

## Improved Minimum Principle for Single-Channel Scattering\*†

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The minimum principle for single-channel scattering obtained previously required the introduction of channel radii for an incident relative kinetic energy  $E$  greater than zero. The channel radii, which greatly complicate the numerical calculations, no longer appear in recent formal theories of reactions and they need not appear in the minimum principle formulation. By projecting out all of the open-channel components from the full wave function, it is possible to eliminate the continuum states of the total Hamiltonian  $H$  originally present below  $E$ . The closed-channel Hamiltonian  $\mathcal{H}$  has only a discrete spectrum below the inelastic threshold. By appropriately subtracting the contributions from the discrete portion of the spectrum,  $\mathcal{H}$  can be used to obtain a minimum principle for  $k \cot \eta$ , where  $\eta$  is the phase shift. This minimum principle provides a rigorous criterion for determining the parameters in a trial function and for choosing among the numerical results obtained with different trial functions. The method requires that one solve exactly the static approximation equation, which plays a particular role in uncoupling the closed-channel equations from the open-channel equation. Finally, contact is made with the results previously obtained at zero energy and a generalized Levinson's theorem is briefly considered.

## 1. INTRODUCTION

IN the minimum principles for scattering theory that have recently been developed,<sup>1-3</sup> a sharp distinction must unfortunately be made between the case for which the incident relative kinetic energy,  $E'$ , of the two systems is zero and that for which it is not. For single-channel scattering at  $E'=0$ , the minimum principle is applicable to the true systems, and the calculations are either precisely of the form of the usual variational principles or only very slightly more complicated, requiring some additional integrations which are no more difficult to perform than those that arise in the variational principles. For  $E'>0$ , the minimum principle is applicable only if some of the various potentials are truncated and if some potential barriers are erected. (The conditions on the potential can be relaxed somewhat, but not significantly.) The minimum principle will not generally, therefore, be applicable to the true problem, but this by itself would not be a serious handicap, for the various potentials can be truncated at such large distances that the effects of the truncation are negligible; the more serious difficulty is that because of the erection of the potential barriers the trial function must satisfy certain rather artificial boundary conditions which can for some problems make the calculations extremely difficult.

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<sup>1</sup> L. Spruch and L. Rosenberg, Phys. Rev. 116, 1034 (1959); 117, 1095 (1960).

<sup>2</sup> L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. 118, 184 (1960).

<sup>3</sup> L. Spruch and L. Rosenberg, Phys. Rev. 120, 474 (1960); L. Rosenberg and L. Spruch, *ibid.* 121, 1720 (1961); 125, 1407 (1962).

The primary purpose of the present article is to develop a minimum principle for single-channel scattering for  $E'>0$  which does not require the introduction of artificial potentials. Before doing so, it will be useful to review briefly the previous work to understand the origin of the need for artificial potentials in that work. Since the need appears even in the simplest cases, it will suffice to consider the zero angular momentum scattering of a spinless particle by a short-range static potential,  $V(q)$ . For potential scattering, the incident relative kinetic energy  $E'$  is, of course, equal to the total energy  $E$  of the system.

For  $E'=0$ , we are interested in the determination of a variational bound on the scattering length,  $A$ . It is simple to prove the identity

$$\frac{\hbar^2}{2\mu}(A - A_t) = \int u_t H u_t dq - \int w H w dq, \quad (1.1)$$

where

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dq^2} + V(q),$$

$u$  is the exact solution,  $u_t$  is the trial function, and  $w = u_t - u$ . Both  $u$  and  $u_t$  vanish at the origin, and they behave asymptotically as

$$u(q) \rightarrow -q + A, \quad u_t(q) \rightarrow -q + A_t.$$

$w(q)$ , therefore, vanishes at the origin and approaches a constant asymptotically. If one knows experimentally or in any other fashion that the potential cannot support a bound state, it is trivial to show that  $(w, Hw) \geq 0$ . (The bound would be an immediate consequence of the Rayleigh-Ritz theorem if  $w$  were a quadratically integrable function. It is a very simple matter, using a limiting process, to extend the theorem to include the class of functions which asymptotically approach a constant.) A bound on  $A$ , or better, a minimum principle for  $A$ , follows immediately, then, on dropping the last term in Eq. (1.1).

The possibility of obtaining a minimum principle for  $A$  is then in the above case a consequence of the fact that the spectrum of  $H$  is bounded from below by the value zero. If  $V(q)$  can support one bound state with an eigenfunction  $\varphi_1$  and an eigenvalue  $E_1$ , then  $H$  is not a positive definite operator and it is not necessarily true that  $(w, Hw) \geq 0$ . We can, however, proceed as follows.<sup>4</sup> We seek an operator inequality of the form  $H \geq B$ , where  $B$  must satisfy the following requirements:

(1)  $B$  must contain only quantities that are actually known, as opposed to quantities that are only known formally.

(2) Since the bound is no longer zero, the inequality relationship

$$(w, Hw) \geq (w, Bw)$$

still involves  $w$ , and we do not have a useful result unless we can eliminate  $w$ . This can be done if an  $H$  appears adjacent to each  $w$ , for we can then eliminate  $w$  by using  $Hw = Hu_t$ .

In summary, then, we seek an inequality of the form

$$H > HCH,$$

where it must be possible to give  $C$  in a usable form; the inequality has meaning for functions  $\omega(q)$  with boundary conditions  $\omega(0) = 0$  and  $\omega(q) \rightarrow \text{constant}$  as  $q \rightarrow \infty$ .

In seeking such a relation, we begin by defining the projection operator  $\Pi_1$  for the compound state  $\varphi_1$ , which, operating on the arbitrary function  $f(q)$ , gives

$$\Pi_1 f(q) \equiv \varphi_1(q) \int \varphi_1(q') f(q') dq',$$

and noting that it, then, follows that  $H(1 - \Pi_1)$  is a positive definite operator, that is, that

$$H \geq H\Pi_1$$

in the space of quadratically integrable functions and of functions that approach a constant asymptotically. Since

$$H\Pi_1 = \Pi_1 H = E_1 \Pi_1,$$

we can write

$$H \geq H\Pi_1 H / E_1,$$

which has the prescribed form, but unfortunately  $\varphi_1$  is practically never known so that we do not really know  $\Pi_1$ . To overcome this difficulty, we introduce the normalizable function  $\varphi_{1t}$ , define  $E_{1t}$  as

$$E_{1t} = (\varphi_{1t}, H \varphi_{1t}) / (\varphi_{1t}, \varphi_{1t}),$$

and define the *known* projection operator  $\Pi_{1t}$ , which,

<sup>4</sup>The proof to be outlined is rather more compact though entirely equivalent to the original proof of reference 2. There we subtracted off approximate bound-state functions from  $w$ , whereas here we subtract from the operator  $H$ . This slightly different viewpoint had its origins in a comment by Dr. B. Lippmann.

operating on the arbitrary function  $f(q)$ , gives

$$\Pi_{1t} f(q) = \varphi_{1t}(q) \int \varphi_{1t}(q') f(q') dq'.$$

It can be shown<sup>2</sup> that

$$H \geq H\Pi_{1t} H / E_{1t},$$

provided only that  $\varphi_{1t}$  is sufficiently accurate to generate a negative  $E_{1t}$ . Since the class of functions for which the above operator is positive definite includes functions which approach a constant asymptotically, we have finally

$$(w, Hw) \geq (w, H\Pi_{1t} Hw) / E_{1t} = |(\varphi_{1t}, Hw)|^2 / E_{1t}.$$

Since the proof depends upon the Rayleigh-Ritz theorem and modifications of that theorem, which are not restricted to static potentials, the generalization of the above results to single-channel scattering by a compound system is trivial.

The extension to the case for which it is known, experimentally perhaps, that there are precisely  $N$  bound states is also straightforward. It is then possible in principle and it will not generally be difficult in practice to find  $N$  orthonormal functions  $\varphi_{nt}$  such that

$$(\varphi_{nt}, H \varphi_{mt}) = E_{nt} \delta_{nm}; \quad E_{nt} < 0; \quad 1 \leq n, m \leq N.$$

It can then be shown that

$$(w, Hw) \geq \sum_{n=1}^N \frac{|(\varphi_{nt}, Hw)|^2}{E_{nt}}, \quad (1.2)$$

so that we have a minimum principle for  $A$  even when an arbitrary but known number of bound states exist.

Now consider an incident energy greater than zero. We again restrict ourselves to the  $L=0$  scattering of a spinless particle by a static central potential. The starting point now is the Kato identity

$$\frac{\hbar^2}{2\mu} [k \cot(\eta - \theta) - k \cot(\eta_t - \theta)] = \int u(H - E)u_t dq, \quad (1.3)$$

or

$$\frac{\hbar^2}{2\mu} [k \cot(\eta - \theta) - k \cot(\eta_t - \theta)] = \int u_t(H - E)u_t dq - \int w(H - E)w dq. \quad (1.4)$$

$u$  and  $u_t$  are the exact and trial scattering functions. They both vanish at  $q=0$ , while asymptotically they behave as

$$u \rightarrow \cos(kq + \theta) + \cot(\eta - \theta) \sin(kq + \theta), \\ u_t \rightarrow \cos(kq + \theta) + \cot(\eta_t - \theta) \sin(kq + \theta),$$

where  $\eta$  and  $\eta_t$  are the exact and trial  $L=0$  phase shifts, respectively, and  $0 \leq \theta < \pi$ .  $w$  is again the difference function, defined by  $w \equiv u_t - u$ . Equation (1.1) is just the  $E=0, \theta \neq 0$  form of Eq. (1.4).

To obtain a minimum principle for  $\cot(\eta - \theta)$ , we must now obtain a bound on  $(w, [H - E]w)$ . Unfortunately, the spectrum of  $H - E$  for  $E \neq 0$  contains negative as well as positive eigenvalues, even when bound states do not appear. Since the spectrum of  $H$  is continuous, there will, in fact, be an infinite number of negative eigenvalues. Now, whereas we know how to "eliminate" a finite number of negative eigenvalues, we do not know how to "eliminate" a continuum of negative eigenvalues. (It is not possible simply to replace the summation by an integration.) The procedure that was used to bypass this difficulty was to truncate the potential and to erect a potential barrier.<sup>3</sup> It was then possible to recast the problem into a form which involved only a finite domain, that within the barrier; not surprisingly, the fact that we are now in a finite domain enables one to work with a discrete spectrum and it is then possible, at least in principle, to "eliminate" the negative eigenvalues.

