

# Through scattering theory with gun and camera: Coping with conventions in collision theory

Michael A. Morrison<sup>a)</sup> and Andrew N. Feldt  
*Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma,  
Norman, Oklahoma 73019-0225*

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Four ambiguities are inherent in time-independent quantum-mechanical scattering theory: two in the normalization of continuum functions, and two in the relation between various scattering matrices. These ambiguities allow the use of different conventions in scattering theory. This freedom has led to inconsistencies among textbooks, monographs, review articles, and research papers. We identify these ambiguities, indicate their context and origin in scattering theory, give the key equations of scattering theory in a form that can be adapted to any convention, and show interrelations between these equations that can lead to confusion and error. We also give several diagnostic approaches for determining the conventions used in a particular source, and reference conventions adopted in widely used books on scattering theory. © 2007 American Association of Physics Teachers.

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## I. INTRODUCTION

If you wish to converse with me, define your terms  
—Voltaire

Practitioners of quantum collision theory sometimes run afoul of ambiguities that are inherent in time-independent continuum-state quantum mechanics. Two of these ambiguities concern the normalization of continuum functions, and two others concern relations between various scattering matrices. The freedom allowed by these ambiguities has resulted in numerous inconsistencies among various textbooks, monographs, review articles, and research papers that treat or use scattering theory. Although many authors are careful about explicitly stating the conventions they adopt, some are not. Even in sources that do give this information, it is often strewn throughout many pages. Research papers rarely state their conventions—a problem exacerbated by the propensity of many authors to change conventions during the course of their career. A further difficulty is posed by research papers whose authors adopt conventions of a given source but do not cite their source, and it is left to the reader to deduce the conventions of such a paper.

This situation holds traps for the unwary. Undergraduate and graduate students are particularly prone to mix and match equations from a variety of sources, unaware that the resulting formalism contains inconsistencies guaranteed to spawn incorrect results. In spite of almost a century of valuable pedagogical resources including many excellent texts (see, for example, those cited in Table I) and a steady stream of valuable papers,<sup>1–16</sup> no one has directly addressed the ambiguities inherent in continuum stationary-state quantum mechanics.

This paper has evolved over 30 years and draws on our notes that encompass over two dozen textbooks and monographs, many tens of review articles, and roughly a thousand research papers. This paper is a codification, synthesis, and condensation of that material. We hope it will heighten readers' awareness of these potential land mines and help them navigate these treacherous waters.

Students usually fail to realize these ambiguities even exist, probably because no such ambiguities appear in bound-state quantum mechanics, which remains the primary focus

of undergraduate and introductory graduate quantum courses. It is necessary to choose a zero of energy, and it is possible to multiply the wave function by an overall global phase factor, and that's about it. Continuum-state quantum mechanics, by contrast, presents four options—all of which, as we shall show, are of great consequence.

This paper has both practical and pedagogical goals. The practical goals are to identify the choices that must be made in setting up and using scattering theory; to express the key equations of scattering theory in a form that facilitates adapting them to any convention; to explicate and illustrate diagnostic approaches that can be used to determine the conventions a particular source uses; and to provide a ready-reference to the choices made in widely used books on scattering theory (see Table I).

The pedagogical goals are to indicate the origin of these conventions in the formulation of scattering theory; to show how these conventions are interrelated by key equations of the theory; and to illustrate the use of simple analytical tools (particularly dimensional analysis; see Appendix A) to determine conventions and to ensure consistency among the key equations. By appreciating these points students gain deeper insight into the structure of scattering theory and ways in which the quantum mechanics of continuum states differs from the more familiar quantum mechanics of bound states.

The most perplexing and frustrating of these differences is the maze of interconnections between key equations in which various conventions appear. We have organized this paper in a series of short sections each of which summarizes a key area of the nonrelativistic quantum collision theory of (primarily) elastic collisions. The application of the guidelines and results of this paper to inelastic and rearrangement collisions, although nontrivial, is reasonably straightforward.

To contextualize this presentation, we use a modicum of formal scattering theory.<sup>17–19</sup> Students can use the guidelines in this paper without knowing this material. In no way is this paper a comprehensive or self-contained presentation of even a part of collision physics. We have relegated detailed derivations, discussions, and examples to standard sources, such as those cited in Table I. We consider primarily elastic scattering in nonrearrangement collisions and omit such topics as Coulomb scattering, dispersion relations, scattering from tar-

Table I. A summary of conventions in selected resources on scattering theory. Entries that contain the notation (NS) were not explicitly stated; these entries were inferred using the methods of this paper. Empty entries mean that either the convention was not discussed in the paper or could not be determined from it.

Reference	$\alpha$	$\beta$	$\gamma$	$\zeta$
This paper	1	1	1	1
19	1	1	1	1
49	1	$-1/\pi$	1	1
21	1	1	1	$e^{-i\delta_\ell(E)}$
23	1	$km/\hbar^2$	$-km\pi/\hbar^2$	$(2/\pi)^{1/2}i^\ell/k$
22	1	$i/2\pi$	1	$e^{-i\delta_\ell(E)}/\cos \delta_\ell(E)$
50	$(2\pi)^{3/2}$	$-1/\pi$	1	1
51	$(2\pi)^{3/2a}$	$-i/2\pi$	1	$e^{-i\delta_\ell(E)}$
52	$(2\pi)^{3/2}$	$2\pi/k$	$1/k$	$1/k$
33	$(2\pi)^{3/2b}$	1	$-\pi$	1
53	1	1 (NS) <sup>c</sup>		$e^{-i\delta_\ell(E)}/k^d$
54	$(2\pi)^{3/2}$	$i/2\pi$	1	$e^{-i\delta_\ell(E)}$
41	$(2\pi)^{3/2}$ (NS)	$-1/\pi$	1	$k^{-1/2}e^{-i\delta_\ell(E)}$
18	$\sqrt{mk\hbar^{2e}}$	1	1	1
55	1 <sup>f</sup>	$k/\pi$	$-k$	$e^{-i\delta_\ell(E)} \cos \delta_\ell(E)$
24	$(2\pi)^{3/2}$	1		$4\pi i^\ell/k$
17	1	1	$-\pi$	$e^{-i\delta_\ell(E)}/k \cos \delta_\ell(E)^g$

<sup>a</sup>Geltman (Ref. 51) uses  $\alpha=(2\pi)^{3/2}$ , Eqs. (1.18) and (8.1), and  $\alpha=1$ , Eqs. (5.2) (11.2), and (15.2).

<sup>b</sup>Rodberg and Thaler (Ref. 33) use a variety of conventions and sometimes absorb the constant  $\alpha$  into the scattering amplitude (for example, Chapters 2 and 3). In chapters on formal scattering theory, they use  $\alpha=(2\pi)^{3/2}$  [for example, their Eqs. (5.4.1) and (6.1.27)]. Elsewhere they use  $\alpha=1$  [for example, in Eq. (4.4.1) and surrounding discussion].

<sup>c</sup>Adhikari (Ref. 53) uses two transition operators, which are denoted by  $\mathbf{t}$  and  $\bar{\mathbf{t}}$ . For equations in which  $\mathbf{t}$  appears, set  $\beta=k/\pi$ ; for equations with  $\bar{\mathbf{t}}$ , set  $\beta=1$ .

<sup>d</sup>The scattering function that Adhikari (Ref. 53) denotes by  $\psi_\ell^{(+)}(r)$  is the auxiliary function  $v_{k\ell}(r)$  defined in our Eq. (85), not the normalized radial function  $u_{k\ell}(r)$ .

<sup>e</sup>For plane wave states Newton (Ref. 18) uses several normalization conventions, including the three discussed in Sec. V C. Like Taylor (Ref. 19), Newton (Ref. 18) sets  $\hbar=1$ .

<sup>f</sup>Khare (Ref. 55) sometimes leaves  $\alpha$  (which is called  $A$ ) unspecified;  $\alpha$  is variously set equal to 1 or  $(2\pi)^{-3/2}$ . The radial function  $f_{\ell k}(r)$  is the auxiliary function  $v_{k\ell}(r)$  of our Eq. (85). In some equations  $\beta=1$  is used [see Eq. (1.109)]; in others  $\beta=k/\pi$  [see Eq. (1.155)].

<sup>g</sup>Joachain (Ref. 17) is one of the few authors to discuss normalization choices. In Sec. 4.1.6 an arbitrary factor  $A(k)$  is introduced in the partial-wave expansion, and in Eqs. (4.84)–(4.86) several widely used choices are listed. In the examples,  $\alpha=1$  is used (see also Ref. 56).

gets with structure, density-matrix formulations, time-dependent scattering, reciprocity and time reversal, complex angular momenta, spin, resonances and other poles of the  $S$  matrix, and analytic properties of the  $S$  matrix. These topics introduce no new choices, and we have found that students who master the four conventions discussed in this paper have little difficulty extending that mastery to more advanced topics.

## II. THE MØLLER AND SCATTERING OPERATORS

The Møller operators  $\hat{\Omega}_\pm$  are defined in terms of the time-evolution operator (see Ref. 19 and Sec. VI C of Ref. 18),

$$\hat{U}(t) \equiv e^{-i\hat{\mathcal{H}}t/\hbar}, \quad (1a)$$

$$\hat{U}^0(t) \equiv e^{-i\hat{\mathcal{H}}^0 t/\hbar}, \quad (1b)$$

where  $\hat{\mathcal{H}}$  is the system Hamiltonian  $\hat{\mathcal{H}} = \hat{\mathcal{H}}^0 + \hat{V}$ , with  $\hat{\mathcal{H}}^0$  the kinetic energy operator, as

$$\hat{\Omega}_\pm \equiv \lim_{t \rightarrow \mp\infty} \hat{U}(t)^\dagger \hat{U}^0(t). \quad (2)$$

These operators relate the in- and out-asymptotes,  $|\psi_{\text{in}}\rangle$  and  $|\psi_{\text{out}}\rangle$ , to the scattering state vector  $|\psi\rangle$  as

$$|\psi\rangle = \hat{\Omega}_+ |\psi_{\text{in}}\rangle = \hat{\Omega}_- |\psi_{\text{out}}\rangle, \quad (3a)$$

where all state vectors refer to  $t=0$ . In terms of the evolution operator, this relation is

$$\hat{U}(t)|\psi\rangle \xrightarrow{t \rightarrow \mp\infty} \hat{U}^0(t)|\psi_{\text{in/out}}\rangle. \quad (3b)$$

### A. The scattering operator

The scattering operator  $\hat{S}$  is defined as

$$\hat{S} \equiv \hat{\Omega}_-^\dagger \hat{\Omega}_+, \quad (4)$$

and maps a given in-asymptote into the corresponding out-asymptote,

$$|\psi_{\text{out}}\rangle = \hat{S} |\psi_{\text{in}}\rangle. \quad (5)$$

The probability for a collision process  $|\psi_{\text{in}}\rangle \rightarrow |\psi_{\text{out}}\rangle$  is

$$P(|\psi_{\text{out}}\rangle \leftarrow |\psi_{\text{in}}\rangle) = |\langle \psi_{\text{out}} | \hat{S} | \psi_{\text{in}} \rangle|^2. \quad (6)$$

The Møller operators and the  $S$  operator preserve normalization.

