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Method of Effective Potentials: Scattering of Positrons and Electrons by Light Atoms[*]

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The theory of effective potentials is developed in a way which lends itself to variational formulations. The positron-helium and electron-helium systems are chosen to illustrate the method. The effective potential is defined in terms of the resolvent operator for a system which has been modified by removal of the open-channel states. Rigorous maximum and minimum principles are derived which should be useful in the computation of the effective potential and which are valid, for sufficiently low energies, even when the target bound-state wave function is not known exactly. A numerical application of this method to positron-hydrogen scattering has been made and results are reported. The effective-potential approach to the scattering problem leads naturally to a model for resonance calculations. This model is reviewed here and formulated variationally. An Appendix is devoted to further elaboration of this approach to resonance calculations in the context of potential scattering, with the aid of Jost-function theory.

I. INTRODUCTION

The analysis of atomic and nuclear scattering processes in terms of effective potentials has been a standard procedure for many years.[1,2] It has lately been recognized[3–5] that appropriately formulated variational methods for the computation of the effective potential have the useful property that in the low-energy domain where the effective potential is Hermitian the error involved in the calculation is of well-defined sign. This provides upper and lower bounds on the eigenphase shifts which, being variational in nature, can be systematically improved. At the same time this approach is well suited for the computation of resonance parameters if the resonance is of the closed-channel type.[2]

Several applications of this variational approach, to atomic and nuclear three-body problems, have already been reported.[6–8] In the case of electron-hydrogen scattering[6] the definition of the effective potential can be taken to be the original one of Feshbach since the required projection operators can be constructed explicitly.[3] In most other cases of interest, however, the projection operators are difficult to construct. Fortunately, the function of the projection operators, which is to remove low-lying states of the bound subsystems which appear in the open channels, can be performed by simple algebraic manipulations of the appropriate integral equation which defines the scattering amplitude.[9] This has been described in detail for the neutrondeuteron system.[7]

In this paper we present a generalization of the basic idea of Ref. 7 to systems containing more than three particles. For definiteness we discuss, in Sec. II, the problems of electron and positron scattering by helium. Explicit definitions of the effective potentials for these systems are provided. In general the effective potential is a matrix in channel space, so that rearrangement, Pauli exchange, and excitation processes are accounted for. For energies below the ionization threshold, maximum and minimum principles can be used as (reliable) approximation methods for the construction of the effective potential, as shown in Sec. III. The phase shifts associated with a given effective potential are obtained by numerical solution of a one-body Lippmann-Schwinger equation, a procedure which offers relatively little difficulty in practice.

In order to generalize the method of Ref. 7 to the case where the target system contains more than two particles it is necessary to introduce a different form for the separable interaction which serves to project out the target bound state. The new method and, for the purpose of comparison, the original one, were applied to the positron-hydrogen system; numerical results are reported in Sec. III.

The close connection between effective potential theory and resonance theory is explored in some detail in Sec. IV. We adopt the model which associates the resonance with an unstable state arising, by perturbation, from a stable state whose energy lies in the scattering continuum. This stable state is identified as an eigenstate of the modified Hamiltonian used in the construction of the effective potential. The level-shift operator[10] can then be defined explicitly. The complex resonant energy, whose real and imaginary parts give the position and width of the resonance, may be determined from the knowledge of the level-shift operator in an energy domain above the real axis by analytic continuation to a region below the real axis on the second Riemann sheet. This formal prescription may also provide the basis for practical calculations. As a first step we write down a Rayleigh-Ritz type of variational principle for the level shift for energies in the upper half-plane. Further discussion of this variational approach to resonance calculations, confined to the two-body problem where the analytic properties of the radial wave functions are well understood, is given in an Appendix. The discussion is based on a Kohn-type variational principle for the Jost function.

II. DEFINITION OF THE EFFECTIVE POTENTIAL

As shown previously,[7,9] an effective potential for three-body scattering can be defined by straightforward manipulation of the Watson-Faddeev equations.[11,12] The same basic approach is applicable to systems containing more than three particles. We illustrate this with specific examples, the first being the problem of elastic positron-helium scattering.

Consider the four-body transition operator T satisfying the Lippmann-Schwinger equation

$$T = V + VG_0T \ , \tag{2.1}$$

where V is the sum of the interparticle Coulomb potentials. G_0 is the free Green's function

$$G_0 = (E - K)^{-1} \ , \tag{2.2}$$

with K representing the total kinetic energy operator (the helium nucleus is treated as a fixed point charge) and E, the total energy, assumed to contain the usual infinitesimal positive imaginary part. In order to exhibit the contribution of the helium ground state, as required in the effective-potential approach, we perform a Watson-type transformation[11] of Eq. (2.1). We write $V = V_1 + V_2$, where V_1 represents the potential energy operator for the helium atom, and V_2 is the positron-helium interaction. In terms of the interparticle potentials we have

$$V_1 = U(2) + U(3) + U(23) \tag{2.3}$$

and

$$V_2 = U(1) + U(12) + U(13) \ . \tag{2.4}$$

Here the $U(i)$ represent the interaction of the positron ($i = 1$) and the electrons ($i = 2, 3$) with the nucleus. The $U(ij)$ represent the positron-electron and electron-electron interactions. Now we define the subsystem scattering amplitudes T_i ($i = 1, 2$) by

$$T_i = V_i + V_i G_0 T_i \ . \tag{2.5}$$

Then with ${}^iT$ defined as

$${}^iT = V_i + V_i G_0 T \ , \tag{2.6}$$

so that

$$T = \sum_{i=1}^{2} {}^iT \ , \tag{2.7}$$

it is easily verified that the ${}^iT$ satisfy the coupled equations

$${}^iT = T_i + T_i G_0 \textstyle\sum_j (1 - \delta_{ij})\, {}^jT \ . \tag{2.8}$$

Similarly, with

$$T^i = V_i + T G_0 V_i \ , \tag{2.9}$$

so that

$$T = \textstyle\sum_i T^i \ ,$$

we have the coupled equations

$$T^i = T_i + \textstyle\sum_j (1 - \delta_{ij}) T^j G_0 T_i \ . \tag{2.10}$$

It is convenient to introduce the further decomposition

$$ {}^{i}T=\sum_j {}^{i}T^{j} \quad , \tag{2.11}$$

$$ T^{i}=\sum_j {}^{j}T^{i} \quad . \tag{2.12}$$

The components ${}^{i}T^{j}$ can then be generated by the coupled equations

$$ {}^{i}T^{j}=T_i\,\delta_{ij}+\sum_k(1-\delta_{ki})\,T_i\,G_0\,{}^{k}T^{j} \tag{2.13}$$

or

$$ {}^{i}T^{j}=T_i\,\delta_{ij}+\sum_k(1-\delta_{kj})\,{}^{i}T^{k}\,G_0T_j \quad . \tag{2.14}$$

