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Improved Minimum Principle for Multichannel Scattering*

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If the open-channel target states are known, the minimum principle formulation of scattering theory provides a systematic approach whereby one can, to arbitrary precision, monotonically approach the reactance matrix **K**. The scattering wave function and the Green's function for the open-channel approximation, that in which the closed channels are not taken into account at all, must be solved numerically. An explicit method for constructing the Green's function is given. The minimum principle approach is probably limited at present, in practice though not in principle, to the three-body problem with just a few open channels. A very useful simplification is possible at the threshold for a new channel; one need not there include the new channel in the equations that must be solved exactly.

1. INTRODUCTION

THE minimum principle formulation of scattering theory was originally restricted to the case for which the initial relative kinetic energy of the two systems, E', was zero.[1] The formulation was a practical one and was applied to a number of scattering problems.[2] The initial extension[3] to $E'>0$ was not quite in a practical form, but recently an improved (and truly rigorous) formalism was derived[4] for $E'>0$ which can and has been applied to single-channel scattering by a compound system. The present paper will be primarily devoted to extending this newer minimum principle formulation to multichannel scattering. It will be useful to begin with a brief outline of the results that were previously obtained. The notation to be used will be that of Ref. 4 and of a paper on bounds on multichannel scattering parameters.[5] (As opposed to some of the earlier usage, we here distinguish between bounds and minimum principles; minimum principles, which might alternatively be called variational bounds, contain variational parameters, while bounds do not.)

For simplicity, we consider the scattering of a particle by a compound system, rather than of one compound system by another, and we take the incident particle to be distinguishable from the target particles, to have no spin or orbital angular momentum and to have no charge; we further assume that no rearrangement processes are possible, and that the ground state and all of the excited states of the target have zero angular momentum. Under most circumstances these restrictions can be trivially relaxed. We also assume this time not for simplicity but because of a basic limitation of the minimum principle approach, that the incident energy is too small to produce breakup.

Let the target have eigenfunctions $\psi_{Tm}(\mathbf{r})$ and associated energy eigenvalues E_{Tm}, where $m=0, 1, 2, \cdots$, and assume that the total energy E lies between $E_{T,N-1}$ and E_{TN}, so that there are N open channels. It will unfortunately be necessary to assume that the open-channel eigenfunctions and energy eigenvalues are known. This is only natural since the eigenfunctions and eigenvalues appear explicitly in the specification of the boundary conditions. We let the index i refer to open channels, and let k_i and μ_i represent the wave number and the reduced mass in channel i. We now introduce for the moment the trial function Ψ_t which is

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[3] L. Spruch and L. Rosenberg, Phys. Rev. **120**, 474 (1960); L. Rosenberg and L. Spruch, *ibid.* **121**, 1720 (1961); **125**, 1407 (1962).

[4] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **130**, 381 (1963).

[5] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **134**, B397 (1964).

regular at the origin and which has the asymptotic form in the ith (open) channel given by

$$\Psi_t \to (\mu_i/k_i)^{1/2}\psi_{Ti}(\mathbf{r})[a_i \sin(k_iq_i+\theta) + b_{it}\cos(k_iq_i+\theta)]/q_i, \quad q_i\to\infty\,. \tag{1.1}$$

The exact wave function has precisely the same asymptotic form, but with b_{it} replaced by the exact (unknown) value b_i. Introducing the vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{b}_t$, with components a_i, b_i, and b_{it}, respectively, the exact and trial reactance matrices $\mathbf{K}_\theta$ and $\mathbf{K}_{\theta t}$ are defined by

$$\mathbf{b}=\mathbf{K}_\theta\mathbf{a} \quad\text{and}\quad \mathbf{b}_t=\mathbf{K}_{\theta t}\mathbf{a}\,, \tag{1.2}$$

respectively. With the error function or difference function Ω defined by

$$\Omega\equiv\Psi_t-\Psi\,, \tag{1.3}$$

which then has the asymptotic form

$$\Omega \to (\mu_i/k_i)^{1/2}\psi_{Ti}(\mathbf{r})(b_{it}-b_i)\cos(k_iq_i+\theta)/q_i\,, \quad q_i\to\infty \tag{1.4}$$

in channel i, one can prove the identity[3]

$$-2\pi\hbar^2\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}=-2\pi\hbar^2\mathbf{a}\cdot\mathbf{K}_{\theta t}\mathbf{a}+\int\Psi_t(H-E)\Psi_t d\tau -\int\Omega(H-E)\Omega d\tau\,, \tag{1.5}$$

where H and E are the total Hamiltonian and total energy of the system. One immediately obtains a variational principle for $\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}$ on dropping the (unknown) second-order error term, $(\Omega,[H-E]\Omega)$, but whereas Ω will hopefully be small, this will never be assumed in the course of the analysis, the objective of which is to obtain an explicit bound on the error term and hence on $\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}$.

The bound is simple to obtain if the incident kinetic energy E' is equal to zero. Approaching this limit, it follows from the assumptions that we have made concerning spins and angular momenta that we have no degeneracy and therefore that there is only one channel open, that labeled by $i=0$. As the wave number k_0 in this channel approaches zero, the asymptotic form of Ω becomes

$$\Omega \to (\mu_0/k_0)^{1/2}\psi_{T0}(\mathbf{r})(b_{0t}-b_0)(\cos\theta-k_0q_0\sin\theta)/q_0\,. \tag{1.6}$$

"Appropriate normalization"[1,2] requires the most rapid possible decay in q_0 so that we want to eliminate the term in the numerator proportional to q_0; this is most simply achieved here[6] by the choice $\theta=0$. The reactance matrices $\mathbf{K}_0(=\mathbf{K})$ and $\mathbf{K}_{0t}(=\mathbf{K}_t)$ reduce to $\tan\eta$ and $\tan\eta_t$, respectively, for single-channel scattering. We now introduce the "threshold reactance matrices" $\boldsymbol{K}$ and $\boldsymbol{K}_t$ defined by

$$\mathbf{K}=k_0\boldsymbol{K} \quad\text{and}\quad \mathbf{K}_t=k_0\boldsymbol{K}_t\,. \tag{1.7}$$