### B. The momentum-space $S$ matrix

The momentum-space  $S$  matrix appears when an initial ( $t=0$ ) scattering state  $|\psi(0)\rangle$  is expanded in plane wave states  $|\mathbf{k}\rangle$ :

$$|\psi(0)\rangle = \int |\mathbf{k}\rangle \langle \mathbf{k} | \psi(0) \rangle d^3k. \quad (7)$$

If we use the time-evolution operator  $\hat{U}(t)$ , we obtain the expansion of the corresponding state at any  $t>0$ ,

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = \int |\mathbf{k}\rangle \langle \mathbf{k} | \psi(0) \rangle e^{-iE_k t/\hbar} d^3k, \quad (8)$$

where  $E_k = \hbar^2 k^2 / 2m$  is the scattering (kinetic) energy of the projectile of mass  $m$ . (For central-potential scattering of two particles, the symbol  $m$  denotes the reduced mass of the two particles.)

To introduce the momentum-space  $S$  matrix elements, we write the definition (5) of the  $S$  matrix in momentum space:

$$\langle \mathbf{k}' | \psi_{\text{out}} \rangle = \int \langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle \langle \mathbf{k} | \psi_{\text{in}} \rangle d^3k, \quad (9)$$

where we have used the identity

$$\hat{1} = \int d^3k |\mathbf{k}\rangle \langle \mathbf{k}|. \quad (10)$$

The matrix element  $\langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle$  is the probability amplitude for the scattering process  $|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle$ .

### C. Plane wave scattering states

#### 1. Wave-vector normalization

We shall take the plane wave states  $|\mathbf{k}\rangle$  to be *wave-vector normalized*,<sup>19</sup>

$$\langle \mathbf{k}' | \mathbf{k} \rangle = \delta(\mathbf{k}' - \mathbf{k}). \quad (11)$$

The coordinate-space projection of  $|\mathbf{k}\rangle$  is therefore

$$\langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (12)$$

The factor of  $(2\pi)^{-3/2}$  in Eq. (12) follows from the integral expression for the Dirac delta function

$$\delta(\mathbf{k}' - \mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{r}\cdot(\mathbf{k}' - \mathbf{k})} d^3r, \quad (13)$$

which must be unaffected by how we choose to normalize  $|\mathbf{k}\rangle$ .

Because the Møller operators preserve normalization, the corresponding *plane wave scattering states*

$$|\mathbf{k}\pm\rangle = \hat{\Omega}_\pm |\mathbf{k}\rangle \quad (14)$$

obey the same normalization condition as the plane wave states,

$$\langle \mathbf{k}' \pm | \mathbf{k} \pm \rangle = \delta(\mathbf{k}' - \mathbf{k}). \quad (15)$$

The scattering function  $\psi_{\mathbf{k}}^\pm(\mathbf{r}) \equiv \langle \mathbf{r} | \mathbf{k}\pm \rangle$  for outgoing waves obeys the boundary condition<sup>8</sup>

$$\psi_{\mathbf{k}}^+(\mathbf{r}) \xrightarrow{r \rightarrow \infty} (2\pi)^{-3/2} \left[ e^{-i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}' \leftarrow \mathbf{k}) \frac{e^{ikr}}{r} \right], \quad (16)$$

which contains the scattering amplitude  $f(\mathbf{k}' \leftarrow \mathbf{k})$ .

#### 2. Alternative normalizations of plane wave states

Although convenient, the choice of wave vector normalization in Eq. (11) is arbitrary. Many quantum mechanics textbooks use *momentum normalization*

$$\langle \mathbf{p}' | \mathbf{p} \rangle = \delta^3(\mathbf{p}' - \mathbf{p}). \quad (17a)$$

(Momentum normalization reduces to wave vector normalization in a set of reduced units in which  $\hbar=1$ , such as atomic units or the units used in Ref. 19.) With this choice the normalized free-particle wave function is

$$\langle \mathbf{r} | \mathbf{p} \rangle = (2\pi\hbar)^{-3/2} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \quad (17b)$$

We can multiply the wave-vector normalized plane wave state  $|\mathbf{k}\rangle$  by any complex constant  $\alpha$ ,

$$|\mathbf{k}\rangle \rightarrow \alpha |\mathbf{k}\rangle, \quad (18a)$$

provided we implement this “renormalization” in all equations where plane wave states appear but  $\alpha$  doesn’t happen to cancel. For example, the renormalized free-particle wave function follows as

$$\frac{1}{\alpha} \langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} \Rightarrow \langle \mathbf{r} | \mathbf{k} \rangle = \alpha (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (18b)$$

Similarly, the generalized normalization condition is

$$\frac{1}{|\alpha|^2} \langle \mathbf{k}' | \mathbf{k} \rangle = \delta(\mathbf{k}' - \mathbf{k}) \Rightarrow \langle \mathbf{k}' | \mathbf{k} \rangle = |\alpha|^2 \delta(\mathbf{k}' - \mathbf{k}). \quad (18c)$$

Equation (18) has corresponding analogs for the plane wave scattering states  $|\mathbf{k}\pm\rangle = \hat{\Omega}_\pm |\mathbf{k}\rangle$ .<sup>20</sup>

Another common alternative to wave vector normalization is  $\alpha = (2\pi)^{3/2}$ , for which

$$\langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (19a)$$

For this choice the normalization condition is

$$\langle \mathbf{k}' | \mathbf{k} \rangle = (2\pi)^3 \delta(\mathbf{k}' - \mathbf{k}) \quad \text{for } \alpha = (2\pi)^{3/2}. \quad (19b)$$

#### 3. Energy normalization of the plane wave states

Older books and papers on scattering theory use yet a third normalization of plane wave states  $|\mathbf{k}\rangle$  (see, for example, Secs. 8.3 and 10.1 of Ref. 18). By choosing  $\alpha = \sqrt{mk\hbar^2}$  we can force these states, which we shall write as  $|E\hat{\mathbf{k}}\rangle$ , to satisfy

$$\langle E'\hat{\mathbf{k}}' | E\hat{\mathbf{k}} \rangle = \delta(E' - E) \delta^3(\hat{\mathbf{k}}' - \hat{\mathbf{k}}). \quad (20)$$

This result follows from

$$\delta^3(\mathbf{k}' - \mathbf{k}) = \frac{1}{k^2} \frac{dE}{dk} \delta(E' - E) \delta^2(\hat{\mathbf{k}}' - \hat{\mathbf{k}}). \quad (21)$$

Unfortunately, many authors use a notation that fails to distinguish  $|\mathbf{k}\rangle$  from  $|E\hat{\mathbf{k}}\rangle$  and so leave their normalization choice ambiguous. We can determine which convention is being used from the fundamental relation for the differential cross section in terms of the momentum-space  $T$  matrix (see Sec. III). For an excitation  $|i\rangle \rightarrow |f\rangle$  of the target accompanied by a change of the projectile’s wave vector from  $\mathbf{k}$  to  $\mathbf{k}'$ , and for wave-vector normalization, this relation reads

$$\frac{d\sigma}{d\Omega} \Big|_{i \rightarrow f} = \left( \frac{m}{4\pi^2\hbar^4} \right) \frac{k'}{k} |\langle \mathbf{k}', f | \hat{T} | \mathbf{k}, i \rangle|^2. \quad (22a)$$

For energy normalization Eq. (22a) reads

$$\frac{d\sigma}{d\Omega} \Big|_{i \rightarrow f} = \frac{(2\pi)^4}{k^2} |\langle E'\hat{\mathbf{k}}' | \hat{T} | E\hat{\mathbf{k}} \rangle|^2. \quad (22b)$$

In both forms the outgoing wave vector for total energy  $E$  is

$$k' = \frac{\sqrt{2m[E - (\epsilon_f - \epsilon_i)]}}{\hbar^2}. \quad (23)$$

The two forms of the differential cross section in Eq. (22) illustrate how choices of conventions that may be unstated or difficult to determine can wreak significant changes on equations for key physical properties—even equations that at first thought should not depend on conventions. These changes often occur in seemingly inexplicable factors, typically involving  $\pi$  (usually  $4\pi^2$ ) and, sometimes, the particle’s mass, in cross sections (see, for example, Sec. 6.7 of Ref. 21; Sec. 1.5 of Ref. 22; Sec. 8.1 of Ref. 18, and Chap. 4 of Ref. 23).

The choice of normalization also affects important formal equations. For instance, the relation between the elastic scattering amplitude and the momentum-space  $T$  matrix (see Sec. IV) is affected not only by how the  $S$  and  $T$  matrices are related (see Sec. III A), but also by how we normalize the plane wave states. For wave-vector normalization, this relation is

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\frac{m}{2\pi\hbar^2} \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle, \quad (24a)$$

and for energy normalization it is

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\frac{4\pi^2}{k} \langle E\hat{\mathbf{k}}' | \hat{T}(E + i0) | E\hat{\mathbf{k}} \rangle. \quad (24b)$$

We must be especially alert for such differences in discussions of dispersion relations and analytic properties of the  $S$  matrix.

The normalization constant  $\alpha$  as well as the other three choices discussed in the following must disappear from a few key invariant equations. This requirement guides users in checking their derivations and in deducing conventions used in various sources. For example, no matter what choice we make, the optical theorem<sup>11</sup> must always relate the scattering amplitude to the total cross section as

$$\sigma^{\text{tot}} \equiv \sum_f \sigma_{f \leftarrow i} = \frac{4\pi}{k_i} \text{Im} f(f, \mathbf{k}' \leftarrow i, \mathbf{k}; 0), \quad (25)$$

where the sum is over all open (energetically accessible) channels  $i \rightarrow f$  (including the elastic channel  $i \leftarrow i$ ), and  $f(f, \mathbf{k}' \leftarrow i, \mathbf{k}; 0)$  is the scattering amplitude for forward scattering.

### III. THE TRANSITION ( $T$ ) MATRIX

In most scattering calculations, cross sections are calculated not from the scattering amplitude but from matrix elements of the transition operator  $\hat{T}$ . We shall define this operator from the Green's operator  $\hat{G}$  as

$$\hat{T}(z) \equiv \hat{V} + \hat{V}\hat{G}(z)\hat{V}. \quad (26)$$

The Green's operator is defined for any complex  $z$  in terms of the system Hamiltonian as

$$\hat{G}(z) \equiv (z - \hat{H})^{-1}. \quad (27)$$

#### A. The $S$ matrix and the $T$ matrix

The crucial relation between elements of the  $S$  matrix and elements of the on-shell  $T$  matrix (see Sec. 8d of Ref. 19) follows solely from the definitions of the  $S$  operator, Eq. (4), and of the  $T$  operator, Eq. (26),

$$\langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle = \delta(\mathbf{k}' - \mathbf{k}) - 2\pi i \delta(E_{k'} - E_k) \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle. \quad (28)$$

The term  $\delta(\mathbf{k}' - \mathbf{k})$  corresponds to the possibility that nothing happens (no scattering); the second term corresponds to the scattering possibility. This term contains an energy-conserving delta function  $\delta(E_{k'} - E_k)$  and the on-shell momentum-space  $T$ -matrix element

$$\langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle \equiv \lim_{\epsilon \rightarrow 0^+} \langle \mathbf{k}' | \hat{T}(E_k + i\epsilon) | \mathbf{k} \rangle. \quad (29)$$

The factor  $-2\pi i$  in the second term of Eq. (28) results from introducing the energy-conserving delta function via

$$\lim_{\epsilon \rightarrow 0} \left( \frac{1}{E_1 - E_2 + i\epsilon} - \frac{1}{E_1 - E_2 - i\epsilon} \right) = -2\pi i \delta(E_1 - E_2). \quad (30)$$

Equation (28) is sometimes taken as the definition of the  $T$  operator. Often this equation is written as an operator equation,

$$\hat{S} = \hat{1} - 2\pi i \hat{T}. \quad (31)$$

This operator form implies that the momentum-space  $T$ -matrix elements must contain (in the second term) both the delta function  $\delta(E_{k'} - E_k)$  and the on-shell restriction. Forgetting this implication can lead to incorrect equations and procedures, such as simply writing Eq. (31) in momentum space as  $\delta(\mathbf{k}' - \mathbf{k}) - 2\pi i \langle \mathbf{k}' | \hat{T} | \mathbf{k} \rangle$ . This expression, versions of which have appeared in the literature, is not the correct momentum-space  $S$ -matrix element.

