Nodal structure and phase shifts of zero-incident-energy wave functions: Multiparticle single-channel scattering

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For potential scattering, with $\delta_L(k)$ the phase shift modulo π for an incident wave number k, Levinson's theorem gives $\delta_L(0)-\delta_L(\infty)$ in terms of N_L, the number of bound states of angular momentum L, for $\delta_L(k)$ assumed to be a continuous function of k. N_L also determines the number of nodes of the zero-energy wave function $u_L(r)$. A knowledge of the nodal structure and of the *absolute* value of $\delta_L(0)$ is very useful in theoretical studies of low-energy potential scattering. Two preliminary attempts, one formal and one "physical," are made to extend the above results to single-channel scattering by a compound system initially in its ground state. The nodal structure will be of greater interest to us here than an extension of Levinson's theorem. The formal approach is applied to e^+-H and e^+-He scattering. Both H and He have zero orbital angular momentum and a nodeless ground-state wave function ψ_T. An effective one-body wave function u_L for the positron incident with zero kinetic energy can be constructed by factoring out the spin and Euler-angle dependence of the full scattering wave function Ψ and projecting the remaining "radial" function R_L onto ψ_T. The nodal surfaces of R_L are shown to divide configuration space into at most N_L+1 subdomains, where N_L is the number of composite bound states of the given L. Since $N_L=0$ for e^+-H and e^+-He, it follows that u_L is nodeless and that $\delta_L(0)=0$, for all L. Partial but useful information on the nodal structure of Ψ for e^--H scattering is also deduced. Interestingly, nodal surfaces exist which are not consistent with a naive generalization of (bound-state) one-dimensional Sturm-Liouville theory. The physical arguments, based on the qualitative concept of an effective central potential seen by each target particle *and* by the incident particle P, strengthen a previous surmise on the value of $\delta_{LJ}(0)$ for $e^{\pm}$-atom scattering and for the scattering of neutrons or protons by a heavy nucleus; L and J are the quantum numbers of the incident P, and ψ_T is assumed to have zero spin and zero orbital angular momentum, but ψ_T need *not* be nodeless, and P need *not* be distinguishable. Roughly, the surmise is that $\delta_{LJ}(0)=K_{LJ}\pi$, where, for the given L and J, K_{LJ} is the number of composite bound states plus the number of one-particle states excluded by the Pauli principle.

I. INTRODUCTION

The low-energy scattering of a particle by a potential $V(r)$ is conveniently described in terms of phase shifts $\delta_L(k)$, where L is the orbital angular momentum and k the wave number. Levinson's theorem[1] relates $\delta_L(0)-\delta_L(\infty)$ to N_L, the number of bound states of that L supported by the potential. If one adopts an absolute definition of the phase [one may, for example, choose $\delta_L(\infty)=0$] the theorem can be expressed in terms of the zero-energy phase shift alone and can then be used to provide information on the nodal structure of the zero-energy wave function. Alternatively, still in the context of a potential problem, one can extend the standard methods used in the analysis of the discrete eigenfunctions of the Sturm-Liouville equation to an analysis of the zero-energy scattering wave function; combined with a knowledge of the threshold behavior of $\delta_L(k)$, one obtains an alternative proof of Levinson's theorem.[2] [We note that one can extend Levinson's theorem from scattering by potentials $V(r)$ for which $r^3V(r)\to 0$ as $r\to\infty$ to potentials which include a long-range repulsive Coulomb tail,[3] the relevant phase shift then being $\delta_{cL}(k)$, the phase shift relative to the Coulomb phase shift.] However arrived at, an absolute definition of $\delta_L(k)$ and a knowledge of the nodal structure of the zero-energy scattering wave function can be very useful as self-consistency checks in a theoretical study of zero-energy and low-energy potential scattering in a fashion which has been discussed previously.[2] (Note that for very low incident momentum $\hbar k$, the nodal structure for most V's will not be expected to vary from its structure at zero energy for distances less than of the order of $1/k$.)

While the potential scattering problem is of considerable interest, one must ultimately address the much more difficult problem of scattering by a system with internal degrees of freedom (the many-body problem). We will consider the possibility of generalizing some of the results obtained for potential scattering to many-body scattering problems. One of the limitations which we will impose upon the many-body problems to be considered is that there be an energy interval—which includes zero incident kinetic energy—which is describable in terms of single-channel scattering processes. We will consider two approaches. In Sec. II we will use a formal approach, rigorous except when noted otherwise. These results are, perhaps, the first rigorous results concerning the nodal structure of the zero-energy wave function obtained for scattering by real compound systems, but the corollary of rigor is, unfortunately, a narrowness of the domain of ap-

plicability. In our rigorous approach, we have restricted our atomic targets to just H and He; these are the only atoms for which, for the ground-state wave functions, the spin dependence appears as a factor and for which the spatial function is nodeless. This in no way implies that the nodal structure of the zero-incident-energy wave function cannot be determined for other targets, but that determination will surely be more difficult. In particular, the Sturm-Liouville differential equation and the associated theory, or rather the extension to the many-body partial differential equation, is applicable when there is only one function to be determined and when the coefficient functions which appear in the differential operator are local; because of the Pauli principle, neither of these conditions is met for either the target wave function or the full scattering wave function for targets other than H or He, and an approach different from that used here will be required. Again to avoid the additional complexities originating in the Pauli principle, in our rigorous approach we have largely restricted our considerations to a distinguishable incident particle. In the case of a nuclear target, we cannot even consider a deuteron in our rigorous approach; for neutron-deuteron or proton-deuteron scattering, the Pauli principle involves an incident particle and a target particle. (This is not the case for e^+-He scattering.) For Λ-d scattering one has a composite bound state to contend with. (This too is not the case for e^+-He scattering.) Except for heavy nuclei, the nuclear case also presents the problem of separating out the center of mass, a problem not present effectively for $e^{\pm}$-atom scattering for any atom.