As already noted, this barrier can introduce serious difficulties. The situation is really not very troublesome for potential scattering, but as one generalizes the barrier technique from potential scattering to single-channel scattering by a compound system and, then, to multichannel scattering, the difficulties become progressively worse. We have, therefore, to seek some other approach. It is, then, worthy of notice that we have done more than was necessary in having truncated the potential and erected a barrier, in that the spectrum was made discrete everywhere, though it would have sufficed to make the spectrum of  $H$  discrete only below  $E$ . The situation is depicted for potential scattering in Fig. 1. Unfortunately, we do not know for potential scattering

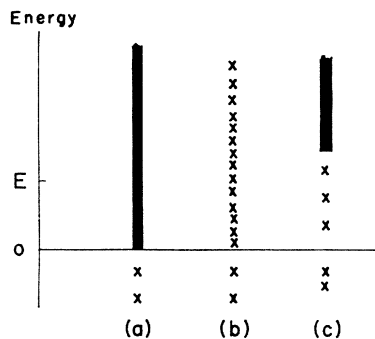


FIG. 1. Spectra for a static potential. Spectrum (a) is that associated with the original  $H$ . Spectrum (b) is that associated with the potential truncated at  $R$ , and with the problem recast into a form that involves only the (finite) interval  $0$  to  $R$ ; for  $R$  large, the negative energy eigenvalues will be very close to those in (a) and the positive energy eigenvalues will be very closely spaced. It would suffice to have a spectrum of the form (c), but we do not know how to obtain such a spectrum for potential scattering.

how to avail ourselves of the less restrictive condition that can be placed upon the modified spectrum.

Let us, however, examine the situation for the single-channel scattering of a particle by a compound system. The spectrum of  $H$ , then, contains discrete eigenvalues if there are composite bound states of the incident particle plus target which lie below the ground-state energy  $E_{T0}$  of the target. In addition, there will be continuous spectra beginning at  $E_{T0}$  and at  $E_{T1}, E_{T2}, \dots$ , the excited-state energies of the target system. We would have the desired situation in which the spectrum of  $H$  could contain at most discrete eigenvalues below the energy  $E$  if it were possible to eliminate the branch of the continuous spectrum bounded from below by  $E_{T0}$ . (See Fig. 2.)

Now it is in fact possible to eliminate this portion of the spectrum by utilizing recent developments in the formal theory of the optical potential.<sup>5</sup> There are two (not unrelated) reasons why these developments might be expected to be helpful for our present purposes. First, in these treatments the term in the expansion of the full scattering wave function that is proportional to the target ground-state function is isolated from all of the other terms, and is treated quite differently from the other terms. Second, channel radii need never be introduced in these treatments. (In our previous work on single-channel and multichannel scattering by systems,<sup>3</sup> an adaptation of the Wigner-Eisenbud formal theory of reactions was used. The truncations that we introduced were similar to those that arise in their theory, where channel radii  $d_0$  appear.) The optical potential formalism has been used previously<sup>6,6a</sup> to show that one

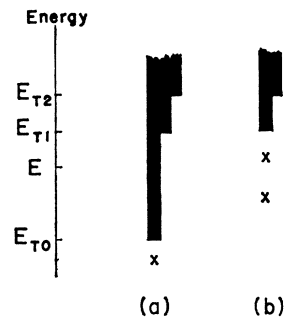


FIG. 2. (a) represents the spectrum of  $H$  for a target system with energies  $E_{T0}, E_{T1}, \dots$ , and an incident particle. (b) represents the spectrum of states with angular momentum  $L=0$  of  $Q\mathcal{H}Q \equiv \mathcal{H}$ , where  $Q$  projects out the ground state of the target. The number of discrete eigenvalues need not be the same for  $H$  and for  $\mathcal{H}$ . The point of primary interest is that the continuous spectrum of  $\mathcal{H}$  begins at  $E_{T1}$  which lies above  $E$  by the assumption that we are dealing with single-channel scattering processes.

<sup>5</sup> H. Feshbach, *Ann. Phys. (N. Y.)* **5**, 357 (1958); **19**, 287 (1962); L. Fonda and R. G. Newton, *ibid.* **10**, 490 (1960).

<sup>6</sup> Y. Hahn, T. F. O'Malley, and L. Spruch, *Phys. Rev.* **128**, 932 (1962).

<sup>6a</sup> Reference 6 overlooked a paper by I. C. Percival, *Phys. Rev.* **119**, 159 (1960), who arrived, using the box-variational principle, at some of the conclusions that were proved in reference 6. Percival's approach contains a number of limitations; in particular, it cannot allow for the Pauli principle and it assumes that various potentials vanish identically beyond some point.

can often obtain a lower bound or a few progressively better lower bounds on the phase shift. (In that paper we restricted ourselves to energies below the first resonances. We have subsequently been able to eliminate this restriction. This point will be elaborated in a future paper.) We are, of course, here interested in obtaining a much more useful result, a minimum principle, that is, a variational bound.

It follows from the above discussion that we can obtain a minimum principle for compound systems that does not involve truncation, while being unable to do the same for the simpler case of potential scattering. The paradox is a spurious one, however, for we shall see that the development of the minimum principle for single-channel scattering by a compound system requires that one first solves a specified static potential problem exactly. (The static potential may, in fact, be nonlocal but with modern computers that need not necessarily be a serious obstacle.)

In the following section, Sec. 2, the minimum principle is derived, and is given by Eq. (2.17). Just as at zero energy, the results are found to be conditional, requiring a certain number of subtractions be made. The extent to which this condition represents a real limitation is discussed in Secs. 3 and 4. Appendix A is a slight generalization of the minimum principle. A simple and quite crude application of the method to the  $e^+H$  problem is given as an example in Appendix B. Further comparisons with the previous results at zero energy are made in Appendix C.

## 2. THE MINIMUM PRINCIPLE

For the purposes of simplicity, we assume that the incident particle is spinless and is distinguishable from the target particles, that the target has a total angular momentum of zero and is infinitely massive as compared to the mass of the incident particle, that there is no net Coulomb force between the target and the incident particle, and that the incident relative orbital angular momentum of the particle is zero. The extensions to include various spins, orbital angular momenta, recoil and Coulomb effects proceed as in our previous paper<sup>6</sup> and will not be repeated. The effects of the Pauli principle are not for present purposes completely contained in that paper since a Green's function will appear here that did not appear there. The construction of the Green's function, which is a matrix, is a tedious but rather straightforward matter, and will be discussed in detail in a future paper on an application of the minimum principle. We will, therefore, no longer concern ourselves with the Pauli principle in the present paper.

We use the same notation as previously.<sup>6</sup>  $\mathbf{r}$  represents the target particle coordinates and  $\mathbf{q}$  the coordinate of the incident particle relative to the (fixed) center of mass of the target.  $\psi_{T_i}(\mathbf{r})$  and  $E_{T_i}$  represent target eigenfunctions and eigenvalues,  $P$  is the projection oper-

ator onto the target ground state,<sup>7</sup> and  $Q=1-P$  projects onto the target excited states. It will be assumed that  $\psi_{T_0}$  and  $E_{T_0}$  are known, but it need not be assumed that the target excited-state wave functions and energies are known.

The problem is to determine the phase shift  $\eta$ , modulo  $\pi$ .  $\eta(\text{mod}\pi)$  is defined by the equation<sup>8</sup>

$$(H-E)\Psi=0, \quad (2.1)$$

where  $\Psi$  is regular at the origin and subject to the boundary condition

$$\Psi(\mathbf{r},\mathbf{q}) \xrightarrow{q \rightarrow \infty} \psi_{T_0}(\mathbf{r})[\cos(kq+\theta) + \cot(\eta-\theta)\sin(kq+\theta)]/q. \quad (2.2)$$

$k$  is defined by  $\hbar^2 k^2/2\mu \equiv E' = E - E_{T_0}$ , where  $E_{T_0}$  is the ground-state energy of the target. Since  $P+Q$  is the unit operator, we have

$$(H-E)P\Psi = -(H-E)Q\Psi,$$

and since  $PQ=0$ , we can write

$$P(H-E)P\Psi = -PHQ\Psi, \quad (2.3a)$$

$$Q(H-E)Q\Psi = -QHP\Psi. \quad (2.3b)$$

Inversion of the operators then leads to

$$P\Psi = \frac{1}{P(E-H)P} PHQ\Psi + P\Psi^P, \quad (2.4a)$$

$$Q\Psi = \frac{1}{Q(E-H)Q} QHP\Psi. \quad (2.4b)$$

$P\Psi^P$  is the exact static approximation scattering wave function defined as that solution of

$$P(H-E)P\Psi^P=0, \quad (2.5)$$

which is regular at the origin and which has the asymptotic form

$$P\Psi^P \xrightarrow{q \rightarrow \infty} \psi_{T_0}(\mathbf{r})[\cos(kq+\theta) + \cot(\eta^P-\theta)\sin(kq+\theta)]/q, \quad (2.6)$$

where  $\eta^P$  is the static approximation phase shift. It will be assumed throughout that  $\Psi^P$  is known, having been determined numerically on a computer. [Since Eq. (2.5) is effectively a one-body Schrödinger equation in the coordinate  $g$ , this is a relatively simple matter.] Substitution of Eqs. (2.4b) and (2.4a) into Eqs. (2.3a)

<sup>7</sup> It should be clear that  $P$  operates in the space of the target particles, while  $\Pi$  used in Sec. 1 operated in the space of all the particles.  $\Pi$  commutes with the full Hamiltonian  $H(\mathbf{r},\mathbf{q})$  while  $P$  commutes with  $H_T(\mathbf{r})$ .

<sup>8</sup> As opposed to the discussion in Sec. 1, the factor  $1/q$  is retained.

and (2.3b), respectively, leads to the results

$$P \left[ H + HQ \frac{1}{Q(E-H)Q} QH - E \right] P \Psi = 0, \quad (2.7a)$$

$$Q \left[ H + HP \frac{1}{P(E-H)P} PH - E \right] Q \Psi = -QHP \Psi^P. \quad (2.7b)$$

Equations (2.7a) and (2.7b) are uncoupled, that is, independent equations, each equivalent to the original Schrödinger equation. Equation (2.7a), which was the basis for the determination of a bound of the phase shift itself,<sup>6</sup> is not used in the present paper where we see a variational bound on  $\cot(\eta - \theta)$ .

