Variational Approach to the Faddeev Equations*

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A variational principle is formulated as a means for obtaining approximate solutions to the Faddeev integral equations for the nonrelativistic three-body scattering problem. Bound states are described by the homogeneous version of the Faddeev equations. In this case a minimum principle for the binding energies is obtained in close analogy with the familiar Rayleigh-Ritz method. An effective potential is defined as the solution of a set of modified Faddeev equations. The variational principle therefore applies to the effective potential. This is shown to be a minimum principle for the eigenphase shifts for energies below the three-particle breakup threshold. Some formal applications of the variational principle are described. These include derivations, within the Faddeev formalism, of a normalization condition for bound-state wave functions, a distorted-wave theory, and a perturbation theory for discrete states.

1. INTRODUCTION

DURING the past few years considerable interest has been shown in the use of the Faddeev equations[1] to formulate the quantum-mechanical three-body problem. Almost all of the numerical calculations, based on the Faddeev formalism, which have been performed up to now have made use of a separable approximation to the two-body input amplitudes.[2] This has the great virtue of leading, after one has separated off the angular variables, to a set of coupled one-dimensional integral equations which can be solved numerically. In spite of the obvious attendant computational difficulties, it is natural at this point to look for approximation techniques which do not require separable input amplitudes. Since variational methods have been quite useful in the usual Hamiltonian approach to the few-body problem, we have set out here to develop analogous methods for treating linear integral equations of the Faddeev type. Variational principles for the scattering amplitude and for the effective potential are derived in Sec. 2. They are valid for all processes, inelastic as well as elastic. The bound-state problem is discussed in Sec. 3, and a minimum principle for calculating binding energies is developed. This result is used, in Sec. 4, to obtain a minimum principle for the effective potential which leads to lower bounds on the eigenphase shifts for energies below the three-particle continuum threshold.

It is known from experience with the Schrödinger equation that the variational approach can be quite useful not only as a calculational device, but also as a formal method for developing a variety of approximation techniques by suitable choice of trial functions. This latter type of application is illustrated in Sec. 2, where a distorted-wave theory, based on the integral equations, is developed. Other formal applications of the variational principle include the derivation of a normalization condition for (bound-state) solutions of the homogeneous Faddeev equations and the development of a perturbation theory for discrete states.

A possible advantage of the present approach, in contrast to methods based on the Schrödinger equation, lies in the fact that the input to the equations consists not of potentials, but rather of subsystem scattering amplitudes. Therefore techniques discussed here can be applied to a relativistic version of the Faddeev equations.[3,4] Many-body generalizations are also possible.[4,5] On the other hand, the operators which enter the theory are relatively unfamiliar. Consequently, it will take some experience before one learns how to choose accurate trial functions in applications of the variational principle. Furthermore, a precise specification of the class of admissible trial functions is necessary with regard both to practical applications and to questions of mathematical rigor. We hope that the approach presented here will prove promising enough so that these problems will eventually receive the attention they require.

2. VARIATIONAL PRINCIPLE FOR SCATTERING

A. Three-Body Integral Equations

The three-body Faddeev equations can be written in the equivalent[6] matrix-operator forms

$$\mathbf{T}=\mathbf{T}_D+\mathbf{T}_D\mathbf{G}\mathbf{T}, \tag{2.1a}$$

$$\mathbf{T}=\mathbf{T}_D+\mathbf{T}\mathbf{G}\mathbf{T}_D. \tag{2.1b}$$

The matrices are 3×3. We suppress the dependence on the total-energy variable E. The disconnected amplitude $\mathbf{T}_D$ is diagonal, with diagonal elements given by the two-body scattering operators. The Green's operator is

$$\mathbf{G}=\begin{bmatrix}0 & G & G\\ G & 0 & G\\ G & G & 0\end{bmatrix}, \tag{2.2}$$

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[1] L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)].

[2] A. N. Mitra, Nucl. Phys. **32**, 529 (1962); R. D. Amado, Phys. Rev. **132**, 485 (1963); L. Rosenberg, *ibid.* **135**, B715 (1964); C. Lovelace, *ibid.* **135**, B1225 (1964).

[3] L. Rosenberg, Phys. Rev. **147**, 1016 (1966).

[4] L. Rosenberg (to be published).

[5] L. Rosenberg, Phys. Rev. **140**, B217 (1965).

[6] The equivalence of Eqs. (2.1a) and (2.1b) is easily demonstrated with the aid of Eq. (2.24) below, with $\Delta\mathbf{T}_D=\Delta\mathbf{G}=0$.

where

$$G=(E+i\eta-K)^{-1}. \tag{2.3}$$

Here K is the total-kinetic-energy operator for the three-body system. The scattering amplitude T which describes the three-body → three-body process is given, in terms of the elements ${}^{(i)}T^{(j)}$ of $\mathbf{T}$, by

$$T=\sum_{i=1}^{3}\sum_{j=1}^{3}{}^{(i)}T^{(j)}. \tag{2.4}$$

Other elements of the T matrix, pertaining to those cases where a pair of particles is bound in the initial or final state, are obtained from T by application of a "residue rule" described previously.[5] A specific application of the rule appears below.

An integral equation for the connected amplitude $\mathbf{T}_C$ is obtained from Eq. (2.1a) with the substitution

$$\mathbf{T}=\mathbf{T}_D+\mathbf{T}_C; \tag{2.5}$$

we obtain

$$\mathbf{T}_C=\mathbf{B}+\mathbf{T}_D\mathbf{G}\mathbf{T}_C, \tag{2.6}$$

where

$$\mathbf{B}=\mathbf{T}_D\mathbf{G}\mathbf{T}_D. \tag{2.7}$$

The bound-state problem is studied with the aid of the homogeneous versions of Eqs. (2.1), which we write as

$$\mathbf{\Gamma}=\mathbf{T}_D\mathbf{G}\mathbf{\Gamma}, \tag{2.8a}$$

$$\mathbf{\Lambda}=\mathbf{\Lambda}\mathbf{G}\mathbf{T}_D. \tag{2.8b}$$

Here $\mathbf{\Gamma}$ and $\mathbf{\Lambda}$ are column and row vectors with elements ${}^{(i)}\Gamma$ and $\Lambda^{(i)}$, respectively. Bound states introduce poles in the scattering amplitude. With E in the neighborhood of a bound-state energy E_B, $\mathbf{T}_C$ takes on the factored form

$$\mathbf{T}_C\approx\mathbf{\Gamma}P\mathbf{\Lambda}, \tag{2.9}$$

where

$$P=(E-E_B)^{-1}. \tag{2.10}$$

In the following, we will make use of the reality properties of the scattering and bound-state functions; we will therefore record these properties here. First, we note the relations

$$\mathbf{T}_D{}^{\dagger(-)}=\mathbf{T}_D, \tag{2.11}$$

$$\mathbf{G}^{\dagger(-)}=\mathbf{G}. \tag{2.12}$$

Here the dagger implies that rows and columns of the matrix are to be interchanged and the operator adjoint of each element is to be taken. The superscript $(-)$ indicates that the energy is to approach the real axis from below rather than above. If we take the adjoint of both sides of Eq. (2.1a), replace $E+i\eta$ by $E-i\eta$, and make use of Eqs. (2.11) and (2.12), we obtain

$$\mathbf{T}^{\dagger(-)'}=\mathbf{T}_D+\mathbf{T}^{\dagger(-)}\mathbf{G}\mathbf{T}_D. \tag{2.13}$$

We conclude, by comparison with Eq. (2.1b), that the relation

$$\mathbf{T}^{\dagger(-)}=\mathbf{T} \tag{2.14}$$

holds. Equation (2.14) implies the well-known reciprocity property

$$T_{\alpha\beta}{}^{*(-)}=T_{\beta\alpha}, \tag{2.15}$$

where α and β are channel labels for the scattering amplitude $T_{\alpha\beta}$. [To go from Eq. (2.14) to Eq. (2.15), one evaluates Eq. (2.14) in momentum space, sums over rows and columns, and makes use of the residue rule.] Similar considerations applied to the homogeneous equations lead to the relation

$$\mathbf{\Lambda}=\mathbf{\Gamma}^{\dagger}. \tag{2.16}$$

Here we make use of the fact that the distinction between $E+i\eta$ and $E-i\eta$ may be dropped for energies below the continuum threshold, i.e., $\mathbf{T}_D$ and $\mathbf{G}$ are self-adjoint at these energies.

