ARTICLES

Absolute determination of zero-energy eigenphase shifts: Applications to n-p, n-d, and p-d scattering

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A generalization of Levinson's theorem, relating the phase shift at zero energy to the number of bound states of the system, previously formulated to apply to the single-channel multiparticle scattering of a particle by a neutral system [L. Rosenberg and L. Spruch, Phys. Rev. A **54**, 4978 (1996)] is further generalized to allow for multichannel scattering. An application to neutron-proton scattering with tensor forces leads to an extension of the existing version of Levinson's theorem for this system by providing information on each of the eigenphases at zero energy rather than just their sum. The effect of the Pauli principle on the absolute determination of the phase shift is illustrated with applications of the method to the scattering of neutrons and protons by deuterons. [S0556-2813(98)02009-3]

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I. INTRODUCTION

Levinson's theorem relates the number of bound states in a given partial wave to the zero-energy partial-wave phase shift. There has been a renewal of interest in recent years in applications of this theorem to nuclear scattering problems [1]. This has been stimulated in part by the need to establish the compatibility of equivalent potentials—those that give rise to the same S matrix—with different numbers of bound states [2]. The original derivation of the theorem [3] was restricted to single-channel potential scattering. An extension to elastic multiparticle scattering, accounting for the effect of the Pauli principle, was conjectured by Swan [4] and has been adopted in the recent literature [2]. Swan's work was based on the independent-particle model and further analysis is required for it to be applied with complete confidence. Moreover, with tensor forces present a multichannel treatment is required, even for scattering at the physical threshold. This is an issue that arises with the use of supersymmetric quantum mechanics to relate phase-equivalent coupled-channel potentials [5]. A closer examination of the applicability to nuclear systems of theorems of the Levinson type therefore seems warranted.

A generalized Levinson theorem, valid for each partial wave, was given recently for multiparticle single-channel scattering of a particle by a neutral compound target [6]. It is formulated without dynamical assumptions (such as the independent-particle model) and avoids reference to a phase shift at infinite energy, nonexistent for scattering by compound targets. The procedure for determining the zero-energy phase shift requires information, not necessarily complete, concerning the target wave function; most significantly, conclusions are reached without the need to solve the scattering problem. The essential feature of the method is the use of the minimum principle for the scattering length, applicable to the wide class of scattering problems for which the scattering length can be defined. Soon after the original version of the minimum principle was derived [7] a useful corollary was proved by Ohmura [8], and it is this version that was applied in Ref. [6]. In addition to the minimum principle a knowledge of the energy-dependence of the phase shift near threshold, as obtained from effective range theory, plays a role in determining the effect of a zero-energy resonance on the phase shift.

Earlier applications were confined to single-channel electron-atom scattering [9]. Motivated partly by revived interest in theorems of the Levinson type we here discuss nuclear applications using an extended version of the approach of Ref. [6]. The manner in which the effects of the Pauli principle and repulsive Coulomb interactions are accounted for is illustrated by our treatment, in Sec. IV, of nucleon-deuteron scattering. The effect of a tensor force is discussed in Sec. III in the context of the neutron-proton system. The existing version for coupled-channel problems relates the sum of the eigenphases to the number of bound states [10]. An extended version, derived here, provides information on individual eigenphases—this should be helpful, for example, in an analysis of equivalent potentials in the problem of n-p scattering with tensor forces [5]. A generalization of the minimum principle applicable to multichannel scattering problems has been available for some time [11], but not a multichannel extension of Ohmura's corollary [8]; a proof suitable for our present purposes is given in Sec. V. To make our presentation reasonably self-contained we begin, in Sec. II, with a summary of our approach to Levinson's theorem in the context of the familiar single-channel potential scattering problem. The remainder of the paper will focus on new features of the theory.

II. PRELIMINARIES: SCATTERING BY A CENTRAL POTENTIAL

Sturm-Liouville theory, usually applied to bound states, has been extended to zero-energy potential scattering [12]. It

was shown that the number of nodes in the wave function, for arbitrary orbital quantum number l, is equal to the number of negative-energy bound states of the same l. This result, used in combination with the nodal definition of the phases shift, some information on its threshold behavior, and the minimum principle for the scattering length [7] leads to Levinson's theorem. Such an approach is not directly applicable to the multiparticle scattering problem since the relevant wave function has a complicated and poorly understood nodal structure. However, it does suggest that nodal properties may still play a role, though less directly, along with the minimum principle and effective range theory, in applications to a wider class of systems. These ideas, developed earlier [6], will now be reviewed. It will be done in the simpler context of potential scattering to provide a suitable background for the discussion to follow.

For definiteness we consider s-wave scattering by a short-range potential. Generalizations are mentioned briefly below. Let us first assume that the scattering length is finite. It then follows from effective range theory that the phase shift δ is a multiple of π in the zero-energy limit since cot δ is infinite. The Kohn variational principle for the scattering length is in fact a minimum principle provided that all bound states are included in the trial function with sufficient accuracy [7]. Ohmura's extension [8] gives a more detailed picture. Thus suppose there are N bound states. With the simplest trial function $\phi(r)=r$ obeying the boundary condition at infinity, the variationally determined scattering length $A^{(0)}$ is just the Born approximation. One considers (in principle) an infinite sequence of variational approximations for the scattering length in which the accuracy of the trial function is steadily improved. The set of approximations $A^{(s)}, s=0,1,...,$ is generated from the variational principle by introducing trial functions

