Minimum Principle for Multi-Channel Scattering*

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The usual variational principles of scattering theory are simply stationary principles. In a recent series of papers, all restricted to single-channel scattering, conditions were established under which variational principles can be found which are much more powerful in that the functional that represents the variational estimate is not simply stationary in the neighborhood of the exact scattering solution but is rather an extremum. A lower bound was obtained on the single real parameter, $\tan\eta_c$, which characterizes the scattering in the (uncoupled) channel c. The conditions previously established allowed for composite bound states, for the Pauli principle, for arbitrary angular momenta, and for long-range and in particular Coulomb potentials; at nonzero energies, the various potentials had to be truncated. The present paper deals with the extension to multi-channel scattering in which each of the open channels contains only two systems. The bounds are now on linear combinations of the elements of the reactance matrix or of the derivative matrix. The potentials must be truncated in a fashion very similar to that used in Wigner-Eisenbud theory.

1. INTRODUCTION

IN a series of papers[1–4] we have treated with increasing generality the problem of establishing the conditions under which a variational principle for scattering has the extremely desirable property of being a minimum principle as well. We present here a further development of the method, the extension to the multi-channel case for which there are two and only two systems in any open channel.

We have previously confined our attention to those problems where the two systems being scattered, and the scattering energies, were such that it was possible to choose a set of uncoupled open channels. Pauli exchange processes were allowed. A lower bound was obtained on the single real parameter, $\tan\eta_c$, which characterizes the scattering in the (uncoupled) channel c. For any incident energy other than zero it was found necessary, in deriving the bound, to restrict our consideration to those interactions which vanish identically or which reduce to a solvable two body potential when the separation of the two scattering systems exceeds some fixed distance.

In the present paper the formalism is extended to include the case where for fixed values of the constants of the motion, which include the total energy, the total angular momentum, J, and the projection, M, of J, there are a finite number, $\mathfrak{N}$, of coupled open channels. It will be necessary to assume that a potential cut off radius exists for each channel. The scattering problem is thereby somewhat restricted, but no more so than that considered in the Wigner-Eisenbud theory of nuclear reactions.[5]

We have in fact adopted almost in its entirety the kinematical description of the scattering process given by Wigner and Eisenbud. Therefore we will refer the reader to their paper, or to the review article by Lane and Thomas,[6] for a discussion of those kinematical details which are only sketched here. Of course, kinematics aside, the approach, purposes, and domains of applicability of the present paper and that of Wigner and Eisenbud are quite different.

As in the case of one-channel scattering, applications will be confined to the domain of low and moderate scattering energies since the amount of labor involved in the calculation increases with increasing values of the relative kinetic energies of the scattering systems.[3] The energy range is of course also limited by the restriction that breakup processes be impossible.

Since a practical application of our method involves the performance of a variational calculation we shall in general be interested in few-body systems where such a calculation is feasible. From the point of view of mathematical rigor we are in fact restricted to problems in which the wave functions of the isolated systems and of their relative motion are known exactly, though in practice there are cases where the requirement may reasonably be relaxed somewhat. [See also the paragraph following Eq. (3.5).] Some of the nuclear scattering processes which would be particularly interesting to study by the present method are nucleon-nucleon scattering with tensor and spin-orbit forces, n-d and p-d scattering with tensor and spin-orbit forces for incident energies below 2.2 Mev, and, to the extent that the H^3 and He^3 ground state wave functions can be assumed to be known, this being an example of the relaxation just referred to,[7] the three-channel process involving a deuteron and a deuteron, a neutron and He^3, and a proton and H^3 (the deuteron-deuteron

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[1] L. Spruch and L. Rosenberg, Phys. Rev. **116**, 1034 (1959); **117**, 1095 (1960).
[2] L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **118**, 184 (1960).
[3] L. Rosenberg and L. Spruch, Phys. Rev. **120**, 474 (1960).
[4] L. Rosenberg and L. Spruch, Phys. Rev. **121**, 1720 (1961).
[5] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947).
[6] A. M. Lane and R. G. Thomas, Revs. Modern Phys. **30**, 257 (1958).
[7] Care must be exercised in this regard. For example, as we have noted previously [L. Spruch and L. Rosenberg, Nuclear Phys. **17**, 30 (1960)], variational calculations of n-d scattering have led to erroneous results when approximate deuteron wave functions were used which were too crude.

channel is of course closed for the total energy below -4.4 Mev). Some of the interesting atomic scattering applications would be to the study of excitation processes for electron scattering by H atoms, as well as excitation and pickup processes for H atoms, positrons or protons on H atoms, where in each case the bombarding energy is below 13.6 ev. To the extent that the He ground state wave function can be considered to be known, one could study elastic scattering of electrons, protons, positrons, H atoms, or He on He. Very often the multi-channel scattering of elementary particles is described in terms of effective potential interactions. Within the context of this model the present method should be quite useful for such problems. In fact there are any number of problems in which simplifying models are introduced which are, however, still sufficiently complicated so that even the model problem cannot be attacked rigorously. One example would be the scattering of a particle by an atomic or nuclear system containing one particle outside of closed shells where in the model the shells would be assumed to contribute only a static potential. Here again a minimum principle would clearly be required if one were to have any assurance of real accuracy, particularly if there were more than one open channel

2. STATEMENT OF THE PROBLEM

For concreteness, the method will be described for the particular example in which there are a total of A nucleons involved, Z protons and N neutrons. (With some minor changes the discussion could just as well be presented for electron-atom or atom-atom scattering, for example.)

