\hat{\mathbf{R}}$ are determined by the q_j and the $2n$ angles in ordinary three-dimensional space determining the directions $\hat{\boldsymbol{r}}_1, \ldots \hat{\boldsymbol{r}}_n$. Then, the probability that particles scatter onto an element of volume $R^{3n-1} dR\, d\Omega$ at the surface of the distant detectors is given by

$$dP = |\Psi_{sc}(\boldsymbol{R})|^2\, R^{3n-1} dR\, d\Omega \tag{46}$$

or

$$\frac{dP}{d\Omega} = |f(\boldsymbol{K})|^2\, \eta_n \left(\frac{R}{\mathcal{R}}\right)^{3n-1} dR. \tag{47}$$

Here, the scattering amplitude from Eq. (21) has been expressed in laboratory coordinates using $\langle\boldsymbol{\mathcal{K}}|\boldsymbol{\mathcal{R}}'\rangle \equiv \langle\boldsymbol{K}|\mathbf{R}'\rangle$ from Eq. (26) so that

$$f(\boldsymbol{K}) = -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,(-i\mathcal{K})^{(3n-3)/2}\,\langle\boldsymbol{K}|V_f|\Psi_i^+\rangle, \tag{48}$$

which gives rise to the dimensionless factor

$$\eta_n \equiv \prod_{j=1}^{n}\left(\frac{m_j}{m}\right)^3 \tag{49}$$

in Eq. (47).

From the results of Sec. III A using $d\boldsymbol{R}_j = \boldsymbol{v}_j dt$ and $\boldsymbol{v}_j = \boldsymbol{R}_j/t = \boldsymbol{R}_j\mathcal{V}/\mathcal{R}$, one sees that

$$dR = \frac{R}{\mathcal{R}}\,\mathcal{V}\,dt \tag{50}$$

to give, again using $v_i dt\, d\sigma \equiv dP$, the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{\mathcal{V}}{v_i}|f(\boldsymbol{K})|^2\eta_n\left(\frac{R}{\mathcal{R}}\right)^{3n}. \tag{51}$$

Equation (51) is the generalization of Eq. (39) to n particles in the exit channel. Now substituting the scattering amplitude Eq. (48) one has

$$\frac{d\sigma}{d\Omega} = \frac{2\pi m}{\hbar^3 v_i}\mathcal{K}^{3n-2}|\langle\boldsymbol{K}|V_f|\Psi_i^+\rangle|^2\eta_n\left(\frac{R}{\mathcal{R}}\right)^{3n}. \tag{52}$$

It is customary to express the cross-section differential in the final vector momenta, that is, we need to transform from the q variables to momentum variables. First, using $q_j = r_j/r_1 = v_j/v_1$ asymptotically, we transform to velocity variables. Evaluating the Jacobian gives

$$\prod_{j=2}^{n} dq_j = \frac{E_{\mathcal{K}}}{\frac{1}{2}m_1 v_1^2}\,\frac{1}{v_1^{n-1}}\prod_{j=2}^{n} dv_j. \tag{53}$$

Transforming further from velocities to momenta we obtain

$$\prod_{j=2}^{n} dq_j = \frac{2E_{\mathcal{K}}}{(\hbar k_1)^{n+1}}\,m_1^n\prod_{j=2}^{n}\frac{\hbar}{m_j}\,dk_j. \tag{54}$$

Putting this transformation in Eq. (52) and equating position angular variables with momentum angular variables results in the simple expression

$$d\sigma = \frac{2\pi m_1}{\hbar^3 v_i}k_1|\langle\boldsymbol{K}|V_f|\Psi_i^+\rangle|^2\,d\Omega_1\prod_{j=2}^{n}d\boldsymbol{k}_j. \tag{55}$$

From the sum rule (29), the total final energy

$$E_f = \sum_{j=1}^{n}\frac{\hbar^2k_j^2}{2m_j} + \mathcal{E}_f \tag{56}$$

is fixed equal to the total initial energy E_i. Taking this into account, one multiplies Eq. (55) by $\delta(E_f - E_i)dE_f$. Then, using the transformation $dE_f = (\hbar^2k_1/m_1)\,dk_1$ gives the final result

$$d\sigma(ab \to n) = \frac{2\pi}{\hbar v_i}|\langle\boldsymbol{K}|V_f|\Psi_i^+\rangle|^2\delta(E_f - E_i)\,d\boldsymbol{K}, \tag{57}$$

or the differential cross section

$$\frac{d\sigma}{d\boldsymbol{k}_1 d\boldsymbol{k}_2 \ldots d\boldsymbol{k}_n} = \frac{2\pi}{\hbar v_i}|\langle\boldsymbol{K}|V_f|\Psi_i^+\rangle|^2\delta(E_f - E_i). \tag{58}$$

Again, this is the standard result and is the n-particle generalization of Eq. (42). By defining an asymptotic position measurement, we have been able to circumvent the complicated many-particle *outgoing* quantum flux calculations of Gerjuoy's derivation [3]. Indeed, it is unnecessary to specify this flux. This has been avoided by defining a detector position which can be associated with a classical time and classical velocity.

