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Generalized Levinson theorem: Applications to electron-atom scattering

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A recent formulation provides an absolute definition of the zero-energy phase shift δ for multiparticle single-channel scattering of a particle by a neutral compound target in a given partial wave l. This formulation, along with the minimum principle for the scattering length, leads to a determination of δ that represents a generalization of Levinson's theorem. In its original form that theorem is applicable only to potential scattering of a particle and relates δ/π to the number of bound states of that l. The generalized Levinson theorem relates δ/π for scattering in a state of given angular momentum to the number of composite bound states of that angular momentum *plus* a calculable number that, for a system described in the Hartree-Fock approximation, is the number of states of that angular momentum excluded by the Pauli principle. Thus, for example, for electron scattering by Na, with its $(1s)^2(2s)^2(2p)^6 3s$ configuration and with one $L=0$ singlet composite bound state, δ would be $\pi+2\pi$ for s-wave singlet scattering, $0+3\pi$ for s-wave triplet scattering, and $0+\pi$ for both triplet and singlet p-wave scattering; the Pauli contribution has been listed first. The method is applicable to a number of $e^{\pm}$-atom and nucleon-nucleus scattering processes, but only applications of the former type are described here. We obtain the absolute zero-energy phase shifts for e^--H and e^--He scattering and, in the Hartree-Fock approximation for the target, for atoms that include the noble gases, the alkali-metal atoms, and, as examples, B, C, N, O, and F, which have one, two, three, four, and five p electrons, respectively, outside of closed shells. In all cases, the applications provide results in agreement with expectations. [S1050-2947(96)03512-3]

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I. INTRODUCTION

The classic Levinson theorem relates the zero-energy phase shift δ, for scattering of a particle of orbital angular momentum l by a short-range potential, to the number of bound states of that l. To generalize the theorem to multiparticle single-channel scattering, it is essential, as first pointed out by Swan [1] in the context of an independent-particle model, that δ be related to the actual number of composite bound states *plus* the number of composite bound states excluded by the Pauli principle. [For $l=0$, for e^--He, for example, there would be a $(1s)^3$ bound state were it not for the Pauli principle.] A recent generalization [2] of Levinson's theorem does exactly that, in a precise and model-independent way. The argument, stripped of details irrelevant for our present purposes and of proofs, is as follows. A zero-energy electron in the lth partial wave is incident on an $M-1$ electron target with an orbital angular momentum L_T and spin S_T. (The validity of LS coupling is assumed here for simplicity; generalizations are possible, as discussed in Ref. [2].) The normalized antisymmetrized target wave function is $\Psi_T(x_2,\ldots,x_M)$, where x_j represents the space and spin coordinates of the jth target electron. We form $\Psi(s_1,\Omega_1;x_2,\ldots,x_M)$, with s_1 and Ω_1 representing the spin and angular coordinates, respectively, of particle 1, by coupling the L_T and S_T of Ψ_T with the l and spin $\frac{1}{2}$ of the incident particle to form an initial state with total orbital and spin angular momenta and projections L, L_z, S, and S_z. [We cite two examples. If $L_T=S_T=0$, as for targets with closed subshells only, and $l=0$, then Ψ is independent of Ω_1 and assumes the simple form

$$\Psi(s_1;x_2,\ldots,x_M)=\Psi_T(x_2,\ldots,x_M)\chi_{1/2}^{\pm 1/2}(1), \quad (1.1)$$

where the one-particle spin function $\chi_{1/2}^{\pm 1/2}$ has a projection $\pm\frac{1}{2}\hbar$ and Ψ has $L=L_z=0$, $S=\frac{1}{2}$, and $S_z=\pm\frac{1}{2}$. (We often label coordinates by particle number to simplify notation.) If $L_T=0$ and/or $l=0$, and $S_T\neq 0$, the coupling would involve only spins. Note that the exact scattering wave function does not enter in this construction.] With $P_{i\leftrightarrow j}$ interchanging x_i and x_j, with

$$\mathcal{A}_1 \equiv 1-\sum_{j=2}^{M} P_{1\leftrightarrow j}, \quad (1.2)$$

and assuming for simplicity that $L_T=0$, we form the fully antisymmetrized function

$$U(x_1,x_2,\ldots,x_M)=\mathcal{A}_1[\Psi(s_1;x_2,\ldots,x_M)r_1^l Y_{l0}(\Omega_1)]. \quad (1.3)$$

