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Absolute determination of zero-energy phase shifts for multiparticle single-channel scattering: Generalized Levinson theorem

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Levinson's theorem relates the zero-energy phase shift δ for potential scattering in a given partial wave l, by a spherically symmetric potential that falls off sufficiently rapidly, to the number of bound states of that l supported by the potential. An extension of this theorem is presented that applies to single-channel scattering by a compound system initially in its ground state. As suggested by Swan [Proc. R. Soc. London Ser. A **228**, 10 (1955)], the extended theorem differs from that derived for potential scattering; even in the absence of composite bound states δ may differ from zero as a consequence of the Pauli principle. The derivation given here is based on the introduction of a continuous auxiliary "length phase" η, defined modulo π for $l=0$ by expressing the scattering length as $A=a\cot\eta$, where a is a characteristic length of the target. Application of the minimum principle for the scattering length determines the branch of the cotangent curve on which η lies and, by relating η to δ, an absolute determination of δ is made. The theorem is applicable, in principle, to single-channel scattering in any partial wave for $e^{\pm}$-atom and nucleon-nucleus systems. In addition to a knowledge of the number of composite bound states, information (which can be rather incomplete) concerning the structure of the target ground-state wave function is required for an explicit, absolute, determination of the phase shift δ. As for Levinson's original theorem for potential scattering, *no additional information concerning the scattering wave function or scattering dynamics is required*. [S1050-2947(96)03612-8]

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I. INTRODUCTION

While only a trigonometric function of the scattering phase shift is required in the evaluation of a single-channel cross section, it can be very useful to have an absolute definition of the phase shift; it can, for example, provide information on the nodal structure of the scattering wave function [1]. (As opposed to the case for bosons, for which the ground-state wave function is known to be nodeless [2], there are no general theorems on the nodal structure of the ground state, or scattering states, of fermions.) Levinson's theorem [3] for scattering by a central potential $V(r)$, satisfying $r^3V(r)\sim 0$ as $r\rightarrow\infty$ and $r^2V(r)\sim 0$ as $r\rightarrow 0$, is of interest in this regard since it relates the zero-energy phase shift δ in a given partial wave (the orbital quantum number l is suppressed here) to the number of bound states of that angular momentum supported by the potential. More precisely, the phase shift is assumed to be a continuous function of the energy and zero at infinite energy and the theorem is as follows. For $l=0$, the phase shift is $\delta=(N+\xi)\pi$, where N is the number of negative-energy bound states and $\xi=\frac{1}{2}$ if there is in addition a zero-energy bound state, while $\xi=0$ if there is no such bound state; for $l>0$ the phase shift is $\delta=N\pi$, where N is the number of bound states, including, when present, a zero-energy bound state. This theorem allows one to determine the number of nodes of the zero-energy scattering wave function. Furthermore, since the theorem provides a fundamental connection between scattering and bound states, generalizations applicable to the more interesting case of scattering by a target with internal degrees of freedom have long been sought for. An early attempt was made by Swan [4]. Many serious objections can be raised with regard to his analysis [5–7]. Nevertheless, his contribution, which included an attempt to obtain a generalized form of Levinson's theorem, *was very suggestive*. Using an approximate antisymmetrized wave function based on an independent-particle model, he derived an integro-differential equation and showed that, in his model, δ satisfied a modified form of Levinson's theorem [4]. Swan's contribution, while restricted to a special model, served to call attention to the distinctive role played by the Pauli principle in determining δ. In the procedure followed here a formal generalized version of Levinson's theorem is developed with reliance on specific models avoided and with the effect of the Pauli principle now formulated in a precise manner. The formal result can be implemented in a few simple cases, leading to explicit results for δ [7]. In general, however, one must introduce a simplified model of the *target*. (In contrast to Swan's method, *no additional assumption concerning the scattering dynamics is required*.) If one describes the target wave function as an antisymmetrized product of one-particle functions, as obtained, for example, by a Hartree-Fock analysis, the results follow with only minimal calculational effort and are applicable both to $e^{\pm}$-atom scattering [7] and to the scattering of neutrons and protons by heavy nuclei. [Some readers may find it helpful, before proceeding to the formal proofs to follow, to read a nonrigorous but intuitive argument, based on the existence of an effective central potential $V_{\text{eff}}(r)$, presented earlier. See Sec. III of Ref. [8]. The essential point is that a reasonably accurate $V_{\text{eff}}(r)$, which may be l dependent, will support the same number N of bound states of the l under consideration as actually exist in the target; Levinson's theorem for potential scattering will therefore give a contribution of $N\pi$ to account for those states.]