An alternative characterization of the operators ${}^{i}T^{j}$ can be given in terms of the resolvent operator

$$ G=(E-H)^{-1} \quad , \tag{2.15}$$

where $H=K+V$ is the full Hamiltonian of the system. One readily finds that

$$ {}^{i}T^{j}=V_i\,\delta_{ij}+V_iG\,V_j \quad . \tag{2.16}$$

At this stage the helium ground-state pole contribution to the amplitude T_1 can be exhibited. (The extension of the following analysis, in which a finite number of excited states are "subtracted out" in addition to the ground state, is straightforward and is omitted here to simplify the discussion.) According to the procedure of Ref. 7 we introduce the decomposition

$$ V_1=V_{1A}+V_{1B} \quad . \tag{2.17}$$

If we define T_{1A} as the solution of

$$ T_{1A}=V_{1A}+V_{1A}G_0T_{1A} \quad , \tag{2.18}$$

and apply the "two-potential" formula,[13] we are led to a representation

$$ T_1=T_{1A}+T_{1B} \quad , \tag{2.19}$$

where, with an appropriate choice of separable interaction V_{1B}, the ground-state pole contribution can be isolated in T_{1B}. The choice of V_{1B} is not unique; in fact the one made in Ref. 7 leads to a form of T_{1B} which is too complicated for our present purposes. Here we choose

$$ V_{1B}=E_{1(0)}\,|\chi_{1(0)}\rangle\langle\chi_{1(0)}| \quad , \tag{2.20}$$

where $|\chi_{1(0)}\rangle$ is the helium ground-state eigenvector, and $E_{1(0)}$ is the corresponding eigenvalue. The amplitude T_{1B} which is fixed by this choice can be found most simply by consideration of the spectrum of the modified helium Hamiltonian $H_{1A}=K_1+V_{1A}$; this is revealed by the relations

$$ \begin{aligned} &H_{1A}|\chi_{1(0)}\rangle=0 \quad , \\ &H_{1A}|\chi_{1(n)}\rangle=E_{1(n)}|\chi_{1(n)}\rangle \quad , \quad n=1,2,\ldots \quad . \end{aligned} \tag{2.21}$$

Here the $|\chi_{1(n)}\rangle$ represent the complete set of helium eigenvectors, and the $E_{1(n)}$ are the corresponding eigenvalues. We see that the spectrum of H_{1A} is identical to the physical helium spectrum with the exception that the ground-state eigenenergy has been raised to zero. By comparison of the eigenfunction expansions of the Green functions

$$ G_1\equiv(E-K-V_1)^{-1}=G_0+G_0T_1G_0 \tag{2.22}$$

and

$$ G_{1A}\equiv(E-K-V_{1A})^{-1}=G_0+G_0T_{1A}G_0 \tag{2.23}$$

we conclude that

$$ \begin{aligned} G_0T_{1B}G_0&\equiv G_1-G_{1A}\\ &=|\chi_{1(0)}\rangle\,[(E-\mathcal{K}_1-E_{1(0)})^{-1}\\ &\qquad -(E-\mathcal{K}_1)^{-1}]\,\langle\chi_{1(0)}| \quad , \end{aligned} \tag{2.24}$$

where $\mathcal{K}_1=K-K_1$ is the kinetic energy operator of the positron. [Note that for $E<0$ the term $(E-\mathcal{K}_1)^{-1}$ is nonsingular.]

Let $\mathcal{T}_{11}$ represent the one-body operator whose matrix elements $\langle\vec{k}'|\mathcal{T}_{11}|\vec{k}\rangle$ in the momentum space of the positron gives the amplitude for elastic positron-helium scattering. To derive an effective one-body integral equation for $\mathcal{T}_{11}$ we first make the identification [see Eq. (2.16)]

$$ \mathcal{T}_{11}=\langle\chi_{1(0)}|{}^{2}T^{2}|\chi_{1(0)}\rangle \quad . \tag{2.25}$$

If we now introduce the decompositon, Eq. (2.19), into Eq. (2.13) and make use of a version of the "two-potential" formula given previously,[9] we obtain the desired one-body integral equation

$$ \mathcal{T}_{11}=\mathcal{V}_{11}+\mathcal{V}_{11}\mathcal{G}_1\mathcal{T}_{11} \tag{2.26}$$

where, from Eq. (2.24), we find that

$$ \mathcal{G}_1=E_{1(0)}/(E-\mathcal{K}_1)(E-\mathcal{K}_1-E_{1(0)}) \quad . \tag{2.27}$$

The operator $\mathcal{V}_{11}$ represents the effective potential for the positron and is defined by

$$ \mathcal{V}_{11}=\langle\chi_{1(0)}|{}^{2}T^{2}_{A}|\chi_{1(0)}\rangle \quad , \tag{2.28}$$

where the operators ${}^{i}T^{j}_{A}$ satisfy the analogs of Eqs. (2.13), with the input amplitude T_1 replaced by T_{1A}. Alternatively, we have, in analogy with Eq. (2.16), the representation

$$ {}^{2}T^{2}_{A}=V_2+V_2G_AV_2 \quad , \tag{2.29}$$

with

$$ G_A=(E-K-V_{1A}-V_2)^{-1} \quad . \tag{2.30}$$

Equation (2.29) is a convenient starting point for the construction of variational principles for the effective potential, as shown in Sec. III.

It is possible to include the pickup process (positronium formation) in the set of open channels, leading to a multichannel generalization of Eq. (2.26). Thus, let the potential energy be decomposed as

$$ V=\sum_{i=1}^{4}V_i \quad , \tag{2.31}$$

with

$$V_1 = U(2) + U(3) + U(23), \quad V_2 = U(3) + U(12) \ ,$$
$$V_3 = U(2) + U(13) \ , \quad V_4 = U(1) - U(2) - U(3) \ . \tag{2.32}$$

The helium ground state is generated by V_1 while V_2 and V_3 each provide for the simultaneous binding of the positronium and He$^+$ systems. Except for the extended range of indices $(i, j = 1, 2, 3, 4)$ the algebra leading to Eqs. (2.13) is unchanged. The bound-state pole contributions to T_2 and T_3 can be separated off in a manner analogous to that shown for T_1 in Eqs. (2.18), (2.19), and (2.24). We need only change the subscripts in these equations, with the understanding that the wave function $\chi_{2(0)}$ is a product of the positronium ground-state function (involving the positron and electron 2) and the He$^+$ ground-state function (involving electron 3); $E_{2(0)}$ is the sum of the corresponding eigenenergies. The operator $\mathcal{K}_2$ represents the kinetic energy of the center of mass of particles 1 and 2 (recall that the nucleus has been taken as fixed). A similar decomposition holds for T_3, the two electrons interchanging their roles.