Simple extensions of formalisms found useful in bound-state problems to analyses of zero-incident-energy scattering problems have proved very fruitful in the past. It is therefore interesting that, as will be shown in Sec. II G, the zero-incident-energy scattering wave function can have a nodal structure different from that predicted by a naive extension of bound-state Sturm-Liouville theory.

In our rigorous analysis we are sometimes able to determine the nodal structure of the full scattering wave function even though we are unable to remove the ambiguity in the multiple of π in the value of $\delta_L(0)$. It should be noted that a knowledge of the nodal structure by itself can be valuable in theoretical studies.

In Sec. III the approach is physical and nonrigorous, and this section can be read independently. Useful insights are obtained by adopting a simple model of the scattering system based on the assumption of an effective central potential seen by each of the particles. This model leads to a prediction concerning the zero-energy phase shift which agrees with one made some years ago by Swan[4] who used a different (and, in our opinion, rather more complicated) argument to arrive at his very interesting result. Our schematic approach depends so little upon the details of the scattering components that its extension to scattering processes in which a repulsive Coulomb interaction is included is immediate. (Examples include proton-nucleus scattering and e^+—positive-ion scattering.) Swan did not consider cases which involve Coulomb interactions.

II. RIGOROUS RESULTS

A. General remarks

In our earlier treatment of potential scattering[2] we showed how classical Sturm-Liouville theory,[5] applicable to systems with a discrete spectrum of energy eigenvalues, could be generalized to the zero-energy scattering problem to provide information on the nodal structure of the zero-energy wave function. The analysis consisted of the following steps.

(i) The minimum principle for the scattering length[6] was used to show that the number of nodes of $u_L(r)$, the zero-energy wave function of angular momentum L, cannot exceed the number N_L of negative-energy bound states of the same L. In particular, it follows, if $N_L=0$, that u_L is nodeless and $\delta_L(0)=0$.

(ii) Discrete eigenfunctions of the radial wave equation have the property that nodes of successive eigenfunctions interlace one another. Since this property may be extended to include the zero-energy wave function it follows that u_L has precisely N_L nodes.

(iii) This information on the nodal structure of u_L, combined with the nodal definition of the phase shift, was shown to provide an alternative derivation of Levinson's theorem.

Since, in going from the one-body to the many-body bound-state problem, the interlacing property is lost, we have no simple generalization of steps (ii) and (iii) above. However, the minimum principle for the scattering length does have a multiparticle generalization so that one may attempt to generalize step (i). While the information to be derived from this approach is necessarily less complete for the multiparticle case than for single-particle scattering it is potentially more useful as a guide to numerical calculations since these are so much more difficult in the former case.

It will be convenient to discuss the extension of step (i) in the context of a few specific scattering systems and we shall do so below. We mention first, however, that we limit our considerations to systems for which only elastic scattering is possible, and for which the spin and Euler angular dependence of the wave function can be factored out, leaving a single "radial" function R_L of internal coordinates. In generalizing step (i) we might adopt as a guide the Courant-Hilbert treatment of the multidimensional Sturm-Liouville problem[5] and attempt to show that for scattering at zero incident kinetic energy of the projectile the number of nodal surfaces in R_L divides the domain in which it is defined into no more than N_L+1 subdomains, where N_L is the number of composite bound states of total orbital angular momentum L. (We assume for simplicity that there is no composite bound state at threshold.) Some of the examples given below satisfy this property but some do not; it follows that the property cannot be valid in general. The reason the property is not necessarily valid in many-body scattering processes is best understood in the context of concrete examples, and we postpone a somewhat more general discussion until the end of this section, after consideration of some of those examples. Basically, the reason is that nodal surfaces may be demanded by antisymmetrization requirements: *not all*

nodes are a consequence of the existence of states of lower energy.

Note though that if only elastic scattering is possible, if the spin and Euler angles can be factored from the wave function, and if the incident particle is distinguishable, we *can* adapt the Courant-Hilbert treatment of the multidimensional Sturm-Liouville problem and we can therefore show that the domain of R_L contains at most N_L+1 subdomains, and, in particular therefore, if there are no composite bound states of the given L, the R_L is nodeless. We will assume initially that the Hamiltonians are spin independent.

B. e^+-H scattering

As a first example we consider the scattering of a positron, incident with zero energy and angular momentum L, by a hydrogen atom in its ground state. The locations of the e^+ and e^- with respect to the proton (assumed to be fixed in space) will be denoted by $\mathbf{r}$ and $\mathbf{r}_1$, respectively, with θ representing the angle between $\mathbf{r}$ and $\mathbf{r}_1$. After factoring out the spin and angular momentum functions we are left with the function $R_L(r_1,r,\theta)$, the radial component of the Lth partial wave. It follows from the discussion in the above subsection that this function is nodeless since, as has been shown,[7] there is no composite e^+-H bound state. [There are no hitches in the argument since the particles are distinguishable and the hydrogenic ground-state wave function $\psi_T(r_1)$ is of course nodeless.]