We will now specify more precisely what is meant by a channel. The channel label, c, will, to begin with, specify which pair of nuclei are involved, that is, the number of neutrons (N_1,N_2) and protons (Z_1,Z_2) in each nucleus. The set of numbers N_1, N_2, Z_1, Z_2 will be denoted by the symbol γ. The quantum states of the two nuclei, the description of which includes the specification of the spins I_1 and I_2, will be labeled by $\alpha(I_1,I_2)$. We shall be interested in the representation in which the system in channel c has a well defined channel spin S, where $S=|\mathbf{S}|=|\mathbf{I}_1+\mathbf{I}_2|$, and a well-defined orbital angular momentum L, where $\mathbf{S}$ and $\mathbf{L}$ are coupled to give the specified values of J and M. Thus each channel c is identified by the set of indices $\{\gamma\alpha(I_1,I_2)\mathrm{SLJM}\}$. Note that the channel label does *not* specify which of the neutrons (or protons) is in the first nucleus and which is in the second, for to do so would be to greatly increase the order of the submatrix of the S matrix referring to open channels for fixed J. We prefer rather to take the Pauli exchange processes into account by using wave functions that are explicitly antisymmetrized in the neutrons and in the protons (representing a departure from the description in reference 5). This will be made clear in the discussion of the boundary conditions to be satisfied by the wave function, Ψ.

We now wish to define precisely the problem for which one obtains a bound. To do so we must give an exact definition of the external and internal regions of our $3A$-dimensional configuration space and to specify the potentials which are assumed to exist in the different regions.

We introduce three mutually exclusive and exhaustive regions. The first region (the "internal region" of Wigner and Eisenbud) is to be finite. While the size of this region is in principle arbitrary a reasonable choice would be such that all the nucleons are within a volume of nuclear dimensions. The potentials in region 1 are arbitrary and may be taken to be of the form of the ordinarily assumed nuclear potentials; in particular, since we are here allowing for multi-channel processes, $\mathbf{L}\cdot\mathbf{S}$ and tensor forces are permitted. Region 2 is divided into a number of subregions, denoted by $2(\gamma j)$, where γ labels the pair of nuclei involved and j is an index which, for a given γ, denotes the particular distribution of neutrons and of protons in each of the nuclei. The total number of subregions is then

$$\sum_{\gamma}\frac{N!}{(N_{1\gamma}!)(N_{2\gamma}!)}\frac{Z!}{(Z_{1\gamma}!)(Z_{2\gamma}!)}.$$

In any of the subregions $2(\gamma j)$ the potential between any two nucleons within a given nucleus can be taken to be one of the standard nuclear two-body potentials, but the interaction, V_c, between the two nuclei must be a function of the separation, $q_{\gamma j}$, of their centers of mass and must further be a solvable potential. (We write V_c rather than V_γ to allow for potentials which depend on the various angular momenta and states of excitation associated with channel c.)

The third region is taken to be the rest of configuration space. The probability of finding the nucleons in this region would be expected to be negligibly small. In order to obtain a rigorous minimum principle, however, it will be necessary to have the probability of finding the nucleons in region 3 identically zero. The potential can therefore be thought of as infinitely repulsive in this region.

It might be worth specifically noting that, as usual, there can be an overlap of different channels in a given region, $2(\gamma j)$, of configuration space. These channels represent different states of excitation, for example, of the two separated nuclei.

It will be useful in the following to have a particular specification of the three regions. The one given below is of course not unique but does have the virtue of leading to boundary conditions with relatively simple analytic forms.

Let us consider a particular partition, $p(A_1,A_2;j)$, of nucleons into two groups of A_1 and A_2 members, where $A_1=N_1+Z_1$, $A_2=N_2+Z_2$, and $A_1+A_2=A$. For this partition we define the parameter $S_1[p(A_1,A_2;j)]$

such that for any configuration of nucleons it is the radius of the smallest sphere centered at the center of mass of the A_1 nucleons in the first group which includes all these nucleons. A similar definition holds for $S_2[p(A_1,A_2;j)]$ and the A_2 nucleons of the second group. We represent the number of nucleons in the two nuclei associated with index γ by $A_{1\gamma}$ and $A_{\gamma 2}$, respectively. In terms of these quantities we now define region 1 by the conditions

$$q_{\gamma j}<R_\gamma, \tag{2.1a}$$

$$\begin{aligned} &S_1[p(A_{1\gamma},A_{2\gamma};j)]<g_{1\gamma},\\ &S_2[p(A_{1\gamma},A_{2\gamma};j)]<g_{2\gamma}, \end{aligned} \tag{2.1b}$$

for all values of γ and j. Subregion $2(\gamma j)$ is defined by

$$q_{\gamma j}>R_\gamma, \tag{2.2a}$$

$$\begin{aligned} &S_1[p(A_{1\gamma},A_{2\gamma};j)]<h_{1\gamma},\\ &S_2[p(A_{1\gamma},A_{2\gamma};j)]<h_{2\gamma}, \end{aligned} \tag{2.2b}$$

for all γ and j. As previously stated, region 3 is taken to be the rest of configuration space. Conditions (2.1a) and (2.2a) guarantee that region $2(\gamma j)$ and region 1 do not overlap. Condition (2.1b) is required for the finiteness of region 1, although in many cases $g_{1\gamma}$ and $g_{2\gamma}$ may be taken to be infinite without violating this finiteness requirement. The parameters $h_{1\gamma}$ and $h_{2\gamma}$ are to be chosen to be sufficiently small such that the subregions $2(\gamma j)$ are nonoverlapping. We shall not choose these numbers here; it shall suffice to remark that in any particular case of interest the maximum allowable values of the parameters $h_{1\gamma}$ and $h_{2\gamma}$ may easily be determined.[8] To approximate the physical problem of interest as closely as possible region 1, and hence the parameters R_γ, $g_{1\gamma}$, and $g_{2\gamma}$, should be large. The limitation is that an increase in the size of region 1 is accompanied by an increase in the number of states with negative eigenvalues in the associated potential strength eigenvalue problem. The computation then involves more labor (see Sec. 3). An optimum choice of the parameters taking into account the above considerations would have to be made for each problem.