It is now a simple matter to obtain the three-channel generalization of Eq. (2.26). We define the operators

$$\mathcal{T}_{ij} = \langle \chi_{i(0)} | (E-K) | \chi_{j(0)} \rangle (1-\delta_{ij}) + \sum_{l=1}^{4} \sum_{k=1}^{4} (1-\delta_{li})(1-\delta_{kj}) \langle \chi_{i(0)} | {}^{l}T^{k} | \chi_{j(0)} \rangle \tag{2.33}$$

for $i, j = 1, 2, 3$, from which the physical elastic and rearrangement scattering amplitudes are obtained by taking matrix elements with respect to the plane-wave states (eigenstates of the kinetic energy operators $\mathcal{K}_j$ which describe the force-free relative motion of the aggregates) for the appropriate channels. The effective potential operators $\mathcal{V}_{ij}$ are defined analogously in terms of the operators ${}^{l}T^{k}_{A}$, solutions of the Watson-type equations with the T_{iA} as input. Finally, with propagators $\mathcal{G}_i$, $i = 1, 2, 3$, defined as in Eq. (2.27) we find, by comparison of the integral equations for the ${}^{l}T^{k}$ and ${}^{l}T^{k}_{A}$, the coupled equations

$$\mathcal{T}_{ij} = \mathcal{V}_{ij} + \sum_{k=1}^{3} \mathcal{V}_{ik} \, \mathcal{G}_k \, \mathcal{T}_{kj} \ . \tag{2.34}$$

The operators $\mathcal{V}_{ij}$ can be expressed in resolvent form with the aid of the representation (we define $V_{4A} \equiv V_4$)

$${}^{l}T^{k}_{A} = V_{lA} \, \delta_{lk} + V_{lA} G_A V_{kA} \ , \tag{2.35}$$

where now, with $V_A = \sum_{i=1}^{4} V_{iA}$ and $H_A = K + V_A$, we have

$$G_A = (E - H_A)^{-1} \ . \tag{2.36}$$

We then find the operators $\mathcal{V}_{ij}$ to be given by

$$\mathcal{V}_{ij} = \langle \chi_{i(0)} | \{ (E-K)(1-\delta_{ij}) + \textstyle\sum_l (1-\delta_{li})(1-\delta_{lj}) V_{lA} + (V_A - V_{lA}) G_A (V_A - V_{jA}) \} | \chi_{j(0)} \rangle \ . \tag{2.37}$$

Of course when the identity of the electrons is taken into account we are left with only two physically distinguishable channels. Correspondingly, the effective potential is reduced to the 2×2 matrix

$$\underline{\mathcal{V}}_{\text{sym}} = \begin{pmatrix} \mathcal{V}_{11} & \sqrt{2}\,\mathcal{V}_{12} \\ \sqrt{2}\,\mathcal{V}_{21} & \mathcal{V}_{22} - \mathcal{V}_{23} \end{pmatrix} \ . \tag{2.38}$$

The properly symmetrized transition matrix[14] connecting these two channels is obtained from a (matrix) Lippmann-Schwinger equation with the above potential as input.

An equivalent method of imposing the symmetry is to compute diagonal expectation values of the original 3×3 $\mathcal{T}$ matrix, of the form $\underline{a}^{\dagger} \underline{\mathcal{T}} \underline{a}$, where the normalized column vector $\underline{a}$ has $a_2 = -a_3$. The advantage of working explicitly with diagonal matrix elements is that the error in the variational calculation can then be shown to have a well-defined sign for energies below the continuum threshold of H_A (see Sec. III).

A quite similar procedure can be used to define an effective potential for the electron-helium system. Let the interelectronic potentials be represented by $U(ij)$ $(i, j = 1, 2, 3)$, and let $U(i)$ $(i = 1, 2, 3)$ represent the interactions of the electrons with the nucleus. The total potential

$$V = \sum_{i=1}^{3} U(i) + \sum_{j=1}^{3} \sum_{i<j} U(ij) \tag{2.39}$$

can be represented as $V = \sum_{i=1}^{4} V_i$ with

$$\begin{aligned} V_1 &= U(2) + U(3) + U(23) \ , \\ V_2 &= U(3) + U(1) + U(13) \ , \\ V_3 &= U(1) + U(2) + U(12) \ , \\ V_4 &= -[U(1) + U(2) + U(3)] \ . \end{aligned} \tag{2.40}$$

A Watson transformation on the Lippmann-Schwinger equation for the scattering operator can now be performed which is formally identical to the one leading to Eq. (2.13). The helium ground-state pole contribution to T_i $(i = 1, 2, 3)$ can be separated off as shown above. Prior to symmetrization we deal with a 3×3 $\mathcal{T}$ matrix describing direct and exchange scattering which can be represented as the solution of an effective one-body equation of the form shown in Eq. (2.34) with the effective potential given by Eq. (2.37). Of course, the symbols must be reinterpreted; each of the V_{iB} is given by the separable form shown in Eq. (2.20) for $i = 1$, and each of the wave functions $\chi_{j(0)}$ represents a helium ground-state function for a particular pair of electrons.

The symmetrized amplitude can be obtained from a single-channel version of Eq. (2.34), with the effective potential $\mathcal{V}_{\text{sym}} = \mathcal{V}_{11} - 2\mathcal{V}_{21}$ taken as input. This construction is equivalent to the determination of the diagonal matrix element $\underline{a}^{\dagger}\underline{\mathcal{T}}\,\underline{a}$, where

$$a_i = 3^{-1/2}(-1)^{i+1}, \quad i = 1, 2, 3 \quad . \tag{2.41}$$

We note that a definition of the effective potential based on four-body Faddeev equations,[15] rather than equations of the Watson type, is also possible, although the derivation would be slightly more complicated. The mathematical virtues of the generalized Faddeev equations, related to the connectivity properties of the kernel, play no role in the present considerations since our objective is to work not with the integral equations but with the resolvent form, Eq. (2.37), using variational methods of the Rayleigh-Ritz type. This is the subject of Sec. III.