Usually the momentum-space  $S$  and  $T$  matrices are related, as in Eq. (28), just like the corresponding operators in Eq. (31). However some authors (especially in nuclear physics<sup>23</sup>) relate the matrices differently than they do the corresponding operators. For example, Sitenko<sup>24</sup> defines the operator as  $\hat{T} \equiv \hat{S} - \hat{1}$ , but introduces a multiplicative factor in the definition of the momentum-space matrix elements of this operator, as  $\langle \mathbf{k}' | \hat{T} | \mathbf{k} \rangle = -2\pi i T_{\mathbf{k}', \mathbf{k}}(E) \delta(E' - E)$ .

#### B. Alternative relations between the $T$ and $S$ operators

As noted, the factor  $-2\pi i$  in Eq. (28) is not arbitrary; it follows from Eq. (30). We can, however, introduce into the scattering term in Eq. (28) an arbitrary multiplicative constant  $\beta$  (which many authors have done, see Table I), as

$$\langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle = \delta(\mathbf{k}' - \mathbf{k}) - 2\pi i \beta \delta(E_{k'} - E_k) \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle. \quad (32a)$$

In terms of operators, this expression reads<sup>25</sup>

$$\hat{S} = \hat{1} - 2\pi i \beta \hat{T}, \quad (32b)$$

Doing so amounts to redefining the  $T$  operator; that is, to making the replacement

$$\hat{T} \rightarrow \beta \hat{T}. \quad (33)$$

We must therefore multiply the  $T$  operator (and hence all  $T$ -matrix elements) by  $\beta$  in any equations in which these quantities appear. For example, the defining equation of the  $T$  operator, Eq. (26), becomes

$$\beta \hat{T}(z) \equiv \hat{V} + \hat{V}\hat{G}(z)\hat{V}. \quad (34)$$

Note that any redefinition of the  $T$  matrix must be implemented so as to leave unchanged the definition of the  $S$  operator,  $\hat{S} = \hat{\Omega}_-^\dagger \hat{\Omega}_+$ .

## IV. THE SCATTERING AMPLITUDE

### A. The scattering amplitude and the $T$ matrix

If we change the normalization of  $|\mathbf{k}\rangle$  via  $\alpha$  or the relation between  $\hat{S}$  and  $\hat{T}$  via  $\beta$ , we must modify several key equations to ensure consistency and dimensional correctness (see Appendix A). The most important of these equations is the definition of the scattering amplitude. Following Taylor<sup>19</sup> we define the scattering amplitude in terms of the on-shell  $T$  matrix element  $\langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle$  as

$$f(\mathbf{k}' \leftarrow \mathbf{k}) \equiv -4\pi^2 \left( \frac{m}{\hbar^2} \right) \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle. \quad (35)$$

Calculations are often based on an integral equation<sup>16</sup> for the scattering amplitude in terms of the potential operator  $\hat{V}$ . To obtain this equation, we first use the definition Eq. (26) of the  $T$  operator to show that on the energy shell,<sup>26</sup>

$$\hat{T}(E_k \pm i0) | \mathbf{k} \rangle = \hat{V} | \mathbf{k} \pm \rangle, \quad (36a)$$

where we note in passing that

$$\hat{V} | \mathbf{k} \pm \rangle = \hat{V} \hat{\Omega}_{\pm} | \mathbf{k} \rangle \hat{T}(E_k \pm i0) = \hat{V} \hat{\Omega}_{\pm}. \quad (36b)$$

Then we insert Eq. (36a) into the definition of the scattering amplitude Eq. (35) to obtain

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -4\pi^2 \left( \frac{m}{\hbar^2} \right) \langle \mathbf{k}' | \hat{V} | \mathbf{k} + \rangle. \quad (37)$$

In configuration space this relation becomes the aforementioned integral equation,

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -(2\pi)^{1/2} \left( \frac{m}{\hbar^2} \right) \int e^{-i\mathbf{k}' \cdot \mathbf{r}} V(\mathbf{r}) \psi_{\mathbf{k}}^+(\mathbf{r}) d^3r, \quad (38)$$

where we have assumed that the potential operator is local,

$$\langle \mathbf{r}' | \hat{V} | \mathbf{r} \rangle = V(\mathbf{r}) \delta^3(\mathbf{r}' - \mathbf{r}). \quad (39)$$

### B. Dimensions of the scattering amplitude and of $T$ matrix elements

We have found dimensional analysis (see Appendix A) to be very useful not only in checking derived equations of collision theory, but also in determining unstated conventions in published equations. For example, the boundary condition (16) on the scattering function reveals the dimension of the scattering amplitude. If the scattering states are subject to wave-vector normalization, the dimension of the scattering amplitude is length  $L$ . If we denote the ‘‘dimension’’ by square brackets, we have

$$[f(\mathbf{k}' \leftarrow \mathbf{k})] = L \times \text{dimension of scattering function } \psi_{\mathbf{k}}^+(\mathbf{r}). \quad (40)$$

Equation (35) shows that the dimensions of the momentum-space  $T$ -matrix elements, if the scattering states are subject to wave-vector normalization, are

$$[\langle \mathbf{k}' | \hat{T} | \mathbf{k} \rangle] = EL^2 \times \text{dimension of scattering amplitude}, \quad (41a)$$

where  $EL^2$  is the dimension of  $\hbar^2/m$ . From Eq. (40), we conclude that

$$[\langle \mathbf{k}' | \hat{T} | \mathbf{k} \rangle] = EL^3 \times \text{dimension of scattering function } \psi_{\mathbf{k}}^+(\mathbf{r}). \quad (41b)$$

For dimensionless scattering functions  $[\langle \mathbf{k}' | \hat{T} | \mathbf{k} \rangle] = EL^3$ .

### C. Effect on the scattering amplitude of renormalizing the plane wave states and redefining $\hat{T}$

If we renormalize the plane wave states via  $|\mathbf{k}\rangle \rightarrow \alpha |\mathbf{k}\rangle$ , we must include a factor of  $1/|\alpha|^2$  in the definition of the scattering amplitude to cancel the factors of  $\alpha$  that are absorbed into the on-shell  $T$  matrix element. If we also redefine the  $T$  operator via  $\hat{T} \rightarrow \beta \hat{T}$ , we must include a factor of  $\beta$  in the scattering amplitude. The general form of this important relation is

$$f(\mathbf{k}' \leftarrow \mathbf{k}) \equiv -4\pi^2 \frac{\beta}{|\alpha|^2} \left( \frac{m}{\hbar^2} \right) \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle. \quad (42)$$

Equation (42) codifies and illustrates the rules for the renormalization of scattering states and/or redefinition of the  $T$  operator:

- (1) Divide plane wave states (and the corresponding bras in dual space) by  $\alpha$ .
- (2) Multiply the  $T$  operator (and all matrix elements of this operator) by  $\beta$ .

The factor  $\beta/|\alpha|^2$  in Eq. (42) ensures that the values of the scattering amplitude are unaffected by our choice of the normalization of plane wave states and/or by our definition of the  $T$  matrix. This invariance is required because the differential cross section, a measurable quantity, is the squared modulus of the scattering amplitude,

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} |f(\mathbf{k}' \leftarrow \mathbf{k})|^2, \quad (43a)$$

where, allowing for inelastic scattering,  $k_f = \sqrt{2mE_f/\hbar^2}$  is the exit-channel wave vector (of the outgoing particle) and  $k_i = \sqrt{2mE_i/\hbar^2}$  is the entrance-channel wave vector (of the incident particle). For elastic scattering  $E_f = E_i$  and  $k_f = k_i$ . The integral cross section is the integral of the differential cross section over the scattering angles,

$$\sigma = \int_{4\pi} \frac{d\sigma}{d\Omega} \sin \theta d\theta d\phi. \quad (43b)$$

The elastic momentum transfer cross section is

$$\sigma = \int_{4\pi} \frac{d\sigma}{d\Omega} (1 - \cos \theta) \sin \theta d\theta d\phi. \quad (43c)$$

We have already noted the importance of the integral equation (38) for the scattering amplitude. The factor  $\beta/|\alpha|^2$  in Eq. (42) does not affect this relation because upon the redefinition of the  $T$  operator, Eq. (36b) becomes  $\beta \hat{T}(E_k \pm i0) = \hat{V} \hat{\Omega}_{\pm}$ , and we have

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -4\pi^2 \frac{1}{|\alpha|^2} \left( \frac{m}{\hbar^2} \right) \langle \mathbf{k}' | \hat{V} | \mathbf{k} + \rangle. \quad (44)$$

The most general form of this integral equation is therefore

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\frac{1}{4\pi} \frac{(2\pi)^{3/2}}{\alpha} \left(\frac{2m}{\hbar^2}\right) \int e^{-i\mathbf{k}' \cdot \mathbf{r}} V(\mathbf{r}) \psi_{\mathbf{k}}^*(\mathbf{r}) d^3r. \quad (45)$$

## V. THE REACTANCE ( $K$ ) MATRIX

For practical reasons many quantum scattering calculations are designed to determine the  $K$  matrix (sometimes called the reactance matrix) rather than the  $S$  or  $T$  matrices.<sup>27</sup> In formulations that impose real boundary conditions the asymptotic form of the scattering function involves the  $K$  matrix, which is also real. (For scattering processes that are invariant under time-reversal, the unitarity of the  $S$  matrix guarantees that the  $T$  matrix is symmetric.) In such an approach a key step is relating the calculated  $K$  matrix to the  $T$  (or  $S$ ) matrix from which cross sections can be calculated. At this point a third ambiguity enters.

### A. The $K$ matrix and the $S$ matrix

The  $K$  matrix consists of momentum-space matrix elements of the operator  $\hat{K}$  that we shall define<sup>19</sup> as the Cayley transform of the  $S$  operator (see p. 232 of Ref. 28)

$$\hat{K} \equiv i(\hat{1} - \hat{S})(\hat{1} + \hat{S})^{-1}. \quad (46)$$

The inverse of this definition gives the  $S$  operator in terms of the  $K$  operator:<sup>29</sup>

$$\hat{S} \equiv (\hat{1} + i\hat{K})(\hat{1} - i\hat{K})^{-1} \quad (47a)$$

$$= [(\hat{1} - \hat{K}^2)(\hat{1} + \hat{K}^2)^{-1}] + i[(2\hat{K})(\hat{1} + \hat{K}^2)], \quad (47b)$$

where the second form isolates the real and imaginary parts of  $\hat{S}$ . This definition ensures that the unitarity of  $\hat{S}$  implies the hermiticity of  $\hat{K}$ . The matrix form of Eq. (47),

$$\mathbf{S} = (1 + i\mathbf{K})(1 - i\mathbf{K})^{-1}, \quad (48)$$

is widely used in scattering calculations. The elements of the  $S$  and  $K$  matrices are explicitly related by

$$\langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle = \frac{\delta(\mathbf{k}' - \mathbf{k}) + i\delta(E_{k'} - E_k) \langle \mathbf{k}' | K | \mathbf{k} \rangle}{\delta(\mathbf{k}' - \mathbf{k}) - i\delta(E_{k'} - E_k) \langle \mathbf{k}' | K | \mathbf{k} \rangle}. \quad (49)$$

Unlike the  $S$  and  $T$  matrices, the  $K$  matrix is defined only on the energy shell.