B. Some Useful Identities

We wish to discuss variational approximations to solutions of the integral equations (2.1). A convenient starting point is the identity

$$O=O_t+O[1-O^{-1}O_t], \tag{2.17}$$

where O is any operator whose inverse is known, and where O_t is some "trial" estimate of O. If we write Eq. (2.17) as

$$O=O_t+O_t[1-O^{-1}O_t]+(\Delta O)O^{-1}(\Delta O), \tag{2.18}$$

where $\Delta O\equiv O-O_t$, we see that the error term $(\Delta O)O^{-1}(\Delta O)$ is of second order in ΔO. Therefore the expression

$$O_v=O_t+O_t(1-O^{-1}O_t) \tag{2.19}$$

provides a variational estimat of O. To make use of this result in the problem at hand, we observe that the integral equations can be written in the form

$$(\mathbf{1}+\mathbf{G}\mathbf{T})(\mathbf{1}-\mathbf{G}\mathbf{T}_D)=\mathbf{1}. \tag{2.20}$$

Then, with O replaced by $(\mathbf{1}+\mathbf{GT})$ and O^{-1} replaced by $(\mathbf{1}-\mathbf{GT}_D)$ in Eq. (2.17), we obtain the identity

$$(\mathbf{1}+\mathbf{G}\mathbf{T})=(\mathbf{1}+\mathbf{G}_t\mathbf{T}_t)+(\mathbf{1}+\mathbf{G}\mathbf{T})\times[\mathbf{1}-(\mathbf{1}-\mathbf{G}\mathbf{T}_D)(\mathbf{1}+\mathbf{G}_t\mathbf{T}_t)]. \tag{2.21}$$

This simplifies to

$$\mathbf{G}\mathbf{T}=\mathbf{G}_t\mathbf{T}_t+(\mathbf{1}+\mathbf{G}\mathbf{T})[\mathbf{G}\mathbf{T}_D\mathbf{G}_t\mathbf{T}_t+\mathbf{G}\mathbf{T}_D-\mathbf{G}_t\mathbf{T}_t]. \tag{2.22}$$

We now consider, for the choice of trial "function" $\mathbf{T}_t$, the exact solution of the integral equation

$$\mathbf{T}_t=\mathbf{T}_{Dt}+\mathbf{T}_{Dt}\mathbf{G}_t\mathbf{T}_t. \tag{2.23}$$

One is often led to approximations of this type by taking the sum of a particular subset of multiple-scattering terms; in Eq. (2.23) the terms to be summed are determined by the choice of $\mathbf{T}_{Dt}$ and $\mathbf{G}_t$. With the aid of Eq. (2.23), and with the definitions $\Delta\mathbf{G}=\mathbf{G}-\mathbf{G}_t$ and $\Delta\mathbf{T}_D=\mathbf{T}_D-\mathbf{T}_{Dt}$, Eq. (2.22) can be written as

$$\mathbf{T}=\mathbf{T}_t+(\mathbf{1}+\mathbf{T}\mathbf{G})\Delta\mathbf{T}_D(\mathbf{1}+\mathbf{G}_t\mathbf{T}_t)+\mathbf{T}\Delta\mathbf{G}\mathbf{T}_t. \tag{2.24}$$

This is a particularly useful identity, which appears frequently, in a variety of forms, in discussions of linear integral equations. As a simple example, we make the choice $\mathbf{T}_{Dt}=\mathbf{T}_D$; Eq. (2.24) then becomes

$$\mathbf{T}=\mathbf{T}_t+\mathbf{T}\Delta\mathbf{G}\mathbf{T}_t. \tag{2.25}$$

With the substitutions

$$\mathbf{T}_t=\mathbf{T}_D(1+\mathbf{G}_t\mathbf{T}_t), \tag{2.26}$$

$$\mathbf{T}=(1+\mathbf{T}\mathbf{G})\mathbf{T}_D, \tag{2.27}$$

Eq. (2.25) takes the form

$$\mathbf{T}=\mathbf{T}_t+(1+\mathbf{T}\mathbf{G})\Delta\mathbf{B}(1+\mathbf{G}_t\mathbf{T}_t). \tag{2.28}$$

Here

$$\Delta\mathbf{B}=\mathbf{T}_D\Delta\mathbf{G}\mathbf{T}_D \tag{2.29}$$

corresponds to a subset of double-scattering terms which contribute to the Born amplitude defined in Eq. (2.7). (Recall that $\mathbf{G}$ is a matrix; $\mathbf{G}_t$ may be chosen by setting certain elements in $\mathbf{G}$ equal to zero. It should also be borne in mind that equations of the above form are valid for the N-body scattering problem and have a relativistic extension.[4]) Consider now a physical collision process dominated by single-particle exchange from one subsystem to another. With the appropriate choice of $\mathbf{G}_t$, these dominant terms will appear in $\Delta\mathbf{B}$. The sum of the remaining terms, which gives rise to the amplitude $\mathbf{T}_t$, will be most significant in the determination of corrections due to initial- and final-state interactions. It is then reasonable to replace $\mathbf{T}\mathbf{G}$ by its trial value $\mathbf{T}_t\mathbf{G}_t$ in Eq. (2.28). This provides a variational expression which is equivalent to the familiar distorted-wave Born approximation.

We now turn to another application of Eq. (2.24) which will serve as preparation for the subsequent derivation of an effective-potential formalism. We take $\mathbf{G}_t=\mathbf{G}$, and for notational convenience rewrite Eq. (2.23) as

$$\mathbf{T}^A=\mathbf{T}_D{}^A+\mathbf{T}_D{}^A\mathbf{G}\mathbf{T}^A. \tag{2.30}$$

Equation (2.24) then becomes

$$\mathbf{T}=\mathbf{T}^A+(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B(1+\mathbf{G}\mathbf{T}^A), \tag{2.31}$$

where we have defined

$$\mathbf{T}_D{}^B=\mathbf{T}_D-\mathbf{T}_D{}^A. \tag{2.32}$$

It will be useful to have an alternative form for Eq. (2.31). We first observe that Eq. (2.31) can be written as

$$1+\mathbf{T}\mathbf{G}=1+\mathbf{T}^A\mathbf{G}+(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B\mathbf{G}^A, \tag{2.33}$$

where

$$\mathbf{G}^A\equiv\mathbf{G}+\mathbf{G}\mathbf{T}^A\mathbf{G}. \tag{2.34}$$

When postmultiplied by $\mathbf{T}_D{}^B$, Eq. (2.33) becomes

$$(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B=(1+\mathbf{T}^A\mathbf{G})\mathbf{T}_D{}^B+(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B\mathbf{G}^A\mathbf{T}_D{}^B, \tag{2.35}$$

which may be viewed as an integral equation for the factor $(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B$. Now we define $\mathbf{T}^{BA}$ as the solution of

$$\mathbf{T}^{BA}=\mathbf{T}_D{}^B+\mathbf{T}^{BA}\mathbf{G}^A\mathbf{T}_D{}^B. \tag{2.36}$$

If we premultiply Eq. (2.36) by $(1+\mathbf{T}^A\mathbf{G})$, we obtain an integral equation for $(1+\mathbf{T}^A\mathbf{G})\mathbf{T}^{BA}$ which is identical to Eq. (2.35) for $(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B$. We conclude that the equality

$$(1+\mathbf{T}\mathbf{G})\mathbf{T}_D{}^B=(1+\mathbf{T}^A\mathbf{G})\mathbf{T}^{BA} \tag{2.37}$$

holds. This allows us to rewrite Eq. (2.31) as

$$\mathbf{T}=\mathbf{T}^A+(1+\mathbf{T}^A\mathbf{G})\mathbf{T}^{BA}(1+\mathbf{G}\mathbf{T}^A). \tag{2.38}$$