III. MAXIMUM AND MINIMUM PRINCIPLES

A. Target Bound-State Functions Known Exactly

It was assumed in the foregoing discussion that the target bound-state wave functions which enter into the definition of the effective potential are known exactly. If this is actually the case, as it is for electron and positron scattering by hydrogen, then variational bounds on the effective potential, leading to rigorous upper and lower bounds on the eigenphase shifts, can be obtained using methods already described.[7,8] For convenience we record here the basic identity for momentum-space elements of the effective potential operators $\mathcal{V}_{ij}$ defined by Eq. (2.37). We have

$$\mathcal{V}_{ij} = \mathcal{V}_{ijv} + \Delta\mathcal{V}_{ij} \quad , \tag{3.1}$$

where the variational estimate is given in momentum space by

$$\begin{aligned}\langle \vec{k}_i | \mathcal{V}_{ijv} | \vec{k}_j \rangle = {} & \langle \chi_{i(0)};\ \vec{k}_i | (E-K) | \chi_{j(0)};\ \vec{k}_j \rangle (1-\delta_{ij}) \\ & + \textstyle\sum_l (1-\delta_{il})(1-\delta_{jl}) \langle \chi_{i(0)};\ \vec{k}_i | V_{lA} | \chi_{j(0)};\ \vec{k}_j \rangle \\ & + \langle \chi_{i(0)};\ \vec{k}_i | (V_A - V_{iA}) | \Psi_{jt} \rangle \\ & + \langle \Psi_{it} | (V_A - V_{jA}) | \chi_{j(0)};\ \vec{k}_j \rangle + \langle \Psi_{it} | (H_A - E) | \Psi_{jt} \rangle .\end{aligned} \tag{3.2}$$

The vector $|\chi_{j(0)};\vec{k}_j\rangle$ represents the bound clusters in a state of relative momentum $\vec{k}_j$. The trial vector $|\Psi_{jt}\rangle$ is thought of as arising from a trial resolvent G_{At} according to

$$|\Psi_{jt}\rangle = G_{At}(V_A - V_{jA}) | \chi_{j(0)};\ \vec{k}_j \rangle \quad . \tag{3.3}$$

The error is given in terms of

$$\Delta G_A = G_A - G_{At} \tag{3.4}$$

as

$$\begin{aligned}\langle \vec{k}_i | \Delta\mathcal{V}_{ij} | \vec{k}_j \rangle = - & \langle \chi_{i(0)};\ \vec{k}_i | (V_A - V_{iA}) \Delta G_A (H_A - E) \\ & \times \Delta G_A (V_A - V_{jA}) | \chi_{j(0)};\ \vec{k}_j \rangle\end{aligned} \tag{3.5}$$

or, after inserting a factor $(H_A - E)G_A = -1$, as

$$\langle \vec{k}_i | \Delta\mathcal{V}_{ij} | \vec{k}_j \rangle = \langle I_{it} | G_A | I_{jt} \rangle \quad , \tag{3.6}$$

where

$$|I_{jt}\rangle = (V_A - V_{jA}) | \chi_{j(0)};\ \vec{k}_j \rangle + (H_A - E) | \Psi_{jt} \rangle \quad . \tag{3.7}$$

We assume that E lies below the continuum threshold E_T of H_A. In this case upper and lower bounds on G_A in Eq. (3.6) lead to *variational* upper and lower bounds on diagonal matrix elements of the error in the effective potential. We have, in particular,[4,16]

$$0 > G_A > (E - E_T)^{-1} \quad , \tag{3.8}$$

provided H_A has no discrete eigenvalues below E_T. If such discrete states exist they must be "subtracted off" in a manner previously described[7] (and reviewed in Sec. IV of this paper).

The above formalism has been applied to the problem of s-wave positron scattering by hydrogen. The incident kinetic energy was taken to be 0.04 Ry which lies below the threshold for positronium formation. The particular value was chosen to facilitate comparison with previous calculations. The trial function was taken to be of the rather simple form

$$\langle \vec{x}, \vec{y} | \Psi_t \rangle = A(k)e^{-\alpha x - \beta y} + B(k)e^{-\gamma y - \delta|\vec{x}-\vec{y}|} \quad , \tag{3.9}$$

where $\vec{x}$ and $\vec{y}$ are the positron and electron coordinates, respectively. The linear parameters A and B were determined variationally in the usual way.[17] For a given set of (momentum-independent) nonlinear parameters the variational estimate of the effective potential thus obtained was used as input to a linear integral equation of the type shown in Eq. (2.26) with the principal-value prescription used to define the singularity in the propagator $\mathcal{G}$. Since the phase shift thus obtained is known to lie below the true value we were able to improve the result systematically by searching for the set of nonlinear parameters which maximizes the phase shift. This powerful validity criterion is the essential feature of the variational approach described here.

A lower bound on the phase shift was also obtained using the alternate method, described in Ref. 7, for subtracting out the target bound state. Comparable accuracy was achieved, although the calculation was more time consuming. Details can be found in Ref. 18.

An upper bound on the phase shift was computed using the lower bound on the modified resolvent G_A given in Eq. (3.8). To limit the already considerable numerical complexity of the computation the trial function was taken to be the same as that used in the calculation of the lower bound on the phase shift [with V_{1B} given by Eq. (2.20)]. In view of the relative simplicity of the trial function and the existence of a strongly attractive polarization force the results, shown in Table I, and compared there with the very accurate variational result of Schwartz,[19] seem encouraging. A more elaborate calculation leading to converged upper and lower bounds now seems to us to be quite feasible with the present method.

The validity of the phase-shift bounds depends on the absence of discrete states of the modified Hamiltonian H_A with energies below the scattering energy E. While a rigorous proof of the absence of such states is lacking, we are reasonably sure that none exist below the pickup threshold E_T; a Rayleigh-Ritz calculation with a trial function of the form

$$\Phi_t(\vec{x},\vec{y}) = (c_1 + c_2 x + c_3 y)e^{-\alpha x - \beta y - \gamma|\vec{x}-\vec{y}|} \tag{3.10}$$

failed to produce an expectation value of H_A below E_T. In fact, when the Hamiltonian is further modified, by subtraction of the appropriate potential, to remove the positronium ground state in addition to the hydrogen ground state we find no evidence for discrete states below the first excitation level of hydrogen. Our calculation therefore supports the view[20] that there exist no additional closed-channel resonances of the positron-hydrogen system below the $n=2$ level of hydrogen, other than those which are known to exist[21] within an electron volt or so of this level. These latter are associated with the degeneracy of the $n=2$ level which leads to dipole interactions not accounted for in our trial function.

B. Target Bound-State Functions Not Known Exactly

The method described in Sec. III A fails to provide rigorous bounds on the eigenphase shifts when the wave functions for the bound subsystems which appear in the entrance and exit channels are not known exactly. Nevertheless, we shall show in the following that the characteristic feature of the above variational method, namely, that trial functions can be systematically improved with the aid of rigorous maximum and mimimum principles, is preserved.