$\boldsymbol{K}$ and $\boldsymbol{K}_t$ are then 1×1 matrices for k_0 sufficiently small, and are given by

$$\boldsymbol{K}=-A \quad\text{and}\quad \boldsymbol{K}_t=-A_t\,, \tag{1.8}$$

respectively, where A is the scattering length and A_t is the trial scattering length. For k_0 sufficiently small, we now have

$$b_0=-k_0Aa_0\,,\quad b_{0t}=-k_0A_ta_0\,, \tag{1.9}$$

and choosing

$$a_0=k_0^{-1/2}\,, \tag{1.10}$$

we have for $k_0=0$, the asymptotic forms

$$\Omega\to\mu_0^{1/2}\psi_{T0}(\mathbf{r})(A-A_t)/q_0\,, \tag{1.11}$$

$$\Psi_t\to\mu_0^{1/2}\psi_{T0}(\mathbf{r})(q_0-A_t)/q_0\,, \tag{1.12}$$

while Eq. (1.5) reduces to

$$2\pi\hbar^2A=2\pi\hbar^2A_t+\int\Psi_t(H-E_{T0})\Psi_td\tau -\int\Omega(H-E_{T0})\Omega d\tau\,. \tag{1.13}$$

If now the incident particle cannot form a composite bound state with the target, it follows that $H-E_{T0}$ is a non-negative operator with respect to any function Ω which satisfies the boundary conditions of Eq. (1.11). We therefore obtain an upper bound on A by simply dropping the error term. Note that for the choice $\theta=\frac{1}{2}\pi$ the asymptotic form of Ω would not decay with q_0 and the knowledge of the nonexistence of a composite bound state would not suffice to determine the sign of the error term.

If there are N composite bound states, one can still obtain a rigorous upper bound on $-\mathbf{a}\cdot\mathbf{K}\mathbf{a}$ if one can find N approximate bound-state functions which are good enough to give binding,[1,2] by effectively subtracting out the contributions to the error term of these bound states. The above considerations are applicable not only to $E'=0$ single-channel scattering but, where the process is possible, to $E'=0$ multichannel scattering; reintroducing spins for the moment, these include, for example, nucleon-nucleon scattering with tensor forces

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[6] In the limiting process $E'\to0$, it was previously found that appropriate normalization corresponded to $\theta=\frac{1}{2}\pi$, as opposed to the result $\theta=0$ obtained here. The difference is due to the fact that the nonzero energy normalization used in some of our recent papers and in the present paper, while allowable, does not reduce in the limit of zero energy to the normalization used in our earlier papers. To have had the same normalization we should not have used

$$a_i\sin(k_iq_i+\theta)+b_i\cos(k_iq_i+\theta),$$

as in the present paper, but

$$a_i\cos(k_iq_i+\theta)-b_i\sin(k_iq_i+\theta)$$

since it is the a_i which are taken to be known and since in our earlier papers it was always the sine function which was multiplied by the unknown number.

and nucleon-deuteron scattering with spin-dependent forces. Similarly, if for the moment we introduce orbital angular momenta, with or without spins, and if the ground state of the target has a nonzero angular momentum and is therefore degenerate, there will be a number of channels open even for $E'=0$ for a fixed total angular momentum, corresponding to different angular momenta of the incident particle and of the target, and the above approach provides bounds on the threshold reactance matrix provided the forces are of sufficiently short range.

The determination of a bound on the error term is a much more difficult matter for $E'>0$, for in addition to any discrete states which give a negative expectation value of $H-E$, there will now be a *continuum* of states, or a number of continua of states, which give a negative expectation value of $H-E$. More precisely, if as before we have

$$E_{T,N-1}\leq E\leq E_{TN} \tag{1.14}$$

there will be associated with $H-E$ a total of N continua whose lower limits, $E_{Ti}-E$ for $i=0, 1, \cdots, N-1$, lie below zero. The problem was first attacked by truncating the various potential and erecting potential barriers,[3] thereby eliminating the continuous spectra, but other than for potential scattering the method is not ordinarily a practical one. It was subsequently realized that the projection technique of the formal theory of reactions,[7] introduced to avoid the truncations of the earlier formal reaction theory formulations, was precisely what was needed for a practical minimum principle formulation for $E'>0$, and the formalism was presented for single-channel scattering.[4] The essential feature was the replacement of the identity of Eq. (1.13) by an identity in which the role of the error term $(\Omega, [H-E]\Omega)$ was played by

$$(Q\Omega, Q[\mathcal{H}-E]Q\Omega)=(Q\Omega, Q[H-E]Q\Omega) +\text{potential term}, \tag{1.15}$$

where Q is projection operator onto the excited states of the target. The potential term does not change the end points of the continuous spectrum, but the appearance of the Q's causes the continuous spectrum of $Q[H-E]Q$ to extend not from $E_{T0}-E$ to ∞ but from $E_{T1}-E$ to ∞, so that, since we have $E<E_{T1}$ by the assumption that we are dealing with single-channel scattering, there are no negative continuum contributions from $(Q\Omega, [H-E]Q\Omega)$ and the situation for $E'>0$ is then of precisely the same form, though algebraically more complex, as that for $E'=0$. The formulation has been applied to the single-channel scattering of positrons by H atoms for angular momenta $L=0$, 1, and 2, with extremely encouraging results,[8] and is currently being applied to the scattering of electrons by hydrogen atoms.

Section 2 will represent a straightforward extension of the projection technique to multichannel scattering processes in which all of the allowed channels contain only two systems. The interesting special case of scattering at the threshold of a new channel will be studied in Sec. 3; it will be shown there that a very useful simplification of the formalism is possible for this case. A concrete method for the construction of the Green's functions that appear in the formalism is presented in an Appendix.

2. THE MINIMUM PRINCIPLE

Let P be a projection operator which projects onto all open channels and possibly some closed ones, and let $Q=1-P$. We then write

$$(H-E)\Psi=0 \tag{2.1}$$

as

$$P(H-E)P\Psi=-PHQ\Psi \tag{2.2}$$

$$Q(H-E)Q\Psi=-QHP\Psi, \tag{2.3}$$

the formal solutions of which are

$$P\Psi=P\Psi^P+PG^PPHQ\Psi, \tag{2.4}$$

$$Q\Psi=QG^QQHP\Psi, \tag{2.5}$$

where

$$P(H-E)P\Psi^P=0. \tag{2.6}$$

G^P is defined by

$$G^P=[P(E-H)P]^{-1} \tag{2.7}$$

and by boundary conditions which follow from taking the asymptotic form of Eq. (2.4) and inserting the asymptotic forms of $P\Psi$ and of $P\Psi^P$; G^Q is defined by

$$G^Q=[Q(E-H)Q]^{-1} \tag{2.8}$$

and by boundary conditions which follow from studying the asymptotic form of Eq. (2.5). We will not actually need G^Q. Substitution of Eqs. (2.5) and (2.4) into Eqs. (2.2) and (2.3), respectively, leads to

$$P(H+HQG^QQH-E)P\Psi=0, \tag{2.9}$$

$$Q(H+HPG^PPH-E)Q\Psi=-QHP\Psi^P. \tag{2.10}$$

The boundary conditions on the various functions are

$$P\Psi\to(\mu_i/k_i)^{1/2}\psi_{Ti}(\mathbf{r})[a_i\sin(k_iq_i+\theta) +b_i\cos(k_iq_i+\theta)]/q_i \tag{2.11}$$

in channel i, with similar forms for $P\Psi^P$ but with b_i replaced by $b_i{}^P$, and

$$Q\Psi\to 0 \tag{2.12}$$

faster than $1/q_i$ asymptotically as $q_i\to\infty$. Multiplying Eq. (2.2) by $P\Psi^P$, Eq. (2.6) by $P\Psi$, subtracting, and

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[7] H. Feshback, Ann. Phys. (N. Y.) **5**, 357 (1958); **19**, 287 (1962); L. Fonda and R. G. Newton, *ibid.* **10**, 490 (1960).