The boundary conditions satisfied by the wave function Ψ are such that Ψ vanishes in region 3 while in region $2(\gamma j)$ it takes the form

$$\Psi=\sum_{\text{open}} P_{\gamma j}D_cF_{cj}[a_c\mathcal{S}_c(q_{\gamma j})+b_c\mathcal{C}_c(q_{\gamma j})]/q_{\gamma j} + \sum_{\text{closed}} P_{\gamma j}c_cF_{cj}f_c(q_{\gamma j})/q_{\gamma j}. \tag{2.3}$$

The first and second sums are taken over all open and closed channels, respectively, corresponding to the pair of nuclei γ, with the particular distribution j, i.e., the sum is over the indices $\alpha(I_1,I_2)$, S, and L for fixed γ and for fixed j. The function F_{cj} is constructed by first forming the product of the wave functions of the two nuclei corresponding to the index γ, each wave function being antisymmetric under interchange either of neutrons or of protons; this product is multiplied by spin and angle functions, and summed over angular momentum projections, to form a state with the appropriate quantum numbers, namely, S, L, J, and M.[9] The orthonormality relation

$$\int F_{cj}{}^*F_{c'j'}dS=\delta_{cc'}\delta_{jj'}, \tag{2.4}$$

with the integral taken over the surface common to regions 1 and 2, will be of use in the following.[10] We assume that the functions F_{cj} satisfy the Wigner reality condition, i.e., that they behave under time reversal, T, as

$$TF_{\gamma\alpha SLJMj}=(-1)^{J-M}F_{\gamma\alpha SLJ-Mj}. \tag{2.5}$$

A complete definition of the functions F_{cj} would require that we specify the ordering of identical nucleons within each of the two nuclei, since an interchange of neutrons, or of protons, induces a change in sign; that is, we should give a particular representation of the j-labeling scheme. For any such specification one can easily convince oneself that the $P_{\gamma j}$ may be given values $+1$ or -1 such that the complete function, Ψ, is antisymmetric, under interchange of any neutron or any proton coordinates, in region 2. The normalization constant, D_c, will be specified later.

The functions $\mathcal{S}_c$ and $\mathcal{C}_c$ are real, linearly independent solutions of the radial equation

$$\left[-\frac{d^2}{dq_{\gamma j}^2}+\frac{L(L+1)}{q_{\gamma j}^2}+\frac{2\mu_\gamma}{\hbar^2}V_c(q_{\gamma j})-k_c^2\right] \times\{\mathcal{S}_c(q_{\gamma j}),\mathcal{C}_c(q_{\gamma j})\}=0; \tag{2.6}$$

k_c is the wave number for the relative motion in channel c and μ_γ is the reduced mass. f_c is the real exponentially decaying solution of Eq. (2.6). We choose $\mathcal{S}_c$ and $\mathcal{C}_c$ such that, for V_c short-ranged,

$$\begin{aligned} &\mathcal{S}_c(q_{\gamma j})\to\sin(k_cq_{\gamma j}-\tfrac{1}{2}L\pi+\theta_c), \quad q_{\gamma j}\to\infty\\ &\mathcal{C}_c(q_{\gamma j})\to\cos(k_cq_{\gamma j}-\tfrac{1}{2}L\pi+\theta_c), \quad q_{\gamma j}\to\infty, \end{aligned} \tag{2.7}$$

where the θ_c are arbitrary phase angles. If V_c contains a Coulomb potential $Z_{1\gamma}Z_{2\gamma}e^2/q_{\gamma j}$, the terms $-\xi_c\ln 2k_cq_{\gamma j}$

[8] One such determination, for the particularly simple one-channel case, with $A_{1\gamma}=1$, appears in reference 4.

[9] See reference 5 for a detailed description of the coupling procedure.

[10] On the surface common to regions 1 and 2 the functions F_{cj} corresponding to different partitions of nuclei have no common domain in which they are nonvanishing, since regions $2(\gamma j)$ do not overlap. This, in addition to the orthonormality of the spin-angle functions and the orthonormality of the nuclear wave functions for different quantum states leads to Eq. (2.4). According to our definition of the various regions of configuration space Eq. (2.4) holds for any value of R_γ, rather than for R_γ "large enough," as is the case in the Wigner-Eisenbud formulation. There the additional precision is not necessary; we have introduced it here to provide a specific problem for which the minimum principle is rigorously valid.

$+\sigma_{cL}$, where $\xi_c=\mu_\gamma Z_{1\gamma}Z_{2\gamma}e^2/\hbar^2k_c$ and $\sigma_{cL}=\arg\Gamma(L+1+i\xi_c)$, must be added to the arguments of both $\mathcal{S}_c$ and $\mathcal{C}_c$.