IV. TIME-DEPENDENT SCATTERING THEORY

Having defined a classical time for asymptotic particle motion, it remains to derive a time dependence for the complete scattering process. To this end, we define a classical time defined by the apparatus, by first integrating the detector into the quantum mechanics and then considering the limit where the detector becomes macroscopic. In this way, we show how time-dependent scattering theory can be derived from our fully time-independent theory. First, we consider that the quantum scattering system with Hamiltonian H together with a quantum apparatus with Hamiltonian $H_{\mathcal{D}}$ giving the total Hamiltonian

$$\mathcal{H} = H(\boldsymbol{r}) + H_{\mathcal{D}}(\boldsymbol{R}) + H_I(\boldsymbol{r},\boldsymbol{R}). \tag{59}$$

Here, for simplicity, we consider only one particle's coordinates $\boldsymbol{r}$. The operator H_I is the time-independent interaction between the two quantum systems, scattering complex, and apparatus. The apparatus position is described first by a quantum variable $\boldsymbol{R}$ which later will go over to a classical position $\boldsymbol{R}(t)$. The total Hamiltonian is time independent so the composite of scattering complex and apparatus has fixed energy E. We wish to solve the time-independent Schrödinger equation (TISE)

$$\mathcal{H}\,\Phi(\boldsymbol{r},\boldsymbol{R}) = E\,\Phi(\boldsymbol{r},\boldsymbol{R}). \tag{60}$$

Although the derivation is perfectly general, to keep the notation simple we will consider the apparatus wave function to depend upon a single "clock" coordinate R, which will be used to define the classical time. The apparatus may consist of timed preparation and/or detection operations. For simplicity, we will refer to both as simply "the detector." After preparation, the total wave function is the entangled linear combination of states

$$\Phi(\boldsymbol{r},R) = \sum_\nu \chi_\nu(R)\psi_\nu(\boldsymbol{r}), \tag{61}$$

where χ_ν is the detector wave function in state ν at fixed energy $\mathcal{E}_\nu$ and ψ_ν and ϵ_ν the corresponding quantities for the scattering system. The total energy is conserved so $E = \mathcal{E}_\nu + \epsilon_\nu$ for all ν, i.e., for a given state ν of the scattering system, the energy of the quantum detector changes such that the total energy is invariant.

A. Detector time

Now, we consider the limit that the detector becomes so large (and its energy and action also large on an atomic scale) that we can use a classical approximation for its action function. That is, we write

$$\chi_\nu(R) = c_\nu(R)\,e^{-\frac{i}{\hbar}W_\nu(R)}, \tag{62}$$

where $W_\nu(R)$ is the *classical* action of the detector, defined by

$$W_\nu(R) = \int^R P_\nu(R')dR' \tag{63}$$

with P_ν the *classical* momentum

$$\begin{aligned} P_\nu &= (2M)^{1/2}(\mathcal{E}_\nu - V_D)^{1/2} \\ &= (2M)^{1/2}(E - \epsilon_\nu - V_D)^{1/2}. \end{aligned} \tag{64}$$

Here, V_D is a detector potential energy which for the purposes of this discussion can be set to zero. Then, we have simply

$$\begin{aligned} W_\nu &= P_\nu R \\ &= (2M)^{1/2}(E - \epsilon_\nu)^{1/2}R. \end{aligned} \tag{65}$$

