

electrons. Clearly, beyond a certain value of δ , the average radius would exceed one-half of the average internuclear separation at a given density and temperature. In this region, the approximation that the electron is bound to a single proton

(or an ionized impurity) is no longer valid and one must take into account systems of the type $(S.C.)_2^+$, $(S.C.)_2$, etc. Here $S.C.$ represents a neutral system (analogous to an H atom) in which the electron is bound in a SSCP.

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Quasiminimum Principle for Multichannel Scattering

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A new variational principle for multichannel scattering is derived which combines certain simplifying features of both Kohn and minimum principles. The rigorous bound property of the latter is relaxed slightly to gain simplifications and efficiency, especially for collisions involving particle rearrangements. The approach is essentially equivalent to treating variationally the open-channel part of the wave function, rather than solving for it exactly as required by the minimum principle. However, variations of parameters for the open and closed channels are carried out separately using a double functional.

I. INTRODUCTION AND SUMMARY

The variational principles for scattering problems of Kohn,¹ Hulthén,² and Schwinger³ types do not provide bounds on scattering parameters. Because of this lack of bound property, scattering parameters calculated may fluctuate, often violently.⁴ Nevertheless, it has been demonstrated⁵ that meaningful stationary values can still be extracted by performing an extensive numerical analysis with large numbers of trial functions. The essential advantage of these methods lies in their simplicity of applications, as *all* the parameters introduced are determined variationally in a uniform fashion. There have also been several modifications of the principles to avoid the violent fluctuations due to spurious singularities. For example, the method developed by Harris⁶ identifies the scattering energy to be one of these spurious points. Another approach⁷ avoids the singularities altogether by analytically continuing to the complex energy

values. These approaches still require a fair number of trial functions and their convergence is not always uniform. However, their applicability for simple scattering systems is reasonably well understood by now. We do not distinguish different versions of the methods and denote them in the following as the variational principles for scattering (VPS).

The minimum principles⁸ and their generalizations⁹ have been successfully applied to many of the low-energy scattering problems,¹⁰⁻¹² with the resulting bounds on scattering parameters. The procedure involved is considerably more complicated than that of the VPS, and gets rapidly worse as more reaction channels open up. Specifically, the complication arises from the requirement that the open-channel part of the scattering equations should be solved *exactly* numerically. Of course, this is necessary if the rigorous bounds are to be maintained. A recent calculation¹² of the positron-hydrogen pickup collision using the generalized varia-

tional bounds (GVB) formulation clearly indicated that the method is too rigid and unwieldy.

It is the purpose of this paper to suggest a new approach which is much simpler to apply than the GVB, but still maintains the bound property in a slightly weakened form. It will also have some fluctuations that the VPS have, but they can be readily controlled or eliminated by one of the alternative VPS. The difficult part of solving a scattering problem involving many particles is the distortion effect, and the important thing here is that this effect of the closed channels will be efficiently treated using the bound property just as with the GVB. We denote this new method as the quasi-minimum principle (QMP) and will show that it is an approach intermediate between the VPS and GVB.

In Sec. II, we discuss the relevant properties of the Kohn principle and the GVB formulation for the development of the QMP. The main result of the paper is contained in (3.1)–(3.4), with the resulting approximate bounds (3.6) on the scattering parameters. Some generalizations and possibilities for further modifications of the QMP are also pointed out.

II. VPS AND GVB

We briefly summarize in this section the specific features¹³ of the VPS and GVB relevant to our discussion of the QMP. We consider a scattering system with L_0 open channels and assume that the explicit forms of projection operators P and $Q = 1 - P$ are available, where P projects onto *all* the open channels. (This strong assumption can be removed,⁹ but we do not consider this possibility here.) With $M_0 \equiv H - E$, we can write the scattering equations as

$$PM_0 P\Psi = -PM_0 Q\Psi, \quad (2.1)$$

$$QM_0 Q\Psi = -QM_0 P\Psi. \quad (2.2)$$

By definition, $Q\Psi$ contains only the closed channels, so that

$$R_i Q\Psi \rightarrow 0 \quad (2.3)$$

as the channel coordinates $R_i \rightarrow \infty$. On the other hand, we have

$$P\Psi - (\mu_i/k_i)^{1/2} \psi_i(\vec{r}_i)[a_i s_i + b_i c_i] \mathcal{Y}_i/R_i \quad (2.4)$$