$$f^{(s)}(r)=\phi(r)+\sum_{s'=1}^{s} b_{s'} f_{s'}(r), \tag{2.1}$$

with $f_1(r)\sim -1$ for $r\to\infty$. The calculated scattering length makes a series of upward jumps as the trial function is steadily improved with the addition of more basis functions and, after having made a total of N jumps, it converges to the exact value from above as s is increased indefinitely. It is then convenient to define a monotonically increasing ''length phase'' by writing $A^{(s)}=a$ cot $\eta^{(s)}$, where a is a characteristic length (a fermi, for example, in a nuclear scattering problem). The phase shift δ (at each stage of the approximation procedure) is defined by requiring that it lie on the same branch of the cotangent curve as η. More precisely, we impose the condition $0\leqslant \eta-\delta<\pi$. To obtain an absolute definition of the length phase, and hence the phase shift itself, we define a reference phase $\delta^{(0)}$ as the phase shift associated with the free wave function $\phi(r)$. Since this function is nodeless we must have, from the nodal definition, $\delta^{(0)}=0$. (A modification of this assignment is required when antisymmetry is accounted for in the multiparticle case; see Sec. IV for an example.) The corresponding length phase $\eta^{(0)}$ must then be chosen to lie between zero and π. This choice for the absolute definition of the phase shift for potential scattering is essentially determined by the requirement that it conform to the nodal definition combined with the relation between bound states and nodes in the zero-energy scattering function deduced earlier [12]. As indicated above, the advantage gained by this reformulation lies in the fact that it requires a nodal count of the free wave function $\phi(r)$ and not the full scattering wave function; it can therefore be applied unambiguously to the multiparticle scattering problem. (See Sec. IV.)

A divergence in the approximate scattering length corresponds to η passing from one branch of the cot η 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 $(N+1)\pi$. Since the scattering length has been assumed to be finite in this first example, the relation $A=a$ cot η implies that η/π is not an integer; it follows that $\delta=N\pi$.

If the scattering length is infinite, corresponding to the existence of an s-wave bound state at zero energy in addition to N negative-energy bound states, the process of minimization will not terminate after N upward jumps and the length phase will approach $(N+1)\pi$. From effective range theory we know that cot δ vanishes at threshold, so that, according to the definition given above, namely, $0\leqslant \eta-\delta<\pi$, we have $\delta=(N+1/2)\pi$. This ''half-bound state'' phenomenon occurs only for s states—cot δ diverges at threshold for higher partial waves. (These results remain valid for potentials that fall off as least as rapidly as $1/r^4$.) The above analysis can be extended to include potentials with a repulsive Coulomb tail. In this case, using the appropriate version of effective range theory, along with the fact that the Coulomb penetration factor decays exponentially as the scattering energy is reduced to zero, one sees that half-bound states do not appear. This conclusion is in agreement with that obtained in two earlier, independent derivations, one based on Jost function theory and the other on a nodal analysis of the wave function [13].

III. POTENTIAL SCATTERING WITH TENSOR FORCES

We consider a scattering system defined by two coupled equations that may be written in the matrix form $Lf=0$, where

$$L_{ji}=-\left[\frac{d^2}{dr^2}+k^2-l_i(l_i+1)/r^2\right]\delta_{ji}+\frac{2\mu}{\hbar^2}V_{ji}, \quad i,j=1,2. \tag{3.1}$$

While greater generality is possible, we assume here that the potential matrix is local, energy independent, and of short range (falling off faster than any power of r). The potential supports a finite number of bound states. As is appropriate to the appearance of a tensor force, the two channels have the same physical threshold, corresponding to energy $E\equiv\hbar^2k^2/2\mu=0$, and the orbital quantum numbers are related by $l_2=l_1+2$. The solution (normalized to have a finite zero-energy limit) has the asymptotic form

$$f_{ji}(r,k)\sim\frac{r}{k^{l_i}}[j_{l_i}(kr)\delta_{ji}-n_{l_j}(kr)K_{ji}], \quad r\to\infty. \tag{3.2}$$

In the neighborhood of threshold the K matrix is known to have the limiting form [10,14] $K=k^{l+1/2}\bar{K}k^{l+1/2}$, where $k^{l+1/2}$ is diagonal, with diagonal elements $k^{l_1+1/2}$ and $k^{l_2+1/2}$, and $\bar{K}$ is analytic in k^2.

We seek a multichannel generalization of Levinson's theorem stated in terms of the zero-energy eigenphase shifts of the scattering system. The basic elements of the procedure outlined in Sec. II for the single-channel case are readily adapted to apply to the case at hand. An absolute determination of these eigenphases is obtained by application of the nodal definition of the phase shifts to particular elements of the multichannel wave function in the representation in which the reaction matrix is diagonal, as described below. The role of the scattering length in the single-channel case is now played by the diagonal elements of a reduced reaction matrix from which threshold singularities have been removed. These elements satisfy a minimum principle (derived in Sec. V) and this may be used to trace the evolution of the eigenphases from their value in the absence of the potential to their true values as the trial function is steadily improved. In this way the value of each zero-energy eigenphase is expressed in terms of the number of bound states in the corresponding eigenchannel. In analogy with the single-channel treatment, the analysis accounts for the special role of zero-energy bound states; here one makes use of the energy dependence of the eigenphases near threshold as determined from an application of effective-range theory [15,16].