For later convenience, we define the symbols

$$K = Q \left[ H + HP \frac{1}{P(E-H)P} PH - E \right] Q, \quad (2.8)$$

$$x = Q \Psi, \quad (2.9)$$

and

$$a = -QHP \Psi^P; \quad (2.10)$$

we can, then, rewrite Eq. (2.7b) as

$$Kx = a. \quad (2.11)$$

Since  $\Psi^P$  is known,  $a$  is also known. It should be noted that the Green's function in  $K$  and, therefore, that  $K$  itself is known; thus, with

$$H(\mathbf{r}, \mathbf{q}) = H_T(\mathbf{r}) + T(\mathbf{q}) + V(\mathbf{r}, \mathbf{q}),$$

with  $H_T$  the target Hamiltonian and  $V(\mathbf{r}, \mathbf{q})$  the interaction between the incident particle and the target particles, we have since

$$H_T P = P H_T = E_{T0} P,$$

that

$$[P(E-H)P]^{-1} = \{P[E' - T(q) - V_{00}(q)]\}^{-1},$$

where

$$V_{00}(q) = \int \psi_{T0}(\mathbf{r}) V(\mathbf{r}, \mathbf{q}) \psi_{T0}(\mathbf{r}) d\mathbf{r}.$$

We are, thus, dealing with the known Green's function for scattering by the static potential  $V_{00}(q)$ , that is, taking into account the boundary conditions on the wave functions,

$$[P(E-H)P]^{-1} = -(2\mu/4\pi\hbar^2 k) [u_{\text{reg}}^P(q_{<}) u_{\text{irreg}}^P(q_{>}) - \cot(\eta^P - \theta) u_{\text{reg}}^P(q_{<}) u_{\text{reg}}^P(q_{>})] P,$$

where  $q_{<}$  and  $q_{>}$  are the smaller and larger, respectively, of  $q$  and  $q'$ .  $u_{\text{reg}}^P$  and  $u_{\text{irreg}}^P$  are solutions of the Schrödinger equation with the potential  $V_{00}(q)$  and with the asymptotic forms

$$u_{\text{reg}}^P(q) \xrightarrow{q \rightarrow \infty} \sin(kq + \eta^P)/q,$$

$$u_{\text{irreg}}^P(q) \xrightarrow{q \rightarrow \infty} \cos(kq + \eta^P)/q.$$

The second term in the definition of the Green's function above is included to make it asymptotically proportional to  $\sin(kq + \theta)$  as is required.  $u_{\text{reg}}^P(q)$  is, of course, the function that appears as the factor of  $\psi_{T0}(\mathbf{r})$  in  $\Psi^P$ .

It follows from a comparison of Eqs. (2.7a) and (2.2) with Eqs. (2.5) and (2.6), and by use of the monotonicity theorem, that  $\eta > \eta^P$  if  $Q(E-H)Q$  is a negative definite operator. This is the bound discussed previously.<sup>6</sup> The minimum principle that we are presently concerned with will be developed not for  $\eta$  but for  $\cot(\eta - \theta)$ . In seeking an explicit expression for  $\cot(\eta - \theta)$ , we will avoid the use of any of the equations which contain the operator  $[Q(E-H)Q]^{-1}$ , for while this operator is perfectly well defined, it cannot actually be written down in a usable form. The most convenient pair of equations to consider is Eq. (2.3a) and Eq. (2.5). We proceed canonically by multiplying Eq. (2.5) by  $\Psi$ , Eq. (2.3a) by  $\Psi^P$ , subtracting, integrating over the full space, applying Green's theorem, and using the boundary conditions as given by Eqs. (2.2) and (2.6) to arrive at an expression of standard form,

$$4\pi(\hbar^2/2\mu) [k \cot(\eta - \theta) - k \cot(\eta^P - \theta)] \\ = (\Psi^P, PHQ\Psi) = (QHP\Psi^P, Q\Psi) = -(a, x), \quad (2.12)$$

where in the last step we used the notation defined by Eqs. (2.9) and (2.10). Since we are seeking a minimum principle, it is natural to attempt to find a form for the quantity of interest,  $k \cot(\eta - \theta)$ , which involves the unknown elements in a quadratic form, the bound following if the operator appears with the unknown element on either side and if the operator can be shown to be negative or positive definite. More precisely, we want the *error* in  $\Psi$  to appear quadratically, so that the term to be bounded will only be of second order. The above remarks make it clear that we should seek a variational formulation of the expression for  $k \cot(\eta - \theta)$  in which the second-order error term is given explicitly. We can easily do this by appealing to the abstract formulation of Marcuvitz<sup>9</sup> of the linear form of the variational principle of Lippmann and Schwinger.<sup>10</sup> Thus, if  $Kx = a$ , where  $K$  and  $a$  are given but  $x$  is not and where  $K$  is a symmetric operator, and if we wish to determine  $\lambda = (a, x)$ , where the inner product does not involve complex conjugation, we have a variational expression  $[\lambda]$  for  $\lambda$  given by

$$\lambda \approx [\lambda] = 2(x_i, a) - (x_i, Kx_i),$$

where  $x_i = x + \delta x$ . For present purposes, where we are explicitly interested in the second-order term, we write the identity

$$\lambda = 2(x_i, a) - (x_i, Kx_i) + (\delta x, K\delta x).$$

It is then obvious that, whereas we have only a variational principle for an arbitrary (symmetric)  $K$ , we

<sup>9</sup> L. Spruch, in *Lectures in Theoretical Physics, Boulder, 1961* [Interscience Publishers, Inc., New York (to be published)], Vol. 4.

<sup>10</sup> B. A. Lippmann and J. Schwinger, *Phys. Rev.* **79**, 469 (1950).

have a minimum principle for  $K$  a non-negative operator. Identifying  $x_i$  with the trial function  $Q\Psi_t(\mathbf{r},\mathbf{q})$ , which vanishes faster than  $1/q$  as  $q \rightarrow \infty$ , and identifying  $\delta x$  with the error term

$$Q\Omega \equiv Q\Psi_t - Q\Psi, \tag{2.13}$$

we have our basic formula

$$4\pi(\hbar^2/2\mu)[k \cot(\eta-\theta) - k \cot(\eta^P-\theta)] \\ = 2(Q\Psi_t, H P \Psi^P) + (Q\Psi_t, [\mathcal{H} - E] Q \Psi_t) \\ - (Q\Omega, [\mathcal{H} - E] Q \Omega), \tag{2.14}$$

where

$$\mathcal{H}(E, \theta) \\ \equiv \mathcal{H} \equiv Q \left[ H + H P \frac{1}{P(E-H)P} P H \right] Q = K + E Q. \tag{2.15}$$

As was our intention, the situation at this stage is very similar to the situation for zero incident kinetic energy. Since the term containing  $[P(E-H)P]^{-1}$  is a potential term which vanishes for large separations, the continuous spectrum of  $\mathcal{H}$  is bounded from below by  $E_{T1}$ , the energy of the first excited state of the target.  $E$  is, of course, less than  $E_{T1}$ . The operator  $\mathcal{H}$  may or may not have discrete eigenvalues below  $E_{T1}$ . If there are no such discrete eigenvalues below  $E$ , we can simply drop the last term in Eq. (2.14) and we remain with a bound on  $k \cot(\eta-\theta)$ . If there are  $\mathfrak{N}^Q = \mathfrak{N}^Q(E, \theta)$  such discrete (real)<sup>11</sup> eigenvalues  $\mathcal{E}_n^Q = \mathcal{E}_n^Q(E, \theta)$  below  $E$ , with eigenfunctions  $\Phi_n^Q = \Phi_n^Q(E, \theta)$ , the effects of the discrete states must be "subtracted out" in a fashion similar to that used in "subtracting out" the effects of the discrete bound states for zero incident kinetic energy. Our result, then, is the following:

If, for a fixed energy  $E$ , there exist  $\mathfrak{N}^Q$  eigenvalues  $\mathcal{E}_n^Q < E$  of  $\mathcal{H}$ , where  $\mathcal{H} = \mathcal{H}(E, \theta)$  is defined by Eq. (2.15), and if one can find  $\mathfrak{N}^Q$  orthonormal functions  $\Phi_{nt}^Q(\mathbf{r}, \mathbf{q})$  such that

$$(\Phi_{nt}^Q, \mathcal{H} \Phi_{mt}^Q) = \mathcal{E}_n^Q \delta_{nm}, \quad \mathcal{E}_n^Q < E, \quad 1 \leq n, m \leq \mathfrak{N}^Q,$$

then, since  $K = \mathcal{H} - E Q$ ,

$$(Q\Omega, [\mathcal{H} - E] Q\Omega) = (\Omega, K\Omega) \geq \sum_{n=1}^{\mathfrak{N}^Q} \frac{|\langle \Phi_{nt}^Q, K\Omega \rangle|^2}{\mathcal{E}_n^Q - E}.$$

Since

$$K\Omega = K\Psi_t - K\Psi = K\Psi_t + QHP\Psi^P$$

<sup>11</sup> The operator  $\mathcal{H}_a$  of Fonda and Newton [see reference 5, Eqs. (2.9) and (2.10)] is not the same as our  $\mathcal{H}$ , even for a partial wave decomposition. The difference lies in the meaning of  $[P(E-H)P]^{-1}$ . For one thing, our Green's function contains an arbitrary  $\theta$ . More significantly, we have used standing waves, whereas it is customary in studies of the formal theory of reactions to use outgoing waves.  $\mathcal{H}_a$  is not, then, Hermitian, and the eigenvalues of  $\mathcal{H}_a$  are complex, with the imaginary component related to the width; the case for which an eigenvalue of  $\mathcal{H}_a$  is real is, then, a very special one and corresponds to a bound state of infinite lifetime (zero width) embedded in the continuum. Our  $\mathcal{H}$ , on the contrary, is Hermitian and its eigenvalues are real; for a partial wave decomposition and for  $\theta = \pi/2$ , the eigenvalues of  $\mathcal{H}$  are the real parts of the eigenvalues of  $\mathcal{H}_a$ .