Next, we recognize that the total energy is now large or $E \gg \epsilon_\nu$ for all ν so that we expand to first order

$$W_\nu \approx (2ME)^{1/2}[1 - \epsilon_\nu/(2E)]R. \tag{66}$$

The detector action still depends on the quantum energy ϵ_ν, which is negligibly small. The final step is the complete disentanglement of detector from scattering system by neglect of this small energy. Then, the detector action becomes independent of the state ν of the scattering system, i.e.,

$$W \equiv (2ME)^{1/2}R = PR. \tag{67}$$

With this classical action the classical time is defined as

$$t = \frac{MR}{\partial W/\partial R} = MR/P. \tag{68}$$

This is where the classical time first enters. Then, the total action from Eq. (66) may be written

$$W_\nu = W - \epsilon_\nu t. \tag{69}$$

Up to an irrelevant overall phase, the total wave function (61) at $R = R(t)$ becomes the now time-dependent wave function *for the scattering system only* in the form

$$\Psi_i^+(\boldsymbol{r},t) = \sum_\nu c_\nu(t)\,e^{-\frac{i}{\hbar}\epsilon_\nu t}\psi_\nu(\boldsymbol{r}). \tag{70}$$

Note that the energy-dependent dynamic phase factor and the coefficients of the expansion arise as remnants of the wave function of the detector. This detector clock time can now be taken as monitoring the time variation of the coordinates $\boldsymbol{r}(t)$ of the asymptotic scattering wave function.

If the detection step involves projection onto some measured state $\psi_f(t)$, then the transition amplitude or T-matrix element is, in prior and post forms,

$$\begin{aligned} T_f(t) &\equiv \langle\psi_f(t)|\Psi_i^+(t)\rangle \\ &= \langle\Psi_f^-(t)|\psi_i(t)\rangle. \end{aligned} \tag{71}$$

By the same procedure as used here it has been shown in Refs. [17,18] in the limit that the detector coordinate $R \to R(t)$ becomes a classical variable, that the full TISE [Eq. (60)] reduces to the time-dependent Schrödinger equation (TDSE) for the scattering system only, i.e.,

$$[H(\boldsymbol{r}) + H_I(\boldsymbol{r},t)]\,\Psi_i(\boldsymbol{r},t) = i\hbar\frac{\partial\Psi_i}{\partial t}, \tag{72}$$

where the operator $\partial/\partial t$ arises from the momentum operator of the detector. Note also that in the interaction Hamiltonian H_I

the parametric dependence on quantum variable $\boldsymbol{R}$ has been replaced by a parametric dependence on classical time t.

Now, if $\psi_f(t)$ satisfies the TDSE with Hamiltonian H_f where $H = H_f + V_f$, then the expressions (71) are equal in prior form to

$$T_f(t) = -\frac{i}{\hbar}\int^t \langle \psi_f(t')|V_f|\Psi_i^+(t')\rangle dt', \tag{73}$$

and in post form with $H = H_i + V_i$ to

$$T_f(t) = -\frac{i}{\hbar}\int^t \langle \Psi_f^-(t')|V_i|\psi_i(t')\rangle dt', \tag{74}$$

which are the standard expressions for the transition-matrix element in time-dependent scattering theory.

The act of preparation and measurement is represented by the interaction $H_I(t)$. Here, we must distinguish two cases. The first case is when the detection simply defines two clock times, one an initiation at time t_0, for example the time where particles enter a collision volume, the other the time of detection t. Then, $H_I(t')$ essentially contains two delta functions $\delta(t'-t_0)$ and $\delta(t'-t)$. Otherwise, $H_I \equiv 0$. Since the scattering system Hamiltonian is still time independent, the time dependence of the wave function is restricted to energy phases. Then, for asymptotically large t, the time integral furnishes an energy-conserving delta function only and, as we show in the following, one could as well use time-independent theory. Nevertheless, if time is defined by the measuring process, the introduction of a clock time is necessary to describe the detection process correctly and to prove the imaging theorem. Also, for most people, a time-developing wave function is physically more intuitive than the idea of a time-independent continuum wave function.

However, the second case is more overtly classical in the origin of time. This is where in addition to the clock interaction defining an initial time and a detection time, the scattering Hamiltonian is not time independent but contains an external interaction potential $V_i(t)$ itself. Such a time-dependent Hamiltonian arises only when an external perturbation, e.g., a particle beam or light source, is treated in a classical approximation from the outset. That is, the time dependence arises from a classical interaction due to an external field obeying Newton or Maxwell equations (particle or light beam). In this case, the transition matrix involves $V_i(t)$ in the form

$$T_f(t) = -\frac{i}{\hbar}\int^t \langle \Psi_f^-(t')|V_i(t')|\psi_i(t')\rangle dt', \tag{75}$$

where again the time is set by the classical measuring apparatus.

Having derived the formal expression for the time-dependent transition-matrix element, we show in the next section how it can be related to a position measurement.