For a particular choice of the real parameters a_c, the values of b_c thus determined contain all the desired information about the scattering process. The relation between these two sets of parameters may be written as

$$b_c=\sum_{c'} K_{cc'}{}^\theta a_{c'}, \quad \text{or} \quad \mathbf{b}=\mathbf{K}^\theta\mathbf{a}.$$

The real, symmetric matrix[11] $\mathbf{K}^\theta$ is related to the reactance matrix $\mathbf{K}(=\mathbf{K}^0)$ by

$$\mathbf{K}^\theta=[-\mathbf{\sin\theta}+\mathbf{\cos\theta}\,\mathbf{K}][\mathbf{\cos\theta}+\mathbf{\sin\theta}\,\mathbf{K}]^{-1}, \quad (2.8)$$

where $\mathbf{\sin\theta}$ and $\mathbf{\cos\theta}$ are diagonal matrices with elements $\sin\theta_c$ and $\cos\theta_c$, respectively. The relation between $\mathbf{K}$ and the submatrix $\mathbf{S}$ corresponding to open channels, for fixed J, of the full scattering matrix is of course

$$\mathbf{K}=i(\mathbf{1}-\mathbf{S})/(\mathbf{1}+\mathbf{S}). \quad (2.9)$$

The Kato identity, as generalized to the scattering system under consideration, plays a central role in our approach. It may be derived by appropriately modifying the procedure of reference 1. Thus, we introduce the trial function, Ψ_t, which vanishes in region 3 and satisfies boundary conditions of the same form as those for Ψ [see Eq. (2.3)], with b_c and c_c replaced by b_{ct} and c_{ct}, respectively; Ψ_t is to be chosen such that the Wigner reality condition, in the form $T\Psi_t(J,M)=(-1)^{J-M}\Psi_t(J,-M)$, is satisfied ($\Psi_t$ is of course taken to be an eigenfunction of the operators $\mathbf{J}^2$ and J_z). This, along with the same reality condition for Ψ, guarantees that the integrals which appear below are real. Ψ is a solution of the Schrödinger equation,

$$(H-E)\Psi=0. \quad (2.10)$$

The expression

$$\int[\Psi^*(H-E)\Psi_t-\Psi_t{}^*(H-E)\Psi]d\tau$$

is evaluated first using Eq. (2.10), and then with the aid of Green's theorem (in $3A$-dimensional space). The calculation proceeds in a manner which is quite similar to that which appears in the development of the Wigner-Eisenbud formalism and we shall merely state the resultant identity. We obtain

$$-\sum_c \frac{N!}{(N_{1\gamma}!)(N_{2\gamma}!)}\frac{Z!}{(Z_{1\gamma}!)(Z_{2\gamma}!)} \times\frac{\hbar^2}{2\mu_\gamma}D_c{}^2W_c a_c(b_c-b_{ct})=\int\Psi^*(H-E)\Psi_t d\tau; \quad (2.11)$$

[11] These properties of $\mathbf{K}^\theta$ follow from Eq. (2.8) and the fact that the reactance matrix $\mathbf{K}$ is itself real and symmetric. The unitarity and symmetry properties of the S matrix which, along with Eq. (2.9) lead to these properties of $\mathbf{K}$ are proved, e.g., in reference 6. We note that the proof makes use of the properties of the functions F_{ci} given by Eqs. (2.4) and (2.5).

W_c is the Wronskian of the two functions $\mathcal{S}_c$ and $\mathcal{C}_c$ and, according to the normalization we have chosen, has the value k_c. The difference function, Ω, defined as $\Omega\equiv\Psi_t-\Psi$, is now introduced; owing to the boundary conditions satisfied by Ψ and Ψ_t, Ω vanishes in region 3 and has the form

$$\Omega=\sum_{\text{open}} P_{\gamma j}D_c F_{cj}(b_{ct}-b_c)\mathcal{C}_c(q_{\gamma j})/q_{\gamma j} + \sum_{\text{closed}} P_{\gamma j}(c_{ct}-c_c)F_{cj}f_c(q_{\gamma j})/q_{\gamma j}, \quad (2.12)$$

in region $2(\gamma j)$. With the choice of D_c such that

$$\frac{N!}{(N_{1\gamma}!)(N_{2\gamma}!)}\frac{Z!}{(Z_{1\gamma}!)(Z_{2\gamma}!)}\frac{\hbar^2}{2\mu_\gamma}D_c{}^2k_c=1,$$

(the normalization of the wave function then differs dimensionally by a factor $[2\times\text{Mass}/\hbar^2]^{\frac{1}{2}}$ from that used in our previous papers), Eq. (2.11) may be written as

$$\mathbf{a}\cdot\mathbf{b}=\mathbf{a}\cdot\mathbf{b}_t-\int\Psi_t{}^*(H-E)\Psi_t d\tau + \int\Omega^*(H-E)\Omega d\tau. \quad (2.13)$$

The integral, $\int\Omega^*(H-E)\Omega d\tau$, is of second order in the error in Ψ; if it is dropped in Eq. (2.13) we obtain a variational expression for $\mathbf{a}\cdot\mathbf{b}=\mathbf{a}\cdot\mathbf{K}^\theta\mathbf{a}$. It is our purpose to do more, namely to obtain a lower bound on $\int\Omega^*(H-E)\Omega d\tau$, thereby providing a lower bound on the form $\mathbf{a}\cdot\mathbf{K}^\theta\mathbf{a}$. (It is recalled that the parameters a_c are real but otherwise arbitrary.) The minimum principle (actually a maximum principle in the form just outlined) is developed in Sec. 3. Before going on to that, however, we wish to make two general remarks. These remarks relate to results which have been obtained previously; they are included to exhibit the ease with which they can be derived from the present formalism.