by Eqs. (2.13), (2.8), and (2.7b), we have, inserting a minus sign,

$$-(\Omega, K\Omega) \leq - \sum_{n=1}^{\mathfrak{N}^Q} \frac{|\langle \Phi_{nt}^Q, K\Psi_t + QHP\Psi^P \rangle|^2}{\mathcal{E}_n^Q - E}. \tag{2.16}$$

The use of this inequality in Eq. (2.14) gives us the sought for variational bound on  $k \cot(\eta-\theta)$

$$4\pi \left( \frac{\hbar^2}{2\mu} \right) [k \cot(\eta-\theta) - k \cot(\eta^P-\theta)] \\ \leq 2(Q\Psi_t, QHP\Psi^P) + (Q\Psi_t, [\mathcal{H} - E] Q\Psi_t) \\ + \sum_{n=1}^{\mathfrak{N}^Q} \frac{|\langle \Phi_{nt}^Q, [\mathcal{H} - E] Q\Psi_t + QHP\Psi^P \rangle|^2}{E - \mathcal{E}_n^Q}. \tag{2.17}$$

Just as for zero incident energy, it is possible to recast the above result into a more appropriate form.<sup>2,9,12</sup> To begin with, one shows that Eq. (2.17) is entirely equivalent to a *variational* principle in which the trial function contains terms proportional to the functions  $\Phi_{nt}^Q$ . Secondly, the functions,  $\Phi_{nt}^Q$  need not be constructed explicitly. Rather, one can introduce trial functions with an increasing number of terms whose coefficients are determined variationally. With the introduction of each term, one sees whether the variational estimate of  $k \cot(\eta-\theta)$  increases or decreases as compared to the previous result. It can be shown that the estimate will increase  $\mathfrak{N}^Q$  times, after which it can only decrease. This procedure is equivalent to the construction of the  $\Phi_{nt}^Q$ .

As a way of picturing how a Kohn-type variational calculation of the type just described converges to the exact value of  $\cot(\eta-\theta)$ , it is most convenient to think of the successive improvements in the trial function as being *continuous* rather than discrete. [This would happen, for example, if one were to introduce an exponential parameter into each term in order to span the gap, and if this parameter were varied in such a way that the estimate of  $\cot(\eta-\theta)$  always moved in a *downward* direction.] The approximation to  $\cot(\eta-\theta)$ , which begins at  $\cot(\eta^P-\theta)$ , will then decrease continuously, apart from  $\mathfrak{N}^Q$  increases which occur when the cotangent function has one of its usual discontinuities, as our approximation to the phase shift increases continuously from  $\eta^P$  toward the exact  $\eta$ . This picture will be discussed further in the following section.

One general remark about the procedure that we have introduced is in order at this time. As contrasted to the zero incident energy case,  $\Psi^P$  plays a fundamental role. It would be preferable to be able to avoid this, for we then immediately require the use of a computer, but it does not appear possible to do so because of the essential way in which  $\Psi^P$  appears in the basic equations upon which the formalism is based.

<sup>12</sup> T. Ohmura, Phys. Rev. 124. 130 (1961).

### 3. POTENTIALITIES OF THE MINIMUM PRINCIPLE— THE ZERO-ENERGY CASE

The results of Sec. 2 represent a rigorous variational bound on  $k \cot(\eta - \theta)$  (a) if and only if the number  $\mathfrak{N}^Q$  of eigenvalues of  $\mathfrak{H}$  which lie below  $E$  is known exactly, and (b) if and only if one can find a trial function which effectively subtracts out the contributions of the associated  $\mathfrak{N}^Q$  eigenfunctions. Point (b) is a limitation in practice but if  $\mathfrak{N}^Q$  is known it will often not be a serious limitation and we will not consider this point further. Point (a), on the other hand, is a limitation in principle since  $\mathfrak{N}^Q$  will rarely be known exactly, and it might seem that the advantages of our approach over a standard variational approach are more formal than real, but this is not the case. While a minimum principle which did not contain any elements of uncertainty whatever would only too obviously be preferable, we would like to discuss why the present approach will often have, from the practical point of view, most of the advantages associated with such an ideal minimum principle.

A consideration of the zero-energy problem will throw some light on this question since a comparable problem has previously been met at zero energy. We shall see that for  $E' = 0$ , and for  $E'$  close to zero, the number  $\mathfrak{N}^Q$  is a rough measure of the failure of the static potential as an approximation to the actual interaction [see Eq. (3.18)]. The experimental evidence of resonances can also provide information about  $\mathfrak{N}^Q$ , but we will not discuss this point.

We will first establish the connection between the present results when specialized to  $E' = 0$  and the results previously obtained at  $E' = 0$ . The connection should be made if only for general interest, but it will also enable us to develop some insight into the question of the number of eigenvalues of  $\mathfrak{H}$  below  $E$  for small incident kinetic energies.

Let  $\Psi_t$  be the  $E' = 0$  trial function in the formulation of the present paper, and let  $\tilde{\Psi}_t$  be the  $E' = 0$  trial function in the previous formulations.<sup>1,2</sup> The connection between the two formulations is then made by choosing, for a given  $\Psi_t$ ,

$$\tilde{\Psi}_t = Q\Psi_t + P\Psi^P + \frac{1}{P(E_{T_0} - H)P} PHQ\Psi_t. \quad (3.1)$$

Before proving the connection, we would like to motivate the above choice somewhat. For one thing, the exact wave function  $\Psi$  satisfies

$$\Psi = Q\Psi + P\Psi = Q\Psi + P\Psi^P + \frac{1}{P(E_{T_0} - H)P} PHQ\Psi, \quad (3.2)$$

where the second form follows from Eq. (2.4a), so that the choice is certainly not an unreasonable one. Secondly, one knows that it is possible to connect the Lippmann-Schwinger variational form, which contains Green's functions, with the Kohn-Hulthén variational form, which contains only differential operators. There,

where the exact function  $\Psi$  satisfies

$$\Psi = \Phi + GV\Psi, \quad (3.2')$$

with  $\Phi$  and  $G$  representing the wave function and the Green's function when the interaction between the incident particle and the target is neglected, one establishes the connection by choosing the Kohn-Hulthén trial function  $\Psi_{tKH}$ , for a fixed Lippmann-Schwinger trial function  $\Psi_{tLS}$ , to be

$$\Psi_{tKH} = \Phi + GV\Psi_{tLS}. \quad (3.1')$$

Since the present minimum principle formulation involves a Green's function,  $[P(E_{T_0} - H)P]^{-1}$ , whereas the previous formulation did not, the choice of  $\tilde{\Psi}_t$  as given in Eq. (3.1) is, then, a very natural one. It should, however, be remarked that, whereas the connection between variational principles neglects second-order terms, the connection between minimum principles that is our present concern does not.

To explicitly exhibit the connection, we start with

$$4\pi(\hbar^2/2\mu)(A - \tilde{A}_t) = (\tilde{\Psi}_t, H\tilde{\Psi}_t) - (\tilde{\Omega}, H\tilde{\Omega}), \quad (3.3)$$

where the inner product is now over the full space (hence the factor  $4\pi$ ), and where

$$\tilde{\Psi}_t \rightarrow \psi_{T_0}(\mathbf{r})(-q + \tilde{A}_t)/q \text{ as } q \rightarrow \infty. \quad (3.4)$$

(The above result is the readily derived generalization<sup>1</sup> to the scattering by a compound system of the results for the special case of potential scattering discussed in Sec. 1.) This is to be compared to the limit as  $E' \rightarrow 0$  of the results of Sec. 2. The form of the limit obtained depends upon the choice of  $\theta$ . To obtain the desired form we can choose any value of  $\theta$  other than  $\theta = 0$ ; it is simplest to choose  $\theta = \frac{1}{2}\pi$ . Dividing by  $k^2$  and letting  $k^2 \rightarrow 0$ , we find<sup>13</sup> from Eqs. (2.14), (2.2), and (2.6), that

$$\begin{aligned} & (4\pi\hbar^2/2\mu)(A - A^P) \\ & = 2(\Psi_t, QHP\Psi^P) + (Q\Psi_t, [\mathfrak{H}_0 - E_{T_0}]Q\Psi_t) \\ & \quad - (Q\Omega, [\mathfrak{H}_0 - E_{T_0}]Q\Omega), \end{aligned} \quad (3.5)$$

where

$$\mathfrak{H}_0 \equiv \mathfrak{H}(E = E_{T_0}, \theta \neq 0)$$

$$= Q \left[ H + HP \frac{1}{P(E_{T_0} - H)P} PH \right] Q, \quad (3.6)$$

and where  $\Psi^P$  and  $A^P$  are the  $E' = 0$  scattering wave function and its associated scattering length in the static approximation.  $\Psi^P$  is normalized as

$$\Psi^P \rightarrow \psi_{T_0}(\mathbf{r})(-q + A^P)/q \text{ as } q \rightarrow \infty, \quad (3.7)$$

<sup>13</sup> In the notation that follows, we will not bother to distinguish between  $k=0$  functions that are the limits of  $k>0$  functions, such as  $u_{\text{irreg}}^P$ , and functions such as  $u_{\text{reg}}^P$  which contain a factor of  $1/k$  in the definition of their  $k=0$  limit, that is, functions defined as

$$u_{\text{reg}}^P(q; k=0) = \lim_{k \rightarrow 0} u_{\text{reg}}^P(q; k)/k.$$

and

$$[P(E_{T_0}-H)P]^{-1} = (-2\mu/4\pi\hbar^2)Pu_{\text{reg}}^P(\mathbf{q}_<)u_{\text{irreg}}^P(\mathbf{q}_>), \quad (3.8)$$

where the regular and irregular functions are solutions of

$$P(H-E_{T_0})Pu^P=0, \quad (3.9)$$

which satisfy

$$u_{\text{reg}}^P(\mathbf{q}) \rightarrow (-q+A^P)/q \text{ as } q \rightarrow \infty,$$

and

$$u_{\text{irreg}}^P(\mathbf{q}) \rightarrow 1/q \text{ as } q \rightarrow \infty.$$

(The term in the Green's function proportional to the product of regular functions vanishes as  $k \rightarrow 0$ .)