### B. The $K$ matrix and the $T$ matrix

Because elements of the  $T$  matrix appear directly in equations for the differential and integral cross sections, the relation between the  $T$  and  $K$  matrices is of vital importance. To relate these matrices, we insert Eq. (47) into  $\mathbf{S} = 1 - 2\pi i\mathbf{T}$  to obtain

$$\mathbf{T} = -\frac{1}{\pi} \mathbf{K}(1 - i\mathbf{K})^{-1}. \quad (50)$$

To illustrate the practical consequence of introducing the  $K$  matrix, we look ahead to scattering from a local central potential  $V(r)$  (see Sec. VII). For this problem, a partial-wave phase shift  $\delta_\ell(E)$  is defined by<sup>7,10</sup>

$$S_\ell(E) \equiv e^{2i\delta_\ell(E)}, \quad (51a)$$

where  $S_\ell(E)$  is an element of the diagonal  $S$  matrix that results from the transformation from plane wave to orbital angular momentum states (see Sec. VII B). We substitute this definition into the angular momentum matrix elements of the  $K$  operator Eq. (46) and obtain the partial-wave  $K$  matrix elements

$$K_\ell(E) = \tan \delta_\ell(E). \quad (51b)$$

Correspondingly, the partial-wave  $T$ -matrix elements are

$$T_\ell(E) = -\frac{e^{i\delta_\ell(E)} \sin \delta_\ell(E)}{\pi}, \quad (51c)$$

where we have used  $1 - e^{2i\delta_\ell(E)} = -2ie^{i\delta_\ell(E)} \sin \delta_\ell(E)$ .

### C. Alternate definitions of the $K$ operator

Almost as various as the relations between the  $S$  and  $T$  operators are the relations between the  $S$  and  $K$  operators.<sup>30</sup> To accommodate these variations we introduce yet another constant  $\gamma$  and write the definition Eq. (46) as

$$\hat{S} \equiv (\hat{1} + i\gamma\hat{K})(\hat{1} - i\gamma\hat{K})^{-1}. \quad (52a)$$

This relation conforms to the requirement that redefinition of the  $K$  matrix must leave the  $S$  matrix unchanged. The corresponding replacement is

$$\hat{K} \rightarrow \frac{1}{\gamma} \hat{K}. \quad (52b)$$

Various authors use various combinations of choices of  $\beta$  (in  $\hat{S} = \hat{1} - 2\pi i\beta\hat{T}$ ) and  $\gamma$ . Consequently there is a range of relations between the  $S$ ,  $T$ , and  $K$  matrices. Equations (48) and (50) correspond to  $\beta=1$  and  $\gamma=1$ .<sup>19</sup> [In partial-wave theory<sup>12</sup> these choices yield Eq. (51).] A common alternative is  $\gamma=1$  and  $\beta=-1/\pi$ .

The general matrix transformation equations when  $\beta$  and/or  $\gamma$  differ from 1 are

$$\mathbf{T} = -\frac{1}{\pi\beta} \mathbf{K}(1 - i\gamma\mathbf{K})^{-1}, \quad (53a)$$

$$\mathbf{T} = -\frac{i}{2\pi\beta} (1 - \mathbf{S}), \quad (53b)$$

$$\mathbf{K} = i\frac{1}{\gamma} (1 - \mathbf{S})(1 + \mathbf{S})^{-1}, \quad (53c)$$

$$\mathbf{K} = -i\frac{\pi\beta}{\gamma} \mathbf{T}(i + \pi\beta\mathbf{T})^{-1}. \quad (53d)$$

The corresponding equations of partial-wave theory are<sup>31</sup>

$$K_\ell(E) = \frac{1}{\gamma} \tan \delta_\ell(E), \quad (54a)$$

$$T_\ell(E) = -\frac{1}{\beta} \frac{e^{i\delta_\ell(E)} \sin \delta_\ell(E)}{\pi}. \quad (54b)$$

Equations (53) and (54) are independent of the normalization of the plane wave states  $|\mathbf{k}\rangle$ , that is, they are independent of the renormalization constant  $\alpha$  [see Eq. (18)].

## VI. THE GREEN'S FUNCTION AND LIPPMANN-SCHWINGER EQUATIONS

### A. The integral equation for the scattering amplitude

We now return to the crucial relation between the boundary conditions on the scattering function, Eq. (16), and the integral equation for the scattering amplitude in terms of the potential, Eq. (37). This relation is founded on the Lippmann-Schwinger equation for the scattering function,

$$\psi_{\mathbf{k}}^+(\mathbf{r}) = \psi_{\mathbf{k}}^0(\mathbf{r}) + \int G_{E_k}^0(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi_{\mathbf{k}}^+(\mathbf{r}') d^3 r', \quad (55)$$

where  $\psi_{\mathbf{k}}^0(\mathbf{r}) \equiv \langle \mathbf{r} | \mathbf{k} \rangle = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}$  is the (wave vector normalized) plane wave function [see Eq. (12)]. The free-particle Green's function in Eq. (55) is defined in terms of the free-particle Green's operator  $\hat{G}^0(z) \equiv (z - \hat{\mathcal{H}}^0)^{-1}$  [see Eq. (27)] as

$$G_{E_k}^0(\mathbf{r}, \mathbf{r}') \equiv \langle \mathbf{r}' | \hat{G}^0(E_k + i0) | \mathbf{r} \rangle = \lim_{\epsilon \rightarrow 0^+} \langle \mathbf{r}' | \hat{G}^0(E_k + i\epsilon) | \mathbf{r} \rangle. \quad (56)$$

To demonstrate consistency between the usual boundary conditions on  $\psi_{\mathbf{k}}^+(\mathbf{r})$  and our definitions of the scattering amplitude, Eq. (35), and the  $T$  operator, Eq. (26), we must evaluate the free-particle Green's function (56), substitute the result into the Lippmann-Schwinger equation (55), and consider the result in the asymptotic limit  $r \rightarrow \infty$ . We first substitute the resolution of the identity [Eq. (10)] into  $\langle \mathbf{r}' | \hat{G}^0(z) | \mathbf{r} \rangle$  twice. We then evaluate the result using free-particle plane wave functions and the action of the free-particle Green's operator on a plane wave state,

$$\hat{G}^0(z) | \mathbf{k} \rangle = \frac{1}{z - E_k} | \mathbf{k} \rangle. \quad (57)$$

These calculations yield

$$\langle \mathbf{r}' | \hat{G}^0(z) | \mathbf{r} \rangle = -\frac{1}{4\pi} \left( \frac{2m}{\hbar^2} \right) \frac{\exp(i\sqrt{2mz/\hbar^2} |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}. \quad (58a)$$

The particular free-particle Green's function that appears in the Lippmann-Schwinger equation (55) requires evaluating Eq. (58a) at  $z = E_k + i\epsilon$  and then taking the limit  $\epsilon \rightarrow 0^+$ . These manipulations lead to

$$G_{E_k}^0(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \left( \frac{2m}{\hbar^2} \right) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \quad (58b)$$

To take the required asymptotic limit, we consider  $r' \gg r$  and expand  $|\mathbf{r} - \mathbf{r}'|$  in powers of  $r'/r$ . Dropping terms of order higher than the first leaves (for details see Sec. 10c of Ref. 19)

$$G_{E_k}^0(\mathbf{r}, \mathbf{r}') \xrightarrow{r \rightarrow \infty} -\frac{1}{4\pi} \left( \frac{2m}{\hbar^2} \right) \frac{e^{ikr}}{r} e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}. \quad (58c)$$

The final step is to substitute this asymptotic form of the free-particle Green's function into the  $r \rightarrow \infty$  limit of the Lippmann-Schwinger equation (55). By matching the result to the boundary conditions (16) on  $\psi_{\mathbf{k}}^+(\mathbf{r})$ , we make the identification

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -4\pi^2 \left( \frac{m}{\hbar^2} \right) \langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle. \quad (59)$$

We thus regain Eq. (37). If we now invoke the definition of the  $T$  operator,  $\hat{T} \equiv \hat{V} + \hat{V} \hat{G}(z) \hat{T}$ , Eq. (26), we can use the resulting on-shell relation  $\hat{T}(E_k \pm i0) | \mathbf{k} \rangle = \hat{V} | \mathbf{k} \pm \rangle$  [Eq. (36a)] to obtain the definition  $f(\mathbf{k}' \leftarrow \mathbf{k}) \equiv -4\pi^2 (m/\hbar) \langle \mathbf{k}' | \hat{T}(E_k + i0) | \mathbf{k} \rangle$  [Eq. (35)] of the scattering amplitude.

This algebra does not constitute a derivation of the boundary conditions in any useful sense, but it justifies our definition (35) of the scattering amplitude in terms of the momentum-space on-shell  $T$ -matrix element.

### B. The partial-wave Green's function

In applications of Lippmann-Schwinger theory based on the expansion of the scattering function in spherical harmonics (such as scattering from a central potential, Sec. VII) the partial-wave Green's function plays a key role. The free-particle partial-wave Green's function  $g_\ell(r', r)$  is defined from

$$G_{E_k}^0(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi} \left( \frac{2m}{\hbar^2} \right) \sum_{\ell=0}^{\infty} (2\ell + 1) g_\ell(r', r) P_\ell(\cos \theta). \quad (60)$$

The function  $g_\ell(r', r)$  consists of a combination of Riccati-Bessel, -Neumann, and -Hankel functions (see Appendix B), depending on the boundary conditions imposed on the radial scattering function. For instance, for complex  $S$ -matrix boundary conditions Eq. (94a) is

$$g_\ell(r', r) = -\frac{1}{k} \hat{j}_\ell(kr_<) \hat{h}_\ell^+(kr_>), \quad (61)$$

where  $r_<$  and  $r_>$  are the minimum and maximum of  $(r', r)$ , respectively.<sup>32</sup>

### C. Consequences for the Green's function of renormalization of plane wave states

Because a derivation of Eq. (58) requires the use of the coordinate-space form  $\langle \mathbf{r} | \mathbf{k} \rangle$  of the plane wave states  $| \mathbf{k} \rangle$ , these equations depend on how we normalize the plane wave states. If we allow for alternatives to wave vector normalization by including the constant  $\alpha$  of Eq. (18), we must multiply the right-hand side of Eq. (58) by  $|\alpha|^2$ . For example, Eq. (58b) becomes

$$G_{E_k}^0(\mathbf{r}, \mathbf{r}') = -\frac{|\alpha|^2}{4\pi} \left( \frac{2m}{\hbar^2} \right) \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \quad (62)$$

Some authors define the free-particle Green's function as the solution of [see, for example, Eq. (6.4.1) of Ref. 33]

$$(\nabla^2 + k^2) G_{E_k}^0(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}'). \quad (63)$$

In effect, this definition absorbs a factor of  $-2m/\hbar^2$  [from the coordinate-space free-particle Hamiltonian  $\hat{\mathcal{H}}^0 = -(\hbar^2/2m)\nabla^2$ ] into the Green's function  $G_{E_k}^0(\mathbf{r}, \mathbf{r}')$ , altering the Lippmann-Schwinger equation, Eq. (55), and the explicit equations for the Green's function, Eq. (58), accordingly.