An effective one-particle wave function

$$F(r_1)=\int d\Omega_1 Y_{l0}(\Omega_1)\int d\mathbf{r}_2\cdots d\mathbf{r}_M \Psi^\dagger(s_1;x_2,\ldots,x_M) \times U(x_1,\ldots,x_M), \quad (1.4)$$

where $\mathbf{r}$ is a spatial coordinate and where there is a summation over the spin coordinates of the target particles and the incident particle, is the projection of U first onto Ψ and then onto the lth partial wave of the incident particle. With N_{Pauli} the number of nodes of $F(r_1)$, the phase shift associated with $F(r_1)$ is defined to be $N_{\text{Pauli}}\pi$. It is then proved that $\delta=(N_{\text{Pauli}}+N)\pi$, where N is the number of bound states of angular momentum l and spin S. (Here we assume that there are no zero-energy bound states; the effect of such states, when they exist, can be accounted for [2].) The treatment of cases in which $L_T\neq 0$ proceeds along similar lines. Circumstances under which only single-channel scattering is possible, so that a real-valued zero-energy phase shift exists, were analyzed in Ref. [2]. Here we merely remark that for $l=0$, the case of greatest interest, the zero-energy phase shift exists for any values of the remaining angular momentum quantum numbers, whether or not LS coupling is valid. With LS coupling assumed, the zero-energy phase shift exists for $L_T=0$; it exists for $L_T=1$ if $L=0$ or 1, but not if $L=2$, a consequence of the existence of a long-range polarization contribution to the effective scattering potential. We return to this point in Sec. II C, below.

The function $r_1^{\,l}$ in Eq. (1.3) is the zero-energy free-particle solution of the radial Schrödinger equation. This form is appropriate for potentials of short range, but an electron scattering from an atom experiences a long-range polarization potential and this requires that, for $l\geqslant 1$, the function $r_1^{\,l}$ be replaced by a more accurate solution accounting for the long-range interaction. The procedure for doing this was developed in detail in Ref. [2]. In the applications below to atoms with $Z>2$, Ψ_T will be replaced by its Hartree-Fock approximation. With the true target Hamiltonian replaced by its Hartree-Fock approximation, the results cited above can be applied for $l\geqslant 1$ as well as for $l=0$. The formalism is readily modified to include the effect of a long-range repulsive Coulomb interaction between projectile and target [2].

Applications of the generalized Levinson theorem to e^--atom scattering are described in Sec. II. Results obtained for H are rigorous and for He they are essentially so: use of more accurate He wave functions than those considered here would be pointless. As mentioned, Hartree-Fock wave functions were used as approximations to the wave functions of the heavier target atoms, with explicit results obtained for the noble gases, the alkali-metal atoms, and, as examples of atoms with one to five p electrons outside closed subshells, B, C, N, O, and F.

II. ELECTRON SCATTERING BY A NEUTRAL ATOM

A. e^--H

As a first application we consider s-wave electron scattering from hydrogen in its ground state. In either the singlet or triplet state the spin function can be factored out so that only the spatial part of the wave function (symmetric in the singlet and antisymmetric in the triplet state) needs to be considered in determining N_{Pauli}. We first consider scattering in the triplet state. While the $1s$ target function is of course known in this case, we present the analysis in a manner that requires less than complete knowledge of this function to illustrate a procedure that will be used in our treatment of e^--He scattering and may be of use in treating still more complex atomic targets and even more so in the study of the scattering of nucleons by nuclei, where the bound-state wave functions are known only very poorly. All that needs to be known of the spatial part $\psi_{1s}(r_2)$ of the target wave function is that it has its maximum value at the origin, decreases monotonically to zero, and satisfies the normalization condition $\int\psi_{1s}{}^2(r)d\mathbf{r}=1$. With the spins omitted, we find that $\Psi(\mathbf{r}_2)=\Psi_T(r_2)=\psi_{1s}(r_2)$, $\quad U=(4\pi)^{1/2}[\psi_{1s}(r_2)-\psi_{1s}(r_1)]$, and

$$F_{\text{triplet}}(r_1)=1-I(r_1), \tag{2.1}$$

where $I(r)=\psi_{1s}(r)\int\psi_{1s}(r')d\mathbf{r}'$. One sees immediately that F_{triplet} has at least one node since it is orthogonal to the nodeless function ψ_{1s}. More explicit information is obtained by noting that the maximum value of $I(r)$ satisfies

$$I_{\max}=I(0)=\psi_{1s}(0)\int\psi_{1s}(r')d\mathbf{r}'>\int\psi_{1s}^2(r')d\mathbf{r}'=1. \tag{2.2}$$

We conclude that $F_{\text{triplet}}(r_1)=1-I(r_1)$ is negative at the origin, increases monotonically, and approaches unity at great distances; it therefore has a single node, so that $N_{\text{Pauli}}=1$. Since no triplet bound state exists for the composite system it follows that $\delta_{\text{triplet}}=\pi$. It should be emphasized that we are able to obtain the precise result $\delta_{\text{triplet}}=\pi$ for the s-wave triplet phase shift by virtue of the fact that our procedure does not require knowledge of the exact scattering wave function; only its Born approximation enters the analysis. In an alternative method proposed some time ago [3,4], the phase shift was defined (in principle) by applying the nodal definition to the equivalent one-body wave function obtained by projecting the exact zero-energy scattering wave function onto the target ground-state function. Then, from the fact that the triplet e^--H wave function is spatially antisymmetric, it follows directly that the equivalent one-body wave function must have at least one node since it is orthogonal to the hydrogenic ground-state function. One can conclude in this way only that the phase shift so defined is at least π.