Taking the asymptotic forms Eqs. (3.4) and (3.7), it follows from Eqs. (3.1) and (3.8) and from the fact that  $\psi_{T_0}(\mathbf{r})u_{\text{reg}}^P(\mathbf{q})=\Psi^P$  that

$$\tilde{A}_t=A^P+(2\mu/4\pi\hbar^2)(\Psi_t, QHP\Psi^P). \quad (3.10)$$

We substitute Eq. (3.1) into Eq. (3.3), use Eq. (3.10), and use the relation

$$\begin{aligned} & \left( \left[ P\Psi^P + \frac{1}{P(E_{T_0}-H)P} PHQ\Psi_t \right], (H-E_{T_0}) \right. \\ & \quad \left. \times \left[ P\Psi^P + \frac{1}{P(E_{T_0}-H)P} PHQ\Psi_t \right] \right) \\ & = \left( \left[ P\Psi^P + \frac{1}{P(E_{T_0}-H)P} PHQ\Psi_t \right], (-)PHQ\Psi_t \right), \end{aligned}$$

which follows from the fact that the square bracket effectively contains a factor of  $P$  and from the subsequent use of Eq. (3.9). We, then, find that Eq. (3.3) becomes identical with Eq. (3.5), but with the last term replaced by  $(\tilde{\Omega}, (H-E_{T_0})\tilde{\Omega})$ , that is, we have

$$(\tilde{\Omega}, [H-E_{T_0}]\tilde{\Omega}) = (Q\Omega, [\mathcal{H}_0-E_{T_0}Q]Q\Omega). \quad (3.11)$$

This relationship can also be established directly; by subtracting Eq. (3.2) from Eq. (3.1), and using

$$\tilde{\Omega} \equiv \tilde{\Psi}_t - \Psi, \quad Q\Omega \equiv Q\Psi_t - Q\Psi,$$

we obtain

$$\tilde{\Omega} = Q\Omega + \frac{1}{P(E_{T_0}-H)P} PHQ\Omega, \quad (3.12)$$

from which Eq. (3.11) can readily be shown to follow.

Having found the connection between the two forms exhibited by Eq. (3.11), we would now like to exploit this connection and any knowledge that we may have of the properties of  $H$  to prove some properties of  $\mathcal{H}_0$ . To begin with, it does not follow from Eq. (3.11) that  $\mathcal{H}_0-E_{T_0}Q$  has as many negative eigenvalues as does  $H-E_{T_0}$ . One reason is that  $\tilde{\Omega}$  is not an arbitrary function, even apart from the usual boundary conditions, but is restricted by Eq. (3.12); thus, for example, operating from the left on Eq. (3.12) first with  $Q$  and

then with  $P$ , we find  $Q\tilde{\Omega}=Q\Omega$  and

$$P\tilde{\Omega} = [P(E_{T_0}-H)P]^{-1}PHQ\tilde{\Omega},$$

the relation between  $P\tilde{\Omega}$  and  $Q\tilde{\Omega}$  clearly exhibiting the lack of arbitrariness of  $\tilde{\Omega}$ . If then  $H-E_{T_0}$  has a given number of negative eigenvalues, it does *not* follow that there exists that number of negative eigenvalues in the restricted space of functions of the form of  $\tilde{\Omega}$ .

There are, nevertheless, properties of  $\mathcal{H}_0$  which do follow from Eq. (3.11). Thus, assume that it is known in any way, experimentally in general, that there are no composite bound states of the target and the incident particle, that is, that  $N=0$ . This result is entirely equivalent to the statement that  $H-E_{T_0}$  is a non-negative operator in the space of functions which decay or approach  $\Psi_{T_0}(\mathbf{r})/q$  as  $q \rightarrow \infty$ .  $H-E_{T_0}$  is, then, *a fortiori* a non-negative operator in the restricted space of functions of the form of  $\tilde{\Omega}$ . Finally then, we see that  $\mathcal{H}_0-E_{T_0}Q$  is a non-negative operator if there are no composite bound states of the target and incident particle.

Now let us assume that it is known that (a) there are  $N$  such composite bound states and (b) that there are  $N^P$  composite bound states in the static approximation; in other words,  $H-E_{T_0}$  has  $N$  negative eigenvalues and  $T(q)+V_{00}(q)$  has  $N^P$  negative eigenvalues. From (a) we expect, in practice, to be able to construct  $N$  orthogonal functions  $\tilde{\Phi}_{nt}$  for which

$$(\tilde{\Phi}_{nt}, [H-E_{T_0}]\tilde{\Phi}_{nt}) = (\tilde{E}_{nt}-E_{T_0})\delta_{mn}, \quad \tilde{E}_{nt}-E_{T_0} < 0, \quad 1 \leq m, n \leq N, \quad (3.13)$$

and we then have

$$(\tilde{\Omega}, [H-E_{T_0}]\tilde{\Omega}) \geq \sum_{n=1}^N \frac{|(\tilde{\Phi}_{nt}, [H-E_{T_0}]\tilde{\Psi}_t)|^2}{\tilde{E}_{nt}-E_{T_0}}. \quad (3.14)$$

It is a one line proof, using Eqs. (3.1) and (3.9), to show that

$$P[H-E_{T_0}]\tilde{\Psi}_t=0;$$

we can, therefore, insert a  $Q$  before  $[H-E_{T_0}]\tilde{\Psi}_t$  in Eq. (3.14). Using Eqs. (3.11) and (3.1), we arrive at the bound

$$\begin{aligned} & (\Omega, [\mathcal{H}_0-E_{T_0}Q]\Omega) \\ & \geq \sum_{n=1}^N \frac{|(\tilde{\Phi}_{nt}, [\mathcal{H}_0-E_{T_0}Q]\Psi_t + QHP\Psi^P)|^2}{\tilde{E}_{nt}-E_{T_0}}. \quad (3.15) \end{aligned}$$

It follows from (b), and from the proof in Appendix D, that it is always possible to choose  $N^P$  of the  $\tilde{\Phi}_{nt}$  to satisfy  $\tilde{\Phi}_{nt}=P\tilde{\Phi}_{nt}$ . Since  $\mathcal{H}_0=Q\mathcal{H}_0$ , the terms in the sum in Eq. (3.15) containing these particular  $\tilde{\Phi}_{nt}$  vanish, leaving only  $N-N^P$  subtraction terms. It almost follows at this point, by comparing Eq. (3.15) with Eq. (2.16) with  $E$  set equal to  $E_{T_0}$  in the latter, that  $\mathcal{R}^Q$  is at most equal to  $N-N^P$ , since a bound on  $(\Omega|\mathcal{H}_0-E_{T_0}|\Omega)$  can be obtained with  $N-N^P$  terms. The



identification of the two equations, however, is not yet complete, since the  $\bar{E}_{nt} - E_{T0}$  which appear in Eq. (3.15) are defined quite differently from the  $\mathcal{E}_{nt}^Q - E_{T0}$  which appear in Eq. (2.16). Thus, from Eq. (3.13), we have

$$\bar{E}_{nt} - E_{T0} = (\tilde{\Phi}_{nt}, [H - E_{T0}]\tilde{\Phi}_{nt}),$$

whereas the  $\mathcal{E}_{nt}^Q - E_{T0}$  were defined by

$$\mathcal{E}_{nt}^Q - E_{T0} = (\Phi_{nt}^Q, [\mathcal{H}_0 - E_{T0}Q]\Phi_{nt}^Q).$$

To complete the identification, we make use of the result, proved in Appendix D, that not only can one find  $N^P$  of the  $N$  functions  $\tilde{\Phi}_{nt}$  which satisfy  $P\tilde{\Phi}_{nt} = \tilde{\Phi}_{nt}$ , but that the remaining  $N - N^P$  of the  $\tilde{\Phi}_{nt}$  can be chosen to satisfy a relationship of the form of Eq. (3.12). In particular, we choose the remaining  $\tilde{\Phi}_{nt}$  to be of the form

$$\tilde{\Phi}_{nt} = Q\Phi_{nt}^Q + \frac{1}{P(E_{T0} - H)P} PHQ\Phi_{nt}^Q. \quad (3.16)$$

(The  $\tilde{\Phi}_{nt}$  are not then normalized, nor need they be for our present purposes.) It is, then, easily verified that

$$(\tilde{\Phi}_{nt}, [H - E_{T0}]\tilde{\Phi}_{mt}) = (\Phi_{nt}^Q, [\mathcal{H}_0 - E_{T0}Q]\Phi_{mt}^Q), \quad (3.17)$$

where  $n$  and  $m$  take on  $N - N^P$  values. Setting  $n = m$ , we have

$$\mathcal{E}_{nt}^Q - E_{T0} = \bar{E}_{nt} - E_{T0},$$

so that the denominators of Eqs. (3.15) and (2.16) are the same. The numerators of these two equations are also the same, since it is only  $Q\tilde{\Phi}_{nt}$  which effectively appears in Eq. (3.15), and from Eq. (3.16),  $Q\tilde{\Phi}_{nt} = Q\Phi_{nt}^Q$ . The identification of the two equations may be regarded as providing a construction at  $E' = 0$  of the required subtraction functions,  $\Phi_{nt}^Q$ , whose number is now seen to be  $N - N^P$ , i.e.,

$$\mathcal{N}^Q(E' = 0) = N - N^P. \quad (3.18)$$

In addition to what this tells us about the zero-energy case itself,<sup>14</sup> Eq. (3.18) will also be true for sufficiently small energies, and should give a good idea of the number of subtractions to be performed at small energies.

### A Generalization of Levinson's Theorem

Returning to zero energy, we shall now show that Eq. (3.18) together with the absolute definition of the phase shift implied at the end of Sec. 2 makes possible a generalization of Levinson's theorem to scattering by a compound system, in the sense of relating the value of the phase shift at zero energy to the number of bound states.