The standard proof [3] of Levinson's theorem for potential scattering is based on the analyticity properties of the partial-wave scattering amplitude. This method is not easily extended to the multiparticle case. An alternative approach [1], based on a count of the number of zeros of the zero-energy wave function, is difficult to generalize owing to the more complex nodal structure of multiparticle wave functions [8]. The method proposed here is based on the minimum principle (a variational bound) for the scattering length [9], a principle that is not restricted to potential scattering, along with a particular absolute definition of δ not requiring that it exist at infinite energy. We apply the method to the potential-scattering problem in Sec. II. Our purpose here is to illustrate certain aspects of this approach in the context of a familiar and relatively simple problem and to show that it reproduces Levinson's theorem in its standard form, including an extension [10] to allow for scattering by potentials with a repulsive Coulomb tail. The problem of electron scattering by a neutral atom is taken up in Sec. III, where the more general statement of the theorem, taking into account the effect of the Pauli principle, is provided. Restrictions on the applicability of the theorem arising from the existence of more than one open channel at zero energy are discussed at the end of Sec. III. The theorem has been used to obtain the zero-energy phase shifts for e^--He scattering and for e^--H scattering in triplet and singlet states. In addition, several applications to electron scattering by heavier targets, including atoms containing only closed subshells, alkali-metal atoms, and atoms with open p-shell configurations, whose wave functions are given not by an independent-particle model but by the Hartree-Fock approximation, have been made [7]. The results confirm and extend (and for $l>0$ correct) those obtained by Swan in an independent-particle model. In all cases studied we verify that the effect of the antisymmetrization requirement on the wave function is to add to the zero-energy phase shift a multiple of π equal to the number of bound states excluded by the Pauli principle.

II. POTENTIAL SCATTERING

In its standard form, Levinson's theorem relates the difference between the phase shifts at zero energy and at infinite energy to the number of bound states. This is not a useful version for our present purposes since the infinite-energy phase shift is not well defined when the target is a compound system. Alternatively, an absolute definition may be adopted for scattering by a potential V by requiring the phase shift $\delta(\lambda)$ for the potential λV to be a continuous function of λ, with $\delta(0)=0$ and $\delta(1)=\delta$. This definition is applicable to the study of the scattering of positrons by neutral atoms. However, adoption of this definition for electron-atom or nucleon-nucleus scattering is problematic since a modification of the strength of the projectile-target interaction without a corresponding rescaling of the interactions of the target particles destroys the symmetry of the Hamiltonian under interchange of particle labels. In the present consideration of potential scattering we confine our attention to procedures that we are able to generalize; we must therefore begin by introducing an appropriate absolute definition of δ. (Note that an absolute definition of δ at zero energy provides, on demanding continuity, an absolute definition of δ up to the energy at which the scattering is no longer single-channel scattering.)

There is clearly an element of arbitrariness in defining the phase shift on an absolute scale since the addition of a multiple of π leaves the scattering amplitude unaltered. A useful definition is one that allows one to extract information, or at least some insight, concerning the dynamics of the scattering process. As mentioned, one based on the nodal structure of the wave function might appear to be a likely candidate, but a straightforward extension of such a definition from single-particle to multiparticle scattering is difficult to implement. More generally, one may envision a sequence of approximations for the zero-energy scattering wave function, starting with one sufficiently simple to which the phase shift may be assigned in an intuitively reasonable way. One would then trace the evolution of the wave function, along with the corresponding phase shift, to its exact form. The resultant phase would then carry information concerning the evolution of the wave function that could be of physical interest.

A simple example, applicable to potential scattering, will clarify this idea. (We emphasize that the approach used in this example is *not* directly applicable to the multiparticle scattering problem. The example is included since it allows us to introduce, in a familiar context, several concepts that will be useful later on.) With the wave function written as $u(r)/r$, the reduced Schrödinger equation is $Hu(r)=0$, where

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}+V(r). \tag{2.1}$$

The reduced wave function satisfies $u(0)=0$ and (for the case of s-wave scattering by short-range potentials, falling off faster than any power of r, to which we confine our attention temporarily) has the asymptotic form $u(r)\sim r-A$. The scattering length A is related to the phase shift $\delta(k)$ for wave number k according to

$$A=-\lim_{k\to 0}\frac{\tan\delta(k)}{k}. \tag{2.2}$$

It satisfies the identity [11]

$$A=A_t+\frac{2m}{\hbar^2}\int_0^\infty u(r)Hu_t(r)dr, \tag{2.3}$$

where the trial function $u_t(r)$ vanishes at the origin and behaves asymptotically as $u_t(r)\sim r-A_t$. A variational approximation for the scattering length is obtained by replacing u by u_t in Eq. (2.3).