[8] Y. Hahn, T. F. O'Malley, and L. Spruch (to be published); C. Kleinman, Y. Hahn, and L. Spruch (to be published).

integrating, we find with the use of Green's theorem that

$$-2\pi\hbar^2(\mathbf{a}\cdot\mathbf{b}_\theta-\mathbf{a}\cdot\mathbf{b}_\theta{}^P)=(P\Psi^P,PHQ\Psi)\,. \tag{2.13}$$

Taking the inner product of Eq. (2.10) with Ψ, we have

$$\begin{aligned}(Q\Psi,[\mathcal{H}-E]Q\Psi)&=-(Q\Psi,HP\Psi^P)\\&=-(P\Psi^P,HQ\Psi)\,,\end{aligned} \tag{2.14}$$

where we have defined the operator $\mathcal{H}(E,\theta)=\mathcal{H}$ by

$$\mathcal{H}=Q[H+HPG^PPH]Q\,. \tag{2.15}$$

From the standing wave boundary conditions for $P\Psi$ as given by Eq. (2.11) and the similar form for $P\Psi^P$, the Green's function G^P is clearly defined with the principal value boundary condition and thus real and symmetric. Consequently the resulting $\mathcal{H}$ is a real and *symmetric* operator. (An elaborate and explicit discussion for the case of single-channel scattering has been given in Ref. 4.) We can therefore write

$$\begin{aligned}-2\pi\hbar^2(\mathbf{a}\cdot\mathbf{b}_\theta-\mathbf{a}\cdot\mathbf{b}_\theta{}^P)=2(P\Psi^P,HQ\Psi)&\\+(Q\Psi,[\mathcal{H}-E]Q\Psi)\,,&\end{aligned} \tag{2.16}$$

where we have chosen that linear combination which is stationary with respect to variations of $Q\Psi$. Introducing the error function $Q\Omega$, defined by

$$Q\Omega=Q\Psi_t-Q\Psi\,, \tag{2.17}$$

where the trial function $Q\Psi_t$ vanishes for any coordinate going to infinity, as does $Q\Psi$, there are then no linear terms in $Q\Omega$ in Eq. (2.16), and we find

$$\begin{aligned}-2\pi\hbar^2(\mathbf{a}\cdot\mathbf{b}_\theta-\mathbf{a}\cdot\mathbf{b}_\theta{}^P)=2(P\Psi^P,HQ\Psi_t)&\\+(Q\Psi_t,[\mathcal{H}-E]Q\Psi_t)-(Q\Omega,[\mathcal{H}-E]Q\Omega)\,.&\end{aligned} \tag{2.18}$$

Since the continuous spectrum of $\mathcal{H}$ runs up to infinity from a value *greater* than E, and since only diagonal elements of $\mathcal{H}-E$ appear, the last term in Eq. (2.18), the only term that cannot be calculated explicitly, can be bounded by the same technique that was used in our previous papers. If, in particular, $\mathcal{H}$ does not have any (discrete) eigenvalues below E, $\mathcal{H}-E$ is a nonnegative operator and we obtain a bound on $\mathbf{a}\cdot\mathbf{b}_\theta$ by simply dropping the term in $\mathcal{H}-E$. More generally, if $\mathcal{H}$ has $\mathfrak{N}^Q$ eigenvalues which lie below E, where $\mathfrak{N}^Q$ then depends upon E and upon θ, we must find $\mathfrak{N}^Q$ orthonormalized functions $\Phi_{nt}{}^Q$ which satisfy

$$\begin{aligned}&(\Phi_{nt}{}^Q,\mathcal{H}\Phi_{mt}{}^Q)=\mathcal{E}_{nt}{}^Q\delta_{nm}\,,\\&\mathcal{E}_{nt}{}^Q<E\,,\quad 1\leq n,\,m\leq\mathfrak{N}^Q\,.\end{aligned} \tag{2.19}$$

We can then bound $(Q\Omega,[\mathcal{H}-E]Q\Omega)$, and we find

$$\begin{aligned}&-2\pi\hbar^2\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}\leq-2\pi\hbar^2\mathbf{a}\cdot\mathbf{K}_\theta{}^P\mathbf{a}+2(Q\Psi_t,HP\Psi^P)\\&\quad+(Q\Psi_t,[\mathcal{H}-E]Q\Psi_t)\\&\quad+\sum_{n=1}^{\mathfrak{N}^Q}\frac{|(Q\Phi_{nt}{}^Q,[[\mathcal{H}-E]Q\Psi_t+QHP\Psi^P])|^2}{E-\mathcal{E}_{nt}{}^Q}\,.\end{aligned} \tag{2.20}$$

Equation (2.20) is almost identical to the corresponding equation for single-channel scattering, and the way in which it will be used will be very similar. Once again one will not normally know the value of $\mathfrak{N}^Q$,[9] and the procedure will be to choose $Q\Psi_t$ to contain more and more terms, ignoring the sum term, until one believes that one has passed through the $\mathfrak{N}^Q$ *decreases* in the right-hand side of Eq. (2.20). From this point on one *does* have a rigorous bound on $\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}$, and the bound will then converge monotonically toward its final value. The "best"[4] choice for the variational parameters that appear in the trial function is the choice which minimizes $-\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}$, though if we have not yet passed through all of the $\mathfrak{N}^Q$ decreases, that is, if we are not yet on the correct "branch," there will be other choices of the parameters which will, accidentally so to speak, give estimates of the elements of $\mathbf{K}_\theta$ which lie closer to the true values.

The vector $\mathbf{a}$ has thus far been completely arbitrary. For the particular choice $\mathbf{a}=\mathbf{a}^{(i)}$, where $\mathbf{a}^{(i)}$ has the components

$$a_j{}^{(i)}=\delta_{ij}\,, \tag{2.21}$$

we immediately obtain a minimum principle for $K_{\theta ii}$ from Eq. (2.20). We cannot however obtain a minimum principle for any individual off-diagonal element, though we can of course obtain a minimum principle for various linear combinations of elements. A minimum principle for a particularly interesting linear combination, related to the eigenphase shifts, can be obtained as follows.