B. Time-dependent transition-matrix element and the imaging theorem

In the fully quantum-mechanical time-independent description we have emphasized particle detection at positions $\mathbf{R} = \boldsymbol{R}$ and shown that the probability amplitude (T-matrix element) for scattering into detectors at $\boldsymbol{R}$ is proportional to $\Psi_{sc}(\boldsymbol{R})$ the scattered wave function at the detector. From Eq. (71), by projecting onto a spatial δ function, we see that this result holds also in the time-dependent case since $T_f(t) = \langle \psi_f(t)|\Psi_i^+(t)\rangle \propto \Psi_i^+(\boldsymbol{R},t)$, where we note that the initial wave function $\psi_i(\boldsymbol{R}) = 0$, i.e., the initial wave function has no overlap with the detector. We remember also that the fully quantum-mechanical theory predicts an asymptotic relation between momenta and position which corresponds to classical motion along $\mathbf{R}(t)$.

For times $t > 0$ following the fragmentation reaction, the free propagation of the scattered fragments is described by

$$|\Psi_i^+(t)\rangle = e^{-iH_0t/\hbar}|\Psi_i^+(0)\rangle, \tag{76}$$

where H_0 is the n-particle free Hamiltonian. It is simplest to express this time development in the hyperspherical coordinates $\boldsymbol{\mathcal{R}}$ and $\boldsymbol{\mathcal{K}}$ from Sec. II B with mass-weighted elements $\boldsymbol{\mathcal{R}}_j \equiv \sqrt{m_j/m}\,\boldsymbol{r}_j$ and $\boldsymbol{\mathcal{K}}_j \equiv \sqrt{m/m_j}\,\boldsymbol{k}_j$, respectively. Then,

$$\langle \boldsymbol{\mathcal{K}}'|e^{-iH_0t/\hbar}|\boldsymbol{\mathcal{K}}\rangle = e^{i\hbar\mathcal{K}^2t/2m}\delta(\boldsymbol{\mathcal{K}}' - \boldsymbol{\mathcal{K}}), \tag{77}$$

and one obtains from Eq. (76) the $3n$-dimensional time-propagated Fourier-integral momentum representation

$$\begin{aligned}\Psi_i^+(\boldsymbol{\mathcal{R}},t) &= \int \tilde{\Psi}_i^+(\boldsymbol{\mathcal{K}}')\frac{e^{i\boldsymbol{\mathcal{K}}'\cdot\boldsymbol{\mathcal{R}}}}{(2\pi)^{3n/2}}e^{-i\hbar\mathcal{K}'^2t/2m}d\boldsymbol{\mathcal{K}}' \\ &= \frac{e^{i\hbar\mathcal{K}^2t/2m}}{(2\pi)^{3n/2}}\int \tilde{\Psi}_i^+(\boldsymbol{\mathcal{K}}')e^{-i(\hbar t/2m)(\boldsymbol{\mathcal{K}}'-\boldsymbol{\mathcal{K}})^2}d\boldsymbol{\mathcal{K}}'.\end{aligned} \tag{78}$$

This result is form identical with the one-particle expression [2,7]. Hence, in the limit $\boldsymbol{\mathcal{R}},t \to \infty$ but with $\mathcal{R}/t \equiv \mathcal{V} = \sqrt{2E/m}$ fixed by the total energy, the integrand is highly oscillatory except at the stationary-phase point $\boldsymbol{\mathcal{K}}' = \boldsymbol{\mathcal{K}} \equiv m\boldsymbol{\mathcal{R}}/\hbar t$. The maximum contributions to the integral come from a small region about this point, and performing the integral in stationary-phase approximation gives

$$\Psi_i^+(\boldsymbol{\mathcal{R}},t) \sim e^{i\hbar K^2t/2m}\left(\frac{m}{i\hbar t}\right)^{3n/2}\tilde{\Psi}_i^+(\boldsymbol{\mathcal{K}})|_{\boldsymbol{\mathcal{K}}=m\boldsymbol{\mathcal{R}}/\hbar t}, \tag{79}$$

which is just the imaging theorem (IT) generalized to n-particle fragmentation.