C. Effective-Potential Formalism

The disconnected amplitude T_D is defined as

$$T_D=\sum_{\alpha=1}^{3}T(S_\alpha), \tag{2.39}$$

where $T(S_\alpha)$ is the scattering operator for the two-body subsystem S_α. The sum runs over the three distinct two-body subsystems. We now choose the amplitude $T_D{}^B$, whose components appear in Eq. (2.36), as

$$T_D{}^B=\sum_{\alpha=1}^{3}T^B(S_\alpha), \tag{2.40}$$

where $T^B(S_\alpha)$ is taken to be of the separable form

$$T^B(S_\alpha)=\Gamma(S_\alpha)G_\alpha\Gamma^\dagger(S_\alpha). \tag{2.41}$$

In the simplest version of the separable approximation, the "propagator" G_α will be a pole in the two-body c.m. energy variable. Since we are interested in matrix elements in the momentum space of three particles, we would express G_α as

$$G_\alpha=(E-K_\alpha-E_{B\alpha})^{-1}, \tag{2.42}$$

where E is the total energy, K_α is the sum of the kinetic energy of the center of mass of the bound cluster plus the kinetic energy of the third particle, and $E_{B\alpha}$ is the eigenenergy of the bound cluster. The vertex functions Γ and $\Gamma^\dagger$ give the correct residue at the pole; they can be obtained, e.g., from a knowledge of the bound-state wave function. More complicated propagators and vertex functions, which take into account continuum effects, can be used to define the separable approximation.[7] [If a number of separable terms are required to give a reasonable approximation to $T(S_\alpha)$, we may take T^B to be a sum of such terms. We may also take $T^B=0$ for a given pair.]

Suppose we are interested in elements $T_{\alpha\beta}$ of the three-body scattering matrix corresponding to entrance and exit channels in which pairs of particles are bound. Suppose further that the poles in the two-body amplitude due to these bound states are contained in $T_D{}^B$, so

[7] See, e.g., S. Weinberg, Phys. Rev. **130**, 776 (1963).

that $T_D{}^A = T_D - T_D{}^B$ has vanishing residues at these poles. According to the residue rule,[5] $T_{\alpha\beta}$ may be obtained from T, as given by Eq. (2.38), by taking residues at the poles in the terminal-state interactions of subsystems S_α and S_β. Now T^A, by construction, has vanishing residue at these poles. Furthermore, when the residue rule is applied to the disconnected amplitude $T_D{}^B$, we obtain a contribution to the S matrix, but not to $T_{\alpha\beta}$. Therefore we need only consider the amplitude

$$\mathbf{T}_C{}^{BA} = \mathbf{T}^{BA} - \mathbf{T}_D{}^B, \tag{2.43}$$

which according to Eq. (2.36) satisfies

$$\mathbf{T}_C{}^{BA} = \mathbf{T}_D{}^B \mathbf{G}^A \mathbf{T}_D{}^B + \mathbf{T}_C{}^{BA} \mathbf{G}^A \mathbf{T}_D{}^B. \tag{2.44}$$

Elements of the leading term are given by

$$^{(\alpha)}[\mathbf{T}_D{}^B \mathbf{G}^A \mathbf{T}_D{}^B]^{(\beta)} = \Gamma(S_\alpha) G_\alpha V_{\alpha\beta} G_\beta \Gamma^\dagger(S_\beta), \tag{2.45}$$

with the effective-potential matrix defined by

$$V_{\alpha\beta} = \Gamma^\dagger(S_\alpha)\, ^{(\alpha)}[\mathbf{G}^A]^{(\beta)} \Gamma(S_\beta). \tag{2.46}$$

This suggests that we look for elements of $\mathbf{T}_C{}^{BA}$ in the form

$$^{(\alpha)}[\mathbf{T}_C{}^{BA}]^{(\beta)} = \Gamma(S_\alpha) G_\alpha T_{\alpha\beta} G_\beta \Gamma^\dagger(S_\beta). \tag{2.47}$$

If we substitute this expression into Eq. (2.44) and apply the residue rule [in this case this amounts to removing the factors $\Gamma(S_\alpha)G_\alpha$ and $G_\beta\Gamma^\dagger(S_\beta)$ which appear in the final- and initial-state interactions, respectively], we obtain the effective two-body integral equation[8]

$$T_{\alpha\beta} = V_{\alpha\beta} + \sum_\gamma T_{\alpha\gamma} G_\gamma V_{\gamma\beta}. \tag{2.48}$$

Once the effective potential is determined, Eq. (2.48) can be readily solved numerically. With $T_{\alpha\beta}$ known, the amplitude for breakup of a bound pair can be determined directly; no additional integral equations need be solved. Thus, if we are interested in a transition from entrance channel β to exit channel f, in which all three particles are free, we substitute the decomposition $\mathbf{T}^{BA} = \mathbf{T}_D{}^B + \mathbf{T}_C{}^{BA}$ into Eq. (2.38) and apply the residue rule to the initial state only. With the definition

$$V_{f\beta} = \sum_\gamma \sum_{\delta \neq \beta} {}^{(\gamma)}[\mathbf{T}^A]^{(\delta)} G \Gamma(S_\beta) + \Gamma(S_\beta), \tag{2.49}$$

we obtain the breakup amplitude in the form

$$T_{f\beta} = V_{f\beta} + \sum_\gamma V_{f\gamma} G_\gamma T_{\gamma\beta}. \tag{2.50}$$

In a similar way we find that $T_{\alpha f}$ is given by

$$T_{\alpha f} = V_{\alpha f} + \sum_\gamma T_{\alpha\gamma} G_\gamma V_{\gamma f}, \tag{2.51}$$

where

$$V_{\alpha f} = \sum_\gamma \sum_{\delta \neq \alpha} \Gamma^\dagger(S_\alpha) G^{(\delta)} [\mathbf{T}^A]^{(\gamma)} + \Gamma^\dagger(S_\alpha). \tag{2.52}$$

Finally, with the definition

$$V_{ff} = \sum_\gamma V_{f\gamma} G_\gamma V_{\gamma f}, \tag{2.53}$$

we have, for three particles free in initial and final states,

$$T \equiv T_{ff} = T^A + \sum_\alpha \sum_\beta V_{f\alpha} G_\alpha T_{\alpha\beta} G_\beta V_{\beta f} + V_{ff}. \tag{2.54}$$

This may be put in the form

$$T_{ff} = T^A + \sum_\beta T_{f\beta} G_\beta V_{\beta f} \tag{2.55}$$

with the aid of Eqs. (2.50) and (2.53).

We conclude this subsection with two general remarks. If we set $\mathbf{T}_D{}^A = 0$ in the above equations, we reproduce the "separable-potential" model which has been studied extensively in recent years.[2] The present formalism provides a convenient basis for systematic improvements in this model due to the nonseparable parts of the input amplitudes. One method for obtaining such improvements, based on a minimum principle, is described in Sec. 4.

As noted by Feshbach,[9,10] an effective-potential formalism has the important feature of providing a model for resonances. Pole terms in the effective potential lead to resonance contributions to the solution of Eq. (2.48) for the T matrix. In the present formalism, poles appear in the effective potential at energies for which the homogeneous version of Eq. (2.30) has solutions. These bound-state solutions will be discussed at greater length in Secs. 3 and 4. In the Feshbach theory the effective potential is defined in terms of projection operators which are difficult to construct in practice. It is an advantage of the present version of the theory that such projection operators are not required. The removal of the pole contributions to the two-body scattering amplitudes in the definition of $T_D{}^A$ plays the role analogous to that played by the projection operators in the Feshbach theory.