It is convenient at this point to introduce [12] an auxiliary phase η, to be referred to as the ''length phase,'' by writing

$$A=a\ \cot\eta, \tag{2.4}$$

where a is some arbitrarily chosen characteristic length, which might be the Bohr radius for scattering by an atomic target—we will mostly be concerned with this case—or a fermi in the case of nuclear scattering. An absolute definition of δ will be obtained by setting up a correspondence between δ and η and providing an absolute definition of η by introducing a procedure for determining the branch of the cotangent curve on which η lies. (A different choice for a leads to different absolute values for η, but the branch of $\cot\eta$ on which η lies and the values of η at which A is singular, the only relevant properties of the nonphysical function η, are not affected by the choice of a.) It will then be shown that this definition reproduces Levinson's theorem in its standard form. Toward this end we consider a sequence of variational approximations for the scattering length in which the accuracy of the trial function is steadily improved. The sequence of approximations $A^{(j)}$, $j=0,1,\ldots,n$, is generated from the variational principle based on Eq. (2.3) by introducing a sequence of trial functions

$$u^{(j)}(r)=\phi(r)+\sum_{i=1}^{j} b_i u_i(r). \tag{2.5}$$

Corresponding to each $A^{(j)}$, we introduce a length phase $\eta^{(j)}$ satisfying $A^{(j)}=a\cot\eta^{(j)}$. To satisfy the boundary conditions we require that $\phi(0)=u_i(0)=0$, and that $\phi(r)\sim r$ and $u_1(r)\sim -1$ for $r\rightarrow\infty$—b_1 then plays the role of a trial scattering length, with the functions $u_i(r)$ for $i>1$ taken to be quadratically integrable. The simplest choice for ϕ is the free wave function $\phi(r)=r$. For short-range potentials with $l>0$ we will require that $\phi(r)\sim r^{l+1}$. (Greater flexibility is required in the treatment, given in the Appendix, of long-range potentials.) The $u_i(r)$ in Eq. (2.5) are assumed to be linearly independent and the linear parameters b_i are determined variationally. The minimum principle for the scattering length [9] may now be invoked to study the behavior of the sequence of approximations for the scattering length and for the associated length phase. The first term in the sequence is obtained by setting the u_i in Eq. (2.5) equal to zero. The trial function is then $\phi(r)=r$ and the associated A_t vanishes. Setting $u=u_t=\phi(r)$ in Eq. (2.3), we then have

$$A^{(0)}=\frac{2m}{\hbar^2}\int_0^\infty \phi(r)H\phi(r)dr=\frac{2m}{\hbar^2}\int_0^\infty r^2V(r)dr. \tag{2.6}$$

If there are no bound states, it follows [9] that $A^{(0)}$ provides an upper bound on the true scattering length; each successive term decreases the value of the approximation obtained at the previous stage. More generally, suppose that N bound states exist; for the moment we assume that there is no zero-energy bound state. Then $A^{(j)}$, $j\geqslant N$, provides a bound on A [9] if N of the basis functions u_i are accurate enough to give binding, that is, if there are N approximate bound-state energies—determined by the Hylleraas-Undheim procedure [13] in which the $N\times N$ Hamiltonian matrix is diagonalized in the basis formed by the u_i—that lie below zero [14]. Once this stage has been reached additional terms in the sequence lead to a steady decrease in the variational approximation for the scattering length, accompanied by a steady increase in the associated length phase. A useful corollary to this theorem was proved by Ohmura [15]: after one verifies N jumps in the sequence of scattering length approximations $A^{(j)}$ for $j=0,1,\ldots,n$, where $n\geqslant N$, the variational method is ensured to give an upper bound on the scattering length.

To obtain a more detailed description of the evolution of the approximate scattering length and its associated phase as the trial function is improved we may imagine that the functions $u_i(r)$ are distorted in such a way that the discrete sequence of scattering-length approximations is replaced by a continuous function that interpolates between adjacent members of the sequence. Since the variational approximation for the scattering length diverges when the Hylleraas-Undheim construction provides zero value for one of the approximate energy eigenvalues, it will be more convenient to trace the continuous, steadily increasing evolution of the length phase. An absolute definition of the length phase is determined by choosing the largest integer contained in $\eta^{(0)}/\pi$ to be equal to $\delta^{(0)}/\pi$, where $\delta^{(0)}$, to be referred to as the reference phase, is here taken to be the phase shift associated with the free wave function $\phi(r)$. Since this function is nodeless, it is natural to set the associated phase shift $\delta^{(0)}$ equal to zero [1]. (A modification of this assignment is necessary when antisymmetry is accounted for in the multiparticle case; see Sec. III.) The corresponding length phase $\eta^{(0)}$ must then be chosen to lie between zero and π. A divergence in the approximate scattering length corresponds to η passing from one branch of the $\cot\eta$ curve to the adjacent one lying to its right as the trial function is improved. From the fact that the scattering length experiences N jumps in this process we may conclude that the true value of η lies between $N\pi$ and $(N+1)\pi$; we suppose for the moment that η/π is not an integer. Since we define the phase shift by equating δ/π to the largest integer contained in η/π, the sought for result $\delta=N\pi$ then follows.