Let $P\Psi^P(\mathbf{a}^{(i)})$ be the uniquely determined solution of Eq. (2.6), with appropriate boundary conditions, associated with $\mathbf{a}^{(i)}$. It follows that

$$P\Psi^P(\mathbf{a}^{(i)})\to\cdots[\delta_{ij}\sin(k_jq_j+\theta)+\cdots]\,,\quad q_j\to\infty\,. \tag{2.22}$$

We now define the vector

$$P\chi=\textstyle\sum_i\mathbf{a}^{(i)}P\Psi^P(\mathbf{a}^{(i)})\,, \tag{2.23}$$

where the sum contains N terms, and choose

$$P\Psi^P(\mathbf{a})=P\chi\cdot\mathbf{a}\,, \tag{2.24}$$

where $\mathbf{a}$ is arbitrary. $P\Psi^P(\mathbf{a})$ is then a solution of Eq. (2.6), while asymptotically it approaches

$$P\Psi^P(\mathbf{a})\to\cdots[a_j\sin(k_jq_j+\theta)+\cdots]\,,\quad q_j\to\infty\,. \tag{2.25}$$

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[9] We showed previously (Ref. 4) that for the incident kinetic energy sufficiently small $\mathfrak{N}^Q$ was the difference between the number of negative eigenvalues of $H-E_{T0}$ and of $P(H-E_{T0})P$, where P is the ground-state projection operator. This is a useful result since the first number can be determined experimentally and the second, which requires the analysis of only a one-body problem, theoretically. It should not be difficult to obtain a similar result, expressing $\mathfrak{N}^Q$ as the difference of two numbers, in the neighborhood of any threshold. The result might not be as useful, however, since it would no longer be possible to experimentally determine either of the two numbers. On the other hand, it is possible that the number which is more or less impossible to determine by a direct theoretical attack would effectively have been determined either theoretically or experimentally by a study of the scattering process at energies below the given threshold energy.

$P\Psi^P(a)$ is then the solution of Eq. (2.6) appropriate to the (arbitrary) vector **a**.

Correspondingly, let $Q\Psi_t{}^{(i)}$ be some choice related to $\mathbf{a}^{(i)}$. $Q\Psi_t{}^{(i)}$ is not uniquely determined by the specification of $\mathbf{a}^{(i)}$. In general, one would choose some $Q\Psi_t{}^{(i)}$ containing variational parameters and then determine the parameters, not necessarily precisely, by trying to minimize the right hand side of Eq. (2.20), with $\mathbf{a}=\mathbf{a}^{(i)}$. We now define

$$Q\zeta=\textstyle\sum_i \mathbf{a}^{(i)}Q\Psi_t{}^{(i)} \tag{2.26}$$

and choose

$$Q\Psi_t=Q\boldsymbol{\zeta}\cdot\mathbf{a}, \tag{2.27}$$

where **a** is arbitrary. Equation (2.20) now becomes

$$-\mathbf{a}\cdot\mathbf{K}_\theta\mathbf{a}\leq-\mathbf{a}\cdot\mathbf{K}_{B\theta}\mathbf{a}, \tag{2.28}$$

where

$$\begin{aligned}-2\pi\hbar^2\mathbf{K}_{B\theta}\equiv{}&-2\pi\hbar^2\mathbf{K}_\theta{}^P\\&+2(Q\zeta,HP\chi)+(Q\zeta,[\mathcal{H}-E]Q\zeta)\\&+\sum_{n=1}^{\mathfrak{N}^Q}\frac{|(Q\Phi_{nt}{}^Q,[[\mathcal{H}-E]Q\zeta+QHP\chi])|^2}{E-\mathcal{E}_{nt}{}^Q},\end{aligned} \tag{2.29}$$

where, though we have not made it obvious notationally, each term in Eq. (2.29) is of course a matrix. We denote the N (calculable) ordered real eigenvalues of the symmetric matrix $\mathbf{K}_{B\theta}$ by $\tan(\eta_{Bs}-\theta)$ and the corresponding real eigenvalues of the symmetric matrix $\mathbf{K}_\theta$ by $\tan(\eta_s-\theta)$.

Since **a** is arbitrary, and since $\mathbf{K}_{B\theta}$ is independent of **a**, Eq. (2.28) becomes

$$-\mathbf{K}_\theta\leq-\mathbf{K}_{B\theta},$$

from which it follows that

$$\tan(\eta_s-\theta)\geq\tan(\eta_{Bs}-\theta),\quad s=1,2,\cdots,N. \tag{2.30}$$

We note in passing that a comparable result can be obtained given any N linearly independent vectors **a** and their associated $\Psi^P(\mathbf{a})$, the particular choice that was made being simply the most convenient.

We close this section with a more general comment. It should be clear that the basic result, Eq. (2.20), can serve as a powerful tool in the anaylsis of the effects of virtual excitation, with potentialities outside of the domain of an approach such as the close coupling approximation.[10] More precisely, the effects of virtual excitation, which include through the G^P term the contribution of $P\Psi-P\Psi^P$, are taken into account through the introduction of $Q\Psi_t$. Thus, as opposed to the close coupling approximation, virtual excitation is accounted for not by including the virtual states (and in particular only the discrete virtual states) one by one, but, for the introduction of each new term in $Q\Psi_t$, by including an arbitrary linear combination of discrete and continuum virtual states, with variational parameters which are to be adjusted to give the "best" possible results, where "best" has the precise meaning noted above. Thus, while the close coupling approximation is often beset by slow convergence difficulties for electron hydrogen scattering in particular[11] and probably rather generally, no such difficulties should ordinarily attend a minimum principle calculation.

3. SIMPLIFICATION AT AN EXCITATION THRESHOLD

The minimum principle formulation just described requires the introduction of the projection operators P and Q, where P must include all open channels. This is also true, in particular, for single-channel scattering. *At* $E'=0$, however, it is unnecessary and therefore undesirable to introduce projection operators; as discussed in the Introduction, the original formulation,[1] valid at $E'=0$, provides a minimum principle which is much simpler to obtain. The relative merits at $E'=0$ of the formulations with and without projection operators, and the connection between them, is discussed in Ref. 4.

The original ($E'=0$) formulation can be thought of as containing projection operators, but with $P=0$ and $Q=1$, that is, with P not containing the ground-state channel. We will show in this section that an analogous simplification is possible *at* any excitation threshold, that is, at exactly that incident energy at which some new channel (or channels) opens up, namely, that it is then unnecessary (and generally undesirable) to include in the P the state which has just opened up. The reduced dimensionality of P and hence of $P\Psi^P$ and even more significantly of PG^P effects a considerable simplification.