D. Variational Principle of the Schwinger Type

If we set $\mathbf{G}_t = \mathbf{G}$ in Eq. (2.22), the identity becomes

$$\mathbf{T} = \mathbf{T}_t + (\mathbf{1} + \mathbf{T}\mathbf{G})(\mathbf{T}_D + \mathbf{T}_D \mathbf{G} \mathbf{T}_t - \mathbf{T}_t). \tag{2.56}$$

As shown by Eq. (2.18), the identity leads directly to a variational principle. Thus, if we replace $\mathbf{T}$ by $\mathbf{T}_\tau + \Delta\mathbf{T}'$ ($\mathbf{T}_\tau$ and $\mathbf{T}_t$ may, in general, be distinct) on the right-hand side of Eq. (2.56), we obtain $\mathbf{T}$ in the form

$$\mathbf{T} = \mathbf{T}_v + \text{error}, \tag{2.57}$$

where

$$\mathbf{T}_v - \mathbf{T}_D \equiv \mathbf{T}_{Cv} = \mathbf{T}_D \mathbf{G} \mathbf{T}_t + \mathbf{T}_\tau \mathbf{G} \mathbf{T}_D - \mathbf{T}_\tau (\mathbf{G} - \mathbf{G}\mathbf{T}_D \mathbf{G}) \mathbf{T}_t. \tag{2.58}$$

The formal expression for the error is found to be

$$\mathbf{T} - \mathbf{T}_v = \Delta\mathbf{T}' \mathbf{G} (\mathbf{T}_D + \mathbf{T}_D \mathbf{G} \mathbf{T}_t - \mathbf{T}_t). \tag{2.59}$$

[8] An effective-potential formalism based on the Faddeev equations has been obtained previously for the case of three identical particles; see Eq. (3.22) of Ref. 15. The formalism has been developed independently by E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. **B2**, 181 (1967).

[9] H. Feshbach, Ann. Phys. (N. Y.) **5**, 337 (1958); **19**, 287 (1962).

[10] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964), Chap. 11.

A more useful form is obtained if we replace $\mathbf{T}_t$ by $\mathbf{T}-\Delta\mathbf{T}$ in Eq. (2.59) and use the integral equation satisfied by $\mathbf{T}$. This gives the error term as

$$\mathbf{T}-\mathbf{T}_v=\Delta\mathbf{T}'(\mathbf{G}-\mathbf{G}\mathbf{T}_D\mathbf{G})\Delta\mathbf{T}. \tag{2.60}$$

The variational nature of the approximation given in Eq. (2.58) is now evident since $\Delta\mathbf{T}$ and $\Delta\mathbf{T}'$ are each assumed to be first-order errors. This variational expression is of the type proposed by Schwinger for the nonrelativistic potential-scattering problem.

Note that the choice

$$\mathbf{T}_r=\mathbf{T}_t^{\dagger(-)} \tag{2.61}$$

guarantees that the variational expression satisfies the correct reality property

$$\mathbf{T}_v^{\dagger(-)}=\mathbf{T}_v. \tag{2.62}$$

Here we have used Eqs. (2.11) and (2.12).

The variational approximation to the physical amplitude is obtained by evaluating Eq. (2.58) in momentum space, summing over rows and columns, and applying the residue rule to pick out the desired elements of the scattering matrix. In numerical applications the trial amplitude will generally be expressed as a linear combination of some conveniently chosen basis functions:

$$\mathbf{T}_t=\sum_{k=1}^{n} c_k\mathbf{T}_k. \tag{2.63}$$

The condition that the variational expression [Eq. (2.58)] be stationary with respect to variation of each of the linear parameters c_k leads to a set of linear equations which can be solved for the unknown parameters. One possible choice of basis functions $\mathbf{T}_k$ is the set obtained from the multiple-scattering expansion of the integral equations, i.e., $\mathbf{T}_1=\mathbf{T}_D$, $\mathbf{T}_2=\mathbf{T}_D\mathbf{G}\mathbf{T}_D$, etc.

We now show how a perturbation theory for discrete states can be deduced from the variational principle for scattering. Suppose that Eqs. (2.8) have solutions at $E=E_B$, the unperturbed binding energy. The disconnected amplitude in the perturbed problem is taken as $\mathbf{T}_D'=\mathbf{T}_D+\delta\mathbf{T}_D$. If the shift in pole position is small enough, the trial amplitudes

$$\mathbf{T}_t=\alpha\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger, \tag{2.64}$$

$$\mathbf{T}_r=\bar{\alpha}\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger, \tag{2.65}$$

with $P^{-1}=E-E_B$, will be appropriate for E near the perturbed energy E_B'. The linear parameters α and $\bar{\alpha}$ are to be determined variationally, as discussed above. The resultant variational expression is

$$\mathbf{T}_{Cv}=\mathbf{\Gamma}'P'\mathbf{\Gamma}'^\dagger, \tag{2.66}$$

with

$$\mathbf{\Gamma}'=\mathbf{T}_D'\mathbf{G}\mathbf{\Gamma}, \tag{2.67}$$

$$\mathbf{\Gamma}'^\dagger=\mathbf{\Gamma}^\dagger\mathbf{G}\mathbf{T}_D', \tag{2.68}$$

and

$$(P')^{-1}=\mathbf{\Gamma}^\dagger(\mathbf{G}-\mathbf{G}\mathbf{T}_D'\mathbf{G})\mathbf{\Gamma}. \tag{2.69}$$

The perturbed energy is found at the zero in $(P')^{-1}$.

We mention another application of the variational principle to the bound-state problem. The statement, contained in Eq. (2.9), that the residue at the pole in $\mathbf{T}_C$ is given by the dyad $\mathbf{\Gamma}\mathbf{\Gamma}^\dagger$ obviously implies a particular normalization of $\mathbf{\Gamma}$. The normalization condition can be deduced as follows. We observe that the trial functions given in Eqs. (2.64) and (2.65), with $\alpha=\bar{\alpha}=1$, are exact for $E=E_B$. Therefore, if these trial functions are inserted in Eq. (2.58), the resultant variational expression must have the correct residue $\mathbf{\Gamma}\mathbf{\Gamma}^\dagger$ at the pole. The residue is given by

$$\lim_{E\to E_B}(E-E_B)[\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger+\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger-\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger\mathfrak{L}\mathbf{\Gamma}P\mathbf{\Gamma}^\dagger],$$

where we have defined

$$\mathfrak{L}=\mathbf{G}-\mathbf{G}\mathbf{T}_D\mathbf{G}, \tag{2.70}$$

and have used Eqs. (2.8), which are valid at the pole. We now expand $\mathbf{\Gamma}^\dagger\mathfrak{L}\mathbf{\Gamma}$ in a Taylor series about $E=E_B$, keeping the first nonvanishing term. The correct residue is obtained provided

$$\frac{\partial}{\partial E}(\mathbf{\Gamma}^\dagger\mathfrak{L}\mathbf{\Gamma})_{E=E_B}=1, \tag{2.71}$$

which is the desired normalization condition. Note the similarity between this condition and the normalization condition for Bethe-Salpeter wave functions.[11]

The normalization condition is equivalent to the statement that the relation

$$P^{-1}=\mathbf{\Gamma}^\dagger(\mathbf{G}-\mathbf{G}\mathbf{T}_D\mathbf{G})\mathbf{\Gamma} \tag{2.72}$$

is valid to first order in $E-E_B$. Now, in deriving Eq. (2.69) as the expression whose root determines the perturbed energy, we assumed that the level shift is small. It is therefore consistent to combine Eqs. (2.69) and (2.72). This leads to the Dyson-like equation

$$(P')^{-1}=P^{-1}-\mathbf{\Gamma}^\dagger\mathbf{G}\delta\mathbf{T}_D\mathbf{G}\mathbf{\Gamma}. \tag{2.73}$$

3. GENERALIZED RAYLEIGH-RITZ PRINCIPLE

The bound-state problem may be defined by the requirement that an energy E and vertex function $\mathbf{\Gamma}$ must be found so that the homogeneous integral equations

$$\mathfrak{L}(E)\mathbf{\Gamma}=0 \tag{3.1}$$

are satisfied. We have indicated explicitly the energy dependence of the operator $\mathfrak{L}$ defined by Eq. (2.70).