as $R_i \rightarrow \infty$, where

$$s_i = \sin(k_i R_i + \gamma_i), \quad c_i = \cos(k_i R_i + \gamma_i),$$

and \mathcal{Y}_i contains the angular and spin factors, the γ_i being additional constant phase factors. For each set of initial conditions $\{a_i\}$, we have the parameters b_i related to the reaction matrix K_{ij} by

$$b_i = \sum_{j=1}^{L_0} K_{ij} a_j. \quad (2.5)$$

For easy comparison of the VPS and GVB, we formulate the VPS in a slightly different way, although one probably never uses this way in practice.

A. VPS

We write the trial function Ψ_t in the form

$$\Psi_t = P\Psi_t + Q\Psi_t, \quad (2.6)$$

with

$$P\Psi_t = \sum_{i=1}^{L_0} \left(\frac{\mu_i}{k_i} \right)^{1/2} \psi_i [a_i f_i s_i + b_{it} g_i c_i] \mathcal{Y}_i/R_i + \sum_{i=1}^{L_p} C_i^P P\chi_{it}, \quad (2.7)$$

$$Q\Psi_t = \sum_{m=1}^{L_Q} C_m^Q Q\chi_{mt}, \quad (2.8)$$

and the Kato identity as

$$\begin{aligned} \lambda &= \lambda_t + (\Psi | M_0 | \Psi_t) \\ &= \lambda_t + (\Psi_t | M_0 | \Psi_t) - \tau, \end{aligned} \quad (2.9)$$

where

$$\tau = (\Omega | M_0 | \Omega), \quad \Omega = \Psi - \Psi_t,$$

$$\lambda_t = -2\pi\hbar^2 \sum_{i=1}^{L_0} a_i b_{it}.$$

In (2.7) and (2.8), both $P\chi_{it}$ and $Q\chi_{mt}$ are square-integrable trial functions of perdetetermined forms, while $f_i(R_i)$ and $g_i(R_i)$ are inserted such that the correct boundary conditions at $R_i = 0$ are satisfied, and both asymptotically approach unity.

The Kohn variational principle is obtained with the functional

$$\begin{aligned} [\lambda] &= \lambda_t + (P\Psi_t | M_0 | P\Psi_t) \\ &\quad + 2(P\Psi_t | M_0 | Q\Psi_t) + (Q\Psi_t | M_0 | Q\Psi_t), \end{aligned} \quad (2.10)$$

and the variations

$$\frac{\delta[\lambda]}{\delta\lambda_t} = 0, \quad \frac{\delta[\lambda]}{\delta C_i^P} = 0, \quad \frac{\delta[\lambda]}{\delta C_m^Q} = 0. \quad (2.11)$$

That is, the stationary value of λ is obtained from a *single functional* $[\lambda]$ by *simultaneous variations of all parameters*. Obviously, this is the most general way in which all the parameters can be varied, but, as mentioned earlier, the VPS do not provide the bound property. Thus, in general it is not possible to judge how small τ should be. Furthermore, the determination of C_m^Q is completely mixed up with the fluctuations, making it difficult to settle the value λ_t . By the QMP given in Sec. III, we uncouple the effect of the fluctuations from C_m^Q . Other variational procedures mentioned earlier have the

similar features as that of Kohn.