Let the total energy E be exactly equal to E_{TN}. There are then $N+1$ open channels, the last of which is just open. In view of the simplifying assumptions noted in the Introduction, and in particular those related to spins and angular momenta, the new channel is nondegenerate. (There would be no difficulty in extending the formalism to include the degenerate case in which the target state associated with the new channels has nonzero angular momentum. The simplification achieved in this case would be even more significant.) The formalism developed in the previous section requires the inclusion of the new channel in P. We will now modify the treatment so that it will be applicable even though the new channel is included in Q rather than in P.

Since one will ultimately be interested in making the connection between the scattering at energies greater than E_{TN} and the scattering at E_{TN}, we consider an energy E just above E_{TN}—in particular, not enough to open up the next channel—and go through a limiting process in which k_N approaches zero. To obtain "ap-

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[10] P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).

[11] P. G. Burke (to be published).

propriate normalization" we set $\theta=0$. The only distinction between the present situation and that considered in the previous section is that $Q\Psi$, because it now contains the new channel, here possesses nonvanishing asymptotic components. More precisely, with k_N not zero, $Q\Psi$ behave asymptotically as

$$Q\Psi\to(\mu_N/k_N)^{1/2}\psi_{TN}(\mathbf{r})(a_N\sin k_Nq_N+b_N\cos k_Nq_N)/q_N\,,\quad q_N\to\infty\,. \tag{3.1}$$

The asymptotic form of $P\Psi$ in the ith channel, where we here restrict i to values from 0 to $N-1$, is given by

$$P\Psi\to(\mu_i/k_i)^{1/2}\psi_{Ti}(\mathbf{r})(a_i\sin k_iq_i+b_i\cos k_iq_i)/q_i\,,\quad q_i\to\infty\,. \tag{3.2}$$

As k_N approaches zero, the asymptotic form of $P\Psi$ changes only in the replacement of k_i by k_{iN}, the (nonzero) value of k_i at $E=E_{TN}$, but the asymptotic form of $Q\Psi$ approaches

$$Q\Psi\to(\mu_N/k_N)^{1/2}\psi_{TN}(\mathbf{r})(a_Nk_Nq_N+b_N)/q_N\,. \tag{3.3}$$

The a_j for $0\leq j\leq N$ are arbitrary, and to simplify the limiting process we introduce the vector $\boldsymbol{a}$, with elements $\boldsymbol{a}_i$, defined by

$$\boldsymbol{a}=\boldsymbol{\omega}^{1/2}\mathbf{a}\,, \tag{3.4}$$

where

$$\boldsymbol{\omega}^{1/2}=\begin{bmatrix} k_{0N}^{1/2} & & & & \\ & k_{1N}^{1/2} & & & \\ & & \ddots & & \\ & & & k_{N-1,N}^{1/2} & \\ & & & & k_N^{1/2}\end{bmatrix}\,. \tag{3.5}$$

Similarly, we introduce the vector $\boldsymbol{b}$, with elements $\boldsymbol{b}_j$, defined by

$$\boldsymbol{b}=\boldsymbol{\omega}^{-1/2}\mathbf{b}\,, \tag{3.6}$$

and the threshold reactance matrix $\boldsymbol{K}$, defined by

$$\mathbf{a}\cdot\mathbf{K}\mathbf{a}=\boldsymbol{a}\cdot\boldsymbol{K}\boldsymbol{a}\,. \tag{3.7}$$

It then follows, since there should of course really be an adjoint on the left element of the dot product, that

$$\mathbf{K}=\boldsymbol{\omega}^{1/2}\boldsymbol{K}\boldsymbol{\omega}^{1/2}\,,\quad\text{or}\quad \boldsymbol{K}=\boldsymbol{\omega}^{-1/2}\mathbf{K}\boldsymbol{\omega}^{-1/2}\,, \tag{3.8}$$

and that

$$\boldsymbol{b}=\boldsymbol{K}\boldsymbol{a}\,.$$

If we now let k_N approach zero, we have asymptotically

$$P\Psi\to\mu_i^{1/2}\psi_{Ti}(\mathbf{r})[\boldsymbol{a}_i(\sin k_{iN}q_i/k_{iN})+\boldsymbol{b}_i\cos k_{iN}q_i]/q_i\,,\quad q_i\to\infty\,, \tag{3.9}$$

$$Q\Psi\to\mu_N^{1/2}\psi_{TN}(\mathbf{r})(\boldsymbol{a}_Nq_N+\boldsymbol{b}_N)/q_N\,,\quad q_N\to\infty\,. \tag{3.10}$$

This completes the limiting process, and we are now in a position to proceed, with the appropriate modifications, as in Sec. 2. We rewrite

$$(H-E_{TN})\Psi=0 \tag{3.11}$$

as

$$P(H-E_{TN})P\Psi=-PHQ\Psi\,, \tag{3.12}$$

$$Q(H-E_{TN})Q\Psi=-QHP\Psi\,. \tag{3.13}$$

The formal solution of these equations is then given by

$$P\Psi=P\Psi^P+PG^PPHQ\Psi\,, \tag{3.14}$$

$$Q\Psi=Q\Psi^Q+QG^QQHP\Psi\,, \tag{3.15}$$

where $P\Psi^P$ is that regular solution of

$$P(H-E_{TN})P\Psi^P=0\,, \tag{3.16}$$

which behaves asymptotically as does $P\Psi$, in Eq. (3.9), but with $\boldsymbol{b}_i$ replaced by $\boldsymbol{b}_i^P$, while $Q\Psi^Q$ is that regular solution of

$$Q(H-E_{TN})Q\Psi^Q=0\,, \tag{3.17}$$

which behaves asymptotically as does $Q\Psi$, in Eq. (3.10), but with $\boldsymbol{b}_N$ replaced by $\boldsymbol{b}_N^Q$. G^P and G^Q are defined in the usual way. It is an essential feature of the present section that neither $Q\Psi^Q$ nor G^Q need actually be constructed explicitly; they appear only in the formal manipulations.