Other authors absorb the factor  $2m/\hbar^2$  into the definition of the potential energy, for example, by defining  $U(\mathbf{r}) \equiv (2m/\hbar^2)V(\mathbf{r})$  and using  $U(\mathbf{r})$  instead of  $V(\mathbf{r})$  in the

Lippmann-Schwinger and related equations (see, for example, Chap. VIII of Ref. 34). Unfortunately, in many papers this redefinition is used along with the symbol  $V(\mathbf{r})$  but without the information that  $V(\mathbf{r})$  denotes not the potential energy but rather the potential energy times  $(2m/\hbar^2)$ . Readers can usually spot this redefinition by finding an integral equation for the scattering amplitude, such as Eq. (37). The presence of  $\pi^2$  instead of  $4\pi^2$  in this equation (even in atomic units) indicates that the author is probably using a scaled potential energy.<sup>35</sup>

## VII. PARTIAL-WAVE SCATTERING STATES

To define the partial-wave scattering states, we first transform the free-particle plane wave states  $|\mathbf{k}\rangle$ , which are eigenfunctions of the linear-momentum operator  $\hat{\mathbf{p}}$ , to eigenfunctions of the free-particle Hamiltonian  $\hat{\mathcal{H}}^0$  and the orbital-angular momentum operators  $\hat{L}^2$  and  $\hat{L}_z$ . The elements of the requisite transformation matrix  $\langle E\ell m|\mathbf{k}\rangle$  are defined by the fundamental expansions<sup>36</sup>

$$|\mathbf{k}\rangle = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \int_0^{\infty} |E\ell m\rangle \langle E\ell m|\mathbf{k}\rangle dE. \quad (64)$$

The coordinate-space projection of Eq. (64) is the familiar expansion of a plane wave function in spherical harmonics,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{kr} \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) \hat{j}_{\ell}(kr) P_{\ell}(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}), \quad (65a)$$

where  $\hat{j}_{\ell}(kr) \equiv kr j_{\ell}(kr)$  is the Riccati-Bessel function<sup>9</sup> (see Appendix B). In scattering theory, the most useful form of this expansion, which follows from the addition theorem of spherical harmonics, is

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi}{kr} \sum_{\ell} \sum_m i^{\ell} \hat{j}_{\ell}(kr) Y_{\ell m}^*(\hat{\mathbf{k}}) Y_{\ell m}(\hat{\mathbf{r}}). \quad (65b)$$

Whatever the normalization for  $|\mathbf{k}\rangle$  and  $|E\ell m\rangle$ , all equations relating to these states must preserve Eq. (65). That is, this expansion is another invariant equation.

Like the plane wave states in Eq. (14), the partial-wave scattering states are related to the corresponding free-particle angular momentum states via Møller operators as

$$|E\ell m \pm\rangle = \hat{\Omega}_{\pm} |E\ell m\rangle. \quad (66)$$

Hence the expansion of the plane wave scattering state in angular momentum scattering states involves the same transformation matrix that appears in the expansion of the corresponding free-particle states:

$$|\mathbf{k} \pm\rangle = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \int_0^{\infty} |E\ell m \pm\rangle \langle E\ell m|\mathbf{k}\rangle dE. \quad (67)$$

The fundamental expansions (64) and (67) follow from the resolution of the identity in angular momentum states

$$\hat{1} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \int_0^{\infty} |E\ell m\rangle \langle E\ell m| dE. \quad (68)$$

Like the resolution of  $\hat{1}$  in plane wave states, Eq. (10), Eq. (68) is valid only for energy-normalized angular momentum states.

## A. Energy normalization

The most convenient normalization for the partial-wave scattering states is energy normalization:<sup>37</sup>

$$\langle E' \ell' m' | E \ell m \rangle = \delta(E_{k'} - E_k) \delta_{\ell', \ell} \delta_{m', m}. \quad (69a)$$

Because the Møller operators preserve normalization, the partial-wave scattering states obey the same condition,

$$\langle E' \ell' m' \pm | E \ell m \pm \rangle = \delta(E_{k'} - E_k) \delta_{\ell', \ell} \delta_{m', m}. \quad (69b)$$

## B. The transformation matrix

If we use plane wave states that obey wave vector normalization and angular momentum states that obey energy normalization, we find for the elements of the transformation matrix

$$\begin{aligned} \langle E\ell m|\mathbf{k}\rangle &= i^{\ell} \left(\frac{\hbar^2}{m}\right)^{1/2} k^{-1/2} Y_{\ell m}^*(\hat{\mathbf{k}}) \delta\left(E - \frac{\hbar^2 k^2}{2m}\right), \\ \langle \mathbf{k}|E\ell m\rangle &= i^{-\ell} \left(\frac{\hbar^2}{m}\right)^{1/2} k^{-1/2} Y_{\ell m}(\hat{\mathbf{k}}) \delta\left(E - \frac{\hbar^2 k^2}{2m}\right). \end{aligned} \quad (70)$$

We can use the transformation matrix in Eq. (70) to transform any equation of scattering theory from the plane wave to the angular momentum representation by inserting resolutions of the identity operator in angular momentum states, Eq. (68), next to each plane wave ket or bra. To illustrate we transform Eq. (35) for the scattering amplitude in terms of the momentum-space  $T$ -matrix elements. If we substitute two resolutions of  $\hat{1}$  and evaluate the integrals over energy, we obtain

$$\begin{aligned} f(\mathbf{k}' \leftarrow \mathbf{k}) &= -4\pi^2 \left(\frac{m}{\hbar^2}\right) \sum_{\ell'=0}^{\infty} \sum_{m'=-\ell'}^{\ell'} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \langle \mathbf{k}' | E \ell' m' \rangle \\ &\quad \times \langle E \ell' m' | \hat{T}(E + i0) | E \ell m \rangle \langle E \ell m | \mathbf{k} \rangle. \end{aligned} \quad (71a)$$

Equation (71a) immediately yields the desired equation for  $f(\mathbf{k}' \leftarrow \mathbf{k})$  in terms of the partial-wave  $T$  matrix,

$$\begin{aligned} f(\mathbf{k}' \leftarrow \mathbf{k}) &= -\frac{(2\pi)^2}{k} \sum_{\ell'=0}^{\infty} \sum_{m'=-\ell'}^{\ell'} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell-\ell'} Y_{\ell' m'}(\hat{\mathbf{k}}') \\ &\quad \times \langle E \ell' m' | \hat{T}(E + i0) | E \ell m \rangle Y_{\ell m}^*(\hat{\mathbf{k}}), \end{aligned} \quad (71b)$$

via the handy result

$$\langle \mathbf{k}' | E \ell' m' \rangle \langle E \ell m | \mathbf{k} \rangle = \frac{i^{\ell-\ell'}}{k} \left(\frac{\hbar^2}{m}\right) Y_{\ell' m'}(\hat{\mathbf{k}}') Y_{\ell m}^*(\hat{\mathbf{k}}). \quad (72)$$

Equation (71) simplifies further if the system is rotationally invariant, in which case the phase shift reappears [see Eq. (51c)]:

$$\begin{aligned} \langle E \ell' m' | \hat{T}(E + i0) | E \ell m \rangle &= T_{\ell}(E) \delta_{\ell', \ell} \delta_{m', m} \\ &= -\frac{1}{\pi} e^{i\delta_{\ell}(k)} \sin \delta_{\ell}(k) \delta_{\ell', \ell} \delta_{m', m}. \end{aligned} \quad (73)$$

For such a system we can evaluate the sums over  $\ell'$ ,  $m'$ , and  $m$  to obtain

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\frac{4\pi^2}{k} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} Y_{\ell m}^*(\hat{\mathbf{k}}') T_{\ell}(E) Y_{\ell m}(\hat{\mathbf{k}}) \quad (74a)$$

$$= -\frac{\pi}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) T_{\ell}(E) P_{\ell}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}), \quad (74b)$$

which implies that

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) e^{i\delta_{\ell}(k)} \sin \delta_{\ell}(k) P_{\ell}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}). \quad (74c)$$

### C. Partial-wave scattering amplitudes and cross sections

Equation (74c) motivates the introduction of the partial-wave scattering amplitude  $f_{\ell}(k)$  via<sup>38</sup>

$$f_{\ell}(k) \equiv -\frac{\pi}{k} T_{\ell}(E) = \frac{1}{k} e^{i\delta_{\ell}(k)} \sin \delta_{\ell}(k) = \frac{i}{2k} [1 - e^{2i\delta_{\ell}(k)}], \quad (75)$$

which implies that

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = \sum_{\ell=0}^{\infty} (2\ell + 1) f_{\ell}(k) P_{\ell}(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}). \quad (76)$$

In the literature, definitions of the partial-wave scattering amplitude vary by additional factors in Eq. (76). But Eq. (74c) for  $f(\mathbf{k}' \leftarrow \mathbf{k})$  in terms of phase shifts is an invariant equation: it is independent of the choices of all four arbitrary constants.

In terms of the partial-wave scattering amplitude, the integral cross section for scattering from a local central potential is

$$\sigma(E) = \sum_{\ell=0}^{\infty} \sigma_{\ell}(E) = \sum_{\ell=0}^{\infty} 4\pi(2\ell + 1) |f_{\ell}(k)|^2 \quad (77a)$$

$$= \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell}(E) \quad (77b)$$

$$= \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) |1 - S_{\ell}(E)|^2, \quad (77c)$$

where in Eq. (77c) we have used the definition of the phase shift Eq. (51a).

### D. Alternate normalization of the angular momentum states

The normalization of angular momentum states is arbitrary. This arbitrariness introduces our fourth (and last) arbitrary constant:

$$|E\ell m\rangle \rightarrow \zeta |E\ell m\rangle. \quad (78a)$$

The renormalization constant  $\zeta$  may be complex and may depend on  $\ell$  and  $k$ ; many authors choose  $\zeta$  to depend on the partial-wave phase shift.<sup>39</sup> The effect of renormalization of the angular momentum states parallels that of the renormal-

ization of the plane wave states in Eq. (18): it changes the normalization condition Eq. (69a) to

$$\langle E' \ell' m' | E \ell m \rangle = |\zeta|^2 \delta(E_{k'} - E_k) \delta_{\ell', \ell} \delta_{m', m}. \quad (78b)$$

We strongly recommend that one not deviate from energy normalization lightly. Transforming from a plane wave representation to an angular momentum representation is the first step in the practical solution of many scattering problems—not just for central potentials.<sup>40</sup> The consequences of the normalization of  $|E\ell m\rangle$  are more far reaching than those of normalization of  $|\mathbf{k}\pm\rangle$ ; correspondingly, the chances for error and (especially) inconsistency are far greater.

To illustrate these consequences, we look ahead to the boundary conditions on the normalized radial function  $u_{k\ell}(r)$  of partial-wave theory (see Sec. VII G). With our conventions these boundary conditions can be written in terms of the phase shift as

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} e^{i\delta_{\ell}(E)} \sin \left[ kr - \ell \frac{\pi}{2} + \delta_{\ell}(E) \right]. \quad (79)$$

In the literature there is a variety of alternative forms of these boundary conditions (see Table II). These forms arise from different normalizations of the orbital angular momentum states. The consequences propagate through several equations (every equation in Table II that contains  $\zeta$  is affected), ranging from the resolution of the identity in these states to the transformation matrix between the plane wave and angular momentum representations.

