Quasiminimum principle for single-channel scattering

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The conventional minimum principle for single-channel scattering is modified to eliminate the requirement that the static part of the open-channel problem must be solved exactly in order to maintain the bound property. The new formulation is easier to apply, at the expense of a slight compromise in the rigor of extremum property.

The minimum principle (MP) for scattering by a composite target system was formulated[1] over 20 years ago. Some applications of the principle to simple systems were carried out since then, providing rigorous bounds on scattering parameters and resonance energies. More importantly, the MP has helped to understand better the effects of dynamic polarization and resonances on the scattering cross sections.

However, direct, literal applications of the MP is complicated in general because of the following requirements. (a) the target wave functions corresponding to all the open channels for given scattering energy E must be known exactly. They are essential in specifying the correct asymptotic boundary conditions. (b) The projection operators P for the open channels and $Q=1-P$ have to be constructed explicitly, including the exchange and possible rearrangement channels. (c) The P component of the problem has to be solved exactly, while the closed Q-channel part is treated approximately by a variational procedure. Of course, these last two parts are related.

The second requirement (b) was resolved[2] completely in terms of the sequential-projection method, in which only P_i for each channel are required. (In general, $P_iP_j\neq 0$ but $P_iP=P_i$.) Extensive use of the static P-component functions, as required in (c), was made in developing the theory. The requirement (a) was examined[3] as to the sensitivity of the scattering amplitude on approximate target functions. It seems that (a) is essential for a rigorous MP. The point (c) was also approximately treated[4] by constructing a quasiminimum principle, in which both the P and Q components are calculated variationally. As a result, the rigor of the bound property was compromised, although the method may still be effective in practice.

In this paper, we eliminate the requirement (c) without too much sacrificing the rigor, for single-channel scattering. The problem (a) is left for some future development. The MP was formulated[1] by dividing the full space into the open- and closed-channel spaces, using the projection operators P and Q, respectively, where $P+Q=1$, $PQ=QP=0$, and $P^+=P=P^2$. The resulting coupled equations[5] are given by

$$P(H-E)P\Psi=-PVQ\Psi\ , \qquad Q(H-E)Q\Psi=-QVP\Psi\ , \tag{1}$$

where $H=H_0+V$ and $[P,H_0]=0$. By formally solving (1),

$$P\Psi=P\Psi^P+G^PPVQ\Psi\ , \qquad Q\Psi=G^QQVP\Psi\ , \tag{2}$$

where

$$P(H-E)P\Psi^P=0\ , \qquad P(H-E)PG^PP=-P,\quad G^P\equiv PG^PP\ , \tag{3}$$

and

$$Q(H-E)QG^QQ=-Q\ ,$$

we have

$$P(H-E+VG^QV)P\Psi=0\ , \tag{4}$$

$$Q(H-E+VG^PV)Q\Psi=-QVP\Psi^P\ . \tag{5}$$

The full scattering solution can be obtained by solving either (4) or (5), together with (2). Of course the asymptotic boundary condition for Ψ is to be imposed on $P\Psi$ while G^P in (5) contains the same information, as $Q\Psi\rightarrow 0$ faster than r^{-1} asymptotically. A variational treatment of G^Q in (4) or $Q\Psi$ in (5) leads to a minimum principle.[1] That is, in order to maintain the bound property of the calculated scattering parameters, either $P\Psi$ in (4) for a given approximate G^Q_t is solved *exactly*, or $Q\Psi_t$ in (5) is variationally estimated for the *exact* $P\Psi^P$ and G^P. These requirements for Eqs. (4) and (5) are of course related, and a careful numerical computation must be carried out in practice to satisfy the requirements. We considered earlier a quasiminimum principle[4] in which both the P and Q components in (1) are treated approximately variationally, but this approach is not always guaranteed to produce a rigorous bound on scattering parameters.

We propose here a simple modification of the MP such that the requirement (c) is approximately eliminated. This will facilitate applications to atomic, molecular, and nuclear scattering problems. From (3), we have

$$P\Psi^P=P\Phi+G_0^PVP\Psi^P\ , \qquad G^P=G_0^P+G_0^PVG^P\ , \tag{6}$$

and where

$$P(H_0-E)P\Phi=0\ ,\quad \Phi\equiv P\Phi\ , \qquad P(H_0-E)PG_0^P=-P\ ,\quad G^P\equiv PG^PP\ . \tag{7}$$

Note that $P\Phi$ and G_0^P involve essentially the "plane-wave" solutions in the limited open-channel space P, so that G_0^P, for example, is extremely simple to construct because of the P projection. By comparison, G_0 is a much more complicated function, although simple in a formal sense. [We can

readily incorporate some of the local, long-range distortion potentials in (7), but this will require numerical work.] Equation (5) then becomes, using (6) and (7),

$$Q(H-E+VG_0{}^PV)Q\Psi=-QVP(P\Psi^P+G_0{}^PVG^PVQ\Psi) \\ =-QVP(P\Phi+G_0{}^PVP\Psi) \ . \tag{8}$$

By further rearranging the terms and using the relations

$$\Psi=\Phi+G_0V\Psi \ ,$$

$$P\Psi=P\Phi+G_0{}^PV\Psi \ ,$$

we obtain

$$[Q(H-E)Q+VG_0{}^PV]\Psi=-VP\Phi+PVP\Psi \ , \tag{9}$$

and thus finally

$$D\Psi=-B_0 \ , \tag{10}$$

where

$$D=Q(H-E)Q+VG_0{}^PV-PVP \ ,$$

$$B_0=VP\Phi \ .$$

Equation (10) is the desired result. The spectrum of D is such that asymptotically it has the same behavior as that of QHQ; D is "essentially closed," although it is not entirely in the Q space. Therefore, Eq. (10) is *not* sensitive to the asymptotic behavior of Ψ.