The substitution of Eqs. (3.15) and (3.14) into (3.12) and (3.13), respectively, gives

$$P(H+HQG^QQH-E_{TN})P\Psi=-PHQ\Psi^Q\,, \tag{3.18}$$

$$Q(H+HPG^PPH-E_{TN})Q\Psi=-QHP\Psi^P\,. \tag{3.19}$$

If now we multiply Eq. (3.12) by $P\Psi^P$ and Eq. (3.16) by $P\Psi$ and subtract, integrate, and use Green's theorem, we find

$$-2\pi\hbar^2{\sum}'_i\,(\boldsymbol{a}_i\boldsymbol{b}_i-\boldsymbol{a}_i\boldsymbol{b}_i^P)=(P\Psi^P,PHQ\Psi)=(QHP\Psi^P,Q\Psi)=-(Q[\mathcal{H}-E_{TN}]Q\Psi,Q\Psi)\,, \tag{3.20}$$

where in the sum i runs from 0 through $N-1$, we used the fact that PHQ vanishes asymptotically to enable us to move PHQ from the right to the left of the comma, and where in the last step we used Eq. (3.19) and introduced

$$\mathcal{H}\equiv Q(H+HPG^PPH)Q\,. \tag{3.21}$$

We rewrite Eq. (3.20) as

$$-2\pi\hbar^2{\sum}'_i\,(\boldsymbol{a}_i\boldsymbol{b}_i-\boldsymbol{a}_i\boldsymbol{b}_i^P)=2(P\Psi^P,PHQ\Psi)+(Q\Psi,Q[\mathcal{H}-E_{TN}]Q\Psi) \tag{3.22}$$

in order to make the right-hand side stationary with respect to variations in $Q\Psi$, and introduce a trial function $Q\Psi_t$ which is regular at the origin and which behaves asymptotically as does $Q\Psi$, in Eq. (3.10), but with $\boldsymbol{b}_N$ replaced by $\boldsymbol{b}_{Nt}$. Defining the error function $Q\Omega$ in the usual way as

$$Q\Omega\equiv Q\Psi_t-Q\Psi\,, \tag{3.23}$$

the asymptotic behavior of $Q\Omega$ is given by

$$Q\Omega\to\mu_N^{1/2}\psi_{TN}(\mathbf{r})(\boldsymbol{b}_{Nt}-\boldsymbol{b}_N)/q_N\,. \tag{3.24}$$

Using the relationship

$$(Q\Omega, Q[\mathcal{H}-E_{TN}]Q\Psi_t)-(Q\Psi_t, Q[\mathcal{H}-E_{TN}]Q\Omega) \\ =2\pi\hbar^2(\boldsymbol{a}_N\boldsymbol{b}_N-\boldsymbol{a}_N\boldsymbol{b}_{Nt}), \quad (3.25)$$

which follows from Green's theorem and Eqs. (3.10) and (3.24), Eq. (3.22) can be rewritten as

$$-2\pi\hbar^2\boldsymbol{a}\cdot\boldsymbol{K}\boldsymbol{a}=-2\pi\hbar^2(\sum{}'_i\,\boldsymbol{a}_i\boldsymbol{b}_i{}^P+\boldsymbol{a}_N\boldsymbol{b}_{Nt}) \\ +2(P\Psi^P,PHQ\Psi_t)+(Q\Psi_t, Q[\mathcal{H}-E_N]Q\Psi_t) \\ -(Q\Omega, Q[\mathcal{H}-E_N]Q\Omega), \quad (3.26)$$

where the threshold reactance matrix $\boldsymbol{K}$ is defined by

$$\boldsymbol{a}\cdot\boldsymbol{K}\boldsymbol{a}\equiv\sum{}'_i\,\boldsymbol{a}_i\boldsymbol{b}_i+\boldsymbol{a}_N\boldsymbol{b}_N\equiv\boldsymbol{a}\cdot\boldsymbol{b}. \quad (3.27)$$

The identity given in Eq. (3.26) is exactly of the form which makes it possible to provide a minimum principle for $\boldsymbol{a}\cdot\boldsymbol{K}\boldsymbol{a}$ and therefore for $\boldsymbol{K}$. If, for example, there are no discrete eigenvalues of $\mathcal{H}$ below E_{TN}—the continuous spectrum of this operator starts at E_{TN}—the only unknown term in Eq. (3.26), the last (second-order error) term, is greater than zero and we obtain a minimum principle for $\boldsymbol{a}\cdot\boldsymbol{K}\boldsymbol{a}$ by simply dropping the error term. Notice that the sign of the error term is known only because we used "appropriate normalization" so that $Q\Omega$ had the asymptotic behavior given by Eq. (3.24). Had we used $\theta=\frac{1}{2}\pi$ rather than $\theta=0$, the asymptotic forms of $Q\Psi$ and of $Q\Psi_t$ would be altered with the consequence that the asymptotic form of $Q\Omega$ would be proportional to $\psi_{TN}(\mathbf{r})$ rather than $\psi_{TN}(\mathbf{r})/q$. The information that $\mathcal{H}$ had no eigenvalues below E_{TN} would *not* then be enough to determine the sign of the error term nor therefore to provide a minimum principle.[12]

If $\mathcal{H}$ has a number of eigenvalues below E_{TN}, we must go through the usual "subtraction" procedure.

The threshold energy dependence of the usual reactance matrix $\mathbf{K}$ follows immediately from a knowledge of the threshold reactance matrix $\boldsymbol{K}$, for Eq. (3.8) can be rewritten as

$$\mathrm{K}_{ij}=(k_{iN}{}^{1/2}k_{jN}{}^{1/2}K_{ij})+\cdots, \quad i\neq N,\ j\neq N,$$

$$\mathrm{K}_{iN}=\mathrm{K}_{Ni}=(k_{iN}{}^{1/2}K_{iN})k_N{}^{1/2}+\cdots, \quad i\neq N,$$

$$\mathrm{K}_{NN}=(K_{NN})k_N+\cdots.$$

APPENDIX A: A CONNECTION BETWEEN THE MINIMUM PRINCIPLE AND A VARIATIONAL PRINCIPLE

It is of interest to see the connection between Eq. (2.20) and the simple variational expression which follows from the identity, Eq. (1.5),

$$-\mathbf{a}\cdot\mathbf{K}\mathbf{a}\approx-\mathbf{a}\cdot\mathbf{K}_{\theta t}\mathbf{a}+(\tilde{\Psi}_t, [H-E]\tilde{\Psi}_t), \quad (\mathrm{A1})$$

where $\tilde{\Psi}_t$ is a trial function which satisfies boundary conditions of the form given by Eq. (1.1). (We use the tilde here in order to distinguish between the trial function $\tilde{\Psi}_t$ to be inserted into the variational principle and the trial function Ψ_t, or rather $Q\Psi_t$, to be inserted into the minimum principle.) Consider the particular choice

$$\tilde{\Psi}_t=P\Psi^P+G^PPHQ\Psi_t+Q\Psi_t, \quad (\mathrm{A2})$$

which satisfies the required boundary conditions and is in fact suggested by the exact relationship

$$\Psi=P\Psi+Q\Psi=P\Psi^P+G^PPHQ\Psi+Q\Psi. \quad (\mathrm{A3})$$

With the insertion of Eq. (A2) into Eq. (A1), we reproduce the first three terms of the right-hand side of Eq. (2.20). We can reproduce the fourth term of Eq. (2.20) by choosing[13]

$$\tilde{\Psi}_t=P\Psi^P+G^PPHQ\Psi_t+Q\Psi_t+\sum_{n=1}^{\mathfrak{N}^P} b_nQ\Phi_{nt}{}^Q, \quad (\mathrm{A4})$$

where the variational parameters b_n do not appear in $Q\Psi_t$ nor in the $\Phi_{nt}{}^Q$, inserting this choice of $\tilde{\Psi}_t$ into Eq. (A1), and setting the variation with respect to the b_n equal to zero.