[11] R. E. Cutkosky and M. Leon, Phys. Rev. **135**, B1445 (1964); D. Lurié, A. J. Macfarlane, and Y. Takahashi, *ibid.* **140**, B1091 (1965).

Since E is below the continuum threshold, we have

$$\mathfrak{L}(E)=\mathfrak{L}^{\dagger}(E), \tag{3.2}$$

and the adjoint of Eq. (3.1) holds in the form

$$\mathbf{\Gamma}^{\dagger}\mathfrak{L}(E)=0. \tag{3.3}$$

It is a simple matter to obtain a variational principle for the bound-state energies. Evidently, the scalar equation

$$\mathbf{\Gamma}^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}=0 \tag{3.4}$$

holds when Eqs. (3.1) and (3.3) are satisfied. With $\mathbf{\Gamma}=\mathbf{\Gamma}_t+\Delta\mathbf{\Gamma}$, where $\mathbf{\Gamma}_t$ is some trial vertex function, Eq. (3.4) reads

$$\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}_t+\Delta\mathbf{\Gamma}^{\dagger}\mathfrak{L}(E)\Delta\mathbf{\Gamma}=0. \tag{3.5}$$

Let E_t be some (real-valued) estimate of E, and suppose that $E-E_t$ and $\mathbf{\Gamma}-\mathbf{\Gamma}_t$ can be considered as small errors. The first term in Eq. (3.5) can be expanded as

$$\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}_t=\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E_t)\mathbf{\Gamma}_t +(E-E_t)(\partial/\partial E)(\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}_t)_{E=E_t}, \tag{3.6}$$

where terms of higher order in $(E-E_t)$ have been dropped. Now the normalization condition [Eq. (2.71)] holds for the correct solution, so that the coefficient of $(E-E_t)$ in Eq. (3.6) differs from unity by a first-order quantity. To first order, then, we have

$$\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}_t=\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E_t)\mathbf{\Gamma}_t+E-E_t. \tag{3.7}$$

When Eqs. (3.5) and (3.7) are combined, and the second-order term in Eq. (3.5) is neglected, we obtain

$$E_v=E_t-\mathbf{\Gamma}_t^{\dagger}\mathfrak{L}(E_t)\mathbf{\Gamma}_t \tag{3.8}$$

as the variational principle for E.

Let $\mathbf{\Gamma}_t$ be represented as a superposition of linearly independent basis functions, i.e.,

$$\mathbf{\Gamma}_t=\sum_{k=1}^{n} c_k\mathbf{\Gamma}_k, \tag{3.9}$$

and let $\mathbf{c}$ represent a column vector with elements c_k. Then, with the $n\times n$ matrix $\mathbf{L}(E)$ defined as

$$L_{ij}(E)=\mathbf{\Gamma}_i^{\dagger}\mathfrak{L}(E)\mathbf{\Gamma}_j, \tag{3.10}$$

the variational principle becomes

$$E_v=E_t-\mathbf{c}^{\dagger}\mathbf{L}(E_t)\mathbf{c}. \tag{3.11}$$

The trial parameters are determined by the requirement that the right-hand side of Eq. (3.11) must be stationary with respect to independent variations of E_t and the components of $\mathbf{c}$. This requirement leads directly to the conditions

$$\frac{\partial}{\partial E}(\mathbf{c}^{\dagger}\mathbf{L}(E)\mathbf{c})_{E=E_t}=1 \tag{3.12}$$

and

$$\mathbf{L}\mathbf{c}=0. \tag{3.13}$$

According to Eqs. (3.11) and (3.13), the variational estimate of E is just E_t, which is determined by

$$\det\mathbf{L}(E_t)=0, \tag{3.14}$$

subject to Eq. (3.12). Of course, a change in normalization of $\mathbf{c}$ will not affect the variational calculation of the energy. Equation (3.12) may be replaced by

$$\frac{\partial}{\partial E}(\mathbf{c}^{\dagger}\mathbf{L}(\mathbf{E})\mathbf{c})_{E=E_t}>0. \tag{3.15}$$

This inequality places a restriction on the choice of trial functions. This is a natural restriction, since it defines a class of allowed trial functions which contains the true function $\mathbf{\Gamma}$.

The roots of Eq. (3.14) yield a set of energies $E_1^{(n)}$, $E_2^{(n)}$, $\cdots$, $E_M^{(n)}$. The superscript (n) denotes the dimension of $\mathbf{L}$, and the subscript implies an ordering such that $E_i^{(n)}\leq E_{i+1}^{(n)}$. We assume that the true energies are bounded from below and that the bottom portion of the spectrum consists of a finite set of isolated points at energies E_i, with $E_i\leq E_{i+1}$.

We have seen that the energies $E_i^{(n)}$ provide variational estimates of the E_i. It is natural to enquire whether these estimates are in fact upper bounds, in analogy with the familiar Rayleigh-Ritz property encountered in the Hamiltonian formulation of the bound-state problem. To investigate this point, we introduce an associated eigenvalue problem in which solutions of

$$[\mathfrak{L}(E)-\lambda\varrho(E)]\mathbf{\Gamma}=0 \tag{3.16}$$

are sought, with E below the continuum threshold. Here ϱ is defined such that $\mathbf{\Gamma}^{\dagger}\varrho\mathbf{\Gamma}$ is positive for any $\mathbf{\Gamma}$. [Equation (3.16) may be thought of physically as arising from Eq. (3.1) by the replacement $\mathbf{T}_D\rightarrow\mathbf{T}_D+\lambda\mathbf{T}_D'$; then $\varrho=\mathbf{G}\mathbf{T}_D'\mathbf{G}$.] With the strength parameter λ fixed at some real value, Eq. (3.16) defines an energy-eigenvalue problem. The inequality

$$\frac{\partial}{\partial E}[\mathbf{\Gamma}^{\dagger}(\mathfrak{L}-\lambda\varrho)\mathbf{\Gamma}]>0 \tag{3.17}$$

is expected to hold for solutions to Eq. (3.16), just as for the case $\lambda=0$. Alternatively, with E fixed, Eq. (3.16) may be used to determine a set of real eigenvalues $\lambda_i(E)$. If this is done for a range of values of E, a set of curves in the λ-E plane is generated; a given point on one of the curves gives a pair of values (λ,E) for which Eq. (3.16) is satisfied. The slope of these curves may be determined to be positive by the following argument. Let

$$Q(\lambda,E)=\mathbf{\Gamma}^{\dagger}(\mathfrak{L}-\lambda\varrho)\mathbf{\Gamma} \tag{3.18}$$

be defined for values of λ and E lying on one of the curves. Since Q vanishes for each point, we have, for

variations in E and λ along the curve,

$$0=dQ(\lambda,E)$$
$$=\frac{\partial Q}{\partial E}dE+\frac{\partial Q}{\partial \lambda}d\lambda. \tag{3.19}$$

If we differentiate Eq. (3.18) with respect to λ and recognize that

$$\mathbf{\Gamma}^\dagger(\mathfrak{L}-\lambda\varrho)\frac{\partial \mathbf{\Gamma}}{\partial \lambda}=0, \tag{3.20}$$

$$\frac{\partial \mathbf{\Gamma}^\dagger}{\partial \lambda}(\mathfrak{L}-\lambda\varrho)\mathbf{\Gamma}=0, \tag{3.21}$$

by virtue of Eq. (3.16) and its adjoint, we find that

$$\frac{\partial Q}{\partial \lambda}=-\mathbf{\Gamma}^\dagger\varrho\mathbf{\Gamma}. \tag{3.22}$$

The expression for the slope is then

$$\frac{d\lambda}{dE}=\frac{\partial Q}{\partial E}\Big/\mathbf{\Gamma}^\dagger\varrho\mathbf{\Gamma}, \tag{3.23}$$

which is positive, since Eq. (3.17) holds for any point on the curve and $\mathbf{\Gamma}^\dagger\varrho\mathbf{\Gamma}$ is positive for any $\mathbf{\Gamma}$. We have assumed that there is an energy E_0 below which there are only a finite number of energy eigenvalues. This, combined with the fact that the λ-versus-E curve has positive slope, implies that for any energy fixed below E_0 there are only a finite number of positive eigenvalues λ associated with the Hermitian operator $\mathfrak{L}$. We therefore assume that these eigenvalues can be characterized by the maximum-minimum property.[12] It is this property which leads to the desired minimum principle for the bound-state energy, as will now be shown.