B. GVB

The GVB formulation completely eliminates the spurious fluctuations in λ_t which occur in the VPS, and provides bounds on scattering parameters. It requires an *exact* solution of (2.1) for $P\Psi_t$ for given $Q\Psi_t$, while (2.2) is treated variationally with adjustable parameters. Thus, we write for (2.1) and (2.2)

$$PM_0 P\bar{\Psi}_t = -PM_0 Q\Psi_t, \quad (2.12)$$

$$[J] = 2(Q\Psi_t | M_0 | P\bar{\Psi}_t) + (Q\Psi_t | M_0 | Q\Psi_t), \quad (2.13)$$

with

$$\frac{\delta[J]}{\delta C_m^Q} = 0. \quad (2.14)$$

Defining the homogeneous solution of (2.12) as

$$PM_0 P\Psi^P = 0, \quad PM_0 PG^P P = -P \quad (2.15)$$

with the resulting parameter λ^P , we have

$$[\bar{\lambda}] = \lambda^P + [J]. \quad (2.16)$$

It is simple to show that as $P\Psi_t \rightarrow P\bar{\Psi}_t$, $[\lambda]$ approaches $[\bar{\lambda}]$. From (2.12) and (2.15), we can write

$$P\bar{\Psi}_t = P\Psi^P + G^P PM_0 Q\Psi_t. \quad (2.17)$$

We have noted previously that (2.17) and (2.8), substituted into the Kohn principle (2.10), result in the GVB. We can also rewrite (2.13) in the form

$$[J] = 2(Q\Psi_t | N_P) + (Q\Psi_t | M_P | Q\Psi_t), \quad (2.18)$$

where

$$M_P \equiv M_0 + M_0 G^P M_0, \quad N_P \equiv M_0 P\Psi^P. \quad (2.19)$$

Using the orthogonality properties⁹

$$\begin{aligned} PM_P &= M_P P = 0, & M_P &= QM_P Q, \\ PN_P &= 0, & N_P &= QN_P, \end{aligned} \quad (2.20)$$

we can write $[J]$ without the Q operator as

$$[J] = (\hat{\Psi}_t | M_P | \hat{\Psi}_t) + 2(\hat{\Psi}_t | N_P), \quad (2.21)$$

where $\hat{\Psi}_t$ is a square-integrable trial function. This form was crucial in treating the rearrangement collisions, where the explicit forms of P and Q are not readily available.

The bound property of the GVB follows essentially from the inequality

$$QM_0 Q > 0 \quad (2.22a)$$

or

$$QM_P Q = M_P > 0, \quad (2.22b)$$

with results in the bound

$$\lambda \leq [\bar{\lambda}]. \quad (2.23)$$

(We neglect here the question of subtractions.)

From (2.14), with (2.8), we have

$$\begin{aligned} [J] &= - \sum_{m,n}^{LQ} (P\bar{\Psi} | M_0 | Q\chi_{mt}) [M_{0t}^{-1}]_{mn} (Q\chi_{nt} | M_0 | P\bar{\Psi}_t) \\ &\equiv (P\bar{\Psi}_t | S_t^Q | P\bar{\Psi}_t), \end{aligned} \quad (2.24)$$

where M_{0t} is a matrix with elements

$$(Q\chi_{mt} | M_0 | Q\chi_{nt}).$$

This result can be combined with (2.12) to obtain

$$P[M_0 + S_t^Q]P\bar{\Psi}_t = 0. \quad (2.25)$$

Thus, the requirement of solving (2.12) exactly, in order to maintain the inequality (2.23), is completely equivalent to solving (2.25) for $P\bar{\Psi}_t$ for a variationally determined S_t^Q , where (2.22) gives immediately

$$S_t^Q \leq S_t^Q < 0. \quad (2.26)$$

The complication of the GVB, compared with the VPS, lies in this requirement for $P\bar{\Psi}_t$. However, we have noted earlier that the physically complicated part in the original scattering problem is contained not in $P\bar{\Psi}_t$, but rather in $Q\Psi_t$ and thus in S_t^Q , and this part *can* be determined effectively using the property (2.26), without the complication of the open channels. The nonlocal operator S_t^Q in (2.24) can also be written in a diagonalized form

$$S_t^Q = - \sum_m^{LQ} M_0 QX_{nt} (E_{nt}^Q - E)^{-1} (QX_{nt} \cdot M_0), \quad (2.27)$$

where $(E_n^Q - E)$ and QX_n are the eigenvalues and eigenfunctions, respectively, of QM_0Q . Some of the low-lying states with E_n^Q may correspond approximately to the resonances. It is clear that S_t^Q can be obtained if we have the explicit Q operator. However, the need for the Q operator in (2.25) may be eliminated only if $P\bar{\Psi}_t$ is obtained exactly from (2.25). On the other hand, this nice feature may still be present to some extent even if (2.25) is treated approximately, so long as the resulting solution is a reasonably good one.