A similar procedure applied in the case of singlet s-wave scattering leads to the form $F_{\text{singlet}}(r_1)=1+I(r_1)$, with $I(r_1)$ defined as above, so that there are no nodes and $N_{\text{Pauli}}=0$; since one and only one singlet bound state exists we conclude immediately that $\delta_{\text{singlet}}=\pi$. An extension of this analysis shows that the zero-energy phase shift vanishes for $l>0$ for both triplet and singlet states. Here one observes that since the H ground state is an s wave, the analog of the function $I(r_1)$ appearing in Eq. (2.1) contains the projection of ψ_{1s} on to a higher partial wave and therefore vanishes.

B. e^--He

Turning now to the s-wave e^--He problem, we take the normalization condition for the spatial part of the target ground-state wave function to be $\int\psi_{\text{He}}^2(\mathbf{r}_2,\mathbf{r}_3)d\mathbf{r}_2d\mathbf{r}_3=1$. The phase shift is independent of the spin projection of the incident electron; we take the projection to be $\hbar/2$ and find that

$$\Psi(s_1;x_1,x_2)=\psi_{\text{He}}(\mathbf{r}_2,\mathbf{r}_3)\chi_0(2{,}3)\alpha(1),$$

where $\chi_0(2{,}3)$ is the spin-zero function for the (2,3) pair, $\alpha(1)$ is $\chi_{1/2}^{1/2}(1)$, and

$$U(x_1,x_2,x_3)=(4\pi)^{1/2}(1-P_{1\leftrightarrow 2}-P_{1\leftrightarrow 3})\Psi(s_1;x_2,x_3).$$

In the evaluation of $F(r_1)$, the unit term in $(1-P_{1\leftrightarrow 2}-P_{1\leftrightarrow 3})$ gives unity and $P_{1\leftrightarrow 2}+P_{1\leftrightarrow 3}$ can be replaced by $2P_{1\leftrightarrow 2}$. The spin factor of the $2P_{1\rightleftarrows 2}$ term is $\frac{1}{2}$ and we find $F(r_1)=1-I(r_1)$ for the effective one-particle wave function, where, since $l=0$,

$$I(r_1)=\int \psi_{\mathrm{He}}(\mathbf{r}_2,\mathbf{r}_3)\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)d\mathbf{r}_2 d\mathbf{r}_3 . \tag{2.3}$$

In arriving at Eq. (2.3), we were able to omit the average $(4\pi)^{-1}\int d\Omega_1$ that is formally required in Eq. (1.4) since this overlap integral is independent of the direction of $\mathbf{r}_1$. This greatly simplifies the analysis, given immediately below, for it enables one to work with the full target wave function ψ_{He}, and all that needs to be known of ψ_{He} is the fact that it is normalized to unity; one does not need to determine the s^2 component of ψ_{He}, that component for which each electron is in an s state. [On the other hand, for the analysis of the p-wave phase shift, for which the angular integration cannot be avoided, we will see shortly that it will be necessary to obtain an (approximate) analytic form of the p^2 component of ψ_{He}.] The direction of $\mathbf{r}_1$ is assumed to have been fixed arbitrarily in Eq. (2.3). An explicit evaluation of this integral using very accurate helium wave functions would allow one to determine (with high confidence) the number of nodes in $F(r_1)$. This, coupled with the fact that there is no stable negative helium ion, would provide us with the value of the zero-energy phase shift. This value is almost certainly π. Thus it is known that $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ is nodeless [5,6], for, the spins having been eliminated and the spatial function being symmetric, the electrons can be treated as bosons. If we make the assumption (which is intuitively reasonable, but thus far not rigorously proved, to our knowledge) that for any fixed values of r_3 and $|\mathbf{r}_3-\mathbf{r}_1|$, the maximum value of $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ is achieved for $r_1=0$ and that $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ is a monotonically decreasing function of r_1, the argument given in the discussion following Eq. (2.1), showing (for e^--H triplet scattering) that $F(r_1)$ has a single node, applies directly to this case, implying that $\delta=\pi$ [7]. We tested the above monotonicity assumption on several variationally determined approximations to $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$, including Kinoshita's ten-parameter trial function [8], and the assumption is verified in these tests [9]. More accurate helium wave functions are available for more stringent tests that are rather simpler to perform than would be an explicit evaluation of the integral appearing in Eq. (2.3).