A variational expression for the eigenvalue λ is given by

$$\mathbf{\Gamma}_t^\dagger(\mathfrak{L}-\lambda_v\varrho)\mathbf{\Gamma}_t=0. \tag{3.24}$$

With $\mathbf{\Gamma}_t$ chosen as in Eq. (3.9), the variational expression becomes

$$\mathbf{c}^\dagger(\mathbf{L}-\lambda_v\mathbf{r})\mathbf{c}=0, \tag{3.25}$$

where $\mathbf{L}$ is given by Eq. (3.10), and

$$r_{ij}=\mathbf{\Gamma}_i^\dagger\varrho\mathbf{\Gamma}_j. \tag{3.26}$$

The requirement that Eq. (3.25) be stationary with respect to variations of $\mathbf{c}$ leads to the set of equations

$$(\mathbf{L}-\lambda_v\mathbf{r})\mathbf{c}=0. \tag{3.27}$$

If the trial function is sufficiently accurate, the inequality

$$\frac{\partial}{\partial E}[\mathbf{c}^\dagger(\mathbf{L}-\lambda_v\mathbf{r})\mathbf{c}]>0 \tag{3.28}$$

will be satisfied along with Eq. (3.27), since Eq. (3.17) is satisfied for the exact solution. Just as in the case $\lambda=0$ discussed above, we reject trial functions for which Eq. (3.28) is violated. It follows from Eqs. (3.27) and (3.28) that curves in the λ_v-E plane will have positive slope; the argument is the same as the one given above for the exact problem.

According to the maximum-minimum property, the variationally determined eigenvalues, now denoted as $\lambda_i^{(n)}$ and ordered so that $\lambda_i^{(n)}\geq\lambda_{i+1}^{(n)}$, lie below the corresponding eigenvalues λ_i, i.e., for a given energy

$$\lambda_i^{(n)}\leq\lambda_i. \tag{3.29}$$

For each curve $C_i^{(n)}$ in the λ-E plane determined by Eq. (3.27) there will be a curve C_i, determined by the exact-eigenvalue problem, which lies above it. Therefore the intersection of C_i with the energy axis lies to the left of the intersection of $C_i^{(n)}$. These points of intersection give the energy eigenvalues E_i and $E_i^{(n)}$, respectively. Furthermore, since each curve has positive slope at $\lambda=0$, it crosses the E axis no more than once. We conclude that for each variational energy eigenvalue there is an exact eigenvalue which lies below it. The inequality

$$E_i\leq E_i^{(n)} \tag{3.30}$$

for the ordered eigenvalues then follows.

As a simple test of the above analysis, we show that well-known results can be recovered when it is applied to the more familiar Hamiltonian theory. Thus we take as our eigenvalue equation

$$\psi=GV\psi, \tag{3.31}$$

where

$$G=(E-K)^{-1} \tag{3.32}$$

and V is the potential. With $\psi\equiv G\Gamma$, Eq. (3.31) becomes

$$\mathfrak{L}(E)\Gamma=0, \tag{3.33}$$

with

$$\mathfrak{L}\equiv G-GVG. \tag{3.34}$$

When Eq. (3.33) is satisfied, we can verify directly that

$$\frac{\partial}{\partial E}(\Gamma,\mathfrak{L}\Gamma)=(\Gamma,(E-K)^{-2}\Gamma)>0. \tag{3.35}$$

Variational estimates of the energy eigenvalues can be obtained from the roots of

$$\det\mathbf{L}(E)=0, \tag{3.36}$$

where

$$L_{ij}=(\Gamma_i,\mathfrak{L}\Gamma_j). \tag{3.37}$$

[12] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1953), Vol. I, Chap. 1; E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1937), Sec. 51. A general rigorous proof of the maximum-minimum property, even for the more familiar energy-eigenvalue problem in the Hamiltonian theory, is apparently lacking. (See remarks in Kemble's text, at the bottom of p. 408.)

If we express the basis functions as $\Gamma_i=G^{-1}\psi_i$, we have

$$L_{ij}=(\psi_i,(E-H)\psi_j), \tag{3.38}$$

with $H=K+V$. To prove that the roots of Eq. (3.36) give upper bounds on the energy eigenvalues, we introduce an associated eigenvalue problem by replacing V with $V+\lambda V'$ in Eqs. (3.33) and (3.34), with V' a positive operator. The proof then proceeds as described above. The minimum principle obtained is, in view of Eqs. (3.36) and (3.38), precisely the Rayleigh-Ritz principle in its usual form.[12] We note, incidentally, that the normalization

$$\frac{\partial}{\partial E}(\Gamma,\mathfrak{L}\Gamma)=1 \tag{3.39}$$

is equivalent to

$$(\psi,\psi)=1. \tag{3.40}$$

4. MINIMUM PRINCIPLE FOR EFFECTIVE POTENTIALS

Minimum principles in scattering theory, based on the nonrelativistic Schrödinger equation, have been known for some time.[13–15] In this section, we show that these previously developed ideas can be applied, with appropriate modifications, to establish a minimum principle for scattering parameters, for reactions of the type $A+B\rightarrow C+D$, based on the integral equations of Sec. 2 and the generalized Rayleigh-Ritz property of Sec. 3.

In order to obtain bounds on scattering parameters, they must be real. We therefore work with the reaction matrix rather than the T matrix.[16] The Green's function G_α, defined by Eq. (2.41), is written as[17]

$$G_\alpha\equiv G_\alpha^{(+)}=G_{\alpha P}+G_{\alpha I}, \tag{4.1}$$

where

$$G_{\alpha P}=\tfrac{1}{2}(G_\alpha^{(+)}+G_\alpha^{(-)}), \tag{4.2}$$

and

$$G_{\alpha I}=\tfrac{1}{2}(G_\alpha^{(+)}-G_\alpha^{(-)}). \tag{4.3}$$

The reaction matrix is defined as the solution of the effective two-body integral equation

$$R_{\alpha\beta}=V_{\alpha\beta}+\sum_\gamma R_{\alpha\gamma}G_{\gamma P}V_{\gamma\beta}, \tag{4.4}$$

or, equivalently,

$$R_{\alpha\beta}=V_{\alpha\beta}+\sum_\gamma V_{\alpha\gamma}G_{\gamma P}R_{\alpha\beta}. \tag{4.5}$$

Equations (2.48) and (4.5) are linear integral equations which differ in the choice of Green's function. The solutions can therefore be compared with the aid of Eq. (2.24); this yields the Heitler equation

$$T_{\alpha\beta}=R_{\alpha\beta}+\sum_\gamma T_{\alpha\gamma}G_{\gamma I}R_{\gamma\beta}, \tag{4.6}$$

which can be solved to give the T matrix once the R matrix is known. If the total energy lies below the three-body continuum threshold (this assumption is maintained throughout this section), then the effective-potential matrix, defined by Eq. (2.46), is Hermitian. This important property follows from the fact that G^A, in Eq. (2.46), has vanishing discontinuity across the branch cut on the real-energy axis below the three-body continuum threshold. The discontinuity which exists for the complete resolvent operator has its origin in the bound-state poles in the two-body scattering amplitudes which appear in T_D. Such poles have been removed in the definition of $T_D{}^A$. Therefore the effect of these poles is missing in the amplitude T^A [see Eq. (2.30)] and in the Green's function G^A [see Eq. (2.34)]. Since $G_{\gamma P}$ in Eq. (4.5) is Hermitian, it follows immediately [e.g., with the aid of Eq. (2.24)] that the reaction matrix is Hermitian. The form

$$\mathbf{a}^\dagger\mathbf{R}\mathbf{a}=\sum_\alpha\sum_\beta a_\alpha{}^*R_{\alpha\beta}a_\beta, \tag{4.7}$$

with $\mathbf{a}$ arbitrary, is therefore real.