III. QUASIMINIMUM PRINCIPLE

In this section, we develop a new variational principle which can improve the VPS insofar as the determination of $Q\Psi_t$ is concerned but still retain the original simplicity, and, at the same time, can simplify the GVB by eliminating the requirement of exact solution of (2.25) and yet retain the inequality approximately. The only *assumption* we have to make for this purpose is that the VPS are perfectly capable of handling a simple potential scattering problem involving several open channels,

such as that described by (2.25), to any desired accuracy.¹⁻⁷

We introduce a double functional of the form

$$[\lambda] = \lambda_t + (P\Psi_t | M_0 | P\Psi_t) + [J], \quad (3.1)$$

with

$$[J] = (Q\Psi_t | M_0 | Q\Psi_t) + 2(P\Psi_t | M_0 | Q\Psi_t), \quad (3.2)$$

where the explicit forms of Ψ_t are given by (2.7) and (2.8). Determination of the parameters is carried out in *two steps*: *first*

$$\frac{\delta[J]}{\delta C_m^Q} = 0, \quad (3.3)$$

followed by

$$\frac{\delta[\lambda]}{\delta \lambda_t} = 0, \quad \frac{\delta[\lambda]}{\delta C_t^P} = 0. \quad (3.4)$$

In this way, we have effectively *isolated* the problem of determining C_m^Q from the rest of the variations involved in the Kohn principle. The double functional (3.1) is constructed to be used precisely in the above sense of (3.3) and (3.4).

Obviously, we immediately recover the usual VPS, (2.11) with (2.10), if (3.3) and (3.4) are combined to a single-step variation. On the other hand, combining (3.3) and (3.1), we can also write

$$[\lambda] = \lambda_t + (P\Psi_t | M_0 + S_t^Q | P\Psi_t), \quad (3.5)$$

which is simply a variational statement of (2.25) and thus the GVB. The form (3.5) also suggests the approximate bound property of the resulting λ_t . That is, from (2.9), we have

$$\tau = (Q\Omega | M_0 | Q\Omega) + 2(Q\Omega | M_0 | P\Omega) + (P\Omega | M_0 | P\Omega),$$

with

$$(Q\Omega | M_0 | Q\Omega) > 0.$$

Therefore, if $Q\Psi_t$ in S_t^Q and $P\Psi_t$ in (3.5) are such that

$$\|Q\Omega\| \gg \|P\Omega'\|$$

where $P\Omega'$ denotes the error involved in (3.5), for given S_t^Q , then we have an approximate inequality

$$\tau \gtrsim 0,$$

and thus

$$\lambda \lesssim \lambda_t, \quad (3.6)$$

which is the desired quasiminimum principle (QMP). [We have to stress at this point that $P\Omega'$ above does *not* include the effect of $Q\Omega$ itself due to the coupling, but *only* that part of the error resulted from (3.5) for given S_t^Q .] It is essential, therefore, that the variations (3.4) should be carried out with a sufficient number of terms (L_P) to yield reliable accuracy.

The two-step variations (3.3) and (3.4) of the QMP cannot be as general variations as those involved in the VPS, but this limitation is more than offset by the advantage gained in the determination of C_m^Q using the inequality (2.26). The past studies on the VPS and GVB indicate that the QMP could yield reliable results with a much fewer number of trial functions. The simplification of the GVB resulting from (3.5), rather than (2.25), will be very significant as the number of open channels goes up. For rearrangement collisions, such as the e^+H system,¹² the exact coupling kernels $P_i M_0 P_j$ as required by the GVB are extremely complicated to evaluate. Although the same quantities also appear in (3.5), for example, they will be immediately integrated out with $P\Psi_t$, and this can simplify the whole calculation as the integration variables can be freely interchanged. This was in fact the partial motivation for the present study. Thus, the essential points to be retained in the QMP are the variations (3.3) and (3.4) from the VPS and the strong inequality (2.26) from the GVB. This latter point will also allow the resonance energy calculations as a part of the program.