The basic equations, such as Eqs. (2.1) and (2.2), define the phase shift  $\eta$  only to within an arbitrary multiple of  $\pi$ . It is only when some procedure is adopted to remove this arbitrariness that we can formulate a

generalization of Levinson's theorem. [The alternative of considering the difference  $\eta(0) - \eta(\infty)$  will not be considered here.] The application of the minimum principle itself, as described at the end of Sec. 2, actually specifies  $\eta$  uniquely once a unique definition of the static phase shift  $\eta^P$  has been adopted. (For our purpose it will not matter what this definition is, since we shall be concerned only with the difference  $\eta - \eta^P$ .) The process of introducing successive terms to our trial function was regarded as a continuous one (in a realizable way) and the approximation to the phase shift itself, determined at any stage of the calculation, was taken to be a continuous (and consequently a monotonically increasing) function of the accuracy of the trial function. In the limit, as the number of terms in the trial function is increased indefinitely, the limiting value of the approximate phase shift is taken to define the exact phase shift  $\eta$  absolutely, that is, it specifies the multiple of  $\pi$  in  $\eta$ . It seems that this procedure for specifying the phase shift is equivalent to varying the optical potential continuously between the static potential and its full value, that is, to "turning on" the second term in Eq. (2.7a) continuously. Since, as pointed out in reference 6, this term represents an attractive interaction, the phase shift would increase monotonically from the already determined  $\eta^P$  to its final value,  $\eta$ .

In the course of this analysis, the number of subtraction terms needed,  $\mathcal{N}^Q$ , was seen to correspond to the number of times that  $\theta \pmod{\pi}$  appears between  $\eta^P$  and  $\eta$  so defined. Now as the energy,  $E'$ , approaches zero, both  $\eta^P$  and  $\eta$  approach multiples of  $\pi$ . Taking  $\theta \neq 0$ , the above interpretation of  $\mathcal{N}^Q$  implies that  $\eta$  will be greater than  $\eta^P$  in this limit by an amount  $\mathcal{N}^Q\pi$ . But combining this with Eq. (3.18) for  $\mathcal{N}^Q$  we have the result

$$\eta - \eta^P = (N - N^P)\pi \quad (3.19)$$

at  $E' = 0$ . This is the sought for generalization of Levinson's theorem for compound systems.

Some general comments should now be made. First, while the most natural definition of  $\eta^P$  would be one which includes the effects of the Pauli principle, the validity of Eq. (3.19) is independent of the absolute definition of  $\eta^P$ . The only effect of the Pauli principle with regard to our generalized Levinson's theorem will then be the influence it exerts in the determination of the number  $N$  of the true bound states.

Second, regarding the possibility of bound states in the continuum, the definition of the phase shift adopted above seems to be equivalent to assuming it to be a continuous function of the (optical) potential strength. It then follows, as mentioned in reference 6, Appendix, that in the remote case there should be a bound state imbedded in the continuum, the phase shift thus defined would, as a function of energy, become discontinuous at that energy, but Levinson's theorem would not be affected.

Finally, it should be noted that generalizations of

<sup>14</sup> Some further comments on the zero energy case itself are contained in Appendix C.

Levinson's theorem have been given previously.<sup>15</sup> Since these generalizations consider phase shifts at  $E'=0$  and at  $E'=\infty$ , they involve the complicated energy domain in which multichannel processes are possible, and the proofs, therefore, necessarily contain statements about the eigenphase shifts. Some of these proofs pertain to more general situations than those which we have considered in that they allow for production processes for example, but they do involve some approximations.

#### 4. POTENTIALITIES OF THE MINIMUM PRINCIPLE—THE GENERAL CASE

At energies sufficiently close to zero, we have seen that the number of subtractions,  $\mathfrak{N}^Q$ , will be known exactly if only we know the number of bound states for the true as well as the static problem; hence our bound on  $\tan\eta$  can be made completely rigorous. We would now like to face up to the more interesting question as to how to proceed in the general case. The natural procedure is to introduce trial scattering functions  $\Psi_t$  with one, then two, etc., terms, which might include nonlinear as well as linear variational parameters, and to proceed as described at the end of Sec. 2, seeking the minimum value of  $k \cot(\eta-\theta)$  for each form of  $\Psi_t$ . We would obtain a bound on  $k \cot(\eta-\theta)$  for the number of parameters "sufficiently large," but if the number of eigenvalues  $\mathfrak{N}^Q$  of  $\mathfrak{H}$  below  $E$  is not known there is no way of actually specifying what "sufficiently large" is to be taken to mean. To put it bluntly, a rigorous bound on  $k \cot(\eta-\theta)$  cannot be obtained. It is, nevertheless, possible to deduce completely rigorous and useful consequences from the minimum principle. When combined with some qualitative ideas, it should, in fact, often be possible not only to obtain good estimates of  $k \cot(\eta-\theta)$  but to be reasonably certain that the estimates are, in fact, good.

Thus, let us assume that we use a trial function of the form

$$\Psi_t = \sum_{j=0}^J C_j g_j(\mathbf{r}, \mathbf{q}),$$

where the  $g_j$  may contain nonlinear parameters. For any fixed  $J$ , we would vary the parameters so as to cause  $k \cot(\eta-\theta)$  to be as small as possible. It is possible, in principle, to pass down through  $-\infty$   $\mathfrak{N}^Q$  times, but of course we do not know what  $\mathfrak{N}^Q$  is. It may be possible in practice to pass through  $-\infty$  by varying the nonlinear parameters, but it is not necessary actually to do so. The passage is signaled if there is a sudden upward jump in  $k \cot(\eta-\theta)$  as we add an additional term, and represents the fact that the trial function now effectively contains one more trial bound state function  $\Phi_{n_t}^Q$  which gives an expectation value of  $\mathfrak{H}$  below  $E$ , and that this state has been "subtracted out." The addition of one

term can at most account for one such state, so that we must have  $J$  at least equal to  $\mathfrak{N}^Q$ , if we are to have accounted for all such states. (The number of terms required to have accounted for all such states may be significantly reduced if we allow the nonlinear parameters to vary, though there must be at least  $\mathfrak{N}^Q$  terms.) From this stage on, the estimate of  $k \cot(\eta-\theta)$  can only decrease.

If then a number of different calculations have been performed, with different  $g_j$  and with different  $J$ , and we wish to judge which of the results is "best," or if we ourselves are performing the calculations and wish to determine the "best" possible values of the parameters, the objective and rigorous criterion for "best" is the following. The "best" result is the one for which the number of passages through  $-\infty$  is the greatest; if the number of passages for a number of calculations is the same, the "best" result is the lowest one. It should clearly be understood that the "best" result as just defined is *not* necessarily the one that is closest to the true value.

The above results can be pictured as the observation of a race in which the path is the curve of  $y = \cot x$  versus  $x$ . (We here choose  $\theta=0$  for convenience.) The starting point of the race for all runners is at  $x = \eta^P$ . When a runner reaches a position  $x$  which is a multiple of  $\pi$ , at which time he is at  $y = -\infty$ , he is moved infinitesimally to the right and then reappears at  $y = +\infty$ . At some unknown point  $x_0, y_0 = \cot x_0$  on the path there is an invisible marker. [This marker will appear on the  $(\mathfrak{N}^Q+1)$ th branch of the curve, but  $\mathfrak{N}^Q$  is not known either.] For some reason the runners can never get beyond the marker. The objective of the observer is to make the "best" possible estimate of the value of  $y_0 = \cot x_0$ . He would clearly only be concerned with the position of the runner who is furthest along. It is, of course, quite possible that some other runners might be closer to  $y_0$  than the front runner but that would be entirely accidental.

As contrasted to ordinary variational calculation, we then have an objective way of judging different results, and a particular "direction" in which to proceed if we ourselves are doing the calculation. We have not given an objective way of deciding when we are close to the true answer. That decision must be made in some qualitative way. For one thing, it should generally be possible to estimate  $\mathfrak{N}^Q$  to within perhaps one. For another, if the runner is approaching the finish line, his motion is necessarily quite slow and will generally be rather smooth. The converse is, of course, not necessarily true. If a particular class of functions have been omitted in the choice of trial functions, the slow and regular motion could signify no more than convergence to the wrong limit.

Though there is no new physical content involved, the above results can be stated much more succinctly in terms of phase shifts. If we let  $\eta_M$  be the phase shift determined at any stage of the variational calculation

<sup>15</sup> R. G. Newton, *J. Math. Phys.* **1**, 319 (1960); M. T. Vaughn, R. Aaron, and R. D. Amado, *Phys. Rev.* **124**, 1258 (1961); L. F. Cook, Jr., and B. W. Lee, *ibid.* **127**, 283 (1962).

in the manner just described (beginning with  $\eta^P$  when  $Q\Psi_l=0$ ), we have that  $\eta_M < \eta$ . It is assumed in this discussion that the multiples of  $\pi$  in the definition of the phase shift are accounted for ( $\eta_M$  and  $\eta$  can actually remain arbitrary to within the *same* multiple of  $\pi$ ). This is, of course, precisely the advantage of talking in terms of phase shifts, for one then knows automatically which branch of the  $\cot x$  vs  $x$  curve one is on. The question of the determination of the appropriate multiple of  $\pi$  is discussed in some detail in references 1 and 6.<sup>16</sup> In references 1 and 16, the definition of the phase shift involves a comparison of the projected wave function with the free wave function. We have subsequently realized that this definition leads to a phase shift which is a discontinuous function of the potential strengths and of the energy when there is a resonance and perhaps under certain other conditions. In reference 6, therefore, where continuity in the potential strengths is assumed throughout the paper, the definition involving the projected wave function should not be used. The main result of that paper, however, that the phase shift increases as additional states are introduced, is still valid, although the application in practice will now be slightly more difficult. The question of the definition of the phase shift will be elaborated upon in a future paper.

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#### APPENDIX A

In the development of the bound on  $\eta$ , it was shown that

$$\eta > \eta^P \quad \text{if} \quad Q(H-E)Q > 0, \quad (\text{A1})$$

where the latter inequality is to be understood to mean that the operator is positive definite. More generally, one can define the target operators  $P^*$  and  $Q^*$ , where  $P^*$  includes not only the ground state but some of the excited states, and where  $Q^*$  includes some but not necessarily all of the excited states not included in  $P^*$ , so that  $P^*$  contains  $P$ ,  $Q^*$  is contained in  $Q$ , and  $P^*Q^*=0$ , but we need not have  $P^*+Q^*$  equal to the unit operator;  $P^*$  and  $Q^*$  must, however, be projection operators.

$$\eta^{P^*+Q^*} > \eta^{P^*} \quad \text{if} \quad Q^*(H-E)Q^* > 0, \quad (\text{A2})$$

which includes Eq. (A1) as a special case.