A straightforward (if not unique) way to assign an absolute value to the phase shift $\delta_L(k)$ is to project the radial wave function (appropriate to scattering with wave number k) on to the target wave function; the phase shift is then chosen to be that which one would assign in a one-body problem whose wave function $u_L(r)$ was given by that projection. [Note that $u_L(r)$ satisfies the boundary conditions at $r=0$ and at $r\sim\infty$ of a one-body scattering wave function.] More explicitly for e^+-H scattering with $k=0$ we define

$$u_L(r)=\int\int \psi_T(r_1)R_L(r_1,r,\theta)r_1^2 dr_1 \sin\theta\, d\theta\ , \qquad (2.1)$$

which is interpreted as the equivalent one-body wave function. Since both $\psi_T(r_1)$ and $R_L(r_1,r,\theta)$ are nodeless functions we conclude that $u_L(r)$ is nodeless from which it follows[2] that $\delta_L(0)=0$ for all L.

The analogous problems involving the systems e^+-He^+, e^+-Li^{2+}, etc., could be treated using considerations very similar to those given above for e^+-H zero-energy scattering. To begin, we note that it can be shown that a positron cannot be bound to any hydrogenlike target with nuclear charge $Z\geq 1$. Furthermore, the modifications in the analysis made necessary by the presence of a repulsive Coulomb tail in the effective e^+-target interaction have been worked out.[3] We shall not elaborate on these matters here, but shall return in Sec. III to a consideration of Coulomb effects in the context of the proton-nucleus scattering problem.

C. e^+-He scattering

We may ignore the spin of the e^+; the spins of the target electrons play a role only in connection with the exclusion principle. The He ground-state wave function is the product of a symmetric function $\Omega(r_1,r_2,\theta_{12})$ of the spatial coordinates of the two electrons (θ_{12} is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$) and of a singlet spin function. The determination of $\Omega(r_1,r_2,\theta_{12})$ is then equivalent to the determination of the ground-state wave function of two bosons interacting with each other and with a center of force, and it is known that the wave function is then nodeless.[8] (In the context of the theorem which we have been using, this can be readily understood if we invoke the nondegeneracy of the ground state of He. The theorem tells us that with no restrictions on symmetry the ground-state wave function is nodeless. Since the Hamiltonian is symmetric in the electron coordinates it follows from the assumption of nondegeneracy that the ground-state wave function is either spatially symmetric or spatially antisymmetric. Since any antisymmetric wave function has a node, it follows that the ground-state wave function is symmetric and nodeless and represents the physical ground state of He.) The full scattering wave function will also have a singlet spin function as a factor, the radial factor R_L being a function of six spatial coordinates. These may be chosen to include, in addition to r_1, r_2, and θ_{12}, the angle θ_{1p} between $\mathbf{r}_1$ and the position $\mathbf{r}$ of the positron, the magnitude r, and an azimuthal angle ϕ_{12} which specifies the rotation of the $\mathbf{r}_1,\mathbf{r}_2$ plane about an axis along $\mathbf{r}_1$; two of the Euler angles would then specify the direction of $\mathbf{r}$ and the third would be the azimuthal angle of $\mathbf{r}_1$ relative to $\mathbf{r}$. It is known[9] that there is no composite e^+-He bound state and it follows from the previous discussion that R_L is nodeless. To determine $\delta_L(0)$ we define the equivalent one-body function u_L as the inner product

$$u_L(r)=\int r_1^2 dr_1 \int r_2^2 dr_2 \int \sin\theta_{12} d\theta_{12} \int \sin\theta_{1p} d\theta_{1p} \int d\phi_{12}\,\Omega(r_1,r_2,\theta_{12})R_L(r_1,r_2,\theta_{12},\theta_{1p},\phi_{12},r)\ . \qquad (2.2)$$

Since each of the functions Ω and R_L is nodeless, u_L is itself nodeless and one deduces here too that $\delta_L(0)=0$ for all L.

D. $L=0$ e^--H scattering, for H in its ground state

With $\delta_0^{(\pm)}(0)$ defined in a manner analogous to that discussed above for e^+-H and e^+-He scattering it has been shown[10] that $\delta_0^{(-)}(0)\geq\pi$ for the spatially antisymmetric $L=0$ triplet state for e^--H scattering. Thus, with $R_0^{(-)}(r_1,r_2,\theta_{12})$ the spatially antisymmetric factor in the full zero-incident-energy scattering wave function, where θ_{12} is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$, and with ψ_{1s} the spatial factor of the hydrogenic $1s$ state, the spatial component $u_0^{(-)}$ of the equivalent one-body $L=0$ zero-energy triplet scattering problem is given by

$$u_0^{(-)}(r_1)=\int\int \psi_{1s}(r_2)R_0^{(-)}(r_1,r_2,\theta_{12}) \times r_2^2 dr_2 \sin\theta_{12} d\theta_{12}\ . \qquad (2.3)$$

It follows that

$$\int \psi_{1s}(r_1)u_0^{(-)}(r_1)r_1^2 dr_1 = 0 , \tag{2.4}$$

since $\psi_{1s}(r_1)\psi_{1s}(r_2)$ is symmetric in r_1 and r_2 while $R_0^{(-)}$ is antisymmetric, and integration is over r_1 and r_2 (and θ_{12}). Since ψ_{1s} is nodeless, $u_0^{(-)}(r_1)$ must have at least one node, which leads to the result quoted; in fact, one would expect to have $\delta_0^{(-)}(0)$ equal to π, but this has not been proved. Of course, one can obtain a rather accurate representation of $R_0^{(-)}(r_1,r_2,\theta_{12})$ in the course of a many-parameter variational calculation of the triplet scattering length $A_0^{(-)}$ for the triplet $L=0$ case, and if this is based on a close-coupling calculation in which one expands $R_0^{(-)}(r_1,r_2,\theta_{12})$ as an antisymmetrized product of hydrogenic functions and arbitrary functions, $u_0^{(-)}(r_1)$ is the function which multiplies $\psi_{1s}(r_2)$. One can then simply examine $u_0^{(-)}(r_1)$ and see how many nodes it has, but it is somewhat unsatisfying to require a heavy calculation to obtain what would seem to be a simple result, namely, that as a consequence of the Pauli principle, one has $\delta_0^{(-)}(0)=\pi$. (We will shortly return to the numerical evaluation of phase shifts when we comment on e^--Li scattering.)

