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# Scattering Theory, Time and Multi-Particle Detection

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We consider the theory of multiple-particle fragmentation processes in the light of modern multi-hit position-sensitive detection. First we give a new formulation of time-independent many-body scattering theory as a direct generalisation of standard text-book two-body potential scattering but in such a way as to emphasise 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 1950's and emphasises 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 wavefunctions arises [2].

At the core of the analysis are three features which are not usually found in text books 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 generalisation of the standard text-book 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 new 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 wavefunction in position space to the momentum space wavefunction at the exit of the reaction zone, which wavefunction can be related to the quantum scattering amplitude [2]. Although proved by Kemble in 1937 [1] and re-discovered 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

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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 wavefunction collapse or the creation of narrow wavepackets.

The establishment of a time-dependent theory is crucial for the proof of the IT, since this relies upon the notion of wavefunctions 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 the IT in connection with modern multi-particle 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 quantised 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 femto- and atto-second 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 text books 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 generalise 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 generalisation 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 Fifties this is the approach adopted by standard text books 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 text-book time-independent two-body scattering theory, such a many-particle theory, formulated in co-ordinate space, is well-suited to one aim of the present paper which is to concentrate on the detection of particles at given positions. Hence in this paper first we give a simple re-formulation of Gerjuoy's theory designed specifically to show the close parallel to the usual text-book 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 quantised 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 wavefunction can be made compatible with the assumed classical interpretation of the particle movement to the detector. Of course, ulti-

mately 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 Section II we present many-particle scattering theory as a direct generalisation 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 Section III we show how the asymptotic behavior of the time-independent wavefunction 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 Section 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 wavefunction is used to prove the many-particle form of the IT, relating the spatial wavefunction to its momentum-space Fourier transform. The conclusions are summarised in Section V.

## II. TIME-INDEPENDENT SCATTERING THEORY

### A. The two-particle case

Since we wish to generalise the simplest two-particle potential scattering theory, first of all we remind ourselves of the salient points of its derivation presented in many text books. Specific equations can then be related to their  $n$ -body counterparts. We consider the elastic collision of two particles of reduced mass  $\mu$ . 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  $\epsilon$  is a positive infinitesimal, and satisfies the equations

$$G^+ = G_0^+ + G_0^+ V G^+ = G_0^+ + G^+ V G_0^+ \quad (1)$$

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

In the standard text-book approach one considers the scattering state  $\Psi_i(\mathbf{r})$ , where  $\mathbf{r}$  is the co-ordinate of relative motion, as a continuum eigenstate of  $H$  at fixed energy  $E$  and so defined as

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

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

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

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

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

It is usual to define the “momentum”  $\hbar \mathbf{k} \equiv \hbar k_i \hat{\mathbf{r}}$ , where  $\hat{\mathbf{r}}$  is the direction of  $\mathbf{r}$ . Hence,  $k = k_i$ . We emphasise that  $\hbar \mathbf{k}$ , 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  $\mathbf{r}$ , 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 centre is infinitely massive so that  $\mathbf{r}$  is the laboratory-fixed coordinate and  $\mu$  the mass of a single scattered particle. In the following we will refer to this as “the one-body case.” However, simply replacing  $\mu$  by a two-body reduced mass and interpreting  $\mathbf{r}$  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 wavefunction is, with  $k_i = k$ ,

$$\begin{aligned} \lim_{r \rightarrow \infty} \Psi_i^+(\mathbf{r}) \\ = \psi_i(\mathbf{r}) - \frac{\mu}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\mathbf{k} \cdot \mathbf{r}'} V(\mathbf{r}') \Psi_i^+(\mathbf{r}') d\mathbf{r}'. \end{aligned} \quad (5)$$

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

$$\lim_{r \rightarrow \infty} \Psi_i^+(\mathbf{r}) = \psi_i(\mathbf{r}) + f(\mathbf{k}) \frac{e^{ikr}}{r} \quad (6)$$

gives the scattering amplitude in the form

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

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

$$\lim_{r \rightarrow \infty} \Psi_{sc}(\mathbf{r}) = f(\mathbf{k}) \frac{e^{ikr}}{r}. \quad (8)$$