Following a standard procedure [10,14] we now diagonalize the (real, symmetric) K matrix with the transformation matrix

$$x=\begin{pmatrix} \cos\varepsilon & -\sin\varepsilon \\ \sin\varepsilon & \cos\varepsilon \end{pmatrix}. \tag{3.3}$$

The eigenvalues are $\tan\delta=x^TKx$, the superscript T denoting transpose. With the potential taken here to be of short range, effective range theory may be applied to give the expansion [15,16]

$$\bar{K}^{-1}\equiv M=-A^{-1}+\frac{1}{2}r_0k^2+O(k^4). \tag{3.4}$$

This information suffices to determine the threshold behavior of the eigenphases and mixture parameter to be $\tan\delta_i \to -k^{2l_i+1}A_i$ (for brevity we write $A_i\equiv A_{ii}$) and $\varepsilon\to mk^{l_2-l_1}$ [17]. With the aid of the relation $(Kx)_{ji}=x_{ji}\tan\delta_i$ along with Eq. (3.2), the asymptotic form of the transformed wave function $u=fx$ is found to be

$$u_{ji}(r,k)\sim(r/k^{l_i})x_{ji}[j_{l_j}(kr)-\tan\delta_i n_{l_j}(kr)]. \tag{3.5}$$

With k fixed and r going to infinity, we see that $(k^{l_i+1}\cot\delta_i)u_{ji}\sim x_{ji}\sin(kr-l_j\pi/2+\delta_i)$. Note that u_{1i} and u_{2i} have the *same* phase shifts; it is then sufficient to examine only the diagonal elements u_{11} and u_{22} to relate A_i and δ_i in a nodal analysis. Using the symbol u_i to denote the column matrix with elements u_{1i} and u_{2i}, and setting $l_1=0$ and $l_2=2$ for definiteness, we find the asymptotic forms

$$u_1(r,0)\sim\begin{pmatrix} r-A_1 \\ -3mA_1/r^2 \end{pmatrix};\quad u_2(r,0)\sim\begin{pmatrix} mr \\ r^3/15-3A_2/r^2 \end{pmatrix}. \tag{3.6}$$

At this stage we must determine the possible values of the eigenphases at threshold. Note first that $\cot\delta=x^TK^{-1}x$ behaves as $x^Tk^{-(l+1/2)}Mk^{-(l+1/2)}x$ near threshold. From the effective range expansion of M, along with the relation $M_{12}=M_{21}$ and the threshold behavior of x, one finds that, with M evaluated at threshold,

$$\cot\delta_1=k^{-1}[M_{11}+2mM_{12}+m^2M_{22}]+O(k). \tag{3.7}$$

Examination of the off-diagonal elements leads to the relation

$$0=k^{-3}[M_{12}+mM_{22}]+O(k^{-1}), \tag{3.8}$$

from which we conclude that $m=-M_{12}/M_{22}$. These relations, along with the identification $\det M/M_{22}=-(A_1)^{-1}$, imply the threshold behavior [15]

$$k\cot\delta_1=-A_1^{-1}+O(k^2). \tag{3.9}$$

Now if A_1 is finite, $\cot\delta_1$ becomes infinite at threshold; thus $\delta_1(0)=0(\mathrm{mod}\ \pi)$. If, on the other hand, A_1 is infinite it follows that $\cot\delta_1\to 0$ and $\delta_1(0)=\pi/2(\mathrm{mod}\ \pi)$. To conclude this preliminary analysis we observe that the relation

$$\cot\delta_2=-k^{-1}M_{11}\sin^2\varepsilon-k^{-3}M_{12}\sin 2\varepsilon+k^{-5}M_{22}\cos^2\varepsilon \tag{3.10}$$

indicates that $\cot\delta_2$ diverges at threshold and therefore $\delta_2(0)=0(\mathrm{mod}\ \pi)$.

To obtain more explicit information on the zero-energy eigenphases we begin by applying the minimum principle, in the form derived in Sec. V, to A_1, the zero-energy limit of $-K_{11}/k$. Since u_{11} has the same asymptotic form as an s-wave single channel wave function, we may adopt the same analysis (described in Sec. II) that relates the phase shift to the number of upward jumps in the scattering length as basis functions are added to the trial function in the variational calculation. A zero-energy resonance, if it exists, must be treated as a ''half-bound'' state as in the single-channel case. Defining

$$u_{1,\mathrm{res}}(r,0)\equiv\lim_{A_1\to\infty}u_1(r,0)/A_1, \tag{3.11}$$

we see that this function has the asymptotic form

$$u_{1,\mathrm{res}}(r,0)\sim\begin{pmatrix} -1 \\ -3m/r^2 \end{pmatrix}, \tag{3.12}$$

corresponding to an ''almost normalizable'' solution, regular at the origin, and is identified as a zero-energy bound state in eigenmode 1. To confirm this identification we determine the asymptotic form of the bound-state wave function by making the replacements $\tan\delta_i\to -i$ and $k\to i\kappa$ in Eq. (3.5). The asymptotic behavior then takes the form $u_{ji}(r,i\kappa)\sim[r/(i\kappa)^{l_i}]x_{ji}h_{l_j}(i\kappa r)$. With $i=1$, we take the limits $\kappa\to 0$, $x_{11}\to 1$, and $x_{21}\to -m\kappa^2$ and conclude that $\kappa u_1(r,i\kappa)$

may be identified with $u_{1,\mathrm{res}}$; the two solutions are regular at the origin and have the same asymptotic forms.