A variational functional for (10) is

$$J_t[\Psi_t]=(\Psi_t|D|\Psi_t)+2(\Psi_t|B_0) \ , \tag{11}$$

and thus $\delta J_t/\delta\Psi_t=0$ gives

$$J=(\Psi|B_0)\sim J_t=-\frac{(B_0|\Psi_t)(\Psi_t|B_0)}{(\Psi_t|D|\Psi_t)} \ . \tag{12}$$

Evidently, the form (10) with D and the full wave function Ψ is not yet quite convenient because of strong involvement of the P component of Ψ, especially in discussing the bound property of J. To improve the situation, we let

$$\Psi=\Phi+w \ , \tag{13}$$

where $w=G_0V\Psi$, and rewrite Eq. (10) as

$$Dw=-B_1 \ , \tag{14}$$

where

$$B_1=VP\Psi_0{}^P-PVP\Phi=QVP\Phi_0{}^P+PVG_o{}^PV\Phi \\ =QVP\Phi+VG_0{}^PV\Phi \ .$$

Here, we used

$$\Psi_0{}^P=P\Phi+G_0{}^PVP\Phi \ ,$$

which is the once-iterated static wave function. The new variational functional for Eq. (14) is

$$J_t'[w_t]=2(B_1|w_t)+(w_t|D|w_t) \ , \tag{15}$$

and thus

$$J_t'=-\frac{(B_1|w_t)(w_t|B_1)}{(w_t|D|w_t)} \ . \tag{16}$$

On the other hand, we have the exact quantity

$$J'=(B_1|w)=K-K_{12B}{}^P \ , \tag{17}$$

where K and $K_{12B}{}^P$ are the exact and once-iterated static Born amplitudes, respectively, and defined by

$$K=(\Phi|V|\Psi) \ ,$$

$$K_{12B}{}^P=(\Phi|V|\Phi)+(\Phi|VG_0{}^PV|\Phi) \\ =(\Phi|V|P\Psi_0{}^P) \ . \tag{18}$$

The exact amplitude can also be written as

$$K=(\Phi|V|P\Psi^P)+(P\Psi^P|V|Q\Psi) \\ \equiv K^P+K^Q \ . \tag{19}$$

Therefore, we finally have, from (17) and (19),

$$J'=K^Q+(K^P-K_{12B}{}^P) \ . \tag{20}$$

It is now obvious that, to the extent that $K_{12B}{}^P$ is close to K^P, J' is essentially the same as K^Q; that is, J_t' given by (16) is close to that of the rigorous MP. Incidentally, we recall that, in the rigorous MP, K^P is evaluated exactly while K^Q is estimated variationally in terms of the trial function $Q\Psi_t$.

In (15) and (16), the trial function w_t may be written as

$$w_t=K_tPC_t+\sum_{n=1}^{n}a_nX_{nt} \ , \tag{21}$$

where C_t satisfies the boundary condition at the origin and asymptotically behaves as a cosine function similar to G_0, $G_0{}^P$, and G^P. (In the T formulation, it would behave as an outgoing wave.) Otherwise, C_t is arbitrary. X_{nt} are a predetermined set of square-integrable functions, which should in general contain both P and Q components. The parameter K_t is a variational approximation to K. Variation of J_t' with respect to K_t and a_n will give an optimum estimate of J', and, according to (20), this will nearly satisfy the bound property $J'\lesssim J_t'$. Unlike with the quasi-MP derived previously,[4] the form (16) has tighter control over the remaining P component in w_t. As is clear from (20), $K_{12B}{}^P\sim K^P$ if the Born series for the static problem of (3) is rapidly convergent, in which case we have $J'\sim K^Q$. We should emphasize however that J_t' estimates mainly the Q part of K, but at the same time the remaining P-part contribution is also being improved.

Recently, a modified form of the Schwinger variational principle was discussed,[6] in which an inhomogeneous scattering equation

$$\mathscr{D}\Psi=-B_0 \tag{22}$$

was treated variationally, where

$$\mathscr{D}=\frac{1}{N+1}(H-E)-\tfrac{1}{2}[P(H-E)+(H-E)P] \\ -\tfrac{1}{2}(PV+VP)+VG_0{}^PV \ , \tag{23}$$

and where N is a constant. It is a simple matter to show that

$$\mathscr{D}=D-\frac{N}{N+1}(H-E) \ . \tag{24}$$

Obviously, this difference of a constant multiple of $(H-E)$ is not going to affect Eq. (10) nor Eq. (22). However, Eqs. (12), (14), and (16) will be very much altered by the addition of such a term. Therefore, it will not be possible to derive a relation such as (20) if $\mathscr{D}$ is used in place of D.

Application of (16) to actual physical systems will not be complicated by the presence of ${G_0}^P$ in D and $P{\Psi_0}^P$ in B_1. Unless some long-range interactions are to be included in H_0, both ${G_0}^P$ and $P{\Psi_0}^P$ can be obtained explicitly analytically in many cases.

The extension of the present formalism to multichannel scattering is straightforward and follows along the line of argument presented in Ref. 7, and the quasibound property should hold here as well since the relationship (20) with ${K_{12B}}^P$ and ${K}^P$ will still be valid. Effectiveness of (16) is being tested by applying it to a number of physical scattering systems.

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