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  $\mathbf{R}$ , then detection implies projection on the wavefunction  $\delta(\mathbf{r} - \mathbf{R})$ . Hence the probability amplitude for detection is given by  $\langle \mathbf{R} | \Psi_{sc} \rangle = \Psi_{sc}(\mathbf{R})$  for asymptotically large  $R$ , that is

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

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

$$dP = |\Psi_{sc}(\mathbf{R})|^2 d\mathbf{R}, \quad (10)$$

or

$$\frac{dP}{d\Omega dR} = |f(\mathbf{k})|^2 \quad (11)$$

for the differential probability of scattering [21]. Here  $d\Omega$  is the solid angle subtended by  $d\mathbf{R}$  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  $f(\mathbf{k}) = f(k\hat{\mathbf{R}})$ , that is, a function dependent on position. This quantity is provided by the theory through the transition matrix element  $\langle \mathbf{k} | V | \Psi_i^+ \rangle$ .

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* wavefunction  $\Psi_i^+(\mathbf{r})$  via a construct involving  $\text{Re}(\Psi_i^{+*} \nabla \Psi_i^+)$ . 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  $r \rightarrow \infty$  limit.

### C. The 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 2-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. Firstly 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.

Secondly 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 wavefunction of the particle by its internal wavefunction and concomitant suitable modification of the energy of the particle. In addition, for re-arrangement 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 centre-of-mass motion and discuss in terms of the 3-dimensional relative coordinate  $\mathbf{r}$ . Then one has an effective one-body problem. For three or more particles, however, the definition of internal co-ordinates is not unique. For this reason, the general case will be analysed in terms of laboratory co-ordinates 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  $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n)$  and *hyperradius*  $R = (r_1^2 + r_2^2 + \dots + r_n^2)^{1/2}$ . Later we use  $\mathbf{R} = (\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_n)$  to denote the collective position co-ordinates of  $n$  detectors. We define also mass-weighted position co-ordinates  $\mathcal{R}_j \equiv \sqrt{m_j/m} \mathbf{r}_j$  and a corresponding  $3n$ -dimensional vector  $\mathcal{R} = (\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_n)$  that defines a mass-weighted hyperradius  $\mathcal{R}$  according to

$$m\mathcal{R}^2 = \sum_j m_j r_j^2, \quad (12)$$

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

As in Section IIA, 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  $\mathcal{R}$  given they started out at  $\mathcal{R}'$  just outside the reaction volume. For  $n$  particles of mass  $m_j$  and total kinetic energy  $E_K \equiv E_f - E_f$ , where  $E_f$  is the total energy and  $E_f$  the total binding energy of the  $n$  fragments, the free Green function is given as [14]

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

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

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 behaviour of  $G_0^+$  is given by

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

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

#### D. Scattering Amplitude and Detection Probability in the $n$ -body Case

In the general case where re-arrangement 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

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

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

$$H = H_i + V_i = H_f + V_f. \quad (16)$$

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

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

$$G^+ = G_f^+ + G_f^+ V_f G^+ \quad (17)$$

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

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

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

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

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

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

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  $\langle \mathcal{K} | V_f | \Psi_i^+ \rangle$ , as we show in Appendix B. Then defining the  $n$ -particle scattering amplitude

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

we re-write Eq. (18) as

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

Eq. (21) and Eq. (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

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

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

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

This is form-identical with the one-particle expression Eq. (11). As in the one-particle case, since  $\mathcal{K} \equiv \mathcal{K}\mathcal{R}/\mathcal{R} = (\mathcal{K}/\mathcal{R})(\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_n)$ , 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  $d\hat{\mathbf{r}}_j$  but also  $n$  additional *hyperangles*, which we will define following Gerjuoy [3] in terms of coordinate length ratios. (See Section III.B below.)