If in addition to N negative-energy bound states there is an s-wave bound state at zero energy, corresponding to a scattering length that is infinite, the process of minimization of the variationally determined scattering length will not terminate after N jumps. This corresponds to the precise value $\eta=(N+1)\pi$ for the length phase. We know from Levinson's theorem that δ is $N\pi$ for η just below $(N+1)\pi$. When the inverse of the scattering length vanishes so does $\cot\delta(k)$ in the limit of vanishing k. This result follows from effective-range theory, which, for $l=0$ *and* $A^{-1}=0$, gives $k\cot\delta(k)=\frac{1}{2}r_0k^2+\cdots$, a result that remains valid even in the presence of a (polarization) potential falling off as r^{-4} [16]. (Long-range potentials, relevant for $e^{\pm}$-atom scattering, are considered in greater detail in the Appendix.) The vanishing of $\cot\delta$ allows us to conclude that $\delta=(N+\frac{1}{2})\pi$ when there exists an s-wave bound state at zero energy in addition to N negative-energy s-wave bound states; we have thus rederived Levinson's theorem. The half-bound-state phenomenon is peculiar to s-wave scattering. Application of effective-range theory for $l>0$ shows that, as opposed to the $l=0$ result, $\cot\delta(k)$ diverges in the limit of vanishing k, either as $k^{-(2l-1)}$ for short-range potentials [17] or, using modified effective-range theory, as k^{-2} for potentials falling off as r^{-4} [16]. It follows for $l>0$ that $\delta=N\pi$ when N bound states exist even when one of them lies at zero energy. We have been considering potentials that vanish more rapidly than r^{-3} asymptotically. A similar analysis may be applied to the case where the potential has a repulsive Coulomb tail. Levinson's theorem, in the form derived previously [10], can be verified this way. (Half-bound states do not appear here, even for $l=0$, as may be verified by application of the appropriate version of effective-range theory.) The absence of the half-bound-state phenomenon may also be traced, in the context of a Jost-function analysis, to the normalizability of a zero-energy bound-state wave function. For short-range potentials, for example, the radial component of the wave function behaves as $1/r^l$ asymptotically and $\int^\infty r^{-2l}dr$ exists for all but $l=0$.

III. ELECTRON SCATTERING BY A NEUTRAL ATOM

We turn now to scattering by a compound target, with consideration here restricted to electron-atom scattering. For the sake of orientation let us first consider a simple model based on the central-field approximation. Since the projectile scatters in a central potential we expect, from Levinson's theorem, that the zero-energy phase shift will be $N\pi$. Now, however, not all of the N bound states are physically realizable. Consider, for example, a helium target in the $(1s)^2$ ground-state configuration. The $l=0$ zero-energy scattering wave function has at least one node since it must be orthogonal to the spatial part of the $1s$ bound-state wave function; a more detailed analysis [1] shows that it has no more than one node. Adopting the nodal definition of the phase shift we conclude that the s-wave zero-energy phase shift is π. This reasoning may be extended, though still within the central-field model, to heavier target atoms, with N representing the number of bound states for the value of l under consideration plus the number for the given l excluded by the Pauli principle. In an attempt to derive a more general version of this theorem for any but the lightest targets, one is faced with the fact that the target wave function is much less precisely known than it is for helium. One can hope, nevertheless, to represent the zero-energy phase shift in terms of the number of bound states for the given l along with information (which can be far from complete) concerning the target structure. In the spirit of Levinson's theorem, an explicit analysis of the scattering problem should not be necessary. We now derive a result of this form by extending the approach, based on the minimum principle for the scattering length, described in Sec. II. We consider the single-channel scattering of an electron by an atom; the target is initially in its ground state, which is assumed to be nondegenerate. Effects of target recoil are ignored. In addition, it is assumed that the effects of the spin-orbit interaction can be neglected, an excellent approximation for scattering by light atoms. (As discussed at the conclusion of this section, this last assumption may be relaxed in most cases of interest.) To simplify the presentation we first consider scattering by target atoms with vanishing orbital angular momentum; more general cases are considered later on.