Our next step is to establish a monotonicity theorem relating changes in the diagonal R-matrix elements induced by increments of definite sign in the effective potential. We consider two versions of Eq. (4.4) in the matrix form

$$\mathbf{R}=\mathbf{V}+\mathbf{R}\mathbf{G}_P\mathbf{V}, \tag{4.8}$$

$$\mathbf{R}'=\mathbf{V}'+\mathbf{V}'\mathbf{G}_P\mathbf{R}', \tag{4.9}$$

where $(\mathbf{G}_P)_{\alpha\beta}=G_{\alpha P}\delta_{\alpha\beta}$. Then, from Eq. (2.24), we find that

$$\mathbf{R}-\mathbf{R}'=(1+\mathbf{R}\mathbf{G}_P)(\mathbf{V}-\mathbf{V}')(1+\mathbf{G}_P\mathbf{R}'). \tag{4.10}$$

To first order in $\Delta\mathbf{V}\equiv\mathbf{V}-\mathbf{V}'$, we can replace $\mathbf{R}'$ by $\mathbf{R}$ on the right-hand side of Eq. (4.10). With $\mathbf{\Omega}\equiv\mathbf{1}+\mathbf{G}_P\mathbf{R}$, Eq. (4.10) leads to

$$\mathbf{R}-\mathbf{R}'=\mathbf{\Omega}^\dagger\Delta\mathbf{V}\mathbf{\Omega}. \tag{4.11}$$

Suppose that $\Delta\mathbf{V}$ is negative, i.e., diagonal matrix elements in any representation are negative. Equation (4.11) then implies the inequality

$$\mathbf{a}^\dagger\mathbf{R}\mathbf{a}\leq\mathbf{a}^\dagger\mathbf{R}'\mathbf{a}, \tag{4.12}$$

where $\mathbf{a}$ is arbitrary, and $\mathbf{R}'$ is obtained from the solution of Eq. (4.9).

The above inequality will break down if $\mathbf{R}$ changes discontinuously with changes in $\mathbf{V}$. It is therefore preferable to express the inequality in terms of the eigenphase shifts, which *do* vary smoothly. We work in a representation in which the total angular momentum is fixed and define the matrix[16]

$$K_{\alpha\beta}=-\pi(\mu_\alpha k_\alpha)^{1/2}R_{\alpha\beta}(\mu_\beta k_\beta)^{1/2}, \tag{4.13}$$

[13] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **134**, B911 (1964).
[14] R. Sugar and R. Blankenbecler, Phys. Rev. **136**, B472 (1964).
[15] L. Rosenberg, Phys. Rev. **138**, B1343 (1965).
[16] M. L. Goldberger and K. M. Watson (Ref. 10), Sec. 7.3.
[17] We allow for the possibility that G_α is given not by Eq. (2.42), but by more elaborate forms which take into account virtual transitions into continuum states (see Ref. 7). The reaction-matrix formalism discussed here is therefore a slight generalization of the standard version discussed in Ref. 16.

where μ_α and k_α are the reduced mass and relative momentum, respectively, in the two-body channel α. The eigenphase shifts are defined by

$$\mathbf{K}\mathbf{x}_i=\tan\delta_i\mathbf{x}_i, \tag{4.14}$$

$$\mathbf{K}'\mathbf{x}_i'=\tan\delta_i'\mathbf{x}_i'. \tag{4.15}$$

In addition to the inequality $\mathbf{x}_i^\dagger\mathbf{K}\mathbf{x}_i\geq\mathbf{x}_i^\dagger\mathbf{K}'\mathbf{x}_i$ which is valid when Eq. (4.12) holds, we also have $\mathbf{x}_i^\dagger\mathbf{K}\mathbf{x}_i\geq\mathbf{x}_i'^\dagger\mathbf{K}'\mathbf{x}_i'$, provided $\mathbf{x}_i$ and $\mathbf{x}_i'$ are both normalized to unity, since $\mathbf{x}_i'^\dagger\mathbf{K}'\mathbf{x}_i'$ changes by a second-order quantity when $\mathbf{x}_i'$ is varied, subject to $\mathbf{x}_i'^\dagger\mathbf{x}_i'=1$. We conclude that $\tan\delta_i\geq\tan\delta_i'$ and, finally,

$$\delta_i\geq\delta_i'. \tag{4.16}$$

This last inequality remains valid even when $\tan\delta_i$ becomes infinite. We can then build $\Delta\mathbf{V}$ up to a finite negative operator, with Eq. (4.16) preserved. In the following, we will show how to obtain a variational approximation to the effective potential whose error is negative. The variationally determined eigenphase shifts then represent lower bounds on the true eigenphases.

To derive a variational principle for the effective potential, we make use of the definition of $V_{\alpha\beta}$ obtained by combining Eqs. (2.34) and (2.46). We find that

$$V_{\alpha\beta}=\Gamma^\dagger(S_\alpha)G\Gamma(S_\beta)(1-\delta_{\alpha\beta}) +\sum_{\gamma\neq\alpha}\sum_{\delta\neq\beta}\Phi^\dagger(S_\alpha)^{(\gamma)}[\mathbf{T}^A]^{(\delta)}\Phi(S_\beta), \tag{4.17}$$

where $\mathbf{T}^A$ is the solution of Eq. (2.30), and where $\Phi(S_\beta)$ is defined as

$$\Phi(S_\beta)=G\Gamma(S_\beta). \tag{4.18}$$

In momentum space, $\Phi(S_\beta)$ reduces, on the energy shell, to the bound-state wave function for subsystem S_β. A variational expression for $\mathbf{T}^A$, with a formal expression for the error, is provided by Eqs. (2.58) and (2.60), respectively; we need only replace $\mathbf{T}_D$ by $\mathbf{T}_D{}^A$. Since $\mathbf{T}^A$ is Hermitian, the choice of an Hermitian trial function $\mathbf{T}_t{}^A$ will guarantee that the variational expression $\mathbf{T}_v{}^A$, as well as the error term, will be Hermitian. [See the discussion leading to Eq. (2.62).] With $\mathbf{T}^A$ replaced by $\mathbf{T}_v{}^A$ in Eq. (4.17), we obtain a variational expression for the effective potential, with an error of the form

$$V_{\alpha\beta}-(V_{\alpha\beta})_v=\mathbf{X}_\alpha^\dagger\mathfrak{U}^A\mathbf{X}_\beta. \tag{4.19}$$

We have defined

$$\mathfrak{U}^A=\mathbf{G}-\mathbf{G}\mathbf{T}_D{}^A\mathbf{G}; \tag{4.20}$$

$\mathbf{X}_\beta$ is a 3×1 matrix operator with elements

$$^{(\gamma)}X_\beta=\sum_{\delta\neq\beta}{}^{(\gamma)}[\Delta\mathbf{T}^A]^{(\delta)}\Phi_\beta, \tag{4.21}$$

where $\Delta\mathbf{T}^A=\mathbf{T}^A-\mathbf{T}_t{}^A$.

According to Eq. (4.19), the error in the variational estimate of the effective-potential matrix will have negative diagonal matrix elements if $\mathbf{X}^\dagger\mathfrak{U}^A\mathbf{X}$ is negative, with $\mathbf{X}=\sum_\alpha a_\alpha\mathbf{X}_\alpha$. To study the circumstances under which this will be true, we turn to the eigenvalue equation

$$[\mathfrak{U}^A(E)-\lambda\mathfrak{o}(E)]\mathbf{\Gamma}=0, \tag{4.22}$$

which is of the type considered in Sec. 3. (Note that, as required, $\mathfrak{U}^A$ is Hermitian, since E lies below the three-particle continuum threshold.) By virtue of the Rayleigh-Ritz principle for the eigenvalues $\lambda_i(E)$ of Eq. (4.22), $\mathbf{X}^\dagger\mathfrak{U}^A\mathbf{X}$ will be negative, provided the $\lambda_i(E)$ are all negative.[18] This is equivalent to the condition that there are no bound-state energy eigenvalues, defined by the eigenvalue equation

$$\mathfrak{U}^A\mathbf{\Gamma}=0, \tag{4.23}$$

below the level E. Here we use the fact that the $\lambda_i(E)$-versus-E curves have positive slope. If there were an energy eigenvalue below E, there would be a positive λ eigenvalue at the energy E. We conclude that if Eq. (4.23) has no solutions for energies below E, then the variationally determined effective potential gives rise to a reaction matrix whose eigenphases lie below the true eigenphases at energy E.