The condition of stationary phase $\hbar\boldsymbol{\mathcal{K}} \equiv m\boldsymbol{\mathcal{R}}/t$ gives $\hbar\boldsymbol{k}_j = m_j\boldsymbol{r}_j/t$ for each and every $j = 1,\ldots,n$, namely, the same classical relationship as emerges from the asymptotic time-independent limit. One sees that the classical large-time limit is equivalent to the quantum large-$\mathcal{R}$ limit. Noting that $d\boldsymbol{\mathcal{K}} = (m/\hbar t)^{3n}d\boldsymbol{\mathcal{R}}$ from this condition, Eq. (79) leads to the asymptotic equality of probabilities

$$|\Psi_i^+(\boldsymbol{\mathcal{R}},t)|^2d\boldsymbol{\mathcal{R}} \sim |\tilde{\Psi}_i^+(\boldsymbol{\mathcal{K}})|^2d\boldsymbol{\mathcal{K}} \tag{80}$$

with $\boldsymbol{\mathcal{R}}$ and $\boldsymbol{\mathcal{K}}$ related by the classical condition $\hbar\boldsymbol{\mathcal{K}} \equiv m\boldsymbol{\mathcal{R}}/t$.

The same time development of the scattering wave function can be carried out in terms of the measured $\mathbf{R}$ and $\boldsymbol{K}$ coordinates and, corresponding to the equation above, leads to equality of measured probabilities

$$|\Psi_i^+(\mathbf{R},t)|^2d\mathbf{R} \sim |\tilde{\Psi}_i^+(\boldsymbol{K})|^2d\boldsymbol{K}. \tag{81}$$

This demonstration of the equivalence of absolutely well-defined momentum and position wave functions at the same time would appear to violate quantum uncertainty. However, this is not so since the above relation is only valid at distances very large on an atomic scale. It is simply a reflection of the

circumstance that asymptotically the accumulated action is much greater than $\hbar$ which leads to classical behavior. Since the exact path integral is decided by a single free-particle classical trajectory, a stationary-phase evaluation [20] of the path integral which is valid asymptotically leads to the well-defined classical relation between distance and momentum, as obtained in the IT. The IT is discussed in detail in our two papers [2,7]. In particular, the conditions for validity of the stationary-phase approximation are defined and the generalization to the important case of extraction of collision fragments from the reaction zone by the use of electric and magnetic fields is given. Also, it is shown that with field extraction the quantum coordinate $\boldsymbol{R}(t)$ obeys the classical equations of motion asymptotically.

Another aspect of the IT which deserves mention concerns the relative orientation or the *shape* of fragment patterns emerging from a collision. For two particles this shape is a line, for three particles a triangle, for four particles a tetrahedron, and so on. This is true both in position and in momentum space. Since, from Eq. (31) one has $r_i/r_j = v_i/v_j$ for all pairs (i,j) of particles and since the angular dependencies are the same, then when the fragments have departed the interaction region the expansion of their shapes in position and *velocity* space will be identical and the shapes time-scale invariant. The IT equates the position shape to the momentum shape exiting the reaction zone, from which the velocity shape can be constructed via $\hbar k_j/m_j = v_j$ for each particle. Hence, data representations such as the Dalitz plot for three particles tracing the shape of a triangle in momentum space can be related to the position shape. Indeed, in the case of the fragmentation of H_3 where momentum space coincides with velocity space, this has been confirmed experimentally by Fechner and Helm [22].

Since we have shown that the *time-independent* position-detection probability $|\Psi_i^+(\boldsymbol{R})|^2 d\boldsymbol{R}$ leads to the cross sections (51) and (58), then from Eq. (81) the momentum-detection probability $|\tilde{\Psi}_i^+(\boldsymbol{K})|^2 d\boldsymbol{K}$ should lead to the same result. This is easily shown. In fact, Eq. (81) embodies in a simple way the *scattering-into-cones theorem* of Dollard [23,24].

Let us take $\psi_f(t)$ to be a product of quantum plane waves with final quantum momenta $\boldsymbol{K}$. This gives

$$\begin{aligned} T_f(t) &= \langle \boldsymbol{K}(t)|\Psi_i^+(t)\rangle \\ &= \tilde{\Psi}(\boldsymbol{K}) e^{i(E_f - E_i)t/\hbar}. \end{aligned} \tag{82}$$

However, this is equivalent to

$$\begin{aligned} T_f(t) &= -\frac{i}{\hbar}\int_0^t \langle \boldsymbol{K}(t')|V_f|\Psi_i^+(t')\rangle dt' \\ &= -\frac{i}{\hbar}\langle \boldsymbol{K}|V_f|\Psi_i^+\rangle \int_0^t e^{i(E_f - E_i)t'/\hbar} dt'. \end{aligned} \tag{83}$$

The probability of detection of particles with momenta between $\boldsymbol{K}$ and $\boldsymbol{K} + d\boldsymbol{K}$ is given by the right-hand side of Eq. (81). Hence, the rate of detection is

$$\frac{dP}{dt} = d\boldsymbol{K}\frac{d}{dt}|T_f(t)|^2 = \left(\frac{dT_f^*}{dt}T_f + \text{c.c.}\right) d\boldsymbol{K}. \tag{84}$$