In the extension of these considerations of e^--He scattering to an arbitrary partial wave it is convenient to introduce the expansion

$$\psi_{\mathrm{He}}(\mathbf{r}_2,\mathbf{r}_3)=\sum_{\Lambda=0}^{\infty}\psi_{\Lambda}(r_2,r_3)\sum_{M_\Lambda=-\Lambda}^{\Lambda}Y_{\Lambda M_\Lambda}(\Omega_2)Y^{*}_{\Lambda M_\Lambda}(\Omega_3). \tag{2.4}$$

The effective one-particle wave function for the lth partial wave then takes the form

$$F(r_1)=r_1^l-\int_0^\infty r_2^2 dr_2\int_0^\infty r_3^2 dr_3\,\psi_l(r_2,r_3)\psi_l(r_1,r_3)r_2^l . \tag{2.5}$$

To study $F(r_1)$ for $l=1$, we evaluated the $l=1$ component ψ_1 of the three-parameter Hylleraas trial function [8] and found that $F(r_1)$ is nodeless, a result that, as expected [10], is consistent with the vanishing of the $l=1$ phase shift [11]. The same result is expected for all higher partial waves, as could now be verified by evaluation of the integral appearing in Eq. (2.5) using a sufficiently accurate trial function. (Presumably, as we have noted previously [2], an *exact* determination of the target wave function is not required since the result sought has a discrete rather than a continuous characterization.)

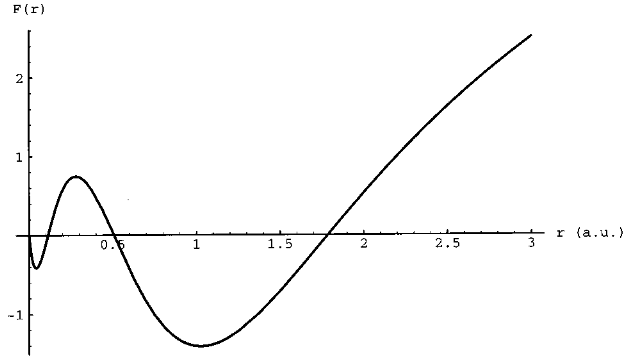

FIG. 1. Plot of the function $F(r)$ [see Eq. (2.6) of the text] for s-wave scattering by argon. The appearance of three nodes (excluding the zero at the origin) shows that the Pauli contribution to the zero-energy phase shift is 3π. An additional factor of r was included in this plot.

C. Heavier targets in the Hartree-Fock approximation

1. Atoms with closed subshells

We now discuss several applications of this procedure to electron scattering by heavier targets, with accurate analytic representations [12] of solutions of the Hartree-Fock equations used to approximate the target ground-state wave functions. We consider scattering in the lth partial wave and denote the target orbitals as $R_{nl}(r)Y_{lm_l}(\Omega)\chi_{1/2}^{m_s}$ with $\int_0^\infty R_{nl}^2(r)r^2dr=1$. It is then found, for targets with closed subshells and therefore with vanishing total spin and orbital angular momentum, that the effective one-body wave function is of the form (see Appendix A)

$$\begin{aligned}F(r)&=r^l-\sum_{n=l+1}^{l+\nu_l}R_{nl}(r)\int_0^\infty R_{nl}(r')r'^l r'^2dr'\\&\equiv\prod_{n=l+1}^{l+\nu_l}(1-P_{nl})r^l.\end{aligned} \tag{2.6}$$

Here ν_l is the number of closed subshells of angular momentum l and P_{nl} is the projection operator $|R_{nl}\rangle\langle R_{nl}|$. Using the data in Ref. [12] for the target atoms Be, Ne, Mg, Ar, and Kr we calculated and then plotted $F(r)$ to determine the number of nodes, N_{Pauli}, in this function and hence the contribution to the zero-energy phase shift originating in the Pauli principle. [As an illustration, we present in Fig. 1 a plot of $F(r)$ for s-wave scattering by Ar.] We found in each case that $N_{\mathrm{Pauli}}=\nu_l$, which determines the zero-energy phase shift as $\delta=(\nu_l+N)\pi$, where N, the number of composite bound states of the given l, is zero for any l for Ne, Ar, and Kr; their s-wave phase shifts are therefore 2π, 3π, and 4π, respectively. It appears [13] that no composite Mg$^-$ bound state exists and that the ^2S state of Be$^-$ is the only stable state of this system, so that $\delta=3\pi$ for the scattering of s-wave electrons from both Mg and Be. Our results for the

s-wave scattering from rare-gas target atoms conform to a prediction made by Swan [1], but we decidedly disagree with his statement that the effect of the Pauli principle may be ignored for $l>0$. We note that the calculated value $N_{\text{Pauli}}=\nu_l$ is the expected one, as it corresponds to the number of states excluded by the Pauli principle [6]. The zero-energy p-wave phase shifts of Be, Ne, Ar, and Kr are therefore 0, π, 2π, and 3π, respectively. Kr has a d-wave phase shift of π. It hardly seems necessary, but if one wished to establish the above results with even greater certainty one would have to show that in each case the same number of nodes is obtained using even more accurate approximations to the ground-state wave function. No scattering calculations need to be performed.