It is a trivial matter to derive a minimum principle which involves  $P^*$  and  $Q^*$  rather than  $P$  and  $Q$ , and which includes the choice  $P^*=P$  and  $Q^*=Q$  as a special

case. In general, there is no point to this generalized form of the minimum principle, for if  $P^*$  includes  $m$  states, one has to solve  $m$  coupled differential (or integro-differential) equations as the starting point of the calculation, rather than simply the one differential (or integro-differential) equation that arises in the  $P$  or static approximation. This is bad enough, but then in all the subsequent calculations that involve the trial function  $\Psi_l$ , the work will be much more laborious. In fact, the great virtue of the minimum principle as opposed to the bound is precisely that the excited states do not have to be introduced one at a time; rather, some arbitrary functions containing variational parameters are to be introduced, where the functions contain the excited states in some perhaps complicated way, and the variational parameters are chosen to minimize  $\cot(\eta-\theta)$ , the contributions of the various excited states being thereby adjusted to produce the best results for the specified form of  $\Psi_l$ . The above remarks are relevant with regard to the determination of numerical values. From a heuristic point of view, however, it is desirable to consider the generalization to  $P^*$  and  $Q^*$ , and we will now proceed to do so.

Starting with the equations satisfied by  $\Psi^{P^*}$  and by  $\Psi^{P^*+Q^*}$ , we arrive at an equation of the form of Eqs. (2.14), with  $\eta$  replaced by  $\eta^{P^*+Q^*}$  and with  $P$  replaced by  $P^*$ , both as an operator and as a superscript, with  $Q$  replaced by  $Q^*$ , and with  $\Psi$  in Eq. (2.1) replaced by  $\Psi^{P^*+Q^*}$ . If then

$$\begin{aligned} & \mathfrak{H}Q^* - Q^*E \\ & \equiv Q^* \left[ H + HP^* \frac{1}{P^*(E-H)P^*} P^*H - E \right] Q^* > 0, \quad (\text{A3}) \end{aligned}$$

we obtain an upper bound on the left-hand side of the analog of Eq. (2.14) by dropping the last line. If the inequality (A3) is not satisfied, we proceed with the subtractions in the usual way. We then have the generalization of Eq. (2.17). If finally we choose  $Q^*\Psi_l=0$ , we have if the inequality (A3) is satisfied that

$$\cot(\eta^{P^*+Q^*}-\theta) \leq \cot(\eta^{P^*}-\theta). \quad (\text{A4})$$

It should be noted that there are conditions on  $\theta$  that follow from the fact that the Green's function in Eq. (A3) is  $\theta$  dependent.

Equations (A3) and (A4) are, of course, analogous to Eq. (A2), the difference between the conditions given by Eqs. (A1) and (A3) being a reflection of the fact that we are obtaining bounds on the one hand on  $\eta^{P^*+Q^*}$  and on the other on a trigonometric function of  $\eta^{P^*+Q^*}$ .

It should be noted that it follows from the above derivation that the best bound that can be obtained on  $\cot(\eta-\theta)$  from a trial function which includes only the  $m$  target states included in  $P^*$  is the value  $\cot(\eta^{P^*}-\theta)$  obtained from an exact (numerical) solution of the set of  $m$  coupled differential equations defined by  $P^*$ .

<sup>16</sup> See also, A. Temkin, J. Math. Phys. 2, 336 (1961).

## APPENDIX B—AN EXAMPLE

A fairly serious calculation of some low energy  $L=0$  and 1 scattering phase shifts for the scattering of positrons by hydrogen atoms is now in progress,<sup>17</sup> in which the target can be excited to superpositions of excited  $s$  states, of  $p$  states, and of  $d$  states, where the superpositions are *not* broken down into states with specified principle quantum numbers, that is, into eigenstates of  $H_T$ . The calculation has not yet been completed and we will, therefore, not discuss the results here other than to say that they are very encouraging. We would, however, like to record the results obtained for  $L=0$  and for an incident energy of 3.4 eV ( $ka_0=0.5$ ) by using the minimum principle in a very simple but very inefficient way, with the static approximation solved numerically and with  $Q^*$  being the very restrictive operator which projects onto the hydrogen  $2s$  state; we then expect to get a bound on the  $1s-2s$  approximation.  $Q^*\Psi_t$  was taken to be the  $2s$  function of  $r$  multiplied by  $Ce^{-\alpha r}$ , giving us one linear and one nonlinear variational parameter. Let us make the reasonable but unproved assumption that, (for  $\theta=\pi/2$  and  $E=3.4$  eV)

$$Q^*\left[H+HP\frac{1}{P(E-H)P}PH-E\right]Q^*>0,$$

in the space of total orbital angular momentum zero, with  $H$  the total Hamiltonian of an electron and a positron in the field of a proton. It then follows from the discussion in Appendix A that the result obtained should be better than the  $1s$  approximation ( $\tan\eta^P = -0.2696$ ), but not as good as the  $1s-2s$  approximation ( $\tan\eta^{1s+2s} = -0.2602$ ).<sup>18</sup> It is very satisfying that with our quite simple trial function we find, using  $\alpha=0.5$ , that  $\tan\eta^{1s+2s} \geq -0.2612$ , which accounts for nearly 90% of the difference. We would like to comment on a recent paper by Rotenberg<sup>19</sup> on  $e^+H$  scattering in which phase shifts are obtained that considerably exceed those of Schwartz.<sup>20</sup> Rotenberg expands in a complete set of functions, Sturmian functions, different from those used in the usual close coupling approach. We want to observe that our proof<sup>6</sup> that for  $Q^*(E-H)Q^* < 0$  in the close coupling approach the phase shift approaches the exact value monotonically is *not* valid in the Sturmian approach.

## APPENDIX C—THE ZERO INCIDENT ENERGY CASE

While the primary purpose of the present paper is to extend the minimum principle to nonzero incident energies without having to alter the potentials, the question naturally arises as to whether the zero incident

energy limit of the present formulation is an improvement over the previous formulation. For  $N^P=N$ , the answer is that in a formal sense it is an improvement, but that from the practical point of view it will almost always be preferable to perform the calculations using the previous formulation. The comparison between the old ( $\alpha$ ) and the new ( $\beta$ ) minimum principle formulations is almost exactly the same as the comparison between the Kohn-Hulthén ( $\alpha$ ) and the Lippmann-Schwinger ( $\beta$ ) variational principle formulations. In both cases formulation  $\beta$  is better in the sense that it generally gives a better answer for a given trial function; as can be seen from Eqs. (3.1) and 3.1'), the trial function for formulation  $\alpha$  that gives the same answer as does formulation  $\beta$  is an iteration of the trial function of formulation  $\beta$ . Nevertheless, since  $\alpha$  does not involve a Green's function while  $\beta$  does, it will generally be preferable to use  $\alpha$  rather than  $\beta$  since one can perform the necessary integrations for trial functions of  $\alpha$  that are so much more complicated than those for which the integrations can be performed for  $\beta$  that the initial advantages of  $\beta$  are more than offset.

There are, nevertheless, some additional remarks that should be made about the zero incident energy limit of the present minimum principle formulation. Thus, from the discussion in Sec. 3 and Eq. (3.16) we obtain the quite pretty result that

$$\mathfrak{H}_0 - E_{T_0}Q \geq 0 \quad \text{if } N^P = N. \quad (C1)$$

It is obviously *not* true that  $H - E_{T_0} > 0$  if  $N^P = N$ , unless  $N=0$ . In the new formulation, therefore, one can obtain a bound on  $A$  for an arbitrary  $\Psi_t$  without having to perform any subtractions. Unfortunately, in order to know that  $N^P = N$ , one would have to construct  $N$  orthonormal trial functions for which the expectation value of  $PHP - E_{T_0}P$  is negative.

The inequality (C1) can be qualitatively understood quite simply. If  $N^P = N$ , the static approximation is a very good one, or, equivalently, excitation from the ground state is not too important. The mathematical equivalent of the above remark is the statement that  $QHP$  and  $V$  are small. But, neglecting only terms of second order in  $QHP$ , we have

$$\mathfrak{H}_0 - E_{T_0}Q \approx Q(H - E_{T_0})Q.$$

Since  $QTQ \geq 0$  and since  $QH_TQ \geq E_{T_1}$ , we then expect that

$$\mathfrak{H}_0 - E_{T_0}Q \gtrsim (E_{T_1} - E_{T_0})Q + QVQ.$$

The remark that  $QVQ$  is small since  $V$  is small concludes the qualitative argument.

We would like finally to record a small generalization of a result obtained previously. It has been shown<sup>21</sup> that

$$A \leq A^P \quad \text{if } N^P = N. \quad (C2)$$

<sup>21</sup> L. Spruch and L. Rosenberg, Nucl. Phys. 17, 30 (1960).

<sup>17</sup> For a preliminary report on this work, see Bull. Am. Phys. Soc. 7, 492 (1962).

<sup>18</sup> K. Smith and P. G. Burke, Phys. Rev. 123, 174 (1961).

<sup>19</sup> M. Rotenberg, Am. Phys. (N. Y.) 19, 262 (1962). See also A. Temkin, Proc. Phys. Soc. (London) A80, 1277 (1962).

<sup>20</sup> C. Schwartz, Phys. Rev. 124, 1468 (1961).

This also follows from Eq. (3.15). If  $N^P$  is less than  $N$ , it may be possible to account for the additional  $N - N^P$  states by including some excited states of the target, that is, by replacing  $P$  by  $P^*$ . Since the entire formalism remains valid under this replacement, we obtain

$$A \leq A^{P^*} \text{ if } N^{P^*} = N, \tag{C3}$$

where  $N^{P^*}$  and  $A^{P^*}$  are, of course, the number of negative eigenvalues and the scattering length associated with  $P^*(H - E_{T_0})P^*$ . If  $N^P = N$ , in which case we automatically also have  $N^{P^*} = N$ , Eq. (C3) simply represents an improvement upon Eq. (C2) rather than an extension which is applicable to new situations.