In the multiparticle generalization of Eq. (2.5) for a zero-energy electron, in the lth partial wave, incident on an $(M-1)$-electron target, we introduce the wave function

$$U(x_1,\ldots,x_M)=\mathcal{A}_1\left[\Psi(s_1;x_2,\ldots,x_M)\,\frac{\phi(r_1)}{r_1}\,Y_{l0}(\Omega_1)\right], \tag{3.1a}$$

where x_j refers to the space and spin variables of the jth target electron and s_1 is the spin coordinate of the projectile. We emphasize that U is not the exact wave function; rather it corresponds to the wave function in the absence of a scattering interaction and plays a role analogous to that of the first term on the right-hand side of Eq. (2.5). For an effective projectile-target interaction of short range, the function $\phi(r)$ in Eq. (3.1a) is chosen to be the free wave function r^{l+1}. As discussed in the Appendix, $\phi(r)$ differs from r^{l+1} for $l>0$ in cases, such as that now under consideration, where the effective potential contains long-range components. [It is more convenient here to work with the full wave function, involving $\phi(r_1)/r_1$, rather than the reduced function introduced in Sec. II. A subscript l on $\phi(r)$ is omitted to simplify notation.] Ψ includes a representation of the target ground-state wave function, antisymmetrized in the space and spin coordinates of the target particles; the target has spin S_T and is coupled with the spin of the projectile to form a state of definite total spin S and projection S_z. (That s_1 appears in Ψ but that l does not is a consequence of our simplifying assumption that the target has zero orbital angular momentum.) The function U is made fully antisymmetric by the residual antisymmetrizer

$$\mathcal{A}_1=1-\sum_{j=2}^{M}P_{1\leftrightarrow j}, \tag{3.1b}$$

where $P_{1\leftrightarrow j}$ interchanges the space and spin coordinates of electrons 1 and j. If the spin S_T of the target is nonvanishing we consider separately scattering states with $S=S_T+\frac{1}{2}$ and $S_T-\frac{1}{2}$; for $S_T=0$ we have only $S=\frac{1}{2}$. In the one-body problem studied in Sec. II, we assigned to the nodeless wave function $\phi(r)$ a phase shift—we referred to it as the reference phase $\delta^{(0)}$—equal to zero. We wish to generalize this assignment in a natural way. Since U, a multiparticle wave function, has no simple nodal structure, we consider instead the one-particle wave function $F(r_1)$ obtained by projecting U onto the function Ψ and then onto the angular component of the lth partial wave of the incident particle. (It should be noted that there is no reason to assume that the function F can be represented as a solution of a wave equation with a well-defined effective one-body Hamiltonian and we make no such assumption.) We have, explicitly,

$$F(r_1)=\int d\Omega_1 Y_{l0}(\Omega_1)\int d\mathbf{r}_2\cdots d\mathbf{r}_M\Psi^{\dagger}(s_1;x_2,\ldots,x_M)\times U(x_1,\ldots,x_M), \tag{3.2}$$

where the second integration is over the spatial variables $\mathbf{r}_j$ of the target and there is an inner product over the spin coordinates of the target particles and of the incident particle. Let N_{Pauli} represent the number of nodes in the function $F(r_1)$. The notation reflects the fact that with $\phi(r)$ in Eq. (3.1a) a nodeless function, any nodes present must be Pauli principle effects. The phase shift associated with $F(r_1)$ is identified as the reference phase $\delta^{(0)}$ and is taken to be $N_{\text{Pauli}}\pi$. (In the central-field model N_{Pauli} may be identified as the number of bound states excluded by the Pauli principle; this is in line with the heuristic remarks made at the beginning of this section and is verified in the applications that we have made to electron-atom scattering [7] based on a Hartree-Fock treatment of the target atom. While such an explicit characterization of this number is not possible under the more general circumstances now under consideration, it is often helpful to keep in mind the physical picture provided by the central-field model.)