We remark that for $\nu_l=1$ the presence of a single node can be deduced without performing the integration indicated in Eq. (2.6). It is sufficient to observe that for such a state the Hartree-Fock function $R_{nl}(r)/r^l$ has some of the same essential properties as the Coulombic $R_{nl}(r)/r^l$, namely, it has its maximum at the origin and decreases monotonically to zero. (One verifies this immediately by noting that functions of this type are represented, in the tables of Ref. [12], as sums of decaying exponentials with positive coefficients [14].) We expect that additional simplifications in the determination of nodal structures could be obtained from an examination of the general features of the radial wave functions. As an example, suppose that each of the functions $R_{nl}(r)$ can be represented, to a good approximation, as the solution of a one-body wave equation for a given potential $V_l(r)$. It can be shown, with the aid of methods described in Ref. [2], that the zero-energy scattering function $\Pi_{i=1}^{N}(1-P_i)r^l$, where P_i projects onto the ith bound state, has N nodes if $V_l(r)$ has N bound states of angular momentum l. Thus there exists a very strong *expectation* that the function defined in Eq. (2.6) has ν_l nodes; this is consistent with numerically determined results that we obtained for several particular cases.

TABLE I. Illustration of the generalized Levinson theorem for s- and p-wave electron scattering by some of the lightest atoms. (See the text for discussion of O, F, and Ne.) Only nonvanishing zero-energy phase shifts are listed. The integer preceding ${}^{2S+1}L$ in the second column is the principal quantum number of the subshell from which the projectile is excluded. The listing of the negative-ion-states includes a labeling of the outer-shell configurations.

Target	Pauli excluded states	Negative-ion states	$\delta\,(l=0)$	$\delta\,(l=1)$
H	$1\,{}^3S$		π	
		$1s^2\ {}^1S$	π	
He	$1\,{}^2S$		π	
Li	$1\,{}^3S$, $2\,{}^3S$		2π	
	$1\,{}^1S$	$2s^2\ {}^1S$	2π	
Be	$1\,{}^2S$, $2\,{}^2S$	$3s\ {}^2S$	3π	
B	$1\,{}^3P$, $2\,{}^3P$		2π	
	$1\,{}^1P$, $2\,{}^1P$		2π	
	$2\,{}^3S$			π
	$2\,{}^1P$			π
		$2p^2\ {}^3P$		π
C	$1\,{}^4P$, $2\,{}^4P$		2π	
	$1\,{}^2P$, $2\,{}^2P$		2π	
	$2\,{}^2S$			π
	$2\,{}^4P$			π
		$2p^3\ {}^4S$		π
N	$1\,{}^5S$, $2\,{}^5S$		2π	
	$1\,{}^3S$, $2\,{}^3S$		2π	
	$2\,{}^5P$			π
		$2p^4\ {}^3P$		π
Na	$1\,{}^1S$, $2\,{}^1S$	$3s^2\ {}^1S$	3π	
	$1\,{}^3S$, $2\,{}^3S$, $3\,{}^3S$		3π	
	$2\,{}^1P$			π
Na	$1\,{}^1S$, $2\,{}^1S$	$3s^2\ {}^1S$	3π	
	$1\,{}^3S$, $2\,{}^3S$, $3\,{}^3S$		3π	
	$2\,{}^1P$			π
	$2\,{}^3P$			π
Mg	$1\,{}^2S$, $2\,{}^2S$, $3\,{}^2S$		3π	
	$2\,{}^2P$			π

2. Atoms with incomplete subshells

We also applied the procedure described above to the scattering of electrons by atoms with incomplete subshells. We first consider the problem of s-wave scattering of electrons by the alkali-metal atom Li in its ground state. The effective one-body wave function for this system is found, assuming the Hartree-Fock approximation for Li, to be

$$\begin{aligned} F(r)&=1-R_{10}(r)\int_0^\infty R_{10}(r')r'^2dr\mp R_{20}(r)\int_0^\infty R_{20}(r')r'^2dr \\ &=1-P_{10}1\mp P_{20}1, \end{aligned} \tag{2.7}$$

where the minus (plus) sign before the second integral corresponds to scattering in the triplet (singlet) spin state. A proof of Eq. (2.7) is provided in Appendix B. We find two nodes in this function for the triplet case and one node in the singlet case. Since the only composite bound state is a singlet, we conclude that $\delta=2\pi$ for each spin state. (This is in agreement with an earlier prediction [6] based on the central-field approximation.) The generalization to heavier alkali-metal targets follows immediately from the derivation of Eq. (2.6) given in Appendix A and from Eq. (2.7). If there are ν_0 closed $l=0$ subshells and there is one s electron with principal quantum number ν_0+1, $F(r)$ for s-wave scattering is given by

$$F(r)=1-\sum_{n=1}^{\nu_0}P_{n0}1\mp P_{(\nu_0+1)0}1. \tag{2.8}$$

Thus $F(r)$ for s-wave scattering by Na will have the structure appropriate to the $F(r)$ for Ne, with an additional term corresponding to the $3s$ valence electron, the sign being negative (positive) for triplet (singlet) scattering. A plot of this function shows, as expected, three nodes for the triplet state and two for the singlet state. We conclude that $\delta=3\pi$ for each spin state since, as for Li, the only composite bound state is a singlet. The function $F(r)$ appropriate to singlet or triplet p-wave scattering by Na has a single node. This conclusion follows from a cursory inspection of the parameters listed in Ref. [12] for the p-wave orbital of Na, which shows that the orbital is a monotonically decreasing function; no calculation is necessary.