For example, the normalization condition on the normalized radial functions becomes

$$\int_0^{\infty} u_{k'\ell}(r) u_{k\ell}(r) dr = |\zeta|^2 \frac{\pi}{2} \delta(k' - k), \quad (80)$$

which no longer corresponds simply to the normalization condition on the Riccati-Bessel functions, Eq. (91). Scaling  $u_{k\ell}(r)$  by  $\zeta$  implies that the corresponding zero-potential (free particle) scattering function is

$$u_{k\ell}(r) \xrightarrow{V \rightarrow 0} \zeta_{\ell} \hat{\zeta}_{\ell}(kr). \quad (81)$$

### E. Transformations using alternate normalization of plane wave and angular momentum states

It is desirable although not required to preserve the mathematical structure of the fundamental transformation Eq. (64) regardless of how  $|\mathbf{k}\pm\rangle$  and  $|E\ell m\rangle$  are normalized. We can do so by multiplying the transformation matrices in Eq. (70) by  $\alpha/\zeta$ :

$$\langle E\ell m | \mathbf{k} \rangle = i^{\ell} \left( \frac{\alpha}{\zeta} \right) \left( \frac{\hbar^2}{m} \right)^{1/2} k^{-1/2} Y_{\ell m}^*(\hat{\mathbf{k}}) \delta \left( E - \frac{\hbar^2 k^2}{2m} \right). \quad (82)$$

With arbitrary normalization constants  $\alpha$  and  $\zeta$  and the constant  $\beta$  in the equation relating the  $T$  matrix to the  $S$  matrix, Eq. (53b), the partial-wave scattering amplitude defined in Eq. (76) becomes

$$f_{\ell}(k) = -\beta \frac{\pi}{k} T_{\ell}(E) = \frac{1}{k} e^{i\delta_{\ell}(k)} \sin \delta_{\ell}(k). \quad (83)$$

All the dependence on  $\alpha$  and  $\zeta$  has canceled. Moreover, the factor of  $1/\beta$  in the generalized equation relating the partial-

Table II. Useful equations for determining conventions. The quantities  $\alpha$ ,  $\zeta$ ,  $\gamma$ , and  $\beta$  are defined in Table III, which contains additional relevant equations.

Relation	Equation
$T$ matrix and $K$ matrix	$T = -\frac{1}{\pi\beta} \mathcal{K}(1 - i\gamma\mathcal{K})^{-1}$
$T$ matrix and $S$ matrix	$T = -\frac{i}{2\pi\beta} (1 - S)$
Scattering amplitude and $T$ matrix	$f(\mathbf{k}' \leftarrow \mathbf{k}) = -4\pi^2 \frac{\beta}{ \alpha ^2} \left(\frac{m}{\hbar^2}\right) \langle \mathbf{k}'   \hat{T}(E_k + i0)   \mathbf{k} \rangle$
$S$ matrix and $K$ matrix	$S = (1 - \gamma^2\mathcal{K}^2)(1 + \gamma^2\mathcal{K}^2)^{-1} + i(2\gamma\mathcal{K})(1 + \gamma^2\mathcal{K}^2)$
$K$ matrix and $S$ matrix	$K = i\frac{1}{\gamma}(1 - S)(1 + S)^{-1}$
$K$ matrix and $T$ matrix	$K = -i\frac{\pi\beta}{\gamma} T(i + \pi\beta T)^{-1}$
Boundary condition on the normalized radial function	$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \zeta e^{i\delta_\ell(E)} \sin\left[kr - \ell\frac{\pi}{2} + \delta_\ell(E)\right]$
Partial-wave expansion of scattering amplitude	$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\beta \frac{\pi}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) T_\ell(E) P_\ell(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}})$
Boundary condition on the radial function	$v_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \zeta \frac{1}{\sqrt{\pi}} \left(\frac{2m}{\hbar^2}\right)^{1/2} k^{-1/2} e^{i\delta_\ell(E)} \sin\left[kr - \ell\frac{\pi}{2} + \delta_\ell(E)\right]$
Partial-wave $T$ matrix	$T_\ell(E) = -\frac{1}{\beta} \frac{e^{i\delta_\ell(E)} \sin \delta_\ell(E)}{\pi}$
Plane wave to angular momentum free-state transformation	$\langle E\ell m   \mathbf{k} \rangle = i^\ell \left(\frac{\alpha}{\zeta}\right) \left(\frac{\hbar^2}{m}\right)^{1/2} k^{-1/2} Y_{\ell m}^*(\hat{\mathbf{k}}) \delta\left(E - \frac{\hbar^2 k^2}{2m}\right)$
Partial-wave $K$ matrix	$K_\ell(E) = \frac{1}{\gamma} \tan \delta_\ell(E)$

wave  $T$  matrix to the phase shift, Eq. (54), results in an equation for  $f_\ell(k)$  in terms of  $\delta_\ell(E)$  that doesn't depend on  $\beta$ . Consequently, the subsequent equations for the differential and integral cross section in terms of phase shifts are also independent of all arbitrary constants. For example, the partial-wave expansion of the scattering amplitude depends on  $\beta$  as

$$f(\mathbf{k}' \leftarrow \mathbf{k}) = -\beta \frac{\pi}{k} \sum_{\ell=0}^{\infty} (2\ell + 1) T_\ell(E) P_\ell(\hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}), \quad (84)$$

so that inserting Eq. (54) gives a scattering amplitude that is independent of  $\beta$ .

## F. The radial scattering function

The radial scattering function  $v_{k\ell}(r)$  is defined via the partial-wave scattering function  $\psi_{E\ell m}^+(\mathbf{r}) \equiv \langle \mathbf{r} | E\ell m \rangle$  as

$$\psi_{E\ell m}^+(\mathbf{r}) \equiv \frac{1}{r} v_{k\ell}(r) Y_{\ell m}(\hat{\mathbf{r}}), \quad (85)$$

where  $\hat{\mathbf{r}} = (\theta, \varphi)$  represents the polar ( $\theta$ ) and azimuthal ( $\varphi$ ) angles of spherical coordinates. We further define the normalized radial function  $u_{k\ell}(r)$  via

$$v_{k\ell}(r) \equiv \frac{1}{\sqrt{\pi}} \left(\frac{2m}{\hbar^2}\right)^{1/2} k^{-1/2} u_{k\ell}(r). \quad (86)$$

The normalized radial function reduces to the Riccati-Bessel function for zero potential energy,  $u_{k\ell}(r) \rightarrow \hat{j}_\ell(kr) = u_{k\ell}^0(r)$  as  $V(r) \rightarrow 0$ .

In coordinate space the partial-wave expansion Eq. (67) becomes

$$\psi_{\mathbf{k}}^+(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \langle E\ell m | \mathbf{k} \rangle \psi_{E\ell m}^+(\mathbf{r}) \quad (87a)$$

$$= \left(\frac{\alpha}{\zeta}\right) \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[ i^\ell \left(\frac{\hbar^2}{mk}\right)^{1/2} Y_{\ell m}^*(\hat{\mathbf{k}}) \right] \psi_{E\ell m}^+(\mathbf{r}) \quad (87b)$$

$$= \left(\frac{\alpha}{\zeta}\right) \left(\frac{\hbar^2}{mk}\right)^{1/2} \frac{1}{r} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell v_{k\ell}(r) Y_{\ell m}^*(\hat{\mathbf{k}}) Y_{\ell m}(\hat{\mathbf{r}}) \quad (87c)$$

$$= \left(\frac{\alpha}{\zeta}\right) \left(\frac{\hbar^2}{mk}\right)^{1/2} \frac{1}{4\pi r} \sum_{\ell=0}^{\infty} i^\ell (2\ell + 1) v_{k\ell}(r) P_\ell(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}). \quad (87d)$$

We can write this expansion in terms of the normalized radial function as

$$\psi_{\mathbf{k}}^+(\mathbf{r}) = \left(\frac{\alpha}{\zeta}\right) \left(\frac{2}{\pi}\right)^{1/2} k^{-1} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^{\ell} Y_{\ell m}^*(\hat{\mathbf{k}}) \left[ \frac{1}{r} u_{k\ell}(r) Y_{\ell m}(\hat{\mathbf{r}}) \right] \quad (88a)$$

$$= \left(\frac{\alpha}{\zeta}\right) (2\pi)^{-3/2} k^{-1} \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) u_{k\ell}(r) P_{\ell}(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}). \quad (88b)$$

We have found the various forms in Eqs. (87) and (88) to be useful templates when trying to deduce choices of  $\alpha$  and  $\zeta$  in various publications.

Both the radial and normalized radial functions satisfy the radial Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r) - E \right] u_{k\ell}(r) = 0. \quad (89)$$

The linearity of Eq. (89) renders its form invariant to the choice of the normalization of the plane wave or partial-wave scattering states.

The scattering function  $\psi_{E\ell m}^+(\mathbf{r})$  must conform to the normalization of the scattering states  $|E\ell m\rangle$ . With energy normalization (69b), this requirement reads

$$\int \psi_{E'\ell'm'}^*(\mathbf{r}) \psi_{E\ell m}^+(\mathbf{r}) d^3r = \delta(E_{k'} - E_k) \delta_{\ell',\ell} \delta_{m',m}. \quad (90)$$

Because the Møller operator in  $|E\ell m\rangle = \hat{\Omega}_+ |E\ell m\rangle$  preserves the normalization, the function  $u_{k\ell}(r)$  obeys the same orthogonality condition as the Riccati-Bessel function,

$$\int_0^{\infty} \hat{j}_{\ell}(k'r) \hat{j}_{\ell}(kr) dr = \frac{\pi}{2} \delta(k' - k), \quad (91a)$$

which implies that

$$\int_0^{\infty} u_{k'\ell}(r) u_{k\ell}(r) dr = \frac{\pi}{2} \delta(k' - k). \quad (91b)$$

Like  $\hat{j}_{\ell}(kr)$ , the normalized radial function  $u_{k\ell}(r)$  is real and dimensionless. The normalized radial function obeys the simple (dimensionless) boundary conditions in Eq. (79).

The (diagonal) partial-wave  $S$ -matrix elements are related to the phase shifts in these boundary conditions by

$$\begin{aligned} \langle E'\ell'm' | \hat{S} | E\ell m \rangle &= S_{\ell}(E) \delta(E_{k'} - E_k) \delta_{\ell',\ell} \delta_{m',m} \\ &= e^{2i\delta_{\ell}(E)} \delta(E_{k'} - E_k) \delta_{\ell',\ell} \delta_{m',m}, \end{aligned} \quad (92)$$

where we have used the conventional definition of the phase shift, Eq. (51a). Equations (91) and (92) are invariant with respect to normalization: Eq. (91) hinges on a property of the Riccati-Bessel functions (Appendix B), and Eq. (92) is the definition of  $\delta_{\ell}(E)$  in terms of the partial-wave  $S$  matrix. As invariants, these equations serve as a check of algebraic and internal consistency. With energy normalization of plane wave and angular momentum states, the definition (86) of the normalized radial function ensures that  $u_{k\ell}(r)$  reduces to  $\hat{j}_{\ell}(kr)$  in the limit of zero scattering potential energy, that  $u_{k\ell}(r)$  is dimensionless (see Appendix A), and that  $u_{k\ell}(r)$  obeys the normalization condition obeyed by  $\hat{j}_{\ell}(kr)$ , Eq. (91).