We first wish to point out that a simple variant of the proof of the Kato identity, Eq. (2.13), may be used to show that the matrix $\mathbf{K}^0\equiv\mathbf{K}$ as defined above is to be identified with the reactance matrix which appears in the standard development of time-dependent scattering theory,[12] with appropriate modifications due to the Pauli principle. Thus, we define the function

$$\Theta_c=\sum_j P_{\gamma j}\left[\frac{\hbar^2}{2\mu_\gamma}\frac{N!}{N_{1\gamma}!N_{2\gamma}!}\frac{Z!}{Z_{1\gamma}!Z_{2\gamma}!}\right]^{-\frac{1}{2}}F_{cj}j_L(k_c q_{\gamma j}),$$

in all configuration space, where j_L is the spherical Bessel function of the first kind. (We here assume the potentials V_c to be short-ranged.) Let $\Psi_{c'}$ be the wave function, normalized according to Eqs. (2.3) and (2.7),

[12] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).

with $\theta_c=0$ for all c. The subscript c' indicates the choice $a_c=\delta_{cc'}$. The expression

$$\int[\Psi_{c'}^*(H-E)\Theta_c-\Theta_c^*(H-E)\Psi_{c'}]d\tau,$$

is evaluated in two ways leading to the result

$$K_{cc'}=-\int\Psi_{c'}^*(H-E)\Theta_c d\tau. \tag{2.14}$$

This would agree with the standard result[12] if it were possible to write $H=H_0+H'$, with $(H_0-E)\Theta_c=0$. The impossibility of doing so is a characteristic of rearrangement collisions which has been discussed by a number of authors, and in some detail by Ekstein.[13] If we write (somewhat schematically) $\Psi_{c'}=\mathcal{A}\Psi_{c'j}$ and $\Theta_c=\mathcal{A}\Theta_{cj}$, where in $\Psi_{c'j}$ and Θ_{cj} the particles are treated as distinguishable and $\mathcal{A}$ is the antisymmetrization operator, then the expression for $K_{cc'}$, Eq. (2.14), can be written as a sum of "direct" and "exchange" contributions. One sees here a justification, in the context of the present approach, of the common procedure of ignoring the Pauli principle in performing the scattering calculation, and antisymmetrizing the resultant expressions for the scattering parameters.

We wish, secondly, to remark that instead of using the boundary conditions for $\mathcal{S}_c$ and $\mathcal{C}_c$ given by Eq. (2.7) it might sometimes be convenient to adopt the conditions

$$\mathcal{S}_c(R_\gamma)=0, \qquad \mathcal{C}_c(R_\gamma)=1,$$
$$\left.\frac{d\mathcal{S}_c}{dq_{\gamma j}}\right|_{q_{\gamma j}=R_\gamma}=1, \quad \left.\frac{d\mathcal{C}_c}{dq_{\gamma j}}\right|_{q_{\gamma j}=R_\gamma}=B_c; \tag{2.15}$$

where B_c is independent of k_c but otherwise arbitrary. The relation between $\mathbf{a}$ and $\mathbf{b}$ is now

$$\mathbf{b}=\mathfrak{R}\mathbf{a},$$

where, for the case where there are no closed channels, the real symmetric matrix $\mathfrak{R}$ is just the derivative matrix, $\mathbf{R}$, of Wigner and Eisenbud.[5] The general relation between $\mathfrak{R}$ and the derivative matrix is given, for example, in the text book by Sachs,[14] as is the connection between $\mathfrak{R}$ and the scattering matrix, $\mathbf{S}$. The fact that the boundary conditions, Eq. (2.15), are energy independent has the consequence that for the case where no closed channels are present (n-p scattering with tensor forces provides an example), the form $\mathbf{a}\cdot\mathfrak{R}\mathbf{a}$ has a positive derivative with respect to the energy, whenever that derivative exists. This interesting property, which is of course the Wigner inequality,[15] may be very simply derived using Eq. (2.13) in its variational form, i.e., with neglect of the second order term, $\int\Omega^*(H-E)\Omega d\tau$. For scattering energy $E+\Delta E$, with ΔE infinitesimal, we write

$$\mathbf{a}\cdot\mathfrak{R}(E+\Delta E)\mathbf{a}\approx\mathbf{a}\cdot\mathfrak{R}_t(E+\Delta E)\mathbf{a}$$
$$-\int\Psi_t^*(E+\Delta E)[H-E-\Delta E]\Psi_t(E+\Delta E)d\tau. \tag{2.16}$$

The formal choice $\Psi_t(E+\Delta E)=\Psi(E)$, where $H\Psi(E)=E\Psi(E)$, is an allowable one due to the energy-independent boundary conditions, Eq. (2.15). Equation (2.16) becomes

$$\frac{\mathbf{a}\cdot[\mathfrak{R}(E+\Delta E)-\mathfrak{R}(E)]\mathbf{a}}{\Delta E}\approx\int|\Psi(E)|^2d\tau.$$

The integral is taken over region 1 and is therefore finite; it is clearly positive, which yields the Wigner inequality.

This inequality provides a distinct advantage in using energy-independent boundary conditions in applying the maximum principle since a lower bound on $\mathbf{a}\cdot\mathfrak{R}\mathbf{a}$ at one energy provides a lower bound for an entire range of higher energies. In the following to be specific we shall assume the boundary conditions of Eqs. (2.7). These boundary conditions have the advantage that the reactance matrix is more directly connected to the scattering matrix than is the derivative matrix.

3. THE MINIMUM PRINCIPLE

In complete analogy with the procedure employed in the one-channel case we begin by considering the equation

$$(H-E)\Phi=\mu\rho\Phi, \tag{3.1}$$

where H is the Hamiltonian of interest in the scattering problem, with potentials defined as in Sec. 2. The auxiliary potential ρ is positive and symmetric in each pair of identical particles but is otherwise arbitrary in region 1, and vanishes elsewhere. (As shown in Sec. 4, ρ plays a purely formal role; calculations may be performed without introducing a specific form for ρ.) The eigenfunctions Φ_n are defined as those regular solutions of Eq. (3.1), obtained by considering the range $-\infty\leqq\mu\leqq\infty$, which satisfy the boundary conditions

$\Phi_n=0$, in region 3;

$$\Phi_n=\sum_{\text{open}}P_{\gamma j}D_cF_{cj}b_{cn}\mathcal{C}_c(q_{\gamma j})/q_{\gamma j}$$
$$+\sum_{\text{closed}}P_{\gamma j}c_{cn}F_{cj}f_c(q_{\gamma j})/q_{\gamma j}, \text{ in region } 2(\gamma j). \tag{3.2}$$

Some features that might be noted are that the b_{cn} and

[13] H. Ekstein, Phys. Rev. **101**, 880 (1956).