Consider the scattering of an electron or positron by a light atom for which a fairly accurate (and improvable) trial bound-state function can be obtained by application of the Rayleigh-Ritz minimum principle. To be specific, and to simplify the discussion, we look at elastic positron-helium scattering. Suppose that we are given a target ground-state function $\bar{\chi}_{1(0)}$, the bar indicating that it differs from the exact eigenfunction $\chi_{1(0)}$. A scattering problem associated with such a trial target function can be defined in precise mathematical terms if we adopt the effective potential formalism described in Sec. II, with the following modifications. The energy conservation condition $E = Q_1 + E_{1(0)}$, where Q_1 is the kinetic energy of the positron in the initial state, is now understood to define E for a given value of Q_1, with $E_{1(0)}$ replaced by the best available approximation to it. (For the very light atoms $E_{1(0)}$ is known essentially exactly to the accuracy sought for in the scattering calculation.) The scattering operator $\mathcal{T}_{11}$ is defined as the solution of a Lippmann-Schwinger equation of the form shown in Eq. (2.26). The effective potential is now defined as

$$\bar{\mathcal{V}}_{11} = \langle\bar{\chi}_{1(0)}|[V_2 + V_2(E - K - V_1 - V_2 + \bar{V}_{1B})^{-1}V_2]|\bar{\chi}_{1(0)}\rangle , \tag{3.11}$$

where, with H_1 representing the helium atom Hamiltonian, we choose

$$\bar{V}_{1B} = H_1|\bar{\chi}_{1(0)}\rangle\langle\bar{\chi}_{1(0)}|H_1/\langle\bar{\chi}_{1(0)}|H_1|\bar{\chi}_{1(0)}\rangle . \tag{3.12}$$

We shall see that for the purpose of obtaining a minimum principle it is necessary to use this form for $\bar{V}_{1B}$ rather than to simply replace $\chi_{1(0)}$ with $\bar{\chi}_{1(0)}$ in Eq. (2.20). The scattering problem thus defined clearly reduces to the exact problem as $\bar{\chi}_{1(0)}$ becomes exact.

The problem of determining $\bar{\mathcal{V}}_{11}$ for a given choice of $\bar{\chi}_{1(0)}$ can be formulated variationally using the method described in Sec. III A. The arguments leading to the establishment of error bounds on the variational approximation to the effective potential can be taken over provided that the total energy E lies below the threshold of the continuous spectrum of the modified Hamiltonian

$$\bar{H}_A = \mathcal{K}_1 + V_2 + H_1 - \bar{V}_{1B} . \tag{3.13}$$

(If there are discrete eigenstates of $\bar{H}_A$ with energies below E they can be subtracted off.) There will be a branch of the continuous spectrum of $\bar{H}_A$ associated with positronium formation. Such states can be removed by subtraction of the appropriate separable potentials. Since the bound-state functions in this channel are known exactly the subtraction procedure is identical to that described in Sec. II, and we do not indicate it explicitly here. It is only the branch of the spectrum associated with a positron free at infinity whose threshold is not precisely known. This threshold is given by the minimum energy of the modified

TABLE I. Upper and lower bounds on the s-wave e^+-H phase shift (in radians) with the initial kinetic energy of the positron taken as 0.04 Ry. The accurate variational result of Schwartz[a] is included for comparison.

Lower bound	Upper bound	Result of Schwartz[a]
0.166	0.226	0.188

[a] See Ref. 19.

helium Hamiltonian

$$\bar{H}_{1A} = H_1 - \bar{V}_{1B} \ . \tag{3.14}$$

We therefore look for a lower bound on the expectation value of $\bar{H}_{1A}$.

Let us consider the matrix

$$\underline{M} = \begin{pmatrix} \langle \bar{\chi}_{1(0)} | H_1 | \bar{\chi}_{1(0)} \rangle & \langle \bar{\chi}_{1(0)} | H_1 | \psi \rangle \\ \langle \psi | H_1 | \bar{\chi}_{1(0)} \rangle & \langle \psi | H_1 | \psi \rangle \end{pmatrix} , \tag{3.15}$$

where ψ and $\bar{\chi}_{1(0)}$ are orthonormal functions. Let $\epsilon_{(0)}$ and $\epsilon_{(1)}$ denote the eigenvalues of $\underline{M}$, with $\epsilon_{(0)} < \epsilon_{(1)}$. According to the Hylleraas-Undheim theorem[22] the inequalities

$$E_{1(0)} < \epsilon_{(0)} < \bar{E}_{1(0)} \tag{3.16}$$

and

$$E_{1(1)} < \epsilon_{(1)} \tag{3.17}$$

are satisfied. We have defined

$$\bar{E}_{1(0)} = \langle \bar{\chi}_{1(0)} | H_1 | \bar{\chi}_{1(0)} \rangle \ . \tag{3.18}$$

Since the determinant of $\underline{M}$ is the product of its eigenvalues we have

$$\langle \psi | \left[H_1 - \frac{H_1 | \bar{\chi}_{1(0)} \rangle \langle \bar{\chi}_{1(0)} | H_1}{\langle \bar{\chi}_{1(0)} | H_1 | \bar{\chi}_{1(0)} \rangle} \right] | \psi \rangle = \frac{\epsilon_{(0)} \epsilon_{(1)}}{\langle \bar{\chi}_{1(0)} | H_1 | \bar{\chi}_{1(0)} \rangle} \ . \tag{3.19}$$

The above inequalities, and the definitions, Eqs. (3.12), (3.14), and (3.18), allow us to write

$$\langle \psi | \bar{H}_{1A} | \psi \rangle > (E_{1(0)} / \bar{E}_{1(0)}) \, E_{1(1)} \ . \tag{3.20}$$

To show that this inequality is preserved when the orthogonality requirement on the test function ψ is dropped we express an arbitrary normalized vector $|\phi\rangle$ as

$$|\phi\rangle = c_1 | \bar{\chi}_{1(0)} \rangle + c_2 | \psi \rangle \ , \tag{3.21}$$

with $|c_1|^2 + |c_2|^2 = 1$. We observe that

$$\langle \phi | \bar{H}_{1A} | \phi \rangle = |c_2|^2 \langle \psi | \bar{H}_{1A} | \psi \rangle \ . \tag{3.22}$$

The desired inequality,

$$\langle \phi | \bar{H}_{1A} | \phi \rangle > (E_{1(0)} / \bar{E}_{1(0)}) \, E_{1(1)} \ , \tag{3.23}$$

then follows from Eqs. (3.20) and (3.22) since $|c_2|^2$ is less than unity, and the right-hand side of Eq. (3.20) is negative. Furthermore, the inequality is preserved if $E_{1(0)}$ and $E_{1(1)}$ are replaced by lower bounds. In the case of helium, lower bounds are known[23] which are sufficiently close to the exact eigenvalues that we may ignore the distinction.

Since we have subtracted out only the ground state the variational bounds can be valid only for scattering energies below the first excitation threshold $E_{1(1)}$. From Eq. (3.23) we conclude that the continuum threshold of $\bar{H}_A$ lies above $fE_{1(1)}$ where $f \equiv E_{1(0)} / \bar{E}_{1(0)}$ differs from unity by about 2% for the simplest one-parameter trial function.[24] A three-parameter Hylleraas trial function gives a value for f which differs from unity by about 0.04%.