Simple evaluation of this expression and division by the incident flux leads to the differential cross section

$$d\sigma = \frac{2\pi}{\hbar v_i}|\langle \boldsymbol{K}|V_f|\Psi_i^+\rangle|^2 \, d\boldsymbol{K}\, \delta(E_f - E_i) \tag{85}$$

or, with $d\boldsymbol{K} = \prod_{j=1}^n d\boldsymbol{k}_j$,

$$\frac{d\sigma}{d\boldsymbol{k}_1 d\boldsymbol{k}_2 \ldots d\boldsymbol{k}_n} = \frac{2\pi}{\hbar v_i}|\langle \boldsymbol{K}|V_f|\Psi_i^+\rangle|^2 \, \delta(E_f - E_i), \tag{86}$$

which is identical to Eq. (58).

The foregoing derivation is much simpler and more direct than that leading to Eq. (58) and could provoke the question as to the need to examine the complicated properties of the many-particle Green function in coordinate space. However, one should not forget that to derive Eq. (86) a projection has been made on *quantum* plane-wave states occupying the whole of space. Only the classical condition contained in the asymptotic spatial Green function and the corollary of identifying spatial and momentum angular variables allows one to associate these momenta with classical momenta deduced from position and time measurements. This identification is also given by the IT. Indeed, precisely this question is what led Kemble [1] to derive the IT in the first place.

So far, we have developed a scattering theory assuming the collision of two composite particles in the incident channel. However, many fragmentation processes such as multiple photoionization or photodissociation are initiated by laser light. This can be thought of as a photon-particle collision. The laser light sources used can be either cw or pulsed and strong or weak depending on the experimental situation. In almost all cases, the light source is treated as a classical electromagnetic field with an explicit time dependence. Then, the transition operator in the form of Eq. (75) is appropriate and a *rate* of photofragmentation is calculated according to Eq. (84). In the special case of a weak cw light source, first-order perturbation theory can be used to eliminate the time and then a cross section analogous to Eq. (86) can be defined.

V. CONCLUSIONS

We have simplified and extended the completely general time-independent multiparticle scattering theory of Gerjuoy, showing how it is a rather straightforward generalization of the treatment of two-body potential scattering theory to be found in many textbooks. In particular, we define a many-body scattering amplitude in analogy to the two-body case. By formulating the differential cross section in terms of the measurement of final particle position rather than momentum, we have derived the cross section without the need to calculate the outgoing flux of scattered waves. This simplifies significantly the derivation of the multiparticle differential cross section.

Further, we have shown that the time-independent theory in spatial coordinates leads naturally for asymptotically large distances to the definition of a classical time and thereby allows association of time-independent quantum "momenta" with measured classical momenta. This justifies proceeding to a time-dependent quantum description of the scattering process where the time is set by the classical apparatus. The time-dependent description of quantum asymptotic fragment

motion leads in turn to the IT, which relates the position and momentum forms of the transition-matrix element. This allows an alternative simpler derivation of the cross section in terms of the probability of a momentum measurement. The asymptotic classical relations occurring in both the time-independent and time-dependent formulations of scattering theory justify the successful use of classical mechanics for such motion as is assumed routinely in experimental data processing.

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APPENDIX A: COMPOSITE PARTICLES AND INTERNAL COORDINATES

For simplicity of notation, we have assumed structureless particles although by definition fragmentation processes involve composite particles. However, the extension of the notation to describe particle aggregates of different character in initial and final states is straightforward, as is the transformation from laboratory to center-of-mass and internal coordinates. We begin with the differential rate expression (58). Then, for a set of particles with final momenta $\boldsymbol{K} = (\boldsymbol{k}_1,\boldsymbol{k}_2 \ldots \boldsymbol{k}_n)$, we write

$$\frac{d\sigma}{d\boldsymbol{K}} = \frac{2\pi}{\hbar v_i}|\langle\psi_f|V_i|\Psi_i^+\rangle|^2\delta(E_f - E_i). \tag{A1}$$