### III. THE PARTICLE MOMENTA

#### A. The definition of time

To re-iterate the development so far; we have presented a fully time-independent scattering theory for multi-particle fragmentation, where the scattering wavefunction 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 wavefunction.

At this stage, to connect directly to measured quantities, we will introduce one-particle momenta  $\hbar\mathbf{k}_j$  but which are defined in terms of the laboratory position coordinates of *all* particles. To this end one notes that the

plane-wave state  $e^{-i\mathbf{K}\cdot\mathbf{R}'}$  of Eq. (20), which derives from the asymptotic form of the Green function Eq. (14), defines an asymptotic wavevector  $\mathbf{k}_j$  of the  $j$ th scattered particle according to

$$\begin{aligned}\mathbf{K}\cdot\mathbf{R}' &= \sum_j \mathbf{K}_j\cdot\mathbf{R}'_j \\ &= \sum_j \frac{\mathcal{K}}{\mathcal{R}} \frac{m_j}{m} \mathbf{r}_j\cdot\mathbf{r}'_j \equiv \sum_j \mathbf{k}_j\cdot\mathbf{r}'_j,\end{aligned}\quad (25)$$

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

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

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

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

$$\mathbf{k}_j \equiv \frac{m_j}{m} \frac{r_j}{\mathcal{R}} \mathcal{K} \hat{\mathbf{r}}_j \quad (27)$$

which correspond to the effective wavevector  $\mathbf{k} = k_i \hat{\mathbf{r}}$  of the  $n = 1$  case. These wavevectors can also be written

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

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

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

Nevertheless, these one-particle “momenta”  $\hbar \mathbf{k}_j$  are a mathematical construct defined in terms of *all* the quantum position variables. That is, the  $k_j(r_j/\mathcal{R})$  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 Eq. (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

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

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

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

for *each and every*  $j = 1, \dots, n$ . 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

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

Then the validity of Eq. (31) is assured at all times by the conditions  $\mathbf{r}_j = \mathbf{v}_j t$  where the  $\mathbf{v}_j$  are constants. Hence each time value defines a different set of positions  $\{\mathbf{r}_j(t)\}$  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  $\{\mathbf{R}_j\} = \{\mathbf{v}_j t_j\}$  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 section 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 co-ordinates for each emitted particle. In Appendix A we show that the cross section is transformed readily to the more usual centre-of-mass and relative co-ordinates. It is interesting that, in the two-body case presented in most text books, the implicit dependence of defined momenta on particle distances is not evident and the necessity to introduce a time via  $\mathbf{r} = \mathbf{v}t$  is not apparent. This is because for two bodies only the effective one-body motion in relative coordinate  $\mathbf{r} \equiv \mathbf{r}_a - \mathbf{r}_b$  with reduced mass  $\mu$  is relevant. Then for the final momentum  $\hbar \mathbf{k}$ , Eq. (28) with  $m_j = \mu$ ,  $E_{\mathcal{K}} = E$  and  $\mathcal{R} = r_j = r$  becomes simply

$$\hbar \mathbf{k} = \sqrt{2mE} \hat{\mathbf{r}} = \hbar k_i \hat{\mathbf{r}}, \quad (33)$$

which expresses  $\mathbf{k}$  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 behaviour of distance with time. In laboratory co-ordinates one has the momenta  $\hbar \mathbf{k}_j$  from Eq. (28), from which follows the sum rule of Eq. (29). Thus one sees that the classical relations established above, i.e.  $\hbar \mathbf{k}_j = m_j \mathbf{v}_j$  with  $\mathbf{r}_j = \mathbf{v}_j t$  are consistent since one obtains from Eq. (28), with  $t = (2E_K / \sum_i m_i r_i^2)^{-1/2}$  from Eq. (32),

$$\hbar \mathbf{k}_j = m_j \frac{\mathbf{r}_j}{t} = m_j \mathbf{v}_j \quad (34)$$