Having established a lower bound $fE_{1(1)}$ on the continuum threshold of $\bar{H}_A$ we can write down upper and lower bounds on the resolvent which appears in the error term in the variational expression for $\bar{\mathcal{V}}_{11}$. We have

$$0 > (E - \bar{H}_A)^{-1} > (E - fE_{1(1)})^{-1} \ , \tag{3.24}$$

valid for $E < fE_{1(1)}$. These inequalities can be used to generate variational upper and lower bounds on diagonal matrix elements of the error in $\bar{\mathcal{V}}_{11}$. The derivation is identical to the one given in Sec. III A for the case of the true effective potential $\mathcal{V}_{11}$. These maximum and minimum principles should appreciably augment the power of the variational approach.

IV. VARIATIONAL METHODS FOR RESONANCE CALCULATIONS

It is well known[2] that bound-state poles in the effective potential lead to Breit-Wigner distributions for cross sections for energies near the pole. Thus, given a calculational scheme for constructing the effective potential, such as the one described in Sec. III, one also has a method for computing resonance parameters. The computational procedure can be formulated variationally as shown in the following. (Numerical applications to the electron-helium system will be reported on in the future.)

We adopt Eq. (2.37) as the definition of the effective potential and assume that G_A has a pole corresponding to a discrete eigenstate of H_A,

$$H_A | a \rangle = E_a | a \rangle \ , \tag{4.1}$$

with E_a lying below the continuum threshold E_T of H_A. Generally $|a\rangle$ will not be known exactly. However, the pole contribution to G_A can be accounted for variationally.[7,25] Thus, let $|\bar{a}\rangle$ be a normalized trial bound-state function leading to the variational upper bound

$$\bar{E}_a = \langle \bar{a} | H_A | \bar{a} \rangle \ , \tag{4.2}$$

with $\bar{E}_a < E_T$. Then the variational approximation to the effective potential given in Eq. (3.2) can be modified, by the addition of a second-order term, to the form

$$\langle \vec{k}_i | \mathcal{V}'_{ijv} | \vec{k}_j \rangle = \langle \vec{k}_i | \mathcal{V}_{ijv} | \vec{k}_j \rangle - \langle \chi_{i(0)}; \vec{k}_i | (V_A - V_{iA}) \Delta G_A \left(\frac{(H_A - E) | \bar{a} \rangle \langle \bar{a} | (H_A - E)}{\langle \bar{a} | (H_A - E) | \bar{a} \rangle} \right) \Delta G_A (V_A - V_{jA}) | \chi_{j(0)}; \vec{k}_j \rangle \ . \tag{4.3}$$

While the right-hand side involves ΔG_A it is nevertheless known since, by virtue of Eqs. (3.3) and (3.4), we have

$$(H_A - E)\,\Delta G_A (V_A - V_{jA}) |\, \chi_{j(0)}; \vec{k}_j \rangle = -\,|I_{jt}\rangle \quad , \tag{4.4}$$

with $|I_{jt}\rangle$ given by Eq. (3.7). Correspondingly, the error is given not by Eq. (3.5) but by the modified form

$$\langle \vec{k}_i | \mathcal{V}_{ij} | \vec{k}_j \rangle - \langle \vec{k}_i | \mathcal{V}'_{ijv} | \vec{k}_j \rangle$$
$$= -\langle \chi_{i(0)}; \vec{k}_i | (V_A - V_{iA})\,\Delta G_A \left(H_A - E - \frac{(H_A - E)|\,\overline{a}\rangle\langle\overline{a}|(H_A - E)}{\langle\overline{a}|(H_A - E)|\overline{a}\rangle} \right) \Delta G_A (V_A - V_{jA}) |\, \chi_{j(0)}; \vec{k}_j \rangle \quad . \tag{4.5}$$

Now it follows from the Hylleraas-Undheim theorem[22] that the operator in large parens is positive for $E < E_T$ provided H_A has no more than one bound state with energy below E. (The subtraction procedure can be generalized if there is more than one bound state with energy below E.[25]) Thus, the minimum property is retained even in the presence of bound states of H_A. It is clear that the method for "subtracting out" these bound states is essentially the same as the one described in Sec. IIIB for subtracting out the target bound states.

It can now be observed that the second term on the right-hand side of Eq. (4.3), which was introduced in order to preserve the minimum principle, is to be interpreted as a variational approximation to the bound-state pole contribution which accounts for the resonance. To show this explicitly one applies the "two-potential" formula[13] to Eq. (2.34) with the two terms on the right-hand side of Eq. (4.3) taken as the two components of the effective potential. The demonstration that this procedure leads to the Breit-Wigner formula is similar to that given in Ref. 2, and becomes identical to it if the trial functions are taken to be exact.[18]

It is useful to have a method for *direct* calculation of the position and width of a resonance as opposed to one, such as that just described, which requires a computation of the scattering amplitude in the neighborhood of the resonance peak. The "direct" method described below is based on the resolvent-operator approach of Watson[10] and Zumino[26] which is here cast in variational form.

We retain the model which relates the resonance to the existence of a discrete state $|a\rangle$ in the modified Hamiltonian H_A. Now, however, we investigate the effect of this state on the scattering amplitude directly, rather than indirectly through the effective potential. The on-shell scattering amplitude can be expressed as

$$\langle \vec{k}_i | \mathcal{T}_{ij} | \vec{k}_j \rangle = \langle \chi_{i(0)}; \vec{k}_i | (V - V_j) |\, \chi_{j(0)}; \vec{k}_j \rangle$$
$$+ \langle \chi_{i(0)}; \vec{k}_i | (V - V_i) G(E) (V - V_j) |\, \chi_{j(0)}; \vec{k}_j \rangle, \tag{4.6}$$

a form which follows, e.g., from Eqs. (2.16) and (2.33) and the relation

$$(H - E) |\, \chi_{j(0)}; \vec{k}_j \rangle = (V - V_j) |\, \chi_{j(0)}; \vec{k}_j \rangle, \tag{4.7}$$

valid on the energy shell. The resolvent $G(z) = (z - H)^{-1}$ can be analyzed in terms of $G_A(z) = (z - H_A)^{-1}$. Thus, with

$$V_B \equiv H - H_A \quad , \tag{4.8}$$

the equation

$$G(z) = G_A(z) + G_A(z) V_B G(z) \tag{4.9}$$

follows directly. To isolate the bound-state contribution to G_A we write

$$G_A(z) = |a\rangle\langle a| / (z - E_a) + \tilde{G}_A(z) \quad . \tag{4.10}$$

We now define $\tilde{G}(z)$ as the solution of

$$\tilde{G}(z) = \tilde{G}_A(z) + \tilde{G}_A(z)\, V_B\, \tilde{G}(z) \quad , \tag{4.11}$$

and observe that the relation between G and $\tilde{G}$ can be expressed in a simple algebraic form since G_A and $\tilde{G}_A$ differ by a separable operator. One easily finds that[27]

$$G(z) = \tilde{G}(z) + [1 + \tilde{G}(z)\, V_B] |\, a\rangle \frac{1}{D(z)} \langle a | [1 + V_B \tilde{G}(z)] \quad , \tag{4.12}$$