In reality, we know more about $R_0^{(-)}$ than that it is antisymmetric. Working in the region defined by $0\le\theta_{12}\le\pi$, $0\le r_1\le\infty$, and $r_1\le r_2<\infty$, and imposing the boundary condition that $R_0^{(-)}(r_1,r_1,\theta_{12})=0$ and the usual boundary conditions elsewhere, it is simple to show that $R_0^{(-)}$ is nodeless within the region just defined. In other words, the *only* nodal surface of $R_0^{(-)}(r_1,r_2,\theta_{12})$ over its entire domain is that at $r_1=r_2$, a nodal surface demanded by the Pauli principle. We have been unable to exploit this information and the knowledge that ψ_{1s} is nodeless to show from Eq. (2.3) that—what we assume to be the case—$u_0^{(-)}$ has only one node.

Correspondingly, we know that $R_0^{(+)}(r_1,r_2,\theta_{12})$, the spatially symmetric $L=0$ zero-incident-energy singlet scattering function, has at most one nodal surface, for there is one and only one singlet state of H^- with an energy below that of the ground state of H. As in the spatially antisymmetric case the proof is based on an application of the basic theorem to the function $R_0^{(+)}(r_1,r_2,\theta_{12})$ in the region $0\le\theta_{12}\le\pi$, $0\le r_1\le\infty$, $r_1\le r_2\le\infty$, but now with the boundary condition $\partial R_0^{(+)}/\partial r_1=\partial R_0^{(+)}/\partial r_2$ to be satisifed on the surface $r_1=r_2$. (The reason for working in the subdomain $r_1\le r_2$ rather than the full space in the e^--H problem will be clarified in Sec. II G below.) The fact that $R_0^{(+)}$ must be orthogonal to the H^- ground-state wave function (which is nodeless) allows us to exclude the possibility that $R_0^{(+)}$ has no nodal surfaces—there is one and only one such surface. Nevertheless, we have been unable to exploit this knowledge to obtain information on the number of nodes of $u_0^{(+)}(r_1)$, defined similarly to the $u_0^{(-)}$ of Eq. (2.3) but with $R_0^{(-)}$ replaced by $R_0^{(+)}$. One should be able to prove that $\delta_0^{(+)}=\pi$, with the origin of the π the bound state, not the Pauli principle.

E. e^--Li scattering

We have no rigorous results to report for this system but we include some remarks on it here, introducing physical considerations developed more fully in Sec. III. The ground state of Li is reasonably well described by the configuration $(1s)^2(2s)$, and, experimentally, it is known that the only composite bound state of Li and an e^- is a spatially symmetric singlet bound state of zero total orbital angular momentum. One might therefore expect—there is no question of a proof here—that $\delta_0^{(+)}(0)=2\pi$ and that $\delta_0^{(-)}(0)=2\pi$, the superscripts $+$ and $-$ referring, as for e^--H scattering, to spatially symmetric singlet scattering and spatially antisymmetric triplet scattering, respectively. In both cases one π should come from the presence of the $1s$ state and the demands of the exclusion principle. In the singlet case the second π should arise because of the singlet bound state, while in the triplet case the second π should again originate in the exclusion principle. These expectations are consistent with numerical computations;[11] the numerically calculated zero-energy scattering wave functions were obtained and projected onto the numerically calculated Li ground-state wave function, and the equivalent one-body singlet and triplet wave functions were each found to have two nodes, a result which gave the authors greater confidence in the accuracy of their calculations.

Since the basic configuration of the ground state of Li has no one-particle state with orbital angular momentum greater than zero, and since there is no bound state of Li^- with total orbital angular momentum greater than zero, one would expect to have $\delta_L^{(\pm)}(0)=0$ for all $L>0$.

F. $L=1$ *even* parity e^--H scattering (H in an excited state)

We have up to this point always assumed the target to be initially in its ground state. The following discussion may be of some interest, in spite of its rather restricted nature, because it deals with the fundamental e^--H system and because it is the only case considered here in which the target is not in its ground state. In general, the problem of scattering from an excited target is a multichannel one and the nature of the discussion thus far limits our considerations to single-channel scattering, characterized by a single partial differential equation containing only one unknown function. Furthermore, the total energy should be at the bottom of that portion of the continuum to which the state is coupled. We now show, however, that by virtue of certain selection rules our analysis can be extended (in at least one case) to allow for an excited target.

In general, in an analysis of e^--H scattering, we do not have one second-order partial differential equation for one function, as we do for $L=0$ singlet and triplet scattering of e^- by H in its ground state. Rather, we have coupled partial differential equations, with the number of equations equal to the number of functions to be determined. More precisely, for both singlet and triplet scattering, with $L_{\rm tot}$ the total orbital angular momentum and Π the parity of the entire system, we have[12]

$L_{\rm tot}$ even, $\Pi=+1$: $L_{\rm tot}+1$ functions

$L_{\rm tot}$ even, $\Pi=-1$: $L_{\rm tot}$ functions

$L_{\rm tot}$ odd, $\Pi=+1$: $L_{\rm tot}$ functions

$L_{\rm tot}$ odd, $\Pi=-1$: $L_{\rm tot}+1$ functions .