[14] R. Sachs, *Nuclear Theory* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1953), pp. 290–297.

[15] The inequality is given in reference 5, in terms of the derivative matrix, $\mathbf{R}$. Wigner subsequently supplied a causal interpretation of the inequality. [See E. P. Wigner, Phys. Rev. **98**, 145 (1955).]

c_{cn} are of course unknown, that the indices γ and j are of course held fixed in the sums over open and closed channels, and that the characteristic feature of these boundary conditions is the absence of the $\mathcal{S}_c$ functions. It is clear that we have generated an Hermitian eigenvalue problem.[16] We restrict the class of potentials to be considered in such a way that the eigenvalues μ_n are bounded from below and only a finite number of negative eigenvalues exist. It seems very likely that this class includes all physically interesting potentials.[17] The assumption is, essentially, that if all the interacting particles were placed in a finite box the energy levels of the system would be discrete and bounded from below. (This last statement is based on the fact that for a sufficiently large box the presence of closed channels is irrelevant; a correspondence between an Hermitian energy eigenvalue problem[5] and our potential strength eigenvalue problem can then be established for the particular choice $\rho=$ constant, and, as is shown below, the bounds we obtain are independent of the choice of ρ.)

It is now noted that the Hylleraas-Undheim theorem[18] may be applied to the associated eigenvalue problem thus defined. Furthermore, the difference function Ω satisfies boundary conditions of the same form as those for the eigenfunctions Φ [compare Eq. (2.12) and (3.2); note that this would not be possible if the functions F_{cj} were not known exactly] and is therefore an allowable trial function in the use of the Hylleraas-Undheim theorem.[19] Consequently, the expression giving a lower bound on the integral $\int\Omega^*(H-E)\Omega d\tau$ which was previously derived for the one-channel scattering case[2-4] may be immediately taken over. This provides us with the inequality

$$\int\Omega^*(H-E)\Omega d\tau \geqq \sum_{n=1}^{T}\left(\int\Phi_{nt}^*(H-E)\Psi_t d\tau\right)^2\Big/\mu_{nt}, \quad (3.3)$$

where

$$\int\Phi_{nt}^*\Phi_{mt}\rho d\tau=\delta_{nm}, \quad (3.4)$$

$$\int\Phi_{nt}^*(H-E)\Phi_{mt}d\tau=\mu_{nt}\delta_{nm}, \quad \mu_{nt}<0; \quad (3.5)$$

T is the number of states with negative eigenvalues μ_n, and is assumed to be known. (Since there is in general no *a priori* way of knowing the number T, our argument encounters a break in rigor at this point. However, as we have mentioned previously in the same connection,[3,4] it should be possible, in practice, on the basis of the numerical calculations involved in determining the Φ_{nt} to be fairly certain that the correct number of states has been included.) The trial eigenfunctions Φ_{nt} satisfy boundary conditions of the form given in Eq. (3.2) with b_{cn} and c_{cn} replaced by trial values b_{cnt} and c_{cnt}, respectively. In many cases there will be an infinite number of closed channels while only a finite number of the functions F_{cj} will be known. As we have mentioned, the method calls for the use of the exact functions. It must then be recognized that the amplitudes of the closed-channel components of the trial function Φ_{nt} and Ψ_t (the c_{cnt} and c_{ct}) are arbitrary. If region 1 is sufficiently large these parameters may be chosen to vanish without significantly affecting the accuracy of the calculation. (This procedure was adopted in a previous calculation[20] of the single-channel scattering of e^+ on H.)

The above inequality, Eq. (3.3), along with the generalized Kato identity, Eq. (2.13), provides us with the basic inequality:

$$\mathbf{a}\cdot\mathbf{K}^\theta\mathbf{a}\geq\mathbf{a}\cdot\mathbf{K}_t^\theta\mathbf{a}-\int\Psi_t^*(H-E)\Psi_t d\tau+\sum_{n=1}^{T}\left(\int\Phi_{nt}^*(H-E)\Psi_t d\tau\right)^2\Big/\mu_{nt}, \quad (3.6)$$

where we have defined the trial reactance matrix by

$$\mathbf{b}_t=\mathbf{K}_t^\theta\mathbf{a},$$

and where the conditions on the Φ_{nt} are given by Eqs. (3.4) and (3.5) and by the assumed form of the boundary conditions.

As we noted previously, we obtain a variational estimate of $\mathbf{a}\cdot\mathbf{K}^\theta\mathbf{a}$, and therefore on linear combinations of the elements of $\mathbf{K}^\theta$, by dropping the second order term in Eq. (2.13). Similarly, the adoption of the conditions of Eq. (2.15) gives a variational expression

[16] It might be thought that an energy eigenvalue problem could be defined, suitable for our purposes, with eigenfunctions satisfying boundary conditions similar to those given above, as is in fact done in the text book by Blatt and Weisskopf [J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, New York, 1952), pp. 544–554]. Such an eigenvalue problem is not Hermitian, however, since for each channel c there is no surface $q_{\gamma j}=$const in region $2(\gamma j)$ for which the two functions $\mathcal{C}_c$ and f_c have logarithmic derivatives independent of the eigenenergy. The relevant discussion in the above-mentioned text book (see, in particular p. 550) is oversimplified, as the authors themselves point out. The energy eigenvalue problem introduced by Wigner and Eisenbud[5] *is* Hermitian, but is inappropriate for our purposes for another reason, mentioned in footnote 19, below.