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

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

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

The conjugate momenta then are, from Eq. (28), the centre-of-mass momentum  $\hbar \mathbf{K}$ ,

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

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

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

where  $\mu$  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 behaviour of the wavefunction. This allows a sharp classical momentum to be associated with a sharp quantum position variable via  $\mathbf{r} = \mathbf{v}t$ . At no stage do we need to invoke wavefunction collapse or narrow wavepackets as Kemble [1] surmised. Our scattering wavefunction occupies all space and we need only interpret detection probability as given by the modulus squared of this wavefunction. 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 wavefunctions.

## B. The differential cross section

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

$$dP = |f(\mathbf{k})|^2 dR d\Omega. \quad (38)$$

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

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

It is standard practice to define a differential cross section with respect to measured momenta  $\mathbf{k}$ . 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 recognising energy conservation. Then one has, reverting to momenta rather than velocity,

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

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

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

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

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

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  $\mathbf{r}$  with that of the final momentum which is justified precisely by the definition of  $\mathbf{k} = k \hat{\mathbf{r}}$ .

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  $\mathbf{r}_j = \mathbf{R}_j$  effect a projection of the scattered wave onto a wavefunction  $\prod_j \delta(\mathbf{r}_j - \mathbf{R}_j)$ . Denoting the  $3n$ -dimensional detector position vector by  $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_n)$ , the detection probability amplitude is given by  $\Psi_{sc}(\mathbf{R})$ .

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

$$d\mathbf{R} = r_1^2 dr_1 d\hat{\mathbf{r}}_1 r_2^2 dr_2 d\hat{\mathbf{r}}_2 \dots r_n^2 dr_n d\hat{\mathbf{r}}_n. \quad (43)$$

We will write this as

$$d\mathbf{R} \equiv R^{3n-1} dR d\Omega, \quad (44)$$

where following Gerjuoy [3] we define

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

with  $d\Omega_j \equiv d\hat{\mathbf{r}}_j$ . The  $n-1$  ratios are defined with respect to an arbitrary coordinate denoted  $r_1$ , i.e.  $q_j = r_j/r_1$  for  $j = 2, \dots, n$ . The directions  $\hat{\mathbf{R}}$  are determined by the  $q_j$  and the  $2n$  angles in ordinary 3-dimensional space determining the directions  $\hat{\mathbf{r}}_1, \dots, \hat{\mathbf{r}}_n$ . 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

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

or

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

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

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

which gives rise to the dimensionless factor

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

in Eq. (47).

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

$$dR = \frac{R}{\mathcal{R}} \mathcal{V} dt \quad (50)$$

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

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

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

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

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

$$\prod_{j=2}^n dq_j = \frac{E\mathcal{K}}{\frac{1}{2}m_1 v_1^2} \frac{1}{v_1^{n-1}} \prod_{j=2}^n dv_j. \quad (53)$$

Transforming further from velocities to momenta we obtain

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

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

$$d\sigma = \frac{2\pi m_1}{\hbar^3 v_i} k_1 |\langle \mathbf{K} | V_f | \Psi_i^+ \rangle|^2 d\Omega_1 \prod_{j=2}^n d\mathbf{k}_j \quad (55)$$

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

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

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  $dE_f = (\hbar^2 k_1/m_1) dk_1$  gives the final result

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

or the differential cross section

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

Again this is the standard result and is the  $n$ -particle generalisation 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  $H_D$  giving the total Hamiltonian

$$\mathcal{H} = H(\mathbf{r}) + H_D(\mathbf{R}) + H_I(\mathbf{r}, \mathbf{R}) \quad (59)$$

Here, for simplicity, we consider only one particle's coordinates  $\mathbf{r}$ . 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  $\mathbf{R}$  which later will go over to a classical position  $\mathbf{R}(t)$ . 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)

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

Although the derivation is perfectly general, to keep the notation simple we will consider the apparatus wavefunction to depend upon a single 'clock' co-ordinate  $R$ , 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 wavefunction is the entangled linear combination of states

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

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

### A. The 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,

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

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

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

with  $P_{\nu}$  the *classical* momentum

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

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

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

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

$$W_k \approx (2ME)^{1/2} (1 - \epsilon_{\nu}/(2E)) R. \quad (66)$$

The detector action still depends on the quantum energy  $\epsilon_{\nu}$ , 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  $\nu$  of the scattering system, i.e.