$\tilde{\Psi}_t$ as given by Eq. (A3) or (A4) represents an iteration on Ψ_t. For the same trial function, Eq. (2.20) will therefore generally give a better result than will Eq. (A1), but of course Eq. (2.20) is much more difficult to apply. For the particular case of zero incident energy, where the potentials need not be truncated, it is preferable to use the result obtained previously,[1] which is just Eq. (A1) with the subtraction terms. Examples of multichannel scattering processes which should be attacked by the older formulation are the zero-energy scattering of nucleons by deuterons or by protons. In the latter case the approach of Sec. 2 is not even applicable because we do not then have scattering by a compound system.

APPENDIX B: CONSTRUCTION OF THE GREEN'S FUNCTION, PG^P

Let P be the projection operator onto the M-dimensional space which includes all N open channels and $M-N$ closed channels. We here assume that the various particles are distinguishable. We furthermore restrict ourselves to excitation, that is, we exclude rearrangement collisions. The problem is to construct PG^P, denoted by PG in this Appendix, which is defined by

$$P(H-E)PG=-P, \quad (\mathrm{B1})$$

and by the appropriate boundary conditions. (Throughout the Appendix we will not actually specify the boundary conditions, which depend upon whether the various channels are open or closed, although they are necessary to uniquely define the different Green's functions.)

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[12] The choice $\theta=0$ is essential in order to obtain a minimum principle at threshold. However, it is more convenient to choose $\theta=\frac{1}{2}\pi$ for the study of reactance matrix near a resonance. [See for example, G. L. Shaw and M. H. Ross, Phys. Rev. **126**, 806 (1962).] The difference of $\frac{1}{2}\pi$ in the choice of θ is a reflection of the fact that the difference in the phase shifts at threshold and at resonance is $\frac{1}{2}\pi$ (mod π).

[13] The situation is very similar to that for $E'=0$. See the third paper of Ref. 1.

We also introduce the projection operators P_i and P_{-i} which project onto the ith target state and all but the ith target state, respectively, that is,

$$P_iP_j=P_i\delta_{ij}\,,\quad P={\sum}'\,P_i\,,\quad P_{-i}=P-P_i\,, \tag{B2}$$

where here and throughout Appendix B all indices take on M values. (To consider rearrangement collision, we would have to deal with elementary projection operators P_i which were not all orthogonal.) We further introduce the associated Green's functions G_i and G_{-i} defined by

$$P_i(H-E)P_iG_i=-P_i\,, \tag{B3}$$

and

$$P_{-i}(H-E)P_{-i}G_{-i}=-P_{-i}\,, \tag{B4}$$

respectively. G_i is the Green's function for an ordinary differential equation and its numerical determination is therefore a simple matter, and will henceforth be assumed to be known.

G_i, G_{-i} and G are similar to one another in that they are the Green's functions for 1, $M-1$, and M channels, respectively. Our expression for G will be recursive in nature, involving G_{-i}, and certain readily constructed Green's functions, including G_i. Let us then assume that G_{-i} is known.

Since $P=P_i+P_{-i}$, Eq. (B1) can be rewritten as a set of coupled equations for P_iG and $P_{-i}G$

$$P_i(H-E)P_iG=-P_i-P_iHP_{-i}G\,, \tag{B5a}$$

$$P_{-i}(H-E)P_{-i}G=-P_{-i}-P_{-i}HP_iG\,. \tag{B5b}$$

The formal solution of these equations is given by

$$P_iG=P_iG_i+P_iG_iP_iHP_{-i}G\,, \tag{B6a}$$

$$P_{-i}G=P_{-i}G_{-i}+P_{-i}G_{-i}P_{-i}HP_iG\,. \tag{B6b}$$

Substitution of Eqs. (B6a) and (B6b) into Eqs. (B5b) and (B5a) respectively, leads to *uncoupled* equations for P_iG and $P_{-i}G$

$$P_i[H+HP_{-i}G_{-i}P_{-i}H-E]P_iG\\=-P_i-P_iHP_{-i}G_{-i}\,, \tag{B7a}$$

$$P_{-i}[H+HP_iG_iP_iH-E]P_{-i}G\\=-P_{-i}-P_{-i}HP_iG_i\,. \tag{B7b}$$

We now introduce two new Green's functions, $\mathcal{G}_i$ and $\mathcal{G}_{-i}$, defined by

$$P_i[H+HP_{-i}G_{-i}P_{-i}H-E]P_i\mathcal{G}_i=-P_i \tag{B8}$$

and

$$P_{-i}[H+HP_iG_iP_iH-E]P_{-i}\mathcal{G}_{-i}=-P_{-i}\,, \tag{B9}$$

respectively. Since G_{-i} is known by assumption, $P_i\mathcal{G}_i$ is the Green's function of an ordinary integrodifferential equation and can therefore be readily constructed numerically. $\mathcal{G}_{-i}$ on the contrary is the solution of a set of $M-1$ coupled equations whose construction it would be very desirable to avoid. We will show in fact that it is not necessary to determine the $\mathcal{G}_{-i}$.

The solution of Eqs. (B7a) and (B7b) is then given by

$$P_iG=P_i\mathcal{G}_i+P_i\mathcal{G}_iP_iHP_{-i}G_{-i}\,, \tag{B10a}$$

$$P_{-i}G=P_{-i}\mathcal{G}_{-i}+P_{-i}\mathcal{G}_{-i}P_{-i}HP_iG_i\,. \tag{B10b}$$

We can now write

$$PG=P_iG+P_{-i}G\,, \tag{B11}$$

but this is only a formal solution since Eq. (B10b) for $P_{-i}G$ involves the $\mathcal{G}_{-i}$ whose determination we would prefer to avoid. We can however write

$$PG={\sum}'\,P_iG={\sum}'\,[P_i\mathcal{G}_i+P_i\mathcal{G}_iP_iHP_{-i}G_{-i}]\,, \tag{B12}$$

where the sum includes M terms. The determination of the M-channel Green's function, PG, has thus been reduced the determination of the M different $M-1$ channel Green's functions, $P_{-i}G_{-i}$, and of the M simple Green's functions $P_i\mathcal{G}_i$.