Following very closely the procedure outlined in Sec. II, we define a length phase η_1 by writing $a\cot\eta_1=A_1$ and introduce an absolute definition of the zero-energy phase shift $\delta_1(0)$ by requiring that $0\leqslant\eta_1-\delta_1(0)<\pi$. We then find that $\delta_1(0)$ itself satisfies a version of Levinson's theorem for coupled-channel scattering. When suitably extended to arbitrary values of l_1 with $l_2=l_1+2$, the theorem states that (i) For $l_1=0$, $\delta_1(0)=(N_1+\xi)\pi$, where N_1 is the number of negative-energy bound states in mode 1 and $\xi=\frac{1}{2}$ if there is in addition a zero-energy bound state in that mode, while $\xi=0$ if there is no such bound state. (ii) For $l_1>0$, application of effective range theory shows that $\cot\delta_1$ diverges at threshold. It follows that $\delta_1(0)=N_1\pi$ where N_1 is the number of bound states in mode 1, including, when present, a zero-energy bound state.

In a similar way we consider the possibility of a zero-energy resonance appearing in eigenmode 2, associated with the divergence of the parameter A_2. We introduce the resonant wave function

$$u_{2,\mathrm{res}}(r,0)=\lim_{A_2\to\infty}u_2(r,0)/A_2 \tag{3.13}$$

with asymptotic form

$$u_{2,\mathrm{res}}(r,0)\sim\begin{pmatrix}0\\-3/r^2\end{pmatrix}. \tag{3.14}$$

This function may be identified with a zero-energy bound state in eigenmode 2. Thus, referring to Eq. (3.5) with $i=2$, we again set $\tan\delta_i\to-i$ and evaluate $\kappa^5u_2(r,i\kappa)$ in the limit $\kappa\to0$. We find that it has the same asymptotic form as $u_{2,\mathrm{res}}(r,0)$ and since the two solutions are regular at the origin their equality is confirmed.

We now consider an application of the minimum principle to the zero-energy limit of $-K_{22}/k^5=-[\tan\delta_1\sin^2\varepsilon+\tan\delta_2\cos^2\varepsilon]/k^5$, which is evaluated as $m^2A_1+A_2$, and is expressed, in terms of a ''length phase'' η_2, as $a^5\cot\eta_2$. Noting that the zero-energy limit of $f_2(r,k)$ has the asymptotic form

$$f_2(r,0)\sim\begin{pmatrix}-mA_1\\ r^3/15-3(m^2A_1+A_2)/r^2\end{pmatrix}, \tag{3.15}$$

we choose a trial function regular at the origin and having a similar behavior at infinity, but with the parameters A_1 and A_2 replaced by trial values. As the number of terms in the trial function is increased, upward jumps in $a^5\cot\eta_2$ appear each time a bound state enters, whether in mode 1 or mode 2. [$f_2(r,k)$ is a mixture of modes, even at zero energy.] For $A_1\to\infty$ we see that the wave function $f_2/(mA_1)$ has the same asymptotic form as $u_{1,\mathrm{res}}$, as shown in Eq. (3.12). This corresponds to the appearance of a zero-energy (non-normalizable) bound state in mode 1. For $A_2\to\infty$ we see that f_2/A_2 has the same asymptotic form as $u_{2,\mathrm{res}}$, as shown in Eq. (3.14). This corresponds to the appearance of a zero-energy (normalizable) bound state in mode 2.

An absolute definition of the sum of zero-energy eigenphase shifts follows from the condition $0\leqslant\eta_2-[\delta_1(0)+\delta_2(0)]<\pi$. A version of Levinson's theorem is then obtained, valid whether or not N_2, the number of bound states in mode 2 includes one at zero energy. It may be stated as follows.

(i) For $l_1=0$, $\delta_1(0)+\delta_2(0)=(N_1+N_2+\xi)\pi$, where N_1 is the number of negative-energy bound states in mode 1 and $\xi=1/2$ if there is in addition a zero-energy bound state in that mode, while $\xi=0$ if there is no such bound state.

(ii) For $l_1>0$, $\delta_1(0)+\delta_2(0)=(N_1+N_2)\pi$, where N_1 is the number of bound states in mode 1, including, when present, a zero-energy bound state. (As in the single-channel version of the theorem, the half-bound state phenomenon appears only if the state is non-normalizable.) Combining this latter result with that obtained above for $\delta_1(0)$, we see that $\delta_2(0)=N_2\pi$, independent of the existence of zero-energy bound states. This result extends that of Newton [10] in that it provides information on each of the zero-energy phase shifts rather than on the sum alone.

IV. EFFECT OF ANTISYMMETRIZATION: *n-d* AND *p-d* SCATTERING

It was shown earlier, in the context of electron-atom scattering [9], how the effect of the Pauli principle can be accounted for in the absolute determination of the zero-energy phase shift. For all but the lightest atoms, phase shifts were determined with the use of Hartree-Fock wave functions to represent the target. Significantly, the procedure does not depend on a knowledge of the structure of the true scattering wave function. While practical difficulties arise due to the more complicated nature of the interactions, as well as reduced-mass effects, the same procedure is applicable, in principle, to nuclear scattering problems. As an illustration, we consider the zero-energy scattering of neutrons and protons by deuterons. As our main focus will be on the effect of antisymmetrization, we simplify the discussion by assuming *s*-wave scattering with central forces.