where, with the level shift defined as

$$R_a(z) = \langle a | [V_B + V_B \tilde{G}(z) V_B] | a \rangle \quad , \tag{4.13}$$

the denominator function $D(z)$ takes the form

$$D(z) = z - E_a - R_a(z). \tag{4.14}$$

A similar decomposition of $\mathcal{T}_{ij}$ follows from Eqs. (4.6) and (4.12), with $z \to E + i0^+$. We have

$$\langle \vec{k}_i | \mathcal{T}_{ij} | \vec{k}_j \rangle = \langle \vec{k}_i | \tilde{\mathcal{T}}_{ij} | \vec{k}_j \rangle$$
$$+ \langle \Omega_i^{(-)} | (H - E) | a \rangle \frac{1}{D(E)} \langle a | (H - E) |\, \Omega_j^{(+)} \rangle , \tag{4.15}$$

where $\tilde{\mathcal{T}}_{ij}$ is defined as in Eq. (4.6) with G replaced by $\tilde{G}$, and

$$|\Omega_j^{(\pm)}\rangle = |\chi_{j(0)};\vec{k}_j\rangle + \tilde{G}(E\pm i0^+)(V-V_j)|\chi_{j(0)};\vec{k}_j\rangle \ . \tag{4.16}$$

In writing Eq. (4.15) in the form shown we have used Eq. (4.7) along with the fact that since $\tilde{G}|a\rangle = 0$ [see Eqs. (4.10) and (4.11)] we can write

$$\tilde{G}V_B|a\rangle = \tilde{G}(H-E)|a\rangle \ . \tag{4.17}$$

Similarly $D(z)$ can be rewritten as

$$D(z) = \langle a|[z-H-(z-H)\tilde{G}(z)(z-H)]|a\rangle. \tag{4.18}$$

Note that with the introduction of the projection operator

$$L = 1 - |a\rangle\langle a| \ , \tag{4.19}$$

the equation defining $\tilde{G}_A(z)$ can be taken as

$$L(z-H_A)L\tilde{G}_A(z) = L \ , \tag{4.20}$$

so that Eq. (4.11), which defines $\tilde{G}(z)$, can be replaced by

$$L(z-H)L\tilde{G}(z) = L \ . \tag{4.21}$$

At this stage everything has been expressed in terms of the state $|a\rangle$ and the original Hamiltonian H. It follows that while the decomposition $H = H_A + V_B$ will generally be helpful in choosing $|a\rangle$, particularly if one has a minimum principle as a guide, this decomposition need not actually be specified. The essential requirement on the choice of $|a\rangle$ which will make the identity, Eq. (4.15), a useful relation is that it shall lead to a resolvent $\tilde{G}(z)$ which has a smooth energy dependence in the neighborhood of the resonance. This allows one to associate the rapid energy variation in the scattering amplitude with the behavior of $D(z)$. We expect[10] that the analytic continuation of $D(z)$ on to the second Riemann sheet vanishes for a value of z just below the real axis; this gives rise to a pole in $G(z)$ and in the scattering amplitude as well. The position of the pole in the complex plane gives us the resonance energy and width. Note that Eq. (4.15) not only describes the Breit-Wigner energy variation near a resonance but also takes into account the background effects contained in $\tilde{G}$.

The remaining computational problem of constructing $|a\rangle$, and then $\tilde{G}$, can be handled variationally. Firstly, improvable approximations to $|a\rangle$ can be obtained by minimization of the expectation value of H_A. If the target bound state which is subtracted off in the definition of H_A is not known exactly the modified procedure described in Sec. III B can be used. One now searches for a discrete state of $\bar{H}_A$ [see, e.g., Eq. (3.13)] with energy $\bar{E}_a$ lying below the continuum threshold $\bar{E}_T$. Since $\bar{E}_T$ may be displaced downward relative to the true continuum threshold E_T of H_A one has a requirement on the accuracy of the trial target wave functions; they must be accurate enough so that $\bar{E}_T$ lies above the resonance energy.[28] According to the discussion of the preceding paragraph the fact that $\bar{\chi}_{j(0)}$ is inexact does not imply that the calculated resonance parameters will reflect this error since a change in the value of E_a is compensated for by a change in the level shift. We emphasize that the decomposition $H = \bar{H}_A + \bar{V}_B$ retains the virtue, from the standpoint of computations, associated with the decomposition $H = H_A + V_B$, namely, that the Rayleigh-Ritz minimum principle can be used to find the discrete state.

Now assuming that the state $|a\rangle$ has been chosen, Eq. (4.21) for $\tilde{G}$ can be solved variationally[7] leading to a variational principle for $D(z)$. Equivalently, we define

$$[D(z)] = \langle a|(z-H)|a\rangle + \langle a|(z-H)|b(z)\rangle + \langle c(z)|(z-H)|a\rangle + \langle c(z)|(z-H)|b(z)\rangle, \tag{4.22}$$

with

$$\langle c(z)|a\rangle = \langle a|b(z)\rangle = 0 \ . \tag{4.23}$$

This functional reduces to the correct expression for $D(z)$, Eq. (4.18), for

$$L(z-H)|b(z)\rangle + L(z-H)|a\rangle = 0 \tag{4.24}$$

or, for

$$\langle a|(z-H)L + \langle c(z)|(z-H)L = 0 \ . \tag{4.25}$$

These two expressions are equivalent to

$$|b(z)\rangle = -\tilde{G}(z)(z-H)|a\rangle \tag{4.24'}$$

and

$$\langle c(z)| = -\langle a|(z-H)\tilde{G}(z) \ , \tag{4.25'}$$

respectively. Furthermore, the stationary property of $[D(z)]$ for independent variations of $|b(z)\rangle$ and $\langle c(z)|$ about their exact values given in Eqs. (4.24') and (4.25'), subject to the orthogonality constraint, Eq. (4.23), is easily verified.

With z taken to lie in the upper half-plane the trial functions will decay asymptotically, guaranteeing convergent integrals. To locate the zero of $D(z)$, and hence the resonance parameters, $D(z)$ must be continued on to the second sheet. This is a trivial procedure if the integrals in the variational expression can be evaluated analytically. Otherwise, a numerical procedure must be adopted, in which values computed at a number of points are matched to a simple analytic function. This procedure has been tested a number of times now for scattering calculations[29] (involving continuation to the real axis) and seems to be quite adequate. The validity of this program rests, of course, on the assumed analytic properties of the level shift.[10] In the Appendix the program is discussed in greater detail in the context of potential scattering in a given partial wave. Here we can take advantage of the well-established analytic properties of the Jost function to provide a firm mathematical basis for the analysis.