[17] We have been informed (J. Berkowitz, private communication) that with the help of a lemma due to Kato [T. Kato, Trans. Am. Math. Soc. **70**, 195 (1951), see Lemma 4] the proof [R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, New York, 1953), Vol. 1, p. 413] for the case where there is only one independent variable can be extended to apply to the present problem provided the potentials are locally square-integrable.

[18] E. A. Hylleraas and B. Undheim, Z. Physik **65**, 759 (1930).

[19] The energy eigenfunctions defined by Wigner and Eisenbud, if continued into the external region (region 2 in our notation) would not behave like scattering functions since they contain exponentially increasing terms. Since Ω *does* behave like a scattering function we may not, in our approach, use the Wigner-Eisenbud energy eigenvalue problem in place of the potential strength eigenvalue problem just defined. For a more detailed discussion of this point see Sec. 5 of reference 4.

[20] L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960).

for linear combinations of the elements of the derivative matrix. Variational principles for quantities that characterize multi-channel scattering go back to the earliest papers on variational principles,[21] but there seems to have been only one other paper on minimum principles in multi-channel scattering.[22] The results obtained were restricted to elastic multi-channel scattering, such as n-p scattering with tensor forces, but the method can probably be extended to include inelastic scattering. Furthermore the potentials need not be truncated, which is a great advantage over the present paper, and one obtains *both* bounds on the scattering parameters. On the other hand the method requires the evaluation of matrix elements of H^2, which is a tremendous disadvantage as compared to the method of the present paper.

4. SIMPLIFICATION OF THE CALCULATIONAL PROCEDURE

We will now show that the calculational procedure is actually simpler than that outlined above. This simplification is not related to the multi-channel feature of the problem but is rather a formal property which had not been realized earlier. To state the procedure, we first convert the inequality, Eq. (3.6), to its equivalent variational form,[2] obtaining

$$\mathbf{a}\cdot\mathbf{K}^{\theta}\mathbf{a}\geq\mathbf{a}\cdot\mathbf{K}_t{}^{\theta}\mathbf{a}-\int\tilde{\Psi}_t{}^*(H-E)\tilde{\Psi}_t d\tau, \qquad (4.1)$$

where now $\tilde{\Psi}_t$ is of the form

$$\tilde{\Psi}_t=\Psi_t+\sum_{n=1}^{T} d_n\Phi_{nt}. \qquad (4.2)$$

Ψ_t is an arbitrary trial scattering function satisfying the proper boundary conditions. The d_n are variational parameters which appear nowhere else and are to be determined by the conditions

$$\frac{\partial}{\partial d_n}\int\tilde{\Psi}_t{}^*(H-E)\tilde{\Psi}_t d\tau=0, \quad n=1, 2, \cdots, T. \qquad (4.3)$$

The simplification arises from the fact that in this variational form the conditions on the functions Φ_{nt} given in Eqs. (3.4) and (3.5) may be replaced, as we shall show immediately, by the equivalent condition that the $T\times T$ matrix, $\mathbf{M}$, with elements $M_{nm}=\int\Phi_{nt}{}^*(H-E)\Phi_{mt}d\tau$, should be negative. It is unnecessary to solve the secular equation to see if all the eigenvalues of $\mathbf{M}$ are negative. According to a theorem of matrix algebra,[23] M will be negative if and only if the principal minors, $M^{(k)}$, defined by

$$M^{(k)}=\begin{vmatrix} M_{11}\cdots M_{1k} \\ \vdots \quad\quad \vdots \\ M_{k1}\cdots M_{kk}\end{vmatrix},$$

satisfy the conditions

$$M^k/|M^k|=(-1)^k, \quad k=1, 2, \cdots, T.$$

This provides the additional simplification that since the orthonormality condition, Eq. (3.4), no longer appears, the weight function ρ need not be introduced in the calculation.

The assertion that in the variational form, Eqs. (4.1)–(4.3), the conditions on the Φ_{nt} given by Eqs. (3.4) and (3.5) may be dropped follows from the observation that the result of a variational calculation of the quantity $\mathbf{a}\cdot\mathbf{K}_t{}^{\theta}\mathbf{a}-\int\tilde{\Psi}_t{}^*(H-E)\tilde{\Psi}_t d\tau$, with $\tilde{\Psi}_t$ of the form given by Eq. (4.2), is invariant under a linear transformation of the functions Φ_{nt}. That is, the replacement of the Φ_{nt} by functions

$$\Phi_{nt}{}'=\sum_{m=1}^{T} C_{nm}\Phi_{mt}$$

in Eq. (4.2) has the same effect as replacing the d_n by

$$d_n{}'=\sum_{m=1}^{T} C_{nm}d_m,$$

while leaving the Φ_{nt} unaltered. This latter transformation preserves the conditions

$$\frac{\partial}{\partial d_n{}'}\int\tilde{\Psi}_t{}^*(H-E)\tilde{\Psi}_t d\tau=0, \quad n=1, 2, \cdots, T.$$

Since the d_n are dummy variables it is clear that the use of the Φ_{nt} and the $\Phi_{nt}{}'$ give rise to the same results.