In particular, therefore, there is no state with $L_{\text{tot}}=0$ and $\Pi=-1$. (That is easy to see; $L_{\text{tot}}=0$ requires a superposition of products of states with the same orbital angular momenta, so that the parity must be even.) To have one and only one function, we must consider (i) $L_{\text{tot}}=0$, $\Pi=+1$ or (ii) $L_{\text{tot}}=1$, $\Pi=+1$. For case (i), one possibility is to have the H atom in its ground state and the incident electron to have zero incident orbital angular momentum, but that is the case considered in Sec. II D; other possibilities are for the target to be in an excited state and for the target and the incident particle to have the same orbital angular momentum, coupled to $L_{\text{tot}}=0$, but these states are coupled to the ground state and must be excluded from our considerations for a number of reasons, one of which is that they represent multichannel situations. We turn to case (ii). This does not allow the target to be initially in its ground state, nor is the state coupled to the ground state. (With the H atom in its ground state the incident particle would have to have $L=1$ and even parity, which is not possible.) There is, however, one interesting example of (ii), a particle incident with unit orbital angular momentum on a H atom in the $2p$ state, so that $\Pi=+1$, with the orbital angular momenta coupled to give $L_{\text{tot}}=1$. The spatial wave functions of the associated states, with angular momentum projections $m=\pm1$ and 0, are the $x\pm iy$ and z components, $Q_{1m}^{(-)}$, of $\mathbf{Q}_1^{(-)}(\mathbf{r}_1,\mathbf{r}_2)=(\hat{\mathbf{r}}_1\times\hat{\mathbf{r}}_2)g$; we assume that $g\equiv g(r_1,r_2,\theta_{12})=g(r_2,r_1,\theta_{12})$, so that the wave functions are spatially antisymmetric and we are concerned with the triplet case. The situation is a single-channel one, describable by one partial differential equation for the one function $g(r_1,r_2,\theta_{12})$—the Euler-angle dependence, contained in the factor $\hat{\mathbf{r}}_1\times\hat{\mathbf{r}}_2$, can be factored out—and the basic theorem is applicable to the region $0\le\theta_{12}\le\pi$, $0\le r_1\le\infty$, $r_1\le r_2\le\infty$ with $\partial g/\partial r_1=\partial g/r_2$ for $r_1=r_2$. We may conclude that the nodal surfaces of $g(r_1,r_2,\theta_{12})$ divide the full domain into no more than $N_1^{(-)}+1$ subdomains, where $N_1^{(-)}$ is the number of triplet bound states of unit orbital angular momentum, where a bound state is here one with an energy below $-\frac{1}{4}$ rydberg, the energy of the $n=2$ level. (We are assuming that the interaction with the radiation field has been turned off, so that we are concerned here with true bound states.) One such state is known to exist.[13] Assuming that there is only one such state, the nodal surfaces of $g(r_1,r_2,\theta_{12})$ divide the full domain into at most two subdomains. The spatial wave functions of the above-mentioned bound state, that with $\Pi=+1$ and $L=1$, with angular momentum projections $m=\pm1$ and 0, are the $x\pm iy$ and z components, $P_{1m}^{(-)}$, of

$$\mathbf{P}_1^{(-)}(\mathbf{r}_1,\mathbf{r}_2)=(\hat{\mathbf{r}}_1\times\hat{\mathbf{r}}_2)h(r_1,r_2,\theta_{12})\ .$$

Since $h(r_1,r_2,\theta_{12})$ and $g(r_1,r_2,\theta_{12})$ are eigenfunctions of the same (modified) Hamiltonian, they must be orthogonal; furthermore, since h is the eigenfunction of that Hamiltonian associated with the lowest eigenvalue, h must be nodeless. It follows that g must have at least one nodal surface. Combined with the upper limit on the number of nodal surfaces discussed just above, it follows that g must have just one nodal surface. It may be helpful to note that the analysis of the nodal structure of g is almost identical to the analysis of the nodal structure of the radial function $R_0^{(+)}(r_1,r_2,\theta_{12})$ introduced in connection with e^--H scattering in Sec. II D.

Considerations of the absolute phase shift for the present problem are also almost identical to those which arose in Sec. II D. The present case is in some regards more interesting, however, for one might have supposed that the zero-incident-energy phase shift would be 2π, with one π arising from the nodal surface along $\hat{\mathbf{r}}_1=\hat{\mathbf{r}}_2$, a nodal surface intimately connected with the Pauli principle, and with the second π having its origins in the existence of a composite bound state. In fact, if one makes the seemingly natural assumption that the absolute phase shift is to be defined by the structure of g, a function with one nodal surface, one would guess that the absolute phase shift would be π, not 2π. (The difficulty in being more precise is the same as that in the case discussed in Sec. II D; a knowledge of the nodal structure of the many-body wave function, by itself, does not determine the absolute value of the phase shift.) The somewhat surprising feature is that the factor $\hat{\mathbf{r}}_1\times\hat{\mathbf{r}}_2$, the Euler-angle factor, plays no role in the dynamics if the absolute phase shift is defined by the properties of g.

In the next section we consider a scattering process under some simplifying assumptions—the target is massive and has no spin or orbital angular momentum, and there exists an "equivalent" one-body central potential. It is then shown that the absolute zero-incident-energy phase shift is a multiple of π, where the multiple contains two contributions, one associated with states excluded by the Pauli principle and one with composite bound states. If that result were always valid, the phase shift in our present problem would be 2π. Since, in fact, that phase shift seems to be π rather than 2π, it is to be expected that the result just quoted, and derived in Sec. III under the specified assumptions, cannot be valid under all circumstances. (There is no contradiction, since the H target under consideration here, having nonzero orbital angular momentum, does not satisfy those specified assumptions.)