To illustrate the application of the generalized Levinson theorem, we present, in Table I, a compilation of zero-energy phase shifts (only nonvanishing phases are listed) for electron scattering by several of the lightest atoms; the necessary information, the number of composite bound states and states excluded by the Pauli principle, is also included. In the absence of zero-energy resonances, the predicted phase shift is $\delta=(N_{\text{Pauli}}+N)\pi$, where N is the number of negative-ion bound states (zero or one in the cases considered) and N_{Pauli} is the number of nodes in the effective one-body wave function $F(r_1)$ defined in Eq. (1.4). [The definition of $F(r_1)$ given in Eq. (1.4) is valid only for $L_T=0$, but the extension to $L_T\neq 0$ is trivial, demanding only the coupling of orbital angular momenta.] The essence of the generalized Levinson theorem is the statement that N_{Pauli} thus defined is equal to the number of bound states excluded by the Pauli principle. By determining the number of nodes in $F(r)$ we are able to confirm this property for the atomic targets listed in Table I. Note that δ depends on the incident orbital angular momentum l and the total orbital and spin angular momenta L and S of the system. (The allowable values of S and L depend upon l, S_T, and L_T.) We have analyzed electron scattering by Li and by atoms with closed subshells, which includes Be, and so we go on to study, in turn, electron scattering by the atoms from B to F, with one to five p electrons.

Consider boron, with its $(1s)^2(2s)^2(2p)$ ^2P configuration. For $l=0$, the excluded ^3P and ^1P states are $(1s)^3(2s)^2(2p)$ $^{3,1}P$ and $(1s)^2(2s)^3 2p$ $^{3,1}P$, while for $l=1$ the excluded ^3S and ^1P states correspond to $(1s)^2(2s)^2(2p)^2$. (A ^3D state is excluded as well, but we omit discussion of p-wave scattering with $L=2$ since, as remarked in Sec. I and discussed in more detail in Ref. [2], the scattering is not restricted to a single channel in this case.) We turn next to C, with its $(1s)^2(2s)^2(2p)^2$ ^3P ground-state configuration. The analysis of δ for $l=0$ is rather similar to that for B. For $l=1$, angular momentum conservation allows S, P, and D singlet and triplet states, while the states that arise from three p electrons (with the same n) are ^4S, ^2D, and ^2P; ^2S, ^4D, and ^4P states are excluded. Reference to p-wave scattering with $L=2$ is omitted in Table I, for the reason mentioned above. Next on the list is N, with its $(1s)^2(2s)^2(2p)^3$ ^4S configuration; the angular factor of the $(2p)^3$ component, totally antisymmetric to minimize the Coulomb repulsion, is $\hat{\mathbf{r}}_1\cdot\hat{\mathbf{r}}_2\times\hat{\mathbf{r}}_3$, with zero total orbital angular momentum. The analysis of s-wave scattering is similar to some of the cases considered above and we consider p-wave scattering. A ^5P state is excluded, since it would demand that four p electrons be in a totally antisymmetric spatial state, but a ^3P state is allowed. (The listing of this state in Table I is tentative since its existence is uncertain [13].) We find that $F(r_1)=(1-P_{21})r_1$ for the excluded ^5P state, so that $\delta=\pi$ for this state, while for the ^3P state we have $F(r_1)=[1+\frac{1}{3}P_{21}]r_1$; there is, therefore, no Pauli contribution to this state, consistent with the fact that it is not excluded. The analysis of scattering by O with its four $2p$ electrons is identical to that for C with its two $2p$ electrons, while the scattering by F with its five $2p$ electrons is identical to that for B with its one p electron.

At this stage we know how to analyze target atoms with closed subshells only and those with closed subshells plus one electron in an s state or one to five electrons in the same p state. This accounts for a large fraction of all of the atoms, and the methodology could readily be extended to other atoms with closed subshells and with only one open subshell.

III. DISCUSSION

The analysis of the zero-energy scattering of positrons by atoms along the lines developed above is particularly simple since the projectile is distinguishable from the particles in the target. The conclusion reached previously [6] that the zero-energy phase shift δ vanishes in each partial wave for e^+-H and e^+-He is confirmed. Since the present approach, unlike that given earlier, does not depend on a knowledge of the structure of the true scattering wave function, it is not only simpler but, more significantly, is applicable to positron scattering by any neutral or positively ionized atomic target. There are some atoms with which an e^+ can form one bound state, with the e^+ in an s state, and for such atoms one would have $\delta=\pi$ for $l=0$ and $\delta=0$ for $l>0$. There is a wide class of problems, including the scattering of electrons by positive ions, which cannot be treated by the present method owing to the presence of an attractive Coulomb tail in the effective projectile-target potential. It had been suggested earlier [15] that it might be possible to establish a connection (involving the quantum defect) between the phase shift generated by the short-range component of the potential and the number of additional bound states that it generates. Such a connection has recently been established (using methods quite different from those employed here) for the one-body potential scattering problem [16]. Subsequently [17], an extension applicable to scattering by a compound target has been developed, thus enlarging significantly the class of problems to which generalized versions of Levinson's theorem can be applied.