In generalizing the treatment of potential scattering outlined in Sec. II the wave function ϕ appearing in Eq. (2.1), and representing the Born approximation, is replaced by an antisymmetrized product of the deuteron wave function $\psi(r_{23})$—taken in some approximation—and the zero-energy free-particle wave function describing the motion of the incident projectile relative to the target. We denote the Born wave function as $\phi(r_{23},q)$, where q is the projectile-target separation. Following the procedure outlined previously [6], an effective single-particle wave function $F(q)$ is obtained by projecting $\phi(r_{23},q)$ onto the target function $\psi(r_{23})$ and a reference phase shift $\delta^{(0)}$ is determined from a nodal analysis of $F(q)$. In contrast to the potential scattering problem, where $\delta^{(0)}$ is determined to be zero, nodes may appear in the function $F(q)$. (In some simplified independent-particle models of the scattering process, the number of nodes in $F(q)$ may be related to the number of composite bound states excluded by the Pauli principle [4]. This may be helpful in forming a physical interpretation but it should be emphasized that the version of the generalized Levinson theorem described here does not depend on the validity of such a model.) It is shown below that in the quartet state, for both *n-d* and *p-d* scattering, a single node appears, so that $\delta^{(0)}$ is set equal to π. For doublet scattering on the other hand, $F(q)$ is found to be nodeless, again for both *n-d* and *p-d* scatter-

ing. With $\phi(r_{23},q)$ as trial function a Born approximation $A^{(0)}$ is determined and a length phase $\eta^{(0)}$ is defined, modulo π, by writing $A^{(0)}=a\ \cot\eta^{(0)}$. To preserve the condition $0\leqslant\eta-\delta<\pi$ at each stage of the variational construction we fix $\eta^{(0)}$ to lie between π and 2π for quartet scattering and between zero and π for doublet scattering. The minimum principle is then used formally, in the manner described earlier in Sec. II, to follow the evolution of the length phase—and with it the zero-energy phase shift—as the accuracy of the trial function is increased through the introduction of an increasing number of basis functions. Since only one composite doublet bound state exists, and no quartet states, the zero-energy phase shift is determined, by this generalized Levinson theorem, to be π for both doublet and quartet scattering of neutrons and protons by deuterons [18].

To illustrate the nodal analysis leading to the determination of the reference phase we first consider n-d quartet scattering. Let χ_Q represent a normalized quartet spin function with a particular (unspecified) projection; it is unchanged when acted on by the interchange operator P_{12}. The zero-energy Born wave function has the form (with particle 1 the incident neutron and particle 2 the bound neutron)

$$\phi(r_{23},q)=(1-P_{12})\psi(r_{23})\chi_Q=[\psi(r_{23})-\psi(r_{13})]\chi_Q. \tag{4.1}$$

(It is more convenient here not to remove a factor $1/q$ from the wave function.) The effective single-particle wave function is

$$F(q)=\int d^3r_{23}\chi_Q^T\psi(r_{23})\phi(r_{23},q)=1-G(q), \tag{4.2}$$

where, with $\psi(r_{23})$ taken to be normalized to unity, we have

$$G(q)=2\pi\int_{-1}^{1}dp\int_0^\infty dr_{23}r_{23}^2\psi(r_{23})\psi(r_{13}), \tag{4.3}$$

with $r_{13}=[(r_{23}/2)^2+q^2-qr_{23}p]^{1/2}$. Given a reasonably accurate deuteron wave function $F(q)$ can readily be determined. We say ''reasonably accurate'' since only the number of nodes in $F(q)$, rather than its detailed form, is required. A sufficient, though not necessary, condition for $F(q)$ to have a *single* node is that $G(q)$ decrease monotonically to zero, with $G(0)>1$. We have verified this property under the assumption that the deuteron wave function can be represented, in the relevant region of bounded interparticle separations, by a sum of Gaussian functions

$$\psi(r)=\sum_{i=1}^{n}c_i\exp(-\alpha_i r^2) \tag{4.4}$$

with positive coefficients c_i. A three-term function of this form was introduced some time ago [19]. The integrals in Eq. (4.3) may then be performed analytically giving

$$G(q)=(4\pi)^{3/2}\sum_i\sum_j c_ic_j(\alpha_i+4\alpha_j)^{-3/2}\times\exp\left[-\frac{4\alpha_i\alpha_j}{\alpha_i+4\alpha_j}q^2\right]. \tag{4.5}$$

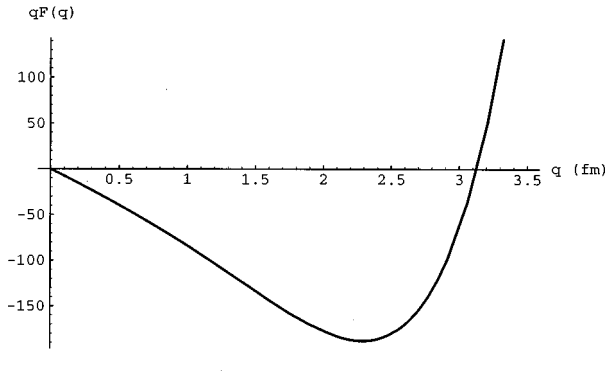

FIG. 1. Plot of the effective single-particle wave function for proton-deuteron scattering in the quartet state showing a single node arising from the antisymmetrization of the zero-energy Born wave function. This implies a value of π for the reference phase shift $\delta^{(0)}$.

This form satisfies the condition stated above for $F(q)$ to have a single node. It is evidently positive. Moreover, at $q=0$ the function $\psi(r_{13})$ in Eq. (4.3) exceeds $\psi(r_{23})$ from which it follows that $G(0)$ exceeds unity, the value of the normalization integral.