G. Special features of the nodal structure of the zero-incident-energy many-body wave function

In a partial-wave analysis of the single-channel scattering of a particle incident with zero kinetic energy on a target, it is often convenient to think of the system as being at the top of the discrete spectrum rather than at the bottom of the continuous spectrum. The convenience lies in the fact that the properties of the continuum state, and in particular its scattering length and its nodal structure, can often be studied by the Sturm-Liouville (SL) methods applicable to bound states. We will now show that this extension of SL bound-state results to the continuum state is *not* always possible. In particular, we will show that the continuum state can have a nodal surface which would not be expected on the basis of SL theory.

Let us return to the study of $L=0$ zero-incident-energy e^--H triplet scattering from the ground state. The antisymmetric spatial wave function $R_0^{(-)}(r_1,r_2,\theta_{12})$ has of course a nodal surface (along $r_1=r_2$). Since e^- and H can form a composite bound state, the existence of a nodal surface of $R_0^{(-)}$ in no way violates the theorems which

might be expected to serve as the natural generalizations of (bound-state) SL theory. However, let us consider a model problem, rather similar to the e^--H problem, but with the two-particle Coulomb interactions modified; we allow them to be short ranged, but they must be local and energy independent. As for e^--H, there would be two indistinguishable spin-$\frac{1}{2}$ particles. With the interaction strengths appropriately chosen, each particle would be capable of forming a bound state with the target, but, as opposed to the physical potentials, the model potentials would be unable to support a composite bound state. The nodal surface along $r_1=r_2$ of the triplet $L=0$ zero-incident-energy wave function, denoted by $R_0^{(-)}(r_1,r_2,\theta_{12})$ as for the true problem, would be present even though there is no state of lower energy. This result is in definite contradiction to what one might expect as a generalization of bound-state SL theory, perhaps the first such contradiction to have been found, and it is important to understand how this comes about.

Nodal surfaces originating in the Pauli principle divide configuration space into subdomains which extend out to infinity and in which the scattering wave function satisfies inhomogeneous boundary conditions. For our model problem we have

$$R_0^{(-)}(r_1,r_2,\theta_{12})\sim\psi_{1s}(r_1)(r_2-A),\quad r_2\sim\infty$$
$$\sim-\psi_{1s}(r_2)(r_1-A),\quad r_1\sim\infty$$

where ψ_{1s} is similar to the hydrogenic $1s$ wave function, and, in particular, is nodeless. It follows that a trial function which vanishes identically in one of the two subdomains of our model problem, the subdomain $r_1>r_2$ or $r_2>r_1$, fails to satisfy the boundary conditions at infinity and is therefore inadmissable. Since in bound-state problems the theorems which place upper limits on the number of subdomains are based on trial functions which vanish identically over subdomains, these theorems are inapplicable to our e^--H problem, for the physical system or for the model system. In other words, for our model system we have a (Pauli-induced) nodal surface in a zero-incident-energy scattering wave function even though there is no state of negative energy. This is contrary to what one might have expected on the basis of SL bound-state theory, but there is no contradiction since the SL proofs are inapplicable.

We note that an analogous situation—the existence of a nodal surface for a state even though there is no state of lower energy—cannot occur for any bound state of our model problem; the lowest state cannot have a node induced by the Pauli principle because whatever the model potentials the ground state will not be spatially antisymmetric, and the (Pauli) node associated with the lowest spatially antisymmetric state will come as no surprise. Indeed, in a SL approach, one ignores all symmetry requirements and (for any number of particles) finds that the state of lowest energy—it might not be physically allowable—is nodeless. For our model problem that excludes the possibility that the ground state is spatially antisymmetric. (One must go further to prove that the state of lowest energy is nondegenerate and is the physically allowed spatially symmetric state, but that is not relevant to the present argument.) A nonmathematically oriented physicist might find more satisfying the following alternative proof that the ground state of the e^--H model problem cannot be spatially antisymmetric. Let the lowest spatially antisymmetric state have an energy $E^{(-)}$ and a normalized spatial wave function

$$\psi^{(-)}(r_1,r_2,\theta_{12})=\phi(r_1,r_2,\theta_{12})-\phi(r_2,r_1,\theta_{12})\equiv\phi-\tilde{\phi}\ ;$$

ϕ is a solution of the Schrödinger equation in the region $0\le r_2\le r_1\le\infty$, which vanishes at $r_1=r_2$ and at $r_1=\infty$. ϕ will be positive for $0\le r_2<r_1<\infty$. [It will be of the form $(r_1-r_2)g(r_1,r_2,\theta_{12})$, with $g>0$ for $0\le r_2<r_1<\infty$.] In a Rayleigh-Ritz estimate $E_t^{(+)}$ of the energy $E^{(+)}$ of the lowest spatially symmetric state with $E^{(+)}\le E_t^{(+)}$, choose as the trial function

$$\psi_t^{(+)}(r_1,r_2,\theta_{12})=|\psi^{(-)}(r_1,r_2,\theta_{12})|\ ;$$

$\psi_t^{(+)}$ is continuous with a piecewise continuous first derivative and is therefore an admissable trial function. With $\Sigma(x)$ a step function, one has

$$\psi_t^{(+)}=(\phi-\tilde{\phi})\Sigma(r_1-r_2)+(\tilde{\phi}-\phi)\Sigma(r_2-r_1)\ ,$$

and, using the fact that $\phi-\tilde{\phi}$ vanishes where $\psi_t^{(+)}$ has a discontinuous derivative, it is simple to show that

$$E^{(+)}\le E_t^{(+)}=\langle\psi_t^{(+)}|H|\psi_t^{(+)}\rangle$$
$$=\langle\,|\psi^{(-)}|\,|H|\,|\psi^{(-)}|\,\rangle$$
$$=\langle\psi^{(-)}|H|\psi^{(-)}\rangle=E^{(-)}\ .$$

Once again, this does not show (though it very strongly suggests) that the ground state is spatially symmetric—as it is—but it does show that it is not spatially antisymmetric.