At this stage, the derivation given in Sec. II, based on the minimum principle for the scattering length, can be extended without difficulty and we briefly outline the steps. The generalization of the minimum principle itself from potential scattering to electron-atom scattering was accomplished some time ago [9]. We recall that the variational identity that generalizes Eq. (2.3) takes the form

$$A=A_t+\frac{2m}{\hbar^2}\int u^\dagger(x_1,\ldots,\quad x_M)(H-E_{\rm tar})$$
$$\times u_t(x_1,\ldots,x_M)d\mathbf{r}_1,\ldots,d\mathbf{r}_M, \qquad (3.3)$$

where $E_{\rm tar}$ is the target ground-state energy; u and u_t are the exact and trial zero-energy wave functions, respectively. A variational approximation for the scattering length is obtained by replacing u by u_t in Eq. (3.3). Let $A^{(0)}$ denote the scattering length obtained from the identity (3.3) by replacing both u and u_t by the zeroth-order trial function, which we take to be the incident wave U; accordingly, the trial scattering length A_t is set equal to zero. A zeroth-order length phase, defined modulo π, is introduced by writing $A^{(0)}=a_0\cot\eta^{(0)}$. An absolute definition of this phase, and hence the phase that evolves from it by subsequent improvement in the trial function, is provided by setting the largest integer contained in $\eta^{(0)}/\pi$ equal to $\delta^{(0)}/\pi$, which has been taken to be $N_{\rm Pauli}$, the number of nodes in the function F of Eq. (3.2). The argument now follows closely that given in Sec. II for potential scattering. Thus we consider the zeroth-order wave function to be supplemented by additional terms, a process that continues until convergence to the exact scattering length is reached. The length phase, now defined absolutely, increases monotonically in this process, with the largest integer contained in η/π increasing by unity each time the variationally determined scattering length diverges as the trial function is made flexible enough to account for the existence of an additional bound state. With η now representing the converged value of the length phase, the value of the zero-energy phase shift is obtained by multiplying by π the largest integer contained in η/π. The generalized Levinson theorem for the zero-energy phase shift in a given partial wave l then takes the form

$$\delta=(N_{\rm Pauli}+N+\xi)\pi. \qquad (3.4)$$

For $l=0$, N is the number of composite negative-energy bound states of zero orbital angular momentum and ξ is zero unless there is a composite bound state of zero energy, in which case $\xi=\frac{1}{2}$; for $l>0$, N is the number of composite bound states of orbital angular momentum l including a bound state of zero energy if one exists.

As an illustration we indicate schematically in Fig. 1 the variation of the scattering length, the length phase, and the phase shift as the trial function in a variational bound calculation of the scattering length is steadily improved, starting with an incident wave of the form (3.1a) and evolving into the exact wave function. The reference phase shift $\delta^{(0)}$, identified as $N_{\rm Pauli}\pi$, is given the value 2π and one composite bound state is assumed to exist. (These values correspond to s-wave scattering of an electron by Na with the composite system in a ${}^1S$ state. Procedures for determining $N_{\rm Pauli}$, in the Hartree-Fock approximation, for a wide class of atomic targets are described in Ref. [7].) The largest integer contained in η/π is 3, and since η/π is not an integer we conclude, using the prescription formulated in Sec. II and summarized above, that $\delta=3\pi$. The same result follows from Eq. (3.4), with $N_{\rm Pauli}=2$, $N=1$, and $\xi=0$.

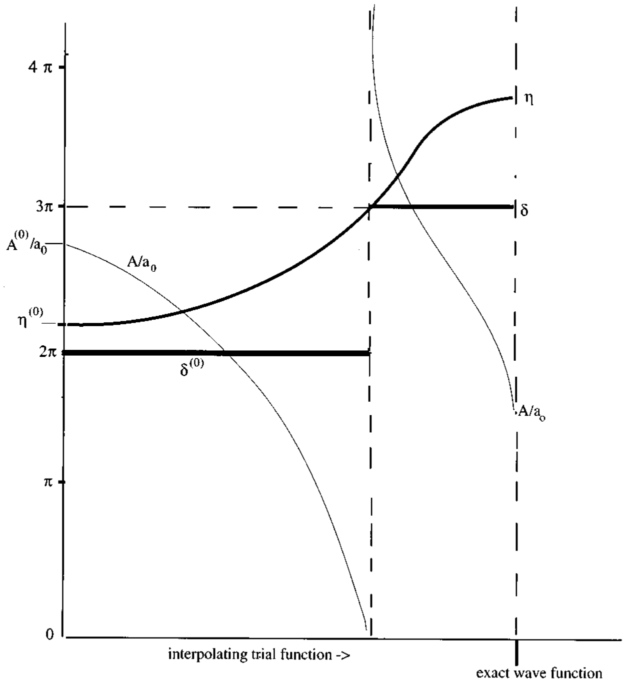

FIG. 1. Schematic plots illustrating the evolution of the scattering length A, the phase shift δ, and the length phase η as the trial function in a variational-bound calculation of A evolves from an antisymmetrized incident wave of the form shown in Eq. (3.1a) to the exact solution. The superscript zero denotes initial values. $\delta^{(0)}$ is assumed to be 2π and $\eta^{(0)}$ must therefore lie between 2π and 3π. A single composite bound state is assumed to exist. The figure illustrates the generalized Levinson theorem, which here predicts that $\delta=\delta^{(0)}+\pi$.