A similar procedure may now be followed for the doublet case. We have

$$\phi(r_{23},q)=(1-P_{12})\psi(r_{23})\chi_D^{(S)}, \tag{4.6}$$

where $\chi_D^{(S)}$ is a doublet spin function symmetric in the spins of particles 2 and 3. The effective single-particle wave function, obtained by projecting the Born wave function onto $\psi(r_{23})\chi_D^{(S)}$, is determined, using the relation $\chi_D^{(S)T}P_{12}\chi_D^{(S)}=-1/2$, to be

$$F(q)=1+\frac{1}{2}G(q). \tag{4.7}$$

This function is seen to be nodeless provided only that the deuteron wave function is nodeless, a property expected to hold under very general conditions [20].

An application to proton-deuteron scattering is complicated somewhat by the need to include the effect of the repulsive Coulomb interaction on the Born wave function. With particle 1 the incident proton and particle 2 the bound proton we introduce the zero-energy Coulomb wave function

$$E(q)=(R/q)^{1/2}I_1[2(q/R)^{1/2}], \tag{4.8}$$

where $R=(3\hbar^2/2Me^2)$ and $I_1(x)$ is the modified cylindrical Bessel function of order unity. The function $E(q)$ is nodeless, goes to unity at the origin and diverges asymptotically. The Born wave function, for the quartet state, is expressed as

$$\phi(r_{23},q)=(1-P_{12})\psi(r_{23})E(q)\chi_Q, \tag{4.9}$$

and the effective single-particle function is

$$F(q)=E(q)-2\pi\int_{-1}^{1}dp\int_0^\infty dr_{23}r_{23}^2\psi(r_{23})\psi(r_{13})E(q'), \tag{4.10}$$

where

$$q'^2=\left(\frac{3r_{23}}{4}\right)^2+\left(\frac{q}{2}\right)^2+\frac{3}{4}qr_{23}p. \tag{4.11}$$

Even with the deuteron function taken as a sum of Gaussians we are unable to evaluate the integral in Eq. (4.10) analytically. A numerical integration was performed with the Christian-Gammel wave function [19]. The result obtained for $qF(q)$ is plotted in Fig. 1 and shows the single node that indicates a value of π for the reference phase $\delta^{(0)}$.

For doublet p-d scattering, taking into account the overlap of doublet spin functions, we have

$$F(q)=E(q)+\frac{1}{2}2\pi\int_{-1}^{1}dp\int_0^\infty dr_{23}r_{23}^2\psi(r_{23})\psi(r_{13})E(q') \tag{4.12}$$

with the deuteron wave function assumed to be nodeless this function is clearly nodeless, from which we conclude that the reference phase is zero.

V. THE MINIMUM PRINCIPLE

Some time ago, a corollary to the minimum principle for the scattering length [7] was derived [8] which proved to be useful in the derivation [6] of a generalized version of Levinson's theorem for single-channel scattering. The sharpened version of the minimum principle obtained by Ohmura states that when the system has N bound states the variationally determined scattering length increases in value precisely N times as the number of adjustable linear parameters in the trial function is increased, and thereafter decreases monotonically with further improvement in the trial function. Here we extend this result to apply to multichannel scattering problems, such as that considered earlier in Sec. III. It will be clear from the derivation that the result applies to arbitrary partial waves, and may also be extended to allow for long-range polarization forces as well as repulsive Coulomb interactions (p-d scattering, for example). The minimum principle is a variant of the Rayleigh-Ritz principle, widely used in bound-state calculations. The present application of the minimum principle is of a formal nature—no numerical calculation need be performed and a particular choice of variational basis need not be specified.

The minimum principle will be formulated in terms of a reduced zero-energy reaction matrix element defined as

$$A_{i'i}=-\lim_{k\to 0}k^{-(l_i+l_{i'}+1)}K_{i'i}. \tag{5.1}$$

We suppose that the scattering problem has been reduced to one defined (in terms of a real, symmetric effective potential matrix V_{ji}) by a set of n coupled radial equations given in matrix form as $Lf_i=0$, where L is given by Eq. (3.1) and f_i is a column matrix corresponding to incident channel i. The asymptotic form of the solution (assuming a short-range potential for simplicity) is obtained by taking the zero-energy limit of Eq. (3.2), leading to

$$f_{ji}(r)\sim\frac{r^{l_i+1}}{(2l_i+1)!!}\delta_{ji}-\frac{(2l_j-1)!!}{r^{l_j}}A_{ji}. \tag{5.2}$$

A trial function $f_{ji,t}$ is introduced, vanishing at the origin as does the true function, and having the same asymptotic form but with A_{ji} replaced by a trial matrix $A_{ji,t}$. A variational identity of the type derived by Kato for potential scattering [21] is readily derived in the matrix form

$$A_{i'i}=A_{i'i,t}+(f_{i'},Lf_{i,t}), \tag{5.3}$$

where the scalar product is defined as

$$(a_{i'},b_i)=\sum_{j=1}^{n}\int_0^\infty a_{ji'}(r)b_{ji}(r)dr. \tag{5.4}$$

The identity is verified by using an integration by parts and applying the wave equation and boundary conditions. A variational approximation is obtained by replacing the exact (row) matrix function $f_{i'}(r)$ by a trial function $\bar{f}_{i',t}(r)$, with this function and $f_{i,t}(r)$ allowed to vary independently.