The use of partial waves through the introduction of angular momentum states is best known for a spherically symmetric interaction potential. For any system the  $S$  operator commutes with the Hamiltonian,  $[\hat{S}, \hat{H}] = 0$ . If the system is rotationally invariant,  $\hat{H}$  commutes with the angular momentum operators  $\hat{L}^2$  and  $\hat{L}_z$ , and  $\hat{S}$  is diagonal in the basis of angular momentum free states  $\{|E\ell m\rangle\}$ . This feature justifies the introduction of the phase-shift via Eq. (92).

Partial waves may be useful even if the system lacks spherical symmetry.<sup>40</sup> If, for example, the system is axially symmetric, then  $\hat{H}$  commutes with  $\hat{L}_z$  but not with  $\hat{L}^2$ . In, for example, charged-particle scattering from a linear molecule, the  $S$  operator is diagonal with respect to  $m$  but not with respect to  $\ell$ ; instead of Eq. (92) we have

$$\langle E'\ell'm' | \hat{S} | E\ell m \rangle = S_{\ell',\ell}^m(E) \delta(E_{k'} - E_k) \delta_{m',m}. \quad (93)$$

## G. Boundary conditions on the normalized radial scattering function

The boundary conditions (79) can be written in various forms that are useful either for practical or interpretive reasons. For example, in terms of the partial-wave  $S$  matrix element of Eq. (92), these boundary conditions are

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \frac{i}{2} [\hat{h}_{\ell}^-(kr) - S_{\ell}(k) \hat{h}_{\ell}^+(kr)]. \quad (94a)$$

In terms of the partial-wave scattering amplitude of Eq. (76), they are

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \hat{j}_{\ell}(kr) + k f_{\ell}(k) \hat{h}_{\ell}^+(kr). \quad (94b)$$

In calculations it is often convenient to use the real boundary conditions

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \hat{j}_{\ell}(kr) + \tan \delta_{\ell}(E) \hat{n}_{\ell}(kr), \quad (94c)$$

which we can derive via a partial-wave expansion of the principal value scattering function rather than the function in Eq. (85) (see Sec. 11.1.2 of Ref. 18). If we normalize the angular momentum states differently from energy normalization via the factor  $\zeta$  in Eq. (78), we must multiply each of these boundary conditions by  $\zeta$ .

## H. Sleuthing out the normalization of angular momentum states

Many books and papers on scattering theory do not explicitly state their normalization convention for the angular momentum or partial-wave scattering states. Knowing the value of this normalization constant,  $\zeta$ , may be vital because it appears in boundary conditions and in equations for the scattering amplitudes. Fortunately, there is a sequence of linear proportionality relations that leads from the defining equation (78) for  $\zeta$  to the boundary condition (86) for the normalized radial scattering function  $u_{k\ell}(r)$ . Each item in this sequence is proportional to  $\zeta$ :

$$|E\ell m\rangle \rightarrow \psi_{E\ell m}^+(\mathbf{r}) \rightarrow v_{k\ell}(r) \rightarrow u_{k\ell}(r). \quad (95)$$

An equation for any quantity in this sequence is a clue to the normalization convention. If, for example, a source states a

Table III. Choices that must be made in setting up and using scattering theory.

Role in collision theory	Symbol	Defining equation	Value in this paper
Normalize asymptotic plane wave states	$\alpha$	$\langle \mathbf{k}'   \mathbf{k} \rangle =  \alpha ^2 \delta(\mathbf{k}' - \mathbf{k})$	1
Relate the $S$ and $T$ operators	$\beta$	$\hat{S} = \hat{1} - 2\pi i \beta \hat{T}$	1
Relate the $S$ and $K$ operators	$\gamma$	$\hat{S} = (\hat{1} + i\gamma \hat{K})(\hat{1} - i\gamma \hat{K})^{-1}$	1
Normalize asymptotic angular momentum states	$\zeta$	$\langle E' \ell' m'   E \ell m \rangle =  \zeta ^2 \delta(E_{k'} - E_k) \delta_{\ell', \ell} \delta_{m', m}$	1

boundary condition on the radial function, we can determine  $\zeta$  from the generic form

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} \zeta e^{i\delta_\ell(E)} \sin \left[ kr - \ell \frac{\pi}{2} + \delta_\ell(E) \right]. \quad (96)$$

Thus we often see (for example, in Ref. 41)

$$u_{k\ell}(r) \xrightarrow{r \rightarrow \infty} k^{-1/2} \sin \left[ kr - \ell \frac{\pi}{2} + \delta_\ell(E) \right], \quad (97)$$

from which we deduce that  $\zeta = k^{-1/2} e^{-i\delta_\ell(E)}$ . This example illustrates that  $\zeta$  may depend on the scattering energy and even on the phase shift.<sup>42</sup>

### VIII. CONCLUSION

We have shown that to define a nonrelativistic scattering theory of nonrearrangement collisions, four quantities must be chosen. These quantities, their defining equations, and the values adopted in this paper are summarized in Table III. Students must be (repeatedly) cautioned that before they take equations from any source, they must determine what choices the author(s) made for the relevant constants. Many authors are careful in this regard and state clearly their choices, although often this information must be tracked down throughout many pages.

Unfortunately, some well-known texts, monographs, reviews, and (especially) research papers do not state this information clearly (or at all) and are not consistent. We have found that the following guidelines usually maximize the chances of success while minimizing the required time and effort:

- (1) Find the key equations that involve only one of the four constants in Table III.
- (2) Keep in mind equations that must not depend on the choices for the constants in Table III. These equations, which we call invariant, include the definition of the scattering operator in terms of Møller operators in Eq. (4), the integral equation for the Dirac-delta function in Eq. (13), the expansion of a plane wave in Eq. (65), and the definition of the partial-wave phase shift in Eq. (51a).
- (3) Use dimensional analysis (see Appendix A) to ensure that all the terms in all equations are dimensionally consistent and that (except for monomial power law functions such as  $x^2$ ), the arguments of all mathematical functions are dimensionless.

Students also must learn how these choices propagate through various equations of scattering theory, a point we have illustrated several times. A ready reference for this de-

fective work appears in Table II. The equations in Tables III and I should also prove useful in checking consistency among different sources.

It would be impractical to tabulate the choices made in the hundreds of resources we have investigated. In the interest of saving readers some of this drudgery, we present in Table I this information for a small number of current, widely used books on collision theory. To further facilitate the use of the transformation equations in this paper, we have prepared a MATHEMATICA notebook<sup>43</sup> that uses replacement rules to generate the key equations in this paper once the user has identified as many of the four constants  $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $\zeta$  as required.

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### APPENDIX A: DIMENSIONAL ANALYSIS

The considerable work often required to determine the conventions used by a particular source is greatly aided by dimensional analysis. Although often marginalized in physics courses and not mentioned in any scattering theory books known to us, dimensional analysis is valuable for deriving and checking equations involving scattering quantities. Not only does dimensional analysis provide an almost foolproof way to check consistency between various equations, it limits (somewhat) the choices that can be made, particularly if partial-wave analysis is used.<sup>44</sup> Table IV lists the dimensions of relevant quantities. Omitted from this table are well-known quantities such as the wave number  $k$  (dimensions  $L^{-1}$ ) and the radius  $r$  (dimensions  $L$ ).

### APPENDIX B: THE RICCATI FUNCTIONS

The Riccati-Bessel, -Neumann, and -Hankel functions are closely related to the familiar spherical Bessel, Neumann, and Hankel functions. The latter functions are defined as

$$j_\ell(z) \equiv \left( \frac{\pi}{2z} \right)^{1/2} J_{\ell+1/2}(z), \quad (B1a)$$

$$n_\ell(z) \equiv (-1)^\ell \left( \frac{\pi}{2z} \right)^{1/2} J_{-\ell-1/2}(z), \quad (B1b)$$

Table IV. Dimensions of quantities in scattering theory. If no entry appears in the third entry in a particular row, then the item in that row has no dimensions. This table assumes our default conventions.

Physical quantity	Symbol	Dimensions
Position eigenstate	$ \mathbf{r}\rangle$	$L^{-3/2}$
Plane wave state <sup>a</sup>	$ \mathbf{k}\rangle$	$L^{3/2}$
Angular momentum state <sup>a</sup>	$ E\ell m\rangle$	$E^{-1/2}$
Transformation matrix	$\langle \mathbf{k}   E \ell m \rangle$	$E^{-1/2} L^{3/2}$
Scattering amplitude	$f(\mathbf{k}' \leftarrow \mathbf{k})$	$L$
Scattering state	$ \psi\rangle$	
Plane wave scattering function	$\psi_{\mathbf{k}}^{\pm}$	$L^{-3/2}$
Partial-wave scattering function	$\psi_{E\ell m}^{\pm}$	$E^{-1/2} L^{-3/2}$
Radial scattering function	$v_{k\ell}(r)$	$E^{-1/2} L^{-1/2}$
Normalized radial scattering function <sup>b</sup>	$u_{k\ell}(r)$	
Partial-wave scattering matrices	$S_{\ell}(E), T_{\ell}(E), K_{\ell}(E)$	
Phase shift	$\delta_{\ell}(E)$	
Green's function <sup>c</sup>	$G_{E_k}(\mathbf{r}, \mathbf{r}')$	$E^{-1} L^{-3}$

<sup>a</sup>Because the Møller operators are dimensionless, these dimensions apply to the scattering state obtained when these operators act on this item.

<sup>b</sup>The zero potential limit of this function is the Riccati-Bessel function  $\hat{j}_{\ell}(kr)$ , which is dimensionless. Note that with our conventions the boundary conditions imposed on  $u_{k\ell}(r)$  must not contain any dimensional quantities.

<sup>c</sup>These dimensions also apply to the free-particle Green's function. Note that these dimensions correspond to our definition of the Green's function as the solution of  $(\hat{H} + E_k)G_{E_k}(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}')$ .

$$h_{\ell}^{\pm}(z) \equiv n_{\ell}(z) \pm ij_{\ell}(z). \quad (\text{B1c})$$

It is easy to overlook the arbitrary phase in the definition of the spherical Neumann function. For the convention we have chosen the asymptotic (for real  $z$ ) behavior of this function as<sup>45</sup>

$$n_{\ell}(z) \xrightarrow{z \rightarrow \infty} \frac{1}{z} \cos \left[ z - \ell \frac{\pi}{2} \right] (\text{real } z). \quad (\text{B2})$$

The Riccati functions corresponding to the spherical functions of Eq. (B1) are these functions times their argument,

$$\hat{j}_{\ell}(z) \equiv zj_{\ell}(z), \quad \hat{n}_{\ell}(z) \equiv zn_{\ell}(z), \quad \hat{h}_{\ell}^{\pm}(z) \equiv zh_{\ell}^{\pm}(z). \quad (\text{B3})$$

The introduction of the Riccati functions simplifies expressing and manipulating the boundary conditions on radial functions, because the Riccati functions have the simple asymptotic forms

$$\hat{j}_{\ell}(kr) \xrightarrow{r \rightarrow \infty} \sin \left[ kr - \ell \frac{\pi}{2} \right], \quad (\text{B4a})$$

$$\hat{n}_{\ell}(kr) \xrightarrow{r \rightarrow \infty} \cos \left[ kr - \ell \frac{\pi}{2} \right], \quad (\text{B4b})$$

$$\hat{h}_{\ell}^{\pm}(kr) \xrightarrow{r \rightarrow \infty} e^{\pm i(kr - \ell \pi/2)}. \quad (\text{B4c})$$

Almost as useful as the asymptotic behavior of these functions is their behavior as  $z \rightarrow 0$ :

$$\hat{j}_{\ell}(kr) \xrightarrow{r \rightarrow 0} \frac{1}{(2\ell + 1)!!} (kr)^{\ell+1} \quad (\text{B5a})$$

$$\hat{n}_{\ell}(kr) \xrightarrow{r \rightarrow 0} \frac{1}{(2\ell - 1)!!} (kr)^{-\ell}. \quad (\text{B5b})$$

Although  $\hat{j}_{\ell}(kr)$  is regular at the origin,  $\hat{n}_{\ell}(kr)$  diverges as  $r \rightarrow 0$ . This behavior is important in the integral equations approach to scattering theory. Extensive information about these functions appears in Refs. 46 (which contains pictures), Ref. 47 (which discusses their calculation), and the “bible” of this subject, Ref. 48.