We once again emphasize that the results obtained are for a function δ, which at zero energy has discrete rather than continuous values. The results therefore tend to be rather robust; the use of imprecise target wave functions and the omission of small perturbations, such as spin-orbit interactions, will not normally affect the value of δ [18]. These remarks, and our continued efforts to provide arguments independent of details, may be of interest, but are not essential in the atomic cases analyzed here since the interactions are well known and Hartree-Fock wave functions are available. However, they have been very useful in our studies (to be reported on subsequently) of nucleon-nucleus scattering, where the interactions and target wave functions are relatively poorly known.

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APPENDIX A: FORMS FOR $F(r_1)$ FOR CLOSED SUBSHELLS ONLY

Rather than proving Eq. (2.6) for an atom with an arbitrary set of closed subshells, we will prove it for Ne, which has all of the physical complexities of the general case and for which the notational details are less cumbersome. We let $\Theta_{n'l'}$ represent the normalized antisymmetric wave function for the $2(2l'+1)$ particles in the closed $n'l'$ subshell. Thus, for example, we have

$$\Theta_{1s}(2,3)=(4\pi)^{-1}R_{1s}(2)R_{1s}(3)\chi_0(2,3). \tag{A1}$$

The symmetrized Ne target wave function is then

$$\Psi_{\rm Ne}(2,\ldots,11)=\hat{\mathcal{A}}[\Theta_{1s}(2,3)\Theta_{2s}(4,5)\Theta_{2p}(6,\ldots,11)], \tag{A2}$$

where $\hat{\mathcal{A}}$ denotes antisymmetrization with respect to electrons in different subshells; the inclusion of an overall normalization factor for $\Psi_{\rm Ne}$ will be seen shortly to be unnecessary. Since $L_T=S_T=0$ for Ne, the wave function Ψ in Eq. (1.3) is given by

$$\Psi=\Psi_{\rm Ne}(2,\ldots,11)\alpha(1), \tag{A3}$$

where, without loss of generality, we have taken the incident particle to have spin up. The unit term in the operator $1-\Sigma_j P_{1\leftrightarrow j}$ appearing in Eqs. (1.2) and (1.3) gives r_1^l and Eq. (1.4) becomes

$$F(r_1)=r_1^l-\sum_{j=2}^{11}\int d\Omega_1 Y_{10}(\Omega_1)\int d\mathbf{r}_2\cdots d\mathbf{r}_{11} \times[\Psi_{\rm Ne}(2,\ldots,11)\alpha(1)]^\dagger[\Psi'_{\rm Ne}\alpha(j)r_j^l Y_{l0}(\Omega_j)], \tag{A4}$$

where $\Psi'_{\rm Ne}\equiv\Psi_{\rm Ne}(2,\ldots,j-1,1,j+1,\ldots,11)$ reflects the effect of $P_{1\leftrightarrow j}$ on Ψ. The integration over Ω_j vanishes unless the jth electron in $\Psi_{\rm Ne}(2,\ldots,11)$ has the quantum number l of the incident particle. [For the Ne atom under consideration we therefore have $F(r_1)=r_1^l$ for $l>1$, so that $F(r_1)$ is nodeless for $l>1$ and there is no Pauli phase shift.] Furthermore, by virtue of the orthogonality of R_{nl} and $R_{n'l}$ for $n\neq n'$, the only nonvanishing contributions come from the same distributions of electrons in the two sets of square brackets; if a term in the first set of brackets contains electrons 2 and 7 in the $1s$ state, the relevant terms in the second set of brackets must also contain electrons 2 and 7 in the $1s$ state, and $\hat{\mathcal{A}}$ in Eq. (A2) can be dropped; the particles in different subshells are effectively distinguishable. The integral over the coordinates in the subshells not containing the jth electron gives unity and we arrive at Eq. (2.6), with the subshells with $l'=l$ contributing separately, with the contribution from a subshell with $l'=l$ coming from the orbital with the quantum numbers $m'_{l'}$, and m'_s, the same as those of the incident electron, namely, $m_l=0$ and $m_s=+\frac{1}{2}$.

APPENDIX B: FORMS FOR $F(r_1)$ FOR ALKALI-METAL ATOMS

We first consider s-wave scattering by Li atoms; the extension to an arbitrary alkali-metal atom follows immediately. The spin projections ± and 0 for triplet scattering must give the same result and we choose to consider the zero projection, for the triplet and singlet scatterings can then be treated together. The normalized Ψ that appears in Eq. (1.3) is given by

$$\Psi(1;2,3,4)=3^{-1/2}(1-P_{2\leftrightarrow 4}-P_{3\leftrightarrow 4})\Gamma(1;2;3;4), \tag{B1}$$

where the coordinate 1 refers only to the spin and where, with Θ_{1s} defined by Eq. (A1),