As stated earlier, the steps involved in (3.5) need not be the Kohn principle, and any other forms of the VPS may serve the purpose equally well so long as the mild restriction on the $P\Omega'$ can be satisfied. Thus, in the application of the Harris method,⁶ the energy values obtained by the diagonalization of the matrix $(P\chi_{it} | M_0 | P\chi_{it'})$ should be adjusted to coincide with the value E , perhaps by varying the nonlinear parameters in $P\chi_{it}$, i. e., zeros of the above matrix. On the other hand, the method of analytic continuation⁷ requires the change of the boundary conditions on $P\Psi_t$ to be the outgoing waves. This will also change the expressions for λ and λ_t but will not affect the above two-step procedure.

The QMP given above can be generalized to cases in which some parts of the open channels may be treated exactly. Thus, we write the open channels in two groups as

$$\Psi_t = P_a \bar{\Psi}_t + P_b \Psi_t + Q\Psi_t, \quad (3.7)$$

where we are again assuming that such projection operators exist, and this new form is substituted into (3.1) and (3.2). The variations (3.3) are the same as before, but (3.4) are replaced now by

$$\begin{aligned} \frac{\delta[\lambda]}{\delta \lambda_t} = 0, \quad \frac{\delta[\lambda]}{\delta C_t^{Pb}} = 0, \\ \frac{\delta[\lambda]}{\delta (P_a \bar{\Psi}_t)} = 0. \end{aligned} \quad (3.4')$$

We then obtain the QMP,

$$\lambda \lesssim \lambda_t, \quad (3.6')$$

if the error made in the variations for C_t^{Pb} is less

than that in (3.3) for C_m^Q , i. e., $\|P_b\Omega'\| \ll \|Q\Omega\|$.

We add two remarks on possible extensions of the QMP.

Remark 1. For some rearrangement collisions, the operators P and Q are not available, so that $[J]$ cannot be constructed. The GVB formulation solved this problem by requiring that the exact G^P and Ψ^P should be calculated. Then, the quantities M_p and N_p of (2.19) can be constructed with the orthogonality properties (2.20).

However, these are precisely the quantities we are trying to avoid in the present formulation: One possible solution to this problem may be that, as $P\Psi_t$ is improved in (3.5) for given S_t^Q , which may contain some P components because of the lack of Q , these undesirable parts will be canceled out through readjustments of C_t^P in the integral $(P\Psi_t | M_0 + S_t^Q | P\Psi_t)$. Thus, even if we do not use the Q projection in the construction of S_t^Q , and, as a result, are without the help of (2.26), the double functional procedure may still give an improved convergence and less fluctuations. This point requires more extensive analysis, however. A more satisfactory solution can be given in terms of the theory of sequential projections,¹⁴ which is in some sense related to the generalization given by (3.7) and (3.4'). This will be discussed more fully elsewhere in connection with the positron-hydrogen pickup collision.¹⁵

Remark 2. Instead of (2.1) and (2.2), we may also study a slightly different set of equations

$$\begin{aligned} PM_0\Psi &= 0 \text{ or } P_i M_0\Psi = 0 \text{ with } P_i P = P_i, \\ QM_0\Psi &= 0, \end{aligned} \quad (3.8)$$

where $P_i = \psi_i \langle \psi_i$. The GVB require that

$$P_i M_0 \bar{\Psi}_t = 0, \quad (\Psi_t, QM_0 \bar{\Psi}_t) \approx 0. \quad (3.9)$$

Although the set (3.9) is very simple, it is not clear at present whether its use will yield further simplifications of the theory.

IV. DISCUSSION

We discuss here briefly the potentialities of the proposed approach and point out where it could be most effective.

(a) In the case of single-channel scattering, such as the positron-hydrogen system, where the exact target function and the open channel projection operator are explicitly available, the QMP may not be needed because the original MP can be carried out by simply integrating numerically the integrodifferential equation for the open channel. In fact, the variational methods of Kohn and Harris are known to be as effective in such cases.^{4,6} As noted earlier, the closed-channel contribution has already been included in (3.5), so that the problem is reduced essentially to a scattering by nonlocal separable po-

tentials. The variational procedure can give reliable result with only a few linear parameters.^{4,6} Now, we consider the multichannel scattering. The GVB require the exact solutions of a set of coupled equations in which the distortion terms have been included as before. Here the numerical solutions require much more effort, although extensive works of this kind have been done in the past. After all, the accuracy of the open-channel solutions can and need not be better than that of the closed-channel distortions.