The scattering state is defined as

$$|\Psi_i^+\rangle = (1 + GV_i)|\psi_i\rangle. \tag{A2}$$

In the case of composite particles a,b in the incident channel, the initial state is defined as

$$|\psi_i\rangle = \left|\boldsymbol{k}_a,\phi_p^a\right\rangle\left|\boldsymbol{k}_b,\phi_q^b\right\rangle, \tag{A3}$$

where $|\boldsymbol{k},\phi_p\rangle$ denotes a particle with momentum $\boldsymbol{k}$ and internal state ϕ_p. Correspondingly, the final state $|\psi_f\rangle$ is defined by a product of such one-particle states. Then, since these states diagonalize H_i and H_f, this fixes the interactions V_i and V_f as those parts of the total Hamiltonian not diagonalized. The initial total energy is

$$E_i = \frac{\hbar^2 k_a^2}{2m_a} + \frac{\hbar^2 k_b^2}{2m_b} + \mathcal{E}_i, \tag{A4}$$

where the $\mathcal{E}_i$ is the sum of the internal binding energies. Similarly, for n particles in the final channel

$$E_f = \sum_j^n \left(\frac{\hbar^2 k_j^2}{2m_j}\right) + \mathcal{E}_f. \tag{A5}$$

The transformation to internal coordinates is made easily since all interactions involve relative coordinates so that the center-of-mass (c.m.) motion may be integrated out. In the incident channel, one transforms to the two-body c.m. and relative coordinates defined in Sec. III. Then,

$$|\psi_i\rangle = \left|\boldsymbol{K}_i,\phi_p^a,\phi_q^b\right\rangle|\boldsymbol{\kappa}_i\rangle \tag{A6}$$

with energy

$$E_i = \frac{\hbar^2\kappa_i^2}{2M} + \frac{\hbar^2 K_i^2}{2\mu} + \mathcal{E}_i. \tag{A7}$$

An equivalent transformation is made on the final state and since all interactions do not involve the c.m. motion, the cross section may be written

$$\frac{d\sigma}{d\boldsymbol{K}'d\boldsymbol{\kappa}_f} = \frac{2\pi}{\hbar v_i}|\langle\psi_f|V_f|\Psi_i^+\rangle|^2\delta(E_f - E_i)\,\delta(\boldsymbol{\kappa_f} - \boldsymbol{\kappa_i}), \tag{A8}$$

where $\boldsymbol{K}' = (\boldsymbol{k}'_1,\boldsymbol{k}'_2 \ldots \boldsymbol{k}'_{n-1})$ are a set of internal momenta. Integrating over c.m. momentum one has

$$\frac{d\sigma}{d\boldsymbol{k}'_1 d\boldsymbol{k}'_2 \ldots d\boldsymbol{k}'_{n-1}} = \frac{2\pi}{\hbar v_i}|\langle\psi_f|V_f|\Psi_i^+\rangle|^2\delta(E'_f - E'_i). \tag{A9}$$

This is the standard result, where the energies now have the c.m. energy subtracted. Similarly, the integrations implied by the matrix element are now over internal coordinates only.

APPENDIX B: REARRANGEMENT COLLISIONS

Since fragmentation always corresponds to rearrangement of the particles involved in collision, here we present some identities satisfied by the various Green operators and T-matrix elements. Appropriate to the three channels, free particle, initial, and final, we have three subdivisions of the total Hamiltonian

$$H = H_0 + V = H_i + V_i = H_f + V_f \tag{B1}$$

and corresponding Green functions

$$G^{\pm}(E) = (E - H \pm i\epsilon)^{-1}, \tag{B2}$$

$$G_\lambda^{\pm}(E) = (E - H_\lambda \pm i\epsilon)^{-1} \tag{B3}$$

with $H_\lambda = H_0, H_i$ or H_f. All Hamiltonians are assumed to be Hermitian.

1. Post and prior equivalence

The equivalence of post and prior forms of the exact T-matrix element is used to derive Eq. (21) of the text. The proof is as follows. Consider the prior form of the T-matrix element

$$T = \langle\psi_f|V_f|\Psi_i^+\rangle = \langle\psi_f|V_f(1 + G^+V_i)|\psi_i\rangle. \tag{B4}$$

We write this as

$$T = \langle\psi_f|V_i + V_fG^+V_i|\psi_i\rangle + \langle\psi_f|V_f - V_i|\psi_i\rangle \tag{B5}$$

or

$$\begin{aligned} T &= \langle(1 + G^-V_f)\psi_f|V_i|\psi_i\rangle + \langle\psi_f|V_f - V_i|\psi_i\rangle \\ &= \langle\Psi_f^-|V_i|\psi_i\rangle + \langle\psi_f|V_f - V_i|\psi_i\rangle. \end{aligned} \tag{B6}$$