The result can be generalized to the case where there is a finite number M of positive eigenvalues $\lambda_i(E)$ defined by Eq. (4.22), or, equivalently, where there are M energy eigenvalues below E. Consider, first, the case $M=1$. According to a previously derived theorem,[19] we can assert that

$$N\equiv\mathbf{X}^\dagger\mathfrak{U}^A\mathbf{X}-\mathbf{X}^\dagger\mathbf{S}\mathbf{X} \tag{4.24}$$

is negative, where

$$\mathbf{S}\equiv\mathfrak{U}^A\mathbf{\Gamma}_t(\mathbf{\Gamma}_t^\dagger\mathfrak{U}^A\mathbf{\Gamma}_t)^{-1}\mathbf{\Gamma}_t^\dagger\mathfrak{U}^A, \tag{4.25}$$

and $\mathbf{\Gamma}_t$ is an approximation to the solution of Eq. (4.22) which is sufficiently accurate, so that $\mathbf{\Gamma}_t^\dagger\mathfrak{U}^A\mathbf{\Gamma}_t$ is positive. To apply this result, we observe that Eq. (4.19) implies

$$\mathbf{a}^\dagger\mathbf{V}\mathbf{a}=\mathbf{a}^\dagger\mathbf{V}_v\mathbf{a}+\mathbf{X}^\dagger\mathfrak{U}^A\mathbf{X}, \tag{4.26}$$

with $\mathbf{X}=\sum_\alpha a_\alpha\mathbf{X}_\alpha$. According to Eq. (4.24), the second term on the right-hand side of Eq. (4.26) can be replaced by $\mathbf{X}^\dagger\mathbf{S}\mathbf{X}$ with negative error, i.e., the matrix

$$(V_{\alpha\beta})_v+\mathbf{X}_\alpha^\dagger\mathbf{S}\mathbf{X}_\beta$$

will provide a variational approximation to the effective potential so that the error is a negative matrix. Now, X_β is unknown, since it involves the unknown matrix $\mathbf{T}^A$ [see Eq. (4.21)]. Nevertheless, $\mathbf{X}_\alpha^\dagger\mathbf{S}\mathbf{X}_\beta$ is known, in

[18] Here we assume that $\mathbf{X}$ is an admissible trial function in the λ-eigenvalue problem. This is quite reasonable, since the eigenvalue problem is essentially a bound-state problem, and $\mathbf{X}$ is a linear combination of (connected) scattering amplitudes appropriate to the energy region below the continuum threshold. The situation is entirely analogous to the one which arises in the Hamiltonian formulation of the minimum principle discussed in Refs. 13–15.

[19] L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **118**, 184 (1960).

terms of $\mathbf{T}_t$ and $\mathbf{T}_D{}^A$. This can be verified from the definitions, Eqs. (4.21) and (4.25), and the relation

$$\mathfrak{L}^A\mathbf{T}^A=\mathbf{G}\mathbf{T}_D{}^A \tag{4.27}$$

which follows from the integral equation satisfied by $\mathbf{T}^A$.

The general case $M\geq 1$ is treated in a similar manner, with Eq. (4.25) replaced by

$$\mathbf{S}=\sum_{i,j=1}^{M}\mathfrak{L}^A\boldsymbol{\Gamma}_{it}(\mathbf{D}^{-1})_{ij}\boldsymbol{\Gamma}_{jt}{}^\dagger\mathfrak{L}^A, \tag{4.28}$$

where the matrix $\mathbf{D}$, with elements

$$D_{ij}=\boldsymbol{\Gamma}_{it}\mathfrak{L}^A\boldsymbol{\Gamma}_{jt}, \tag{4.29}$$

is positive. This is to be achieved by appropriate choice of the trial functions $\boldsymbol{\Gamma}_{it}$.

As a simple application of the formalism, we take the trial function $T_t{}^A$ to be zero. The variational expression for the effective potential then becomes

$$(V_{\alpha\beta})_v=\Gamma^\dagger(S_\alpha)G\Gamma(S_\beta)(1-\delta_{\alpha\beta})+\Phi^\dagger(S_\alpha)\sum_{\gamma\neq\alpha,\beta}T^A(S_\gamma)\Phi(S_\beta), \tag{4.30}$$

where the amplitudes $T^A(S_\gamma)$ are the diagonal elements of $\mathbf{T}_D{}^A$. Now the complete two-body scattering operator for subsystem γ can be written as

$$T(S_\gamma)=V(S_\gamma)+V(S_\gamma)G(S_\gamma)V(S_\gamma), \tag{4.31}$$

where $V(S_\gamma)$ is the potential-energy operator, and $G(S_\gamma)$ is the resolvent operator for S_γ. According to the eigenfunction expansion of the resolvent operator, we have

$$G(S_\gamma)=G^A(S_\gamma)+G^B(S_\gamma), \tag{4.32}$$

where $G^B(S_\gamma)$ contains the bound-state pole contributions, and $G^A(S_\gamma)$ represents a sum over continuum states. We remark that $G^A(S_\gamma)$ is a negative operator, since the total energy E lies below the continuum threshold. Our separable approximation for the two-body scattering amplitude is taken as

$$T^B(S_\gamma)=V(S_\gamma)G^B(S_\gamma)V(S_\gamma), \tag{4.33}$$

so that

$$T^A(S_\gamma)=V(S_\gamma)+V(S_\gamma)G^A(S_\gamma)V(S_\gamma). \tag{4.34}$$

Equation (4.30) then becomes

$$\mathbf{V}_v=\mathbf{V}_s+\mathbf{V}_r, \tag{4.35}$$

where

$$(V_{\alpha\beta})_s=\Gamma^\dagger(S_\alpha)G\Gamma(S_\beta)(1-\delta_{\alpha\beta})+\sum_{\gamma\neq\alpha,\beta}\Phi^\dagger(S_\alpha)V(S_\gamma)\Phi(S_\beta), \tag{4.36}$$

and

$$(V_{\alpha\beta})_r=\sum_{\gamma\neq\alpha,\beta}\Phi^\dagger(S_\alpha)V(S_\gamma)G^A(S_\gamma)V(S_\gamma)\Phi(S_\beta). \tag{4.37}$$

Now diagonal matrix elements of $\mathbf{V}_r$ can be put in the form

$$\mathbf{a}^\dagger\mathbf{V}_r\mathbf{a}=\sum_\gamma Q_\gamma{}^\dagger G^A(S_\gamma)Q_\gamma, \tag{4.38}$$

where

$$Q_\gamma=V(S_\gamma)\sum_\epsilon(1-\delta_{\gamma\epsilon})a_\epsilon\Phi(S_\epsilon). \tag{4.39}$$

Since $G^A(S_\gamma)$ is negative, we see that $\mathbf{a}^\dagger\mathbf{V}_r\mathbf{a}$ is negative for arbitrary $\mathbf{a}$.

Let us assume that there are no bound-state solutions of Eq. (4.23), so that the error in $\mathbf{V}_v$ is negative. The previous discussion then shows that the error made in replacing $\mathbf{V}$ by $\mathbf{V}_s$ is negative. The use of $\mathbf{V}_s$ as the effective potential is equivalent to the well-known resonating-group (or static) approximation. We have shown that this approximation gives rise to lower bounds on the eigenphase shifts under the above assumption.[20]

[20] The analog of this theorem in the Hamiltonian formulation of the minimum principle is given in Ref. 13.