APPENDIX D

From the assumption that there exist  $N^P$  bound states in the static approximation, it follows that one can choose  $N^P$  functions of the form

$$\psi^{(1)} = P\psi^{(1)} \tag{D1}$$

which satisfy Eq. (3.13) with  $N$  replaced by  $N^P$ . It is not immediately clear, however, once one has chosen  $N^P$  such functions that it is always possible to find  $N - N^P$  additional functions such that the entire set of  $N$  functions satisfies (3.13). We will now show that not only is this always possible, but that the  $N - N^P$  additional functions can even be chosen to be of the particular form

$$\psi^{(2)} = Q\psi + \frac{1}{P(E_{T_0} - H)P}PHQ\psi. \tag{D2}$$

To begin with, we note that the totality of functions  $\psi^{(1)}$  and  $\psi^{(2)}$  form a complete set of functions in the space of functions which are regular and which vanish at least as rapidly as  $1/q$  as  $q \rightarrow \infty$ . Secondly, we notice that

$$(\psi^{(1)}, [H - E_{T_0}]\psi^{(2)}) = (\psi^{(2)}, [H - E_{T_0}]\psi^{(1)}) = 0.$$

If then we place all the functions of form  $\psi^{(1)}$  before those of form  $\psi^{(2)}$ , the matrix of  $H - E_{T_0}$  reduces to block diagonal form; more precisely, we find

$$(H - E_{T_0}) = \begin{pmatrix} H^{(1)} - E_{T_0} & 0 \\ 0 & H^{(2)} - E_{T_0} \end{pmatrix}, \tag{D3}$$

where the superscript indicates the class of functions with respect to which the submatrix is constructed.

A useful consequence of this is that, for a finite  $H$  matrix, the determinant may be written

$$\text{Det}(H - E_{T_0}) = \text{Det}(H^{(1)} - E_{T_0}) \cdot \text{Det}(H^{(2)} - E_{T_0}). \tag{D4}$$

Now we know that the operator  $H - E_{T_0}$  has  $N$  nega-

tive eigenvalues and that  $H^{(1)} - E_{T_0}$  has  $N^P$ , since there are  $N$  bound states and  $N^P$  static bound states. What we would like to know is how many negative eigenvalues the submatrix  $H^{(2)} - E_{T_0}$  has. We will show that it has exactly  $N - N^P$  of them, as might have been suspected. The method of proceeding will be to take the functions one at a time and consider first the  $1 \times 1$  matrix, then the  $2 \times 2$  and so on. At each stage, we will look at the determinant,  $\text{Det}(H - E_{T_0})$  and use the theorem that a change in sign of the determinant as an additional function is introduced is equivalent to the introduction of an additional negative eigenvalue to the matrix. Since the operator  $H - E_{T_0}$  has  $N$  exact negative eigenvalues, and our set of  $\psi^{(1)}$ 's and  $\psi^{(2)}$ 's is complete, exactly  $N$  such changes in sign will eventually be observed, as functions are added one at a time.

We begin by introducing only functions of the type  $\psi^{(1)}$  until the changes in sign of the determinant indicate that  $N^P$  approximate negative eigenvalues of  $H - E_{T_0}$  (which is the same as  $H^{(1)} - E_{T_0}$  at this stage) have been introduced. Since  $H^{(1)} - E_{T_0}$  has only  $N^P$  exact negative eigenvalues, from this point on introducing any number of additional  $\psi^{(1)}$  functions cannot cause  $\text{Det}(H^{(1)} - E_{T_0})$  to change sign again. Now since  $\text{Det}(H - E_{T_0})$  must ultimately change sign  $N$  times, it follows from Eq. (D4) that the remaining  $N - N^P$  changes in sign must come from  $\text{Det}(H^{(2)} - E_{T_0})$ . Therefore, the infinite submatrix  $H^{(2)} - E_{T_0}$  has exactly  $N - N^P$  negative eigenvalues, which is the desired result.

To complete the proof in the form required in the text, one further thing should be shown. So far, it has been seen that it is possible to find  $N^P$  approximate negative eigenvalues of  $H - E_{T_0}$  of the form  $\psi^{(1)}$  and also  $N - N^P$  of the form  $\psi^{(2)}$ . If  $N$  such functions have been constructed, one simply repeats the procedure of the last paragraph with these  $N$  functions and, thus, finds that  $\text{Det}(H - E_{T_0})$  changes sign  $N$  times, and hence that these  $N$  functions taken together generate  $N$  negative eigenvalues.

In the light of the foregoing procedure, the reduction of the original Hamiltonian,  $H$ , by means of the functions  $\psi^{(1)}$  and  $\psi^{(2)}$  into the form Eq. (D3), a certain insight can be gained into the minimum principle as derived in Sec. 2, where we begin with the Schrödinger equation (2.1) and proceed through Eqs. (2.5) and (2.7b) to the final result, Eq. (2.17). First, it has been pointed out already that the submatrix  $H^{(1)} - E$  in Eq. (D3) is equivalent to the static Hamiltonian of Eq. (2.5). (The present discussion will not be confined to the zero-energy problem.) Further, if one looks at Eq. (3.17) where the  $\Phi_{n,t}$  were all functions of the form  $\psi^{(2)}$ , it will be seen that this equation states that our submatrix,  $H^{(2)} - E$ , is equal, element by element, to the matrix  $\mathcal{H} - EQ$ . That is, the operator  $\mathcal{H} - EQ$  which is used in the minimum principle corresponds to the submatrix,  $H^{(2)} - E$  of the original Hamiltonian, based on functions of the class  $\psi^{(2)}$ . What was done in Sec. 2

can then be summed up in this way. The Hamiltonian matrix was effectively reduced to the form Eq. (D3). The first submatrix,  $H^{(1)} - E$  corresponds to a simple operator, and represents a problem which can be solved exactly. The second submatrix,  $H^{(2)} - E$  ( $\mathcal{H} - EQ$ ),

though more complicated, has the property that its spectrum is discrete below the inelastic threshold, and so it can readily be bounded. Consequently, in terms of an exact solution of  $H^{(1)}$  and a bound on  $H^{(2)}$  a bound is found on  $k \cot(\eta - \theta)$ .

## Collision Lifetimes in Many-Body Processes\*

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Collision lifetimes and the lifetime matrix are expressly formulated so as to include three-body and many-body collision and breakup processes. The many-body states are expressed in the generalized angular momentum representation, in which the principal radial coordinate is proportional to the square root of the trace of the inertia tensor for the  $N$ -body configuration. The physical significance of the (energy-dependent) three-body collision lifetime  $Q^{(3)}(E)$  is clarified by considering the special case where the three-body breakup occurs by way of a metastable two-body intermediate. If the metastable occurs with an internal energy  $E_m$  and a decay time  $\tau_m$ , and the process creating it has a collision lifetime  $Q^{(2)}(E - E_m)$ , the connection with  $Q^{(3)}$  is:  $Q^{(3)}(E) = Q^{(2)}(E - E_m) + \tau_m E_m / E$ . This result holds both classically and quantumly.

### A. INTRODUCTION

THE breakup of an unstable particle into three or more fragments is an important process in many areas of physics and chemistry: high-energy particles, compound nuclei, and highly excited molecules provide a variety of examples. The inverse process of three-body collision can also be important in chemical reactions and in the nuclear reactions of stellar interiors. The lifetime of the unstable particle or collision complex is one of its principal characteristics. It is the purpose of this note to examine some general features of such lifetimes when three-body processes are present.

For a two-body collision in the simplest case (elastic scattering, classical nonrelativistic mechanics, forces of range shorter than Coulomb), the collision lifetime is conveniently defined as the limit, as  $R \rightarrow \infty$ , of the difference between the time the particles spend within a distance  $R$  of each other in the actual collision and the time they would have spent there in a hypothetical trajectory without any interaction<sup>1,2</sup>:

$$Q_{\text{el}} = \lim_{R \rightarrow \infty} [t(R) - t_0(R)]. \quad (1)$$

This definition can be readily translated to quantum mechanics, and leads to the result that the collision lifetime is proportional to the energy derivative of the phase shift, and thus also to the statistical density of

available states; for isolated resonances and slowly decaying states, there is a simple relation between the collision lifetime, the width of the resonance, and the characteristic decay time of the state.<sup>3</sup> The definition is also easily extended to inelastic collisions—in the quantum case there results the lifetime matrix  $\mathbf{Q}$  related to the energy derivative of the scattering matrix  $\mathbf{S}$ .<sup>1</sup> Classically, the lifetime for an inelastic collision is defined by subtracting from the actual collision duration that of a hypothetical trajectory with two portions, the asymptotic incoming and outgoing paths extended as straight lines to their respective points of closest approach.

The development of a new description for three-body and many-body collisions<sup>4</sup> was initially motivated by a desire to include these processes in the formulation of the lifetime matrix. This note will carry out that program explicitly.

In treating three-body and  $(N+1)$ -body events, it is most helpful to use a center-of-mass coordinate system normalized so that all internal coordinates involve a common reduced mass  $\mu^{(3)}$  or  $\mu^{(N+1)}$  such that

$$\mu^{(3)} = \prod_{i=1}^3 m_i / \sum_{i=1}^3 m_i, \quad \mu^{(N+1)} = \prod_{i=1}^{N+1} m_i / \sum_{i=1}^{N+1} m_i. \quad (2)$$

The internal coordinates characterize a space of  $3N$

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<sup>1</sup> F. T. Smith, Phys. Rev. **118**, 349 (1960), referred to below as "LM"; also **119**, 2098(E) (1960). See also A. Krzywicki and J. Szymanski, Progr. Theoret. Phys. (Kyoto) **23**, 376 (1960).

<sup>2</sup> Such a definition is implicit in L. Eisenbud, dissertation, Princeton, June, 1948 (unpublished) and E. P. Wigner, Phys. Rev. **98**, 145 (1955).

<sup>3</sup> T. Ohmura has pointed out an error of a factor of 2 in LM. The decay time  $\tau_m$  is  $\frac{1}{2}$  the average value  $\bar{Q}$  near the resonance and  $\frac{1}{4}$  the value  $Q_{\text{max}}$  at the resonance; physically this is reasonable since the average collision lifetime  $\bar{Q}$  involves two passages through a barrier, while the decay time  $\tau_m$  involves only one. [See also the Appendix in F. T. Smith, J. Chem. Phys. **36**, 248 (1962).]

<sup>4</sup> F. T. Smith, Phys. Rev. **120**, 1058 (1960), referred to below as "GAM"; See also L. M. Delves, Nucl. Phys. **9**, 391 (1958-1959).