<sup>a</sup>Electronic mail: morrison@nhn.ou.edu

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<sup>20</sup>The resolution of the identity operator, Eq. (10), holds only for wave vector normalized plane wave states  $|\mathbf{k}\rangle$ . The form appropriate for arbitrary normalization via  $|\mathbf{k}\rangle \rightarrow \alpha|\mathbf{k}\rangle$  is  $\hat{1} = |\alpha|^2 \int d^3k |\mathbf{k}\rangle \langle \mathbf{k}|$ . This point can be seen by taking matrix elements of Eq. (10) in configuration space and noting that the resulting equation then becomes a representation of the Dirac delta function  $\langle \mathbf{r}' | \mathbf{r} \rangle = \delta^3(\mathbf{r}' - \mathbf{r})$  analogous to the momentum-space Eq. (13).

<sup>21</sup>I. E. McCarthy and E. Weigold, *Electron-Atom Collisions* (Cambridge U.P., New York, 1995).

<sup>22</sup>P. G. Burke and C. J. Joachain, *Theory of Electron-Atom Collisions. Part I: Potential Scattering* (Plenum, New York, 1995).

<sup>23</sup>M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

<sup>24</sup>A. G. Sitenko, *Lectures in Scattering Theory* (Pergamon Press, New York, 1971).

<sup>25</sup>Many authors choose  $\beta$  to depend on  $k$ ; see, for example, Chap. 3 of Ref. 52 and Ref. 57 in which  $\beta = 1/k$ .

<sup>26</sup>Equation (36a) follows by applying the definition Eq. (26) of the  $T$  operator to the relation (Eq. 10.8 of Ref. 19,  $|\mathbf{k}\pm\rangle = |\mathbf{k}\rangle + \hat{G}(E_k + i0)\hat{V}|\mathbf{k}\rangle$ ).

Note that the Green's operator in this equation is not the free-particle Green's operator; rather it is  $\hat{G}(z)=(z-\hat{\mathcal{H}})^{-1}$  evaluated on the energy shell. Note also that it is not correct to write  $\hat{T}|\mathbf{k}\rangle=\hat{V}|\mathbf{k}\rangle$ , because this relation is valid only on the energy shell. In some papers, this (incorrect) relation is taken as the definition of the  $T$  operator.

<sup>27</sup>Early treatments of scattering theory—especially in nuclear physics—denoted the reactance matrix by  $\mathbf{R}$ , a notation that spawned endless confusion with the  $R$ -matrix of  $R$ -matrix theory.

<sup>28</sup>W. O. Amrein, J. M. Jauch, and K. B. Sinha, *Scattering Theory in Quantum Mechanics* (Benjamin, Reading, MA, 1977).

<sup>29</sup>Because the scattering operator is unitary ( $\hat{S}^\dagger\hat{S}=\hat{1}$ ), the operators  $(\hat{1}+i\hat{K})$  and  $(\hat{1}-i\hat{K})^{-1}$  in Eq. (47) commute.

<sup>30</sup>For example, Adhikari (Ref. 53) adopts the unconventional relation  $\mathbf{S}=[1-(i/2)\mathbf{K}][1+(i/2)\mathbf{K}]^{-1}$ . Rodberg and Thaler (Ref. 33) define the  $K$  matrix from  $\mathbf{S}=[1-(i/2)\mathbf{K}][1+(i/2)\mathbf{K}]^{-1}$ .

<sup>31</sup>Some authors write these and many other equations in terms of the density of states per unit energy  $\rho(E)\equiv k^2/[dE(k)/dk]$ , which for a free particle equals  $mk/\hbar^2$ . For example, in Sec. 6.2 of Ref. 23 we find  $K_\ell(E)=-\tan\delta_\ell(E)/\pi\rho(E)$ , which for a free particle (and in atomic units, which are used in Ref. 23) equals  $-\tan\delta_\ell(E)/\pi k$ . See also Chaps. XIV–XVII of Ref. 60.

<sup>32</sup>A useful account of the relation between  $g_\ell(r',r)$  and the boundary conditions along with a clever prescription for adapting this function to any boundary condition we might choose to impose on the radial scattering function appears in Sec. IV B of Ref. 33.

<sup>33</sup>L. S. Rodberg and R. M. Thaler, *Introduction to the Quantum Theory of Scattering* (Academic, New York, 1967).

<sup>34</sup>C. Cohen-Tannoudji, B. Diu, and F. Lalöe, *Quantum Mechanics* (Wiley-Interscience, New York, 1977).

<sup>35</sup>For example, Adhikari (Ref. 53) uses this convention (in atomic units  $\hbar=1$ ,  $m_e=1$ ).

<sup>36</sup>Here and elsewhere, all sums over partial-wave order  $\ell$  run from zero to  $\infty$ . All sums over the magnetic quantum number  $m$  run from  $-\ell$  to  $+\ell$ .

<sup>37</sup>Energy normalization is especially convenient because with this choice, the diagonal elements of the  $S$  matrix for scattering via a central local potential  $V(r)$  automatically obey Eq. (51a).

<sup>38</sup>Although very widely used, this definition of the partial-wave scattering amplitude is not universal. For example, Friedrich (Ref. 58) absorbs the factor of  $2\ell+1$  into this amplitude and writes the expansion in the form  $f(\mathbf{k}'\leftarrow\mathbf{k})=\sum_{\ell=0}^{\infty}f_\ell(E)P_\ell(\cos\theta)$ . This choice forces the factor of  $2\ell+1$  into the expression relating  $f_\ell(E)$  to the phase shift and into the asymptotic form of the radial function, resulting in the correct but unfamiliar boundary condition  $u_{k\ell}(r)\xrightarrow{r\rightarrow\infty}(1/k)(2\ell+1)i^\ell e^{i\delta_\ell(E)}\sin[kr-\ell\pi/2+\delta_\ell(E)]$ .

<sup>39</sup>We recommend against this choice, because it results in a phase-shift dependence in quantities that describe the free particle ( $V=0$ ) case; for example, the eigenfunctions of  $\hat{\mathcal{H}}^0$ ,  $\hat{L}^2$ , and  $\hat{L}_z$  that define partial-wave theory will depend on  $\delta_\ell(E)$ .

<sup>40</sup>A. Ziegler, "Scattering by spherically symmetric and nonspherically symmetric potentials," *Am. J. Phys.* **57**, 518–524 (1989).

<sup>41</sup>R. K. Nesbet, *Variational Methods in Electron-Atom Scattering Theory* (Plenum, New York, 1980).

<sup>42</sup>Jochain (Ref. 17) notes in Chap. 4 that we can codify the infinity of choices for normalizing the radial function by writing its asymptotic

boundary conditions as  $u_{k\ell}(r)\xrightarrow{r\rightarrow\infty}\cos[kr-\ell\pi/2+\xi]+\cot[\delta_\ell(k)-\xi]\sin[kr-\ell\pi/2+\xi]$ , where  $\xi$  is a constant in the half-open interval  $\xi\in[0,\pi)$ . See also Ref. 56.

<sup>43</sup>From [www.nhn.ou.edu/~morrison/Research/Papers/MF06](http://www.nhn.ou.edu/~morrison/Research/Papers/MF06). There you will find download links for the accompanying MATHEMATICA materials. We welcome feedback from users of these materials and may post revised versions in response.

<sup>44</sup>Special systems of units, such as atomic units and relativistic units, which correspond to setting various physical constants equal to dimensionless numerical values (as, for example,  $\hbar=1$  in atomic units) preclude use of dimensional analysis. Authors of many research papers and some textbooks use units in which  $\hbar=1$  but  $\mu\neq 1$ . This choice can lead to confusion because some of these authors replace the linear momentum  $\mathbf{p}$  with  $\mathbf{k}$ , while others do not (see, for example, Refs. 19 and 18). To avoid this confusion and to enable easy use of dimensional analysis, we adopt no particular system of units in this paper.

<sup>45</sup>Many authors omit the phase factor  $(-1)^\ell$  in the definition of the spherical Neumann function, in which case this factor appears in the asymptotic form of this function; other use  $(-1)^{\ell+1}$  in Eq. (B1b). This phase factor then appears in all scattering boundary conditions that involve the spherical Neumann function (see, for example, Ref. 59). This flexibility explains, for example, why we often see  $K$ -matrix boundary conditions on the radial scattering function  $u_{k\ell}(r)$  written with a minus sign multiplying the  $K$  matrix. Note also that a variety of notations and definitions are used for the spherical Hankel function.

<sup>46</sup>J. Spanier and K. B. Oldham, *An Atlas of Functions* (Hemisphere, New York, 1987).

<sup>47</sup>W. J. Thompson, *Atlas for Computing Mathematical Functions* (Wiley-Interscience, New York, 1997).

<sup>48</sup>M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1965).

<sup>49</sup>M. A. Morrison and W. Sun, "How to calculate rotational and vibrational cross sections for low-energy electron scattering from diatomic molecules using close-coupling techniques," in *Computational Methods for Electron-Molecule Collisions*, edited by W. Huo and F. Gianturco (Plenum, New York, 1995), pp. 131–190.

<sup>50</sup>B. H. Bransden, *Atomic Collision Theory* (Benjamin/Cummings, Reading, MA, 1983), 2nd ed.

<sup>51</sup>S. Geltman, *Topics in Atomic Collision Theory* (Academic, New York, 1969).

<sup>52</sup>G. F. Drukarev, *Collisions of Electrons with Atoms and Molecules* (Plenum, New York, 1997).

<sup>53</sup>S. K. Adhikari, *Variational Principles and the Numerical Solution of Scattering Problems* (Wiley, New York, 1998).

<sup>54</sup>P. G. Burke, *Potential Scattering in Atomic Physics* (Plenum, New York, 1977).

<sup>55</sup>S. P. Khare, *Introduction to the Theory of Collisions of Electrons with Atoms and Molecules* (Kluwer Academic/Plenum, New York, 2003).

<sup>56</sup>T. Kato, "Upper and lower bounds of scattering phases," *Prog. Theor. Phys.* **6**, 394–407 (1951).

<sup>57</sup>L. I. Schiff, *Quantum Mechanics* (McGraw Hill, New York, 1968), 3rd ed.

<sup>58</sup>H. Friedrich, *Theoretical Atomic Physics* (Springer, New York, 2006), 3rd ed.

<sup>59</sup>G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists* (Elsevier, New York, 2005), 6th ed.

<sup>60</sup>A. Bohm, *Quantum Mechanics: Foundations and Applications* (Springer-Verlag, New York, 1993), 3rd ed.