We close this section with just one remark on systems containing more than two electrons, noting that even the meaning of a nodal surface must be reexamined. It will be sufficient to consider a three-electron system, which might be the ground state of Li or an e^--He scattering state. Since the spin dependence cannot in general be factored out for a system with three electrons, the wave function will be an antisymmetrized sum of products of spatial functions and spin functions and may well not have any nodal surface of sufficiently high dimensionality—dimensionality eight in the nine-dimensional problem under consideration—to separate the full volume into subdomains. For such a system, any theorems on nodal structure which one might hope to obtain would refer to the nodal structure of one of the spatial factors in the sum of products.

III. NONRIGOROUS RESULTS: A PHYSICAL ARGUMENT

When we consider the scattering of positrons by atoms heavier than helium we no longer have the pleasant situation that the target ground-state wave function factors into a spin function and a nodeless spatial function. We now turn our attention to the scattering of electrons and positrons by atoms, and neutrons and protons by heavy nuclei, in the context of some simple models.

A. $e^{\pm}$-atom scattering

Some very interesting speculations on $\delta_L(0)$ for the scattering of an electron by a neutral atom were made by Swan.[4] Using approximate antisymmetrized wave functions based on an independent-particle model, he derived an integro-differential equation and showed that the related (approximate) $\delta_L(0)$ satisfied a modified form of Levinson's theorem. (This approach has been developed further, though still within the context of a specific scattering model, by Glöckle and Le Tourneux.[14] The distinction between a rigorous proof and one based on a model should be kept clearly in mind throughout this discussion.) We will here adopt a much simpler and less mathematical viewpoint, also approximate, one which would be expected to be most useful for heavy atoms; our simple viewpoint will reproduce Swan's results for e^--atom scattering. We assume that the ground state of the neutral atom has a total orbital angular momentum of zero and a total spin of zero, and for the moment, that the e^- and the atom cannot form a negative ion. We assume in addition that there exists an effective short-range central potential $V(r)$ which, in an independent-particle model, generates an approximate target ground-state wave function $\psi_{T,\text{app}}$, an antisymmetrized product of one-particle states, which provides a good description of the properties of the atom. To be concrete, we will choose a particular atom ($Z=30$) with a particular configuration, $(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^{10}(4s)^2$. We must then also assume, since for the moment we wish to exclude cases for which a negative ion can be found, that $V(r)$ supports only $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, and $4s$ states. Finally, we assume that the scattering of the incident electron can be reasonably described by assuming that the problem is a one-body problem with the *same* potential $V(r)$. Since, in the above example, $V(r)$ can support four $L=0$ states, two $L=1$ states, one $L=2$ state, with all bound states assumed to have negative energy, and no states with $L>2$, it follows from Levinson's theorem as originally derived, that

$$\delta_0(0)=4\pi,\quad \delta_1(0)=2\pi,\quad \delta_2(0)=\pi,\quad \delta_L(0)=0 \quad \text{for } L>2\ . \tag{3.1}$$

In obtaining Eq. (3.1), we used results obtained from an analysis of the radial equation for a particle of angular momentum L in a potential $V(r)$, and it follows that the degeneracy with respect to projections of the spin or orbital angular momenta of the individual target electrons does not enter in the determination of $\delta_L(0)$.

We now drop our assumption that a negative ion cannot exist and assume, to be concrete, that one and only one negative-ion state, a $5s$ state, does exist. We would then demand of $V(r)$ that it be capable of supporting one and only one additional state, a $5s$ state, and one would expect to have $\delta_0(0)=5\pi$; *very* crudely, one might think of 4π as the contribution arising from Pauli effects and π as arising from the bound state. The phase shifts $\delta_L(0)$ for $L\neq 0$ would not be affected.

In the same approximate spirit, one might assume that the potential seen by a e^+ incident on an atom is equal but opposite to the $V(r)$ seen by an e^- incident on an atom. Since $V(r)$ is expected to be attractive for all r, that would imply that $-V(r)$ is repulsive everywhere. The e^+ could not then be bound to any atom, and one would have $\delta_L(0)=0$ for all L for all atoms. [In fact, there are some atoms with which an e^+ can form one bound state, with the e^+ in an s state, and for such atoms the assumption that the effective potential is everywhere repulsive is of course incorrect and one would expect to have $\delta_0(0)=\pi$ and $\delta_L(0)=0$ for $L>0$.] Looking at the problem slightly differently, it would not be *too* unreasonable to assume, for a e^+ incident on an atom to which it cannot be bound, that the e^+ has little effect on the target atom, and that the zero-energy scattering wave function is therefore a product of the target ground-state wave function $\psi_T(\boldsymbol{\rho})$ and a function of $u(r)$ of the positron coordinate; this is the static approximation. The inner product of $\psi_T(\boldsymbol{\rho})u(r)$ and $\psi_T(\boldsymbol{\rho})$ would then be $u(r)$. Since the effective e^+-atom interaction has been assumed to be weak, we expect $u(r)$ to be nodeless, and it follows that $\delta_L(0)=0$ for all L. In this slightly different approach, we made three assumptions: that there was no composite bound state, that the static approximation was a good approximation, and that the factor $u(r)$ in the static approximation was nodeless. In fact, once we have made the static approximation the other results follow, for the nodelessness follows if the equivalent one-body potential cannot support a bound state and, following Ore,[15] one can easily prove that in the static approximation the e^+ cannot form a composite bound state. Thus, the e^+ satisfies a one-body equation with an effective potential

$$V_{\text{eff}}(r)=\int \psi_T(\boldsymbol{\rho})\left[\sum_{i=1}^{Z}\frac{-e^2}{|\mathbf{r}_i-\mathbf{r}|}+\frac{Ze^2}{r}\right]\psi_T(\boldsymbol{\rho})d\boldsymbol{\rho}\ . \tag{3.2}$$