APPENDIX

In the case of scattering of a particle by a static potential $v(r)$, the S matrix (for simplicity we confine our attention here to s-wave scattering) can be represented as a ratio of Jost functions[30]:

$$S(k)=\mathcal{F}_-(k)/\mathcal{F}_+(k) \quad . \tag{A1}$$

The Jost functions can be defined in terms of the regular solution of the Schrödinger equation

$$\phi''(r)+k^2\phi(r)+u(r)\phi(r)\equiv L\phi=0 \quad , \tag{A2}$$

where $u(r)=-(2m)/\hbar^2 v(r)$. The boundary conditions at $r=0$ are

$$\phi(0)=0 \quad , \tag{A3}$$

$$\phi'(0)=1 \quad , \tag{A4}$$

and at infinity ϕ satisfies

$$\phi(r)\sim\frac{1}{2ik}\left[\mathcal{F}_-(k)e^{ikr}-\mathcal{F}_+(k)e^{-ikr}\right] \quad . \tag{A5}$$

An alternate definition of the Jost functions is obtained from the irregular solutions of Eq. (A2), which have the asymptotic form

$$f_\pm(r)\sim e^{\pm ikr} \quad , \tag{A6}$$

while at the origin

$$f_\pm(0)=\mathcal{F}_\pm \quad . \tag{A7}$$

By virtue of Eq. (A1) and the relation

$$\mathcal{F}_-(k)=\mathcal{F}_+^*(k^*) \tag{A8}$$

we see that the scattering problem is reduced to a computation of $\mathcal{F}_+(k)$. In particular, the zeros of $\mathcal{F}_+(k)$ give the bound-state energies if k is on the positive imaginary axis and give the resonance positions if k is just below the positive real axis.

Consider now a variational approach to the computational problem. We introduce a trial regular function $\phi_t(r)$ which satisfies Eqs. (A3) and (A4) and has the asymptotic form

$$\phi_t(r)\sim\frac{1}{2ik}\left[\mathcal{F}_{-t}(k)e^{ikr}-\mathcal{F}_{+t}(k)e^{-ikr}\right] \quad , \tag{A9}$$

where $\mathcal{F}_{\pm t}$ are trial Jost functions. Now

$$J\equiv\int_0^\infty f_+L\,\phi_t\,dr-\int_0^\infty \phi_t\,Lf_+\,dr \tag{A10}$$

is given, on the one hand, by

$$J=\int_0^\infty f_+L\,\phi_t\,dr \quad , \tag{A11}$$

since $Lf_+=0$. On the other hand, integration by parts gives

$$J=(f_+\phi_t'-f_+'\phi_t)\Big|_0^\infty \quad , \tag{A12}$$

which can be evaluated with the aid of the boundary conditions. The identity

$$\mathcal{F}_+(k)=\mathcal{F}_{+t}(k)-\int_0^\infty f_+L\,\phi_t\,dr \tag{A13}$$

follows immediately. The replacement of the unknown function f_+ by a trial function f_{+t} which has the correct outgoing wave form at infinity introduces only a second-order error since $L\phi_t$ is itself a first-order quantity. Note that $f_t(0)\equiv\hat{\mathcal{F}}_{+t}$ is a trial Jost function which need not be equal to $\mathcal{F}_{+t}$. Similar arguments lead to the identity

$$\mathcal{F}_+(k)=\hat{\mathcal{F}}_{+t}(k)-\int_0^\infty \phi\,Lf_{+t}\,dr \quad , \tag{A14}$$

but the variational expression obtained from it gives nothing new since

$$\mathcal{F}_{+v}\equiv\mathcal{F}_{+t}-\int_0^\infty f_{+t}\,L\,\phi_t\,dr=\hat{\mathcal{F}}_{+t}-\int_0^\infty \phi_t\,Lf_{+t}\,dr \quad , \tag{A15}$$

as can be seen by integration by parts.

For a wide class of short-ranged potentials the Jost function $\mathcal{F}_+(k)$ can be continued into a domain below the real k axis.[31] In many cases this domain will extend well below the values of Imk for which the integral in Eq. (A13) begins to diverge. Let us assume that $\mathcal{F}_+(k)$ vanishes for some k within the domain of analyticity below the real positive axis. Then the position of this zero, and hence the resonance parameters, can be determined variationally from an examination of $\mathcal{F}_{+v}(k)$. If the zero is located in a region where the integral in Eq. (A15) converges then no analytic continuation is necessary. Otherwise, $\mathcal{F}_{+v}(k)$ must be evaluated for Imk sufficiently large and continued downward in the complex k plane. Numerical methods are available to achieve this continuation.[29,32] A possible advantage of the variational approach, as opposed to direct numerical computation of the Jost function at selected points in the upper half-plane, is that in many cases the trial function can be chosen such that the integrals can be performed exactly; the process of analytic continuation is then trivial.

A perturbation theory for the Jost function is easily obtained from the variational formulation. Thus, suppose we can write $u(r)$ as the sum of two potentials $u_0(r)$ and $u_1(r)$, where $u_0(r)$ is solvable. If $u_1(r)$ is effectively small the exact solutions associated with $u_0(r)$ are reasonable trial functions. We have the identity (analogous to the "two-potential" formula of scattering theory)

$$\mathcal{F}_+(k)=\mathcal{F}_{+0}(k)-\int_0^\infty f_+u_1\,\phi_0\,dr \quad , \tag{A16}$$

from which we derive the first-order perturbation formula

$$\mathcal{F}_{+v}(k)=\mathcal{F}_{+0}(k)-\int_0^\infty f_{+0}\,u_1\,\phi_0\,dr \quad . \tag{A17}$$

For the particular case $u_1(r)=\lambda\,\delta(r-a)$ we have the amusing result that the perturbation formula

$$\mathcal{F}_{+v}(k)=\mathcal{F}_{+0}(k)-\lambda f_{+0}(a)\phi_0(a) \tag{A18}$$

is exact; the value of the irregular solution at $r = a$ depends only on the potential for $r > a$, i.e., $f_{+0}(a) = f_+(a)$.

Recently, a perturbation formula for the shift in a resonance position was derived by More.[33] To verify that More's result is contained in the above perturbation formula for the Jost function we set $k = K_0$ in Eq. (A17), where $\mathcal{F}_{+0}(K_0) = 0$. We expand the left-hand side as

$$\mathcal{F}_{+v}(K_0) = \mathcal{F}_{+v}(K) + (K_0 - K)\,\mathcal{F}'_{+v}(K_0) + \cdots \tag{A19}$$

and observe that the zero of $\mathcal{F}_+(K)$ is given, to first order in the perturbation, by

$$K - K_0 = [\mathcal{F}'_{+0}(K_0)]^{-1} \int_0^\infty f_{+0}\, u_1\, \phi_0\, dr \ . \tag{A20}$$

This can be put in the form given by More. Actually, we now see that More's assumption that the potential vanishes beyond some finite point can be relaxed somewhat. It is required only that the integral in Eq. (A20) be convergent.

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