In an extension of the procedure outlined in Sec. II, we consider a sequence of variational calculations in which trial functions $f_{i,t}$, now labeled as $f_i^{(s)}$ to indicate the number of linear parameters they contain, are chosen in the form

$$f_{ji}^{(s)}(r)=\phi_{ji}(r)+\sum_{s'=1}^{s}b_{ji,s'}f_{ji,s'}(r). \tag{5.5}$$

Here $\phi(r)$ and $f_{s'}(r)$ are matrix functions vanishing at the origin and behaving at infinity in a manner consistent with Eq. (5.2). In particular, $b_{ji,1}$ is identified as the trial reaction matrix element $A_{ji,t}$. The trial function $\bar{f}^{(s)}(r)$ is similarly constructed, with the matrix parameters $b_{s'}$ replaced by $\bar{b}_{s'}$. The variational approximation for the A matrix obtained with this set of trial functions is denoted as $A^{(s)}$. Its form is simplified by application of the identity

$$b_{ii',1}+(\phi_{i'},Lf_{i,1})=(L\phi_{i'},f_{i,1}), \tag{5.6}$$

obtained [as in the derivation of Eq. (5.3)] by integration by parts and use of the boundary conditions. For $s'>1$ the functions $f_{s'}$ are assumed to fall off fast enough for the relation $(\phi_{i'},Lf_{i,s'})=(L\phi_{i'},f_{i,s'})$ to hold, without the appearance of surface terms. For $s=1$ and $l_j=0$, $f_{ji,1}(r)\sim -1$ asymptotically. To allow for the applicability of Rayleigh-Ritz methods we insert a cutoff factor in the definition of $f_{ji,1}$ which is ultimately removed, this justified by a demonstration of continuity in the limiting procedure [7]. Now with all basis functions of the bound-state type we may replace the linear parameters $b_{ji,s'}$ by $\bar{b}_{i,s'}$, with no reference to an exit channel; a similar replacement is made for $\bar{b}_{s'}$. With these parameters determined variationally, and with the introduction of the notation $L\phi_i(r)=w_i(r)$ and $A_{i'i}^{(0)}=(\phi_{i'},L\phi_i)$, the variational approximation for the A matrix takes the form [22]

$$A_{i'i}^{(s)}=A_{i'i}^{(0)}-\sum_{s',s''=1}^{s}(w_{i'},f_{i,s'})\left[\frac{1}{L^{(s)}}\right]_{s's''}(f_{i',s''},w_i), \tag{5.7}$$

where $L^{(s)}$ (channel labels i,i' are omitted in this definition) is the matrix with elements $L^{(s)}_{s's''}=(f_{i',s'},Lf_{i,s''})$ for $1 \leqslant s',s'' \leqslant s$.

We wish to determine the conditions under which the variational approximation for one of the diagonal elements A_{ii} either increases or decreases when an additional basis function is included in the trial function. This information is most easily obtained from the identity

$$A^{(s+1)}-A^{(s)}=-\frac{[D^{(s)}]^2}{|L^{(s)}||L^{(s+1)}|}, \tag{5.8}$$

where the channel index i has been omitted and we have defined

$$D^{(s)}=\begin{vmatrix} L_{11} & \cdots & L_{1s} & (f_1,w) \\ \vdots & & \vdots & \vdots \\ L_{s1} & \cdots & L_{ss} & (f_s,w) \\ L_{s+1,1} & \cdots & L_{s+1,s} & (f_{s+1},w) \end{vmatrix}. \tag{5.9}$$

To cover the case $s=0$ we apply Eq. (5.7) directly to obtain

$$A^{(1)}-A^{(0)}=-(w,f_1)(f_1,Lf_1)^{-1}(f_1,w). \tag{5.10}$$

Thus the change in going from the Born approximation $A^{(0)}$ to the first-order approximation $A^{(1)}$ is positive—an upward jump—if at least one bound state exists and the function f_1 is accurate enough to support it, that is if (f_1,Lf_1) is negative. Otherwise there is a downward jump. For $s=1$, Eq. (5.8) is verified without difficulty by direct calculation. To treat the general case [23] it is convenient to transform to a new basis in which the matrix elements $(f_{s'},w)$ vanish for $1 \leqslant s' \leqslant s$. In this basis we have $A^{(s)}=A^{(0)}$ for $s \geqslant 2$ and

$$A^{(s+1)}-A^{(s)}=-(w,f_{s+1})\left[\frac{1}{L^{(s+1)}}\right]_{s+1,s+1}(f_{s+1},w). \tag{5.11}$$

This can be put in the form

$$A^{(s+1)}-A^{(s)}=-(w,f_{s+1})\,\frac{|L^{(s)}|}{|L^{(s+1)}|}\,(f_{s+1},w). \tag{5.12}$$

Noting that in this system $D^{(s)}=|L^{(s)}|(f_{s+1},w)$, we arrive at Eq. (5.8), a result which remains valid upon transformation back to the original basis.

Now following the argument in Ref. [8] one notes that each of the determinants in the denominator of Eq. (5.8), one of dimension s and the other dimension $s+1$, may be expressed as a product of eigenvalues of the corresponding Hamiltonian matrix. From the Hylleraas-Undheim theorem [24] the two sets of eigenvalues satisfy the interlacing property

$$E_1^{(s+1)} \leqslant E_1^{(s)} \leqslant E_2^{(s+1)} \leqslant E_2^{(s)} \leqslant \cdots E_s^{(s)} \leqslant E_{s+1}^{(s+1)}. \tag{5.13}$$

From this property it may be seen that the number of negative eigenvalues C_{s+1} in the $(s+1)$th approximation is either C_s+1 or C_s. In the first case the sign of $|L^{(s)}|L^{(s+1)}|$ is negative and in the second case it is positive. Since C_s cannot be larger than N, the number of physical bound states, the number of values of s for which the right-hand side of Eq. (5.8) is positive cannot exceed N. Furthermore, under the assumption that the basis functions can be properly chosen to assure convergence to the true solution, the number of positive values of $A^{(s+1)}-A^{(s)}$ that is encountered as s is increased arbitrarily must be precisely N. Once N positive jumps in the zero-energy scattering parameter have been observed one is assured that with further improvement in the trial function $A^{(s)}$ will decrease monotonically. This sharpened version of the minimum principle is just the property needed in the development of the generalized Levinson theorem, as discussed in Sec. II.