$$\Gamma(1;2,3;4)=\Theta_{1s}(2,3)\psi_{2s}(4)\chi(1,4), \tag{B2}$$

where $\chi(1,4)$ is $\chi_0(1,4)$ for the singlet case and the spin-1 state with zero projection for the triplet case. The $3^{-1/2}$ factor reflects the orthonormality of the terms containing 1, $P_{2\leftrightarrow 4}$, and $P_{3\leftrightarrow 4}$. In fact, we note for later purposes that each pairing of two different terms of these three is orthogonal in each of two variables. [The pairing 1Γ and $P_{2\leftrightarrow 4}\Gamma$, for example, contains the factors $\psi_{1s}(3)\psi_{2s}(3)$ and $\psi_{1s}(4)\psi_{2s}(4)$.] Since $l=0$, the U of Eq. (1.3) is

$$U=\left(1-\sum_{j=2}^{4}P_{1\leftrightarrow j}\right)[\Psi(1;2,3,4)Y_{00}(\Omega_1)]. \tag{B3}$$

We can now write

$$F(r_1)=\int d\Omega_1\int d\mathbf{r}\;Y_{00}(\Omega_1)\Psi^\dagger(1;2,3,4)\left(1-\sum_{j=2}^{4}P_{1\leftrightarrow j}\right) \times[\Psi(1;2,3,4)Y_{00}(\Omega_1)], \tag{B4}$$

where $d\mathbf{r}\equiv d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4$. The unit term in $1-\Sigma_j P_{1\leftrightarrow j}$ makes a contribution of one to $F(r_1)$ and the integration over Ω_1 is trivial. Furthermore, since $P_{1\leftrightarrow j}$ changes only one of the j coordinates, the only nonvanishing contributions to $F(r_1)$ are those for which, for a given term in $\Psi^\dagger$, proportional to 1, $P_{2\leftrightarrow 4}$, or $P_{3\leftrightarrow 4}$, the corresponding term is taken in Ψ. The three terms 11, $P_{2\leftrightarrow 4}P_{2\leftrightarrow 4}$, and $P_{3\leftrightarrow 4}P_{3\leftrightarrow 4}$ make the same contribution and we arrive at

$$F(r_1)=1-3\times(3^{-1/2})^2\int d\mathbf{r}\;\Gamma^\dagger(1;2,3;4)(2P_{1\leftrightarrow 2}+p_{1\leftrightarrow 4}) \times\Gamma(1;2,3;4); \tag{B5}$$

we used the symmetry in 2 and 3 of $\Gamma(1;2,3;4)$ to replace $P_{1\leftrightarrow 3}$ by $P_{1\leftrightarrow 2}$. The remainder of the calculation is now trivial and gives Eq. (2.7).

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[7] The conditions assumed for $\psi_{1s}(r)$ and $\psi_{\rm He}(\mathbf{r}_1,\mathbf{r}_3)$ are sufficient but not necessary for the proofs that followed. The nec-

essary conditions on $\psi_{1s}(r)$, for example, are that its maximum value be greater than unity and that it achieve that value once and only once.

[8] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Plenum/Rosetta, New York, 1977), p. 151.

[9] We observed that for r_1 and r_3 fixed, $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ has its maximum for $|\mathbf{r}_3-\mathbf{r}_1|=r_3+r_1$, that is, for electrons 1 and 3 as far apart as possible. This property, along with the fact that $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ has its maximum at $r_1=0$ for any fixed values of $|\mathbf{r}_3-\mathbf{r}_1|$ and r_3, implies that $\psi_{\mathrm{He}}(\mathbf{r}_1,\mathbf{r}_3)$ has a ridge at $r_1=0$.

[10] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon, Oxford, 1965), p. 569.

[11] Rather than evaluate the integral in Eq. (2.5) explicitly, we found it sufficient to obtain an upper bound on it. With the magnitude of the second term on the right-hand side in Eq. (2.5) determined to be less than 3% of the first, there appears to be little urgency in repeating the calculation with more accurate trial functions. The function r_1^l appearing in Eq. (2.5) should have been replaced by the (nodeless) function accounting for the presence of a long-range polarization interaction. One can do so by following the prescription given in the Appendix of Ref. [2]. However, since the integral is so small, we have, for simplicity, ignored this replacement.

[12] E. Clementi and C. Roetti, *Atomic Data and Nuclear Data Tables* (Academic, New York, 1974), Vol. 177.

[13] H. S. W. Massey, *Negative Ions* (Cambridge University Press, London, 1976), p. 61.

[14] At least for low-lying levels, the monotonic decrease of the wave function is hardly surprising. If, for a given n and l, the size of the orbit is rather less than the length scale of the atom, which we take to be the Thomas-Fermi length scale $a_0/Z^{1/3}$, that is, roughly speaking, $n^2a_0/Z<a_0/Z^{1/3}$ or $n<Z^{1/3}$, the wave function will be at least roughly Coulombic. For Kr with $Z=36$, for example, $Z^{1/3}=3.3$ and the low-lying states include $1s$, $2s$, $3s$, $2p$, $3p$, and $3d$ states.

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