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

With this classical action the classical time is defined as

$$t = \frac{MR}{\partial W / \partial R} = MR/P, \quad (68)$$

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

$$W_k = W - \epsilon_k t. \quad (69)$$

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

$$\Psi_i^+(\mathbf{r}, t) = \sum_k c_k(t) e^{-\frac{i}{\hbar} \epsilon_k t} \psi_k(\mathbf{r}). \quad (70)$$

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

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

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

By the same procedure as used here it has been shown in Refs. [17, 18] in the limit that the detector coordinate  $R \rightarrow R(t)$  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.

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

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  $\mathbf{R}$  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 Eq. (71) are equal in prior form to

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

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

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

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 wavefunction is restricted to energy phases. Then, for asymptotically large  $t$ , the time integral furnishes an energy-conserving delta function only and, as we show below, 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 wavefunction is physically more intuitive than the idea of a time-independent continuum wavefunction.

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

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

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 emphasised particle detection at positions  $\mathbf{R} = \mathbf{R}$  and shown that the probability amplitude ( $T$ -matrix element) for scattering into detectors at  $\mathbf{R}$  is proportional to  $\Psi_{sc}(\mathbf{R})$  the scattered wavefunction at the detector. From Eq. (71), by projecting onto a spatial  $\delta$ -function, we see that this result holds also in the time-dependent case since  $T_f(t) = \langle \psi_f(t) | \Psi_i^+(t) \rangle \propto \Psi_i^+(\mathbf{R}, t)$ , where we note that the initial wavefunction  $\psi_i(\mathbf{R}) = 0$ , i.e. the initial wavefunction 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

$$| \Psi_i^+(t) \rangle = e^{-iH_0 t/\hbar} | \Psi_i^+(0) \rangle, \quad (76)$$

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

$$\langle \mathcal{K}' | e^{-iH_0 t/\hbar} | \mathcal{K} \rangle = e^{i\hbar \mathcal{K}^2 t/2m} \delta(\mathcal{K}' - \mathcal{K}), \quad (77)$$

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

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

This result is form identical with the one-particle expression [2, 7]. Hence in the limit  $\mathcal{R}, t \rightarrow \infty$  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  $\mathcal{K}' = \mathcal{K} \equiv m\mathcal{R}/\hbar t$ . The maximum contributions to the integral come from a small region about this point, and performing the integral in stationary-phase approximation gives

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

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

The condition of stationary phase  $\hbar \mathcal{K} \equiv m\mathcal{R}/t$  gives  $\hbar \mathbf{k}_j = m_j \mathbf{r}_j/t$  for each and every  $j = 1, \dots, n$ , 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  $d\mathbf{K} = (m/\hbar t)^{3n} d\mathbf{R}$  from this condition, Eq. (79) leads to the asymptotic equality of probabilities

$$|\Psi_i^+(\mathbf{R}, t)|^2 d\mathbf{R} \sim |\tilde{\Psi}_i^+(\mathbf{K})|^2 d\mathbf{K}. \quad (80)$$

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

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

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

This demonstration of the equivalence of absolutely well-defined momentum and position wavefunctions 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 behaviour. 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 Ref. [2] and Ref. [7]. In particular the conditions for validity of the stationary phase approximation are defined and the generalisation 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  $\mathbf{R}(t)$  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 dependences 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  $|\Psi_i^+(\mathbf{R})|^2 d\mathbf{R}$  leads to the

cross-sections Eq. (51) and Eq. (58), then from Eq. (81) the momentum detection probability  $|\tilde{\Psi}_i^+(\mathbf{K})|^2 d\mathbf{K}$  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  $\mathbf{K}$ . This gives