Now, consider the first Born elements on the right-hand side of this result. One has

$$\langle\psi_f|V_f|\psi_i\rangle = \langle\psi_f|H - H_f|\psi_i\rangle = \langle\psi_f|H - E_f|\psi_i\rangle. \tag{B7}$$

From energy conservation, $E_f = E_i$ so we can write $\langle\psi_f|H - E_f|\psi_i\rangle = \langle\psi_f|H - E_i|\psi_i\rangle$ to give equivalence of post-prior first-Born terms

$$\langle\psi_f|V_f|\psi_i\rangle = \langle\psi_f|H - H_i|\psi_i\rangle = \langle\psi_f|V_i|\psi_i\rangle. \tag{B8}$$

Hence, the second term on the right-hand side of Eq. (B6) vanishes identically and we have the post form of the exact T-matrix element

$$T = \langle\Psi_f^-|V_i|\psi_i\rangle. \tag{B9}$$

2. Alternative form of the scattered wave

In Eq. (15), the exact scattering state is written

$$|\Psi_i^+\rangle = |\psi_i\rangle + |\Psi_{sc}\rangle = |\psi_i\rangle + G^+(E_i)V_i|\psi_i\rangle. \tag{B10}$$

Now, we employ the equivalent form with

$$|\Psi_i^+\rangle = |\psi_i\rangle + G_i^+(E_i)V_i|\Psi_i^+\rangle. \tag{B11}$$

Using the identity

$$G_i^+(E_i) = G_f^+(E_i)[1 + (V_f - V_i)G_i^+(E_i)] \tag{B12}$$

which can be proved by letting both sides operate on $[G_i^+(E_i)]^{-1}$, we have, noting that all Green operators are at energy E_i,

$$\begin{aligned}|\Psi_{sc}\rangle &= G_f^+[1 + (V_f - V_i)G_i^+]V_i|\Psi_i^+\rangle \\ &= G_f^+V_i|\Psi_i^+\rangle + G_f^+(V_f - V_i)(|\Psi_i^+\rangle - |\psi_i\rangle) \\ &= G_f^+V_f|\Psi_i^+\rangle - G_f^+(V_f - V_i)|\psi_i\rangle. \end{aligned}\tag{B13}$$

The second term of this equation involves a contribution from the initial state. However, when we project the scattering state onto the final state and recognize energy conservation, we have

$$\langle\psi_f|G_f^+(V_f - V_i)|\psi_i\rangle = \frac{\langle\psi_f|(V_f - V_i)|\psi_i\rangle}{E_f - E_i + i\epsilon} \equiv 0 \tag{B14}$$

from the equivalence of post and prior first-Born matrix elements [Eq. (B8)]. Hence, that part of the scattered wave with nonzero overlap with the final state is simply $G_f^+V_f|\Psi_i^+\rangle$. Accordingly, instead of Eq. (18) we could write, choosing $G_f^+ = G_0^+$,

$$\begin{aligned}&\lim_{\mathcal{R}\to\infty}\Psi_{sc}(\boldsymbol{\mathcal{R}}) \\ &= \lim_{\mathcal{R}\to\infty}\langle\boldsymbol{\mathcal{R}}|G_0^+V_f|\Psi_i^+\rangle \\ &= \lim_{r\to\infty}\int\langle\boldsymbol{\mathcal{R}}|G_0^+|\boldsymbol{\mathcal{R}}'\rangle\langle\boldsymbol{\mathcal{R}}'|V_f|\Psi_i^+\rangle\,d\boldsymbol{\mathcal{R}}' \\ &= -\sqrt{2\pi}\,\frac{m}{\hbar^2}\,(-i\mathcal{K})^{(3n-3)/2}\,\eta_n\,\frac{e^{i\mathcal{K}\mathcal{R}}}{\mathcal{R}^{(3n-1)/2}}\,\langle\boldsymbol{\mathcal{K}}|V_f|\Psi_i^+\rangle,\end{aligned}\tag{B15}$$

which is a more direct derivation of Eq. (21) and analogous to the one-particle case of Eq. (7).

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[21] Due to our using delta-function normalization of wave functions, the physical dimensions in Eq. (11) appear incorrect as the square of the scattering amplitude has dimensions of area. This is remedied by multiplying the right-hand side by a normalization factor L^{-3} as for a box of volume L^3. However, in Secs. II B and III B, we assume one particle in the incident beam per unit volume and take $L^{-3} \equiv 1$, so that the final cross-section expressions do have the correct physical dimensions. Note that the scattering amplitude for n particles also has dimensions of length.
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