The preceding formalism is readily extended to allow for many target atoms that are not spherically symmetric. Rather than present the details we confine our remarks to the question of the existence of the zero-energy phase shift. The question is whether, through a change in target orientation in the course of the collision, the projectile, originally in a state with orbital quantum number l, could emerge with quantum number $l'\neq l$; if so, this would violate the restriction to single-channel scattering if the transition were allowed. We neglect spin-orbit interactions, let L and $L_{\rm tar}$ represent the total and target orbital quantum numbers, and let l and l' represent the orbital quantum numbers of the projectile in its initial and final states. Considerations of angular momentum conservation are standard, as are considerations of parity, but the treatment of centrifugal barrier effects requires some care. For short-range potentials the l to l' transition amplitude for fixed $L_{\rm tar}$ and L is proportional to $k^{l+l'}$ in the neighborhood of $k=0$ [18]; transitions to $l'>l$ are suppressed relative to the l to l transition and one has single-channel scattering for $l=0$ or 1, cases of primary importance. For $l\geqslant 2$, however, transitions to $l'=l-2$ are not ruled out by centrifugal-barrier effects; if such transitions are not otherwise forbidden, the restriction to single-channel scattering will be violated. We conclude that cases for which only single-channel reactions occur include $L_{\rm tar}=0$ for any l and, for $L_{\rm tar}>0$, $l=0$ or 1. For $L_{\rm tar}>0$ and $l\geqslant 2$, single-channel scattering will occur at threshold provided $L=L_{\rm tar}+l$ or $L=L_{\rm tar}+l-1$. As will be discussed elsewhere, the case for long-range potentials, behaving as $1/r^4$ for electron-atom scattering, is somewhat different. Centrifugal-barrier effects rule out $l'>0$ for $l=0$, but do not rule out $l'>l$ for $l>0$. The restriction to single-channel scattering will be satisfied for $L_{\mathrm{tar}}=0$ for any l. For $l>0$, the conditions that guarantee single-channel scattering are more restrictive. For example, suppose $L_{\mathrm{tar}}=1$, $l=1$, and $L=2$. A transition to $l'=3$ is allowed by parity and angular momentum conservation and the amplitude has the same (k^2) energy dependence near threshold as the p-wave to p-wave transition, so that more than one channel is open. For $L_{\mathrm{tar}}=1$, $l=1$, and $L=0$ or 1, however, the transition to $l'=3$ is forbidden and the zero-energy p-wave phase shift exists. The argument is easily extended. Thus, for $L_{\mathrm{tar}}=2$, the zero-energy p-wave phase shift exists for $L=0$, but not for higher L, and similarly, for $L_{\mathrm{tar}}=1$, the zero-energy d-wave phase shift exists for $L=0$, but not for higher L.

IV. SUMMARY

An absolute definition of the zero-energy phase shift for multiparticle single-channel scattering has been introduced that removes the ambiguity concerning multiples of π that would otherwise be present. With this as a starting point, a formal procedure, valid for each partial wave, was provided for determining the phase shift. This procedure requires a knowledge of the number of composite bound states that exist—the composite bound-state wave functions need not be known—along with some information, not necessarily complete, concerning the target wave function; knowledge of the exact zero-energy scattering wave function is not required. The result represents a generalization of Levinson's theorem, derived many years ago for potential scattering, that accounts for the effect of the Pauli principle in a well-defined way and that is applicable to a wide variety of atomic and nuclear scattering problems. It was possible to arrive at this generalization by basing the derivation not on the analytic properties of the wave function, which are difficult to determine for multiparticle systems, but rather on the minimum principle for the scattering length, which does apply to this more general class of problems. In view of current interest in atomic scattering at very low energies, which is spurred by recent developments in techniques for atomic cooling, the analysis given here of the behavior of the phase shift in the zero-energy limit—a problem of long standing in formal scattering theory—may be particularly timely.