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

However this is equivalent to

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

The probability of detection of particles with momenta between  $\mathbf{K}$  and  $\mathbf{K} + d\mathbf{K}$  is given by the r.h.s. of Eq. (81). Hence the rate of detection is

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

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

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

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

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

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 multi-particle scattering theory of Gerjuoy, showing how it is a rather straightforward generalisation of the treatment of two-body potential scattering theory to be found in many text books. 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 multi-particle 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 Co-ordinates.

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 centre-of-mass and internal co-ordinates. We begin with the differential rate expression Eq. (58), which is trivially extended to any number of particles in the final state simply by adding more momenta differentials on the left hand side. Then, for a set of particles with final momenta  $\mathbf{K} = (\mathbf{k}_1, \mathbf{k}_2 \dots \mathbf{k}_n)$ , we write

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

The scattering state is defined as

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

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

$$|\psi_i\rangle = |\mathbf{k}_a, \phi_p^a\rangle |\mathbf{k}_b, \phi_q^b\rangle \quad (\text{A3})$$

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

$$E_i = \frac{\hbar^2 k_a^2}{2m_a} + \frac{\hbar^2 k_b^2}{2m_b} + \mathcal{E}_i \quad (\text{A4})$$

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

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

The transformation to internal co-ordinates is made easily since all interactions involve relative co-ordinates so that the centre-of-mass (CM) motion may be integrated out. In the incident channel one transforms to the two-body CM and relative co-ordinates defined in Section III. Then,

$$|\psi_i\rangle = |\mathbf{K}_i, \phi_p^a, \phi_q^b\rangle |\boldsymbol{\kappa}_i\rangle \quad (\text{A6})$$

with energy

$$E_i = \frac{\hbar^2 \kappa_i^2}{2M} + \frac{\hbar^2 k_i^2}{2\mu} + \mathcal{E}_i \quad (\text{A7})$$

An equivalent transformation is made on the final state and since all interactions do not involve the CM motion,

the cross section may be written

$$\frac{d\sigma}{d\mathbf{K}'d\mathbf{k}_f} = \frac{2\pi}{\hbar v_i} |\langle \psi_f | V_f | \Psi_i^+ \rangle|^2 \delta(E_f - E_i) \delta(\mathbf{k}_f - \mathbf{k}_i) \quad (\text{A8})$$

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

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

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

## Appendix B: Re-arrangement Collisions

Since fragmentation always corresponds to re-arrangement 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

$$H = H_0 + V = H_i + V_i = H_f + V_f \quad (\text{B1})$$

and corresponding Green functions

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

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

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

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

We write this as

$$T = \langle \psi_f | V_i + V_f G^+ V_i | \psi_i \rangle + \langle \psi_f | V_f - V_i | \psi_i \rangle, \quad (\text{B5})$$

or

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

Now consider the first Born elements on the r.h.s. of this result. One has

$$\langle \psi_f | V_f | \psi_i \rangle = \langle \psi_f | H - H_f | \psi_i \rangle = \langle \psi_f | H - E_f | \psi_i \rangle. \quad (\text{B7})$$

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,

$$\langle \psi_f | V_f | \psi_i \rangle = \langle \psi_f | H - H_i | \psi_i \rangle = \langle \psi_f | V_i | \psi_i \rangle. \quad (\text{B8})$$

Hence the second term on the r.h.s. of Eq. (B6) vanishes identically and we have the post form of the exact  $T$  matrix element

$$T = \langle \Psi_f^- | V_i | \psi_i \rangle. \quad (\text{B9})$$

### 2. Alternative form of the Scattered Wave

In Eq. (18) the exact scattering state is written

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

Now we employ the equivalent form with

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

Using the identity

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

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  $E_i$ ,

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

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 recognise energy conservation, we have

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

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

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

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

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