Now let us choose for the transformation matrix, $\mathbf{C}$, the product $\mathbf{C}_1\mathbf{C}_2$, where $\mathbf{C}_1$ converts the set $\{\Phi_{nt}\}$ into one which is orthonormal with respect to some weight function ρ, while $\mathbf{C}_2$ takes the set into one which diagonalizes the matrix $\mathbf{M}$. (That C_2 exists follows from a well-known theorem. C_1 may be constructed, for any given ρ, using what is essentially the Schmidt orthogonalization procedure.) If the diagonal elements are all negative the new set of trial eigenfunctions satisfy, according to our previous result, the necessary conditions to assure that the variational form lies below the form $\mathbf{a}\cdot\mathbf{K}^{\theta}\mathbf{a}$. The same will then be true using the original set of functions $\{\Phi_{nt}\}$. The condition that $\mathbf{M}$ be negative is unaltered by the transformation from one set of functions to the other[24] and may be checked,

[21] W. Kohn, Phys. Rev. **74**, 1763 (1948), and ref. 12.
[22] R. Bartram and L. Spruch, J. Math. Phys. (to be published).
[23] K. Hoffmann and R. Kunze, *Linear Algebra* (Prentice-Hall, Inc., Englewood Cliffs, 1961), p. 249.

[24] We have

$$\int\Phi_{nt}{}'^*(H-E)\Phi_{nt}{}'d\tau=\sum_{ij} C_{ni}C_{nj}M_{ij}, \quad n=1, 2, \cdots, T,$$

which is negative since, by assumption, the matrix $\mathbf{M}$ is negative definite.

for the original set, by examining the signs of the principal minors of **M**.

The simplification of the present section is the elimination of the requirement of orthonormality with respect to ρ of the trial functions Φ_{nt} and of the requirement that the Φ_{nt} diagonalize $(H-E)$, and the replacement by the simpler requirement on the signs of the minors of the determinant. The two requirements which were imposed in the problem of zero-energy scattering[2] were completely analogous but with the exception that ρ did not appear. It is however trivial, proceeding along lines almost identical to those above. to simplify the auxiliary conditions on the trial bound state functions.

The fact that the results are entirely independent of ρ suggests that ρ need never have been introduced, and it is indeed simple enough to derive bounds rather more directly than we have done by a derivation with ρ set equal to a constant. The details are given in a set of lectures[25] which also include the simplifications with regard to the zero energy case that were noted above.

The simplification at zero energy, which in turn was the starting point of the investigation of Sec. 4, is due to T. F. O'Malley (unpublished), to whom we would wish to express our thanks. The simplification at zero energy was obtained independently by Ohmura,[26] in a slightly different form.

[25] L. Spruch, in *Lectures in Theoretical Physics, Boulder, 1961* [Interscience Publishers, Inc., New York (to be published)], Vol. 4. The portion of these lectures devoted to variational minimum principles is basically a review of the present series of papers.
[26] T. Ohmura, Phys. Rev. **124**, 130 (1961).

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Coherent Photoproduction of π^0 from Deuterium*

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The calculation of elastic photoproduction of π^0 mesons from deuterium, $\gamma+d\rightarrow\pi^0+d$, is carried out in the impulse approximation at photon energies around 500 Mev. The single nucleon photoproduction amplitudes are taken from dispersion formulas and are corrected for kinematic effects due to internal momentum of the nucleons in the deuteron. We include the D-state part of the deuteron wave function and use different models with Yukawa type or repulsive core wave functions. We give formulas connecting the cross section with the deuteron form factors. For small momentum transfers the formulas are of course model independent and reduce to the usual ones. The presence of a 7% D state in a repulsive-core model leads to a cross section which falls typically more slowly at high momentum transfers, e.g., at a momentum transfer 2.74 f^{-1}, the cross section is larger by about 40% than the cross section calculated in the absence of the D state. The experimental points favor this model.

I. INTRODUCTION

THIS work is a calculation of the elastic photoproduction of π^0 mesons from deuterium, $\gamma+d\rightarrow\pi^0+d$, at photon energies around 500 Mev.[1] Chew and Lewis[2] and Lax and Feshbach[3] first calculated the cross section for such a process in the impulse approximation. De Wire *et al.*[4] applied these results to analyze the $\gamma+d\rightarrow\pi^0+d$ cross section at energies 250–300 Mev, normalizing the theoretical formulas with the free-nucleon photoproduction cross sections. Multiple scattering corrections to the impulse approximation have been considered by Chappelear[5] but the analyses so far have taken the static limit of infinite nucleon mass.

The present work can be described as follows: (1) As a refinement in the calculation we put much effort into maintaining relativistic covariance, at least on all kinematic quantities. For this we borrowed the free-nucleon dispersion formulas[6] and used them in the deuteron case. Of course the nucleons in the deuterium do not satisfy the free-particle energy-momentum relation $\mathbf{p}^2+m^2=E^2$; this is a familiar limitation to impulse approximation. (2) The transition matrix T will be a function of the two kinematic invariants $S=(k+P)^2$, the "invariant total energy" of the photon+deuteron, and $t=(k-q)^2$ the momentum transfer:

$$T=T(S,t). \tag{1.1}$$

k, P, and q are the photon, deuteron, and pion four-momenta, respectively.

Now we want to relate T to the photoproduction from single nucleons. Since the nucleons in the deuteron will be distributed over the internal momentum **p**, we write

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[1] Experiment of J. Friedman and H. Kendall (to be published).
[2] G. F. Chew and H. W. Lewis, Phys. Rev. **84**, 779 (1951).
[3] M. Lax and H. Feshbach, Phys. Rev. **88**, 509 (1952).
[4] J. W. De Wire, A. Silverman, and B. Wolfe, Phys. Rev. **92**, 520 (1953).
[5] John Chappelear, Phys. Rev. **99**, 254 (1955).
[6] G. F. Chew, F. E. Low, M. L. Goldberger, and Y. Nambu, Phys. Rev. **106**, 1345 (1957).