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APPENDIX: LONG-RANGE POTENTIALS

The analysis given in Sec. II for s-wave scattering by short-range potentials is easily extended to include higher partial waves, but the necessary modifications are more substantial if the potential has a long-range component. Here we consider potentials of the form $V(r)=V_{\mathrm{sh}}(r)+V_l(r)$, where V_{sh} falls off faster than any power of r and V_l is a long-range component that vanishes for $r<R$ and is represented as

$$V_l(r)=-\frac{\hbar^2}{2m}\left(\frac{d_4}{r^4}+\frac{d_6}{r^6}+\cdots\right) \tag{A1}$$

for $r>R$. The distance R is chosen to be large enough so that V_l cannot support a bound state even when all components are attractive. If only a single long-range component were present in Eq. (A1) it would be possible to obtain exactly, in terms of Bessel functions [19], the regular and irregular zero-energy solutions of the Schrödinger equation for the potential V_l. While analytic solutions are not available, to our knowledge, for a superposition of long-range components, an approximate solution $\phi(r)$ is easily developed in the form of an expansion in decreasing powers of r for $r>R$, which may then be continued smoothly in to the inner region, such that it vanishes at the origin. Since we require only that $\phi(r)$ be nodeless, that it contain no component that can give binding [20], and that $H\phi(r)$ vanish sufficiently rapidly at great distances so that the variational approximation is well defined, we may assume that by taking sufficiently many terms in the expansion of $\phi(r)$, these requirements may be met. A sufficiently accurate approximation $\zeta(r)$ to the irregular solution of the zero-energy Schrödinger equation for the potential V_l may be constructed in a similar way; these functions behave as

$$\phi(r)\sim r^{l+1}/(2l+1)!!,$$

$$\zeta(r)\sim(2l-1)!!/r^l,$$

$$(2l+1)!!\equiv 1\times 3\times 5\times\cdots\times(2l+1) \tag{A2}$$

asymptotically and have been normalized to give a unit Wronskian. The solution appropriate to the full potential $V(r)$ has the asymptotic form

$$u(r)\sim\phi(r)-B\zeta(r), \tag{A3}$$

where the parameter B plays the role of a modified scattering length. In analogy with the identity (2.3) we have, with the Hamiltonian given by Eq. (2.1),

$$B=B_t+\frac{2m}{\hbar^2}\int_0^\infty u(r)Hu_t(r)dr; \tag{A4}$$

here u_t vanishes at the origin and has the asymptotic form shown in Eq. (A3) with B replaced by B_t. This identity provides the basis for the derivation of a minimum principle for B [1,9]. At this point the discussion given earlier for scattering by a short-range potential may be taken over, *mutatis mutandis*, to provide a definition of the zero-energy phase shift that satisfies Levinson's theorem. In particular, the ''length phase'' is defined by setting $B=a^{2l+1}\cot\eta$ and the first term in the sequence of approximations for B is given as $B^{(0)}=(2m/\hbar^2)\int_0^\infty\phi(r)H\phi(r)dr$. Note that for s-wave scattering this integral is convergent if one makes the choice $\phi(r)=r$. For $l=1$, the form $\phi(r)=r^2/3+d_4/6$ accounts for the effect of the long-range component V_l for $r>R$ to sufficient accuracy. The smooth continuation of this function into the region $r<R$ as $(1+3d_4/2R^2)r^2/3-(d_4/3R^3)r^3$ defines $\phi(r)$ as a nodeless function for $d_4>0$, the attractive case of greatest interest in applications to $e^{\pm}$-atom scattering. (In such applications one would set $d_4=\alpha/a_0$, with α denoting the dipole polarizability of the target.) For $d_4<0$, $\phi(r)$ will be nodeless provided $R>(-3d_4/2)^{1/2}$. For higher partial waves more terms in the expansion of the function $\phi(r)$ must be included.

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[6] The literature on zero-energy electron-atom phase shifts with $l>0$ is mostly from earlier times and is rather confusing. References to the original papers can be found, for example, in H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Clarendon, Oxford, 1952) and in N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon, Oxford, 1965), where some of the graphs of those papers are reproduced. Some of the results cited are inconsistent. (Compare Fig. 64, p. 117, of Massey and Burhop with Table IV, p. 578, of Mott and Massey.) Further, some of the results were obtained using potentials for which $r^2V(r)$ is nonvanishing as $r\rightarrow 0$. (See Fig. 61, p. 114, of Massey and Burhop.) Such potentials are unrealistic. (The true potentials behave as $1/r$ for $r\rightarrow 0$.) Since the potentials used do not satisfy the conditions of validity of Levinson's theorem, it is not surprising that some of the phases obtained (in particular, the p-wave phase shifts for Ar and Kr) are incorrect. Our analysis [7] of the zero-energy phase shifts for p-wave scattering of electrons by the rare gases He, Ne, Ar, and Kr leads to the predictions (assuming the incident electron cannot form a composite bound state) 0, π, 2π, and 3π.

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