For the two-channel case we have, in particular, labeling the target states 1 and 2,

$$PG=\sum_{i=1}^{2}\,[P_i\mathcal{G}_i+P_i\mathcal{G}_iP_iHP_jG_j]\,, \tag{B13}$$

where $j=2$ if $i=1$ and $j=1$ if $i=2$, where we have used the fact that for the two-channel case $G_{-i}=G_j$ and $P_{-i}=P_j$, and where G_i and $\mathcal{G}_i$ are defined by

$$P_i(H-E)P_iG_i=-P_i\,, \tag{B14}$$

$$P_i(H+HP_jG_jP_jH-E)P_i\mathcal{G}_i=-P_i\,. \tag{B15}$$

In the more transparent matrix form, we have

$$PG=PGP\\=\begin{pmatrix} P_1\mathcal{G}_1P_1 & P_1\mathcal{G}_1P_1HP_2G_2P_2 \\ P_2\mathcal{G}_2P_2HP_1G_1P_1 & P_2\mathcal{G}_2P_2 \end{pmatrix}. \tag{B16}$$

The Pauli case, which requires some modifications, will be treated in the course of an actual application.

APPENDIX C: A CONNECTION BETWEEN MINIMUM PRINCIPLES AT AND ABOVE THRESHOLD ENERGIES

As in Appendix A, a connection between the two forms of minimum principle for energies at and above the new excitation threshold can be easily shown by constructing a suitable trial function $Q\Psi_t$. For $N+1$ open channels, we define the projection operators

$$P=P_0+P_1+\cdots+P_{-N-1}+P_N\equiv P_{-N}+P_N\,, \tag{C1}$$

and

$$Q=1-P=Q_{-N}-P_N\,. \tag{C2}$$

The two minimum principles derived in Secs. 3 and 2 can then be rewritten as

$$-\mathbf{a}\cdot\mathbf{b}\leq-\mathbf{a}_{-N}\cdot\mathbf{b}_{-N}{}^{P-N}-a_N\cdot b_{Nt}+2(Q_{-N}\tilde{\Psi}_t,HP_{-N}\Psi^{P-N})\\+(Q_{-N}\tilde{\Psi}_t,[H-E_{TN}+HG^{P-N}H]Q_{-N}\tilde{\Psi}_t)\,, \tag{C3}$$

and

$$-\mathbf{a}\cdot\mathbf{b}\leq-\mathbf{a}\cdot\mathbf{b}^P+2(Q\Psi_t,HP\Psi^P)\\ +(Q\Psi_t,[H-E_{TN}+HG^PH]Q\Psi_t)\,,\quad\text{(C4)}$$

where we have neglected the possible subtraction terms for simplicity. [Usually Eq. (C4) contains fewer subtractions than Eq. (C3). When there are infinite number of resonances below the Nth threshold, thus requiring an infinite number of subtractions in Eq. (C3), then Eq. (C3) would no longer be useful.]

Now, from the exact form of the solution Ψ given by

$$\begin{aligned}\Psi&=P\Psi^P+G^PHQ\Psi+Q\Psi\\ &=P_{-N}\Psi^P+P_N\Psi^P+\mathcal{G}_{-N}HQ\Psi+\mathcal{G}_NHQ\Psi\\ &\quad+G_{-N}H\mathcal{G}_NHQ\Psi+G_NH\mathcal{G}_{-N}HQ\Psi+Q\Psi\,,\end{aligned}\quad\text{(C5)}$$

it is possible to construct a function $Q_{-N}\tilde{\Psi}_t$ of the form

$$\begin{aligned}Q_{-N}\tilde{\Psi}_t&=P_N\Psi_t+Q\Psi_t\\ &=P_N\Psi^P+\mathcal{G}_NHQ\Psi_t+G_NH\mathcal{G}_{-N}HQ\Psi_t+Q\Psi_t\,.\end{aligned}\quad\text{(C6)}$$

Substitution of Eq. (C6) into Eq. (C3) and simplifying the resulting expression, one obtains Eq. (C4). The calculation is tedious but perfectly straightforward, and the following relations prove useful:

$$G^P=\mathcal{G}_{-N}+G_{-N}H\mathcal{G}_N+G_NH\mathcal{G}_{-N}+\mathcal{G}_N\,,\quad\text{(C7)}$$

$$\mathbf{a}_{-N}\cdot\mathbf{b}_{-N}{}^{P-N}=a_{-N}\cdot b_{-N}{}^P+(P_{-N}\Psi^{P-N},HP_N\Psi^P)\,,\quad\text{(C8)}$$

$$a_N\cdot b_{Nt}=a_N\cdot b_N{}^P+(P_N\Psi_t,HP_{-N}\Psi^P)\\ +(P_N\Psi^P,[H-E_{TN}]P_N\Psi_t)\,,\quad\text{(C9)}$$

$$\mathcal{G}_NHG_{-N}=G_NH\mathcal{G}_{-N}\,,\quad\text{(C10)}$$

$$G_{-N}-\mathcal{G}_{-N}=-G_{-N}HG_NH\mathcal{G}_{-N}\,.\quad\text{(C11)}$$

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Measurement of Time Correlations for Quantum-Mechanical Systems*

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Measurements that are of limited accuracy, are incomplete, or require a finite time to make do not generally permit one to construct a wave function for describing a physical system. The use of such partial information to predict the results of subsequent measurements is studied here. There are several practical applications of this problem, including the use of the autocorrelation function for a particle counter in a scattering experiment.

I. INTRODUCTION

It is customary in the pedagogical development of quantum mechanics and field theory to mention the limitations on correlated measurements of observables at different space-time points. Little attention has been given, however, to actual experiments for making such observations, or their usefulness. In this paper and in a subsequent one, we shall discuss both of these subjects from a general point of view and with particular applications to scattering processes.

This work is an outgrowth from a recent paper on the correlated counting rate of two detectors recording particles scattered from a target.[1] There it was shown that by such an observation both the magnitude *and* phase of a scattering amplitude can be determined. Such an observation of spatial correlations is only one of a much broader class of experiments to measure time and space-time correlations in a particle beam. For example, as we shall show in a subsequent paper, the time-dependent autocorrelation function for a single counter can provide information on the coherence of, say, a laser beam.[2] If a beam has been scattered, the autocorrelation function yields a measure of relaxation processes in the target.

In this paper we make some general comments on the theory of measurement for quantum-mechanical systems and illustrate the theory with some conceptually simple examples: (a) measurement of the spin of either one of two interacting particles at a time t_2 following the measurement of the spin of one of them at an earlier time t_1, and (b) the theory of intensity correlations of the Hanbury Brown-Twiss variety.

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[1] M. L. Goldberger, H. W. Lewis, and K. M. Watson, Phys. Rev. **132**, 2764 (1963).

[2] See, for example, C. H. Townes and R. Serber, *Quantum Electronics* (Columbia University Press, New York, 1960), p. 233.