Since $\psi_T(\boldsymbol{\rho})$ is a state of zero total orbital angular momentum, we can replace $|\mathbf{r}_i-\mathbf{r}|^{-1}$ by $1/r_{i>}$, where $r_{i>}$ is the larger of r_i and r. V_{eff} then becomes

$$V_{\text{eff}}(r)=e^2\int \psi_T^2(\boldsymbol{\rho})\sum_{i=1}^{Z}\left[\frac{1}{r}-\frac{1}{r_{i>}}\right]d\boldsymbol{\rho}\ , \tag{3.3}$$

a repulsive potential. [Note that in the static approximation the nodal structure of $u(r)$, namely, its nodelessness, follows without any information about $\psi_T(\boldsymbol{\rho})$ other than that it has zero total orbital angular momentum; in particular, the nodal structure of $\psi_T(\boldsymbol{\rho})$ does not enter the argument.] The assumption made in the second viewpoint, that the target is unaffected by the e^+, is surely a more restrictive assumption than one would like to make, but the argument does provide some physical insight.

It is important to recognize that while $V(r)$ must give all of the appropriate one-particle states (and only those states) for the atom under consideration, $V(r)$ need *not* give the correct energies of those states. It follows from the above remark and from one's experience of effective central potential studies that an adequate $V(r)$ is available for almost all of the atoms, those with zero spin and zero total orbital angular momentum, under consideration. On the other hand, if it is because we do not need a $V(r)$ which is precisely defined that we can readily accept the

validity of the surmise on $\delta_L(k)$, it is for that very same reason that we do not have a proper proof of that surmise. Stated somewhat differently, the requirement that $V(r)$ generate a $\psi_{T,\text{app}}$ "which provides a good description of the properties of the atom" can hardly be the starting point of a rigorous proof of the surmise. The point is that ψ_T is not one configuration but a superposition of configurations, and that the zero-incident-energy wave function Ψ is not the product (antisymmetirzed if the incident particle is an e^-) of a one-particle function and of the one configuration for ψ_T but a sum of products of one-particle functions and of target configurations, and that the surmise involves the assumption that the superposition of configurations in ψ_T and in Ψ alters neither the nodal structure of Ψ nor $\delta_L(0)$ from the results obtained using just one configuration for ψ_T and for Ψ. (One can hope, as we do, to use an approximate theory to obtain an exact result if the result has a discrete rather than continuous characterization.)

B. Neutron and proton scattering by heavy nuclei

The physical argument for the value of $\delta_L(0)$ just given for $e^{\pm}$-atom scattering can be applied with essentially no change to neutron—heavy-nucleus scattering. We here allow for spin-orbit coupling, since that coupling is generally more significant in the nuclear case; allowance for that coupling could just as easily have been made in the $e^{\pm}$-atom case.

We consider a nucleus heavy enough so that the neutron mass can be neglected with respect to the nuclear mass. We assume that no composite bound state can be found, that the ground state has zero total spin and zero total orbital angular momentum, and that there exists an effective one-body potential of the form $V(r)+\mathbf{L}_i\cdot\mathbf{S}_i U(r)$, where $\mathbf{L}_i$ and $\mathbf{S}_i$ refer to the ith particle, such that the ground-state wave function is adequately described by a product of one-particle states determined by this potential. The potential is such that it supports all of those and only those one-particle states which generate a wave function providing a good description of the properties of the ground state. We assume further that the incident neutron experiences precisely the same effective one-body potential, which we can rewrite as $V(r,L,J)$, with L and J referring to the quantum numbers of the incident neutron. It follows that the phase shift at zero energy, $\delta_{LJ}(0)$, is, in this approximation, a multiple of π, the multiplicative factor K_{LJ} being equal to the number of neutrons in the target in states with the given L and J, degeneracy playing no role. In analogy with the discussion in the previous subsection, one would expect K_{LJ}, for the case in which $V(r)$ can support ν_{LJ} additional states of the given L and J, to be increased by ν_{LJ}. (The additional states would represent composite bound states.)

It has recently been shown[3] that Levinson's theorem is satisfied for potential scattering, where the potential is the sum of a repulsive Coulomb field and a short-range potential; the relevant phase shift is $\delta_{cLJ}(k)$, the phase shift relative to the Coulomb phase shift. We therefore expect the argument just given for the value of $\delta_{LJ}(0)$ for the scattering of a neutron by a heavy nucleus to be valid for the $\delta_{cLJ}(0)$ which appears in the scattering of a proton by a heavy nucleus. The effective one-body central potential would now include the component Ze^2/r, where Z is the atomic number of the target nucleus.

Note added in proof. Sturm-Liouville theory has been used to obtain a Levinson-like theorem for the Dirac equation. See Z. Q. Ma, Phys. Rev. D **32**, 2213 (1985) and references therein.

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