VI. SUMMARY

Levinson's theorem for potential scattering is usually stated in terms of the difference between the phase shift at zero energy and at infinite energy in which case the question of an absolute determination of the phase shift does not arise. With composite targets, however, scattering at infinite energy is not characterized by a single phase shift and while a version of the theorem has been given that involves the scattering matrix at infinite energy [25], a formulation involving only zero-energy scattering can be useful. The version given earlier [6,9], and extended here to allow for multichannel scattering, removes the ambiguity in multiples of π that would otherwise be present through the introduction of an absolute definition of the phase shift that incorporates the effect of the Pauli principle in a relatively simple fashion. This feature was illustrated in the context of nucleon-deuteron scattering in Sec. IV. The theorem can be applied to other nuclear scattering problems provided a reasonably accurate model of the target wave function is available; the eigenphase shifts at zero energy take on discrete rather than continuous values, so that results tend to be rather robust. A knowledge of the full scattering wave function is not required.

An application to a two-channel problem (n-p scattering with tensor forces is the prototype) was described in Sec. III. It led to a relation, for each of the two eigenmodes, between the zero-energy eigenphase shift and the number of bound states in the corresponding mode, with the contribution of zero-energy bound states properly accounted for. The proof of this relation required application of a particular version of the zero-energy minimum principle, the derivation of which was given in Sec. V. Results obtained here may find use in current studies of multichannel scattering involving phase equivalent potentials that generate different numbers of bound states.

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[1] See, for example, D. Baye, Phys. Rev. Lett. **58**, 2738 (1987).
[2] F. Michel and G. Reidemeister, J. Phys. G **11**, 835 (1985).
[3] See, for example, R. G. Newton, *Scattering Theory of Waves and Particles*, 2nd ed. (Springer, New York, 1982), p. 356. A list of references relating to Levinson's theorem and various generalizations can be found on p. 397 of Newton's book.
[4] P. Swan, Proc. R. Soc. London, Ser. A **228**, 10 (1955).
[5] J.-M. Sparenberg and D. Baye, Phys. Rev. Lett. **79**, 3802 (1997).
[6] L. Rosenberg and L. Spruch, Phys. Rev. A **54**, 4978 (1996).
[7] L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **118**, 184 (1960).
[8] T. Ohmura, Phys. Rev. **124**, 130 (1961).
[9] L. Rosenberg and L. Spruch, Phys. Rev. A **54**, 4985 (1996).
[10] R. G. Newton, Phys. Rev. **100**, 412 (1955).
[11] L. Rosenberg and L. Spruch, Phys. Rev. **125**, 1407 (1962).
[12] Z. R. Iwinski, L. Rosenberg, and L. Spruch, Phys. Rev. A **31**, 1229 (1985).
[13] Z. R. Iwinski, L. Rosenberg, and L. Spruch, Phys. Rev. Lett. **54**, 1602 (1985). A different conclusion (with which I disagree) was reached by P. Swan, Nucl. Phys. **46**, 669 (1963). The half-bound-state phenomenon is associated with zero-energy bound states that are not normalizable; the zero-energy bound-state functions decay exponentially in the repulsive Coulomb case.
[14] J. M. Blatt and L. C. Biedenharn, Phys. Rev. **86**, 399 (1952).
[15] L. C. Biedenharn and J. M. Blatt, Phys. Rev. **93**, 1387 (1954).
[16] M. H. Ross and G. L. Shaw, Ann. Phys. (N.Y.) **13**, 147 (1961).
[17] It was shown in Ref. [15] that for the n-p system, the coefficient m is, in good approximation, proportional to the quadrupole moment of the deuteron.
[18] This conclusion confirms that obtained in Ref. [4] in the context of an independent-particle model of the scattering process.
[19] R. A. Christian and J. L. Gammel, Phys. Rev. **91**, 100 (1953).
[20] As an indication that these nodal properties are not trivially satisfied, we remark that if the doublet spin function antisymmetric in the spins of particle 2 and 3 were used in place of the symmetric function, then $F(q)$ would develop a node. However, use of the antisymmetric doublet function would violate the boundary condition on the scattering wave function at infinity.
[21] T. Kato, Prog. Theor. Phys. **6**, 394 (1951).
[22] An alternative derivation of Eq. (5.7) may be based on a representation of the resolvent operator as a sum of kernels of finite rank with coefficients determined variationally.
[23] The procedure of Ref. [8], starting with Eq. (14) of that paper, is not sufficiently precise and we here modify the argument appropriately.
[24] E. A. Hylleraas and B. Undheim, Z. Phys. **65**, 759 (1930).
[25] S. P. Merkuriev, V. V. Kostrykin, and A. A. Kvitsinsky, Sov. J. Part. Nucl. **21**, 553 (1990). The effect of the Pauli principle was not included in this work.