(b) The second real advantage of the QMP would be in the scattering by a more complex system where the exact target function is not available, as in the electron-atom and electron-molecular collisions (e.g., $e\text{-He}$, $e\text{-N}$, $e\text{-H}_2$, and $e\text{-N}_2$). An elaborate attempt to solve a set of coupled open-channel equations would be less meaningful here since the original GVB no longer provides rigorous bounds on scattering parameters. The scattering solution is useful only to the extent that the approximate target function is reliable. The question of precisely how an approximate target function would affect the resulting amplitude is only beginning to be understood.¹⁵

Therefore, the modification of the GVB in the form of QMP would allow wider applications to the electron-atom and electron-molecule scatterings, by not requiring an exact solution of the open-channel problem. Incidentally, we note here that, because of the exchange and rearrangement channels, we do not in general have the exact channel projections even if the exact target functions are known. Of course, the GVB formulation takes care of this difficulty by requiring an exact evaluation of the shift operators of the form $P_i M_0 G^P M_0 P_j$, with $[P_i P_j] \neq 0$. However, this procedure will also be affected if P_i are not known exactly.

(c) The *main* reason for the QMP is of course in the treatment of the rearrangement processes. Here, even if the target and residual bound-state functions are available, the open-channel projection operators cannot readily be constructed. Thus, as assume that we have to apply the GVB formulation, as in the positron-hydrogen pickup collision.¹² The first step is to solve a set of coupled equations in the coupled-static approximation, in which the coupling kernels of the form $P_1 K_{12} P_2 = P_1 (H - E) P_2$ appear. The integral kernel $K_{12}(r_2, R)$ is a function of two variables for the positron-proton and positronium center of mass proton coordinates \vec{r}_2 and \vec{R} , respectively. The evaluation of K_{12} is extremely complicated because of the Coulomb singularities and multiple integrals to be performed numerically.¹² The final accuracy of the amplitude turned out to be limited mainly by the accuracy of K_{12} . On the other hand, any matrix elements involving $P_1 (H - E) P_2$ are much easier to evaluate, because we can then

interchange the variables of integrations. This seems to be a very trivial point, but happens to be the main difficulty in the actual calculation of the rearrangement collisions. In fact, this is the main motivation for the formulation of QMP, and ob-

viously we no longer have to evaluate the kernels such as K_{12} . An improved calculation of the e^+H pickup collision is in progress using the QMP and incorporating some additional simplifications peculiar to this particular system.¹⁴

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Forcing Conservation of Particle Flux in Perturbation-Theory Calculations of Inelastic Scattering

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Two approximations to Seaton's unitarization scheme are described which make it possible to impose the conservation-of-particle-flux requirements on an approximate calculation of inelastic scattering without making calculations of elastic scattering in the two channels which the transition connects. One approximation is based on the black-sphere model of Feshbach and Weisskopf. Another approximation corrects only for back coupling and can be equivalent to a method of Levine. The methods are illustrated by applying them to the Born approximation for the $1s-2s$ excitation of the hydrogen atom by electron impact.

I. INTRODUCTION

It is well known that as a consequence of time-reversal invariance and particle-flux conservation for a scattering process, we can assign phases to the wave functions in such a way that the scattering matrix S is symmetric and unitary, the transition matrix T is symmetric and satisfies the generalized optical theorem, and the reactance matrix R is symmetric and real.¹⁻³ Cross sections and scattering amplitudes calculated by many theoretical approximations to the S and T matrices do not satisfy these requirements, even within an artificially limited subset of open channels. Although cross sections can be most directly calculated from S and T , it has often been recognized that it is advantageous to make approximations to R (or to the reaction matrix $K=2R$) rather than directly to S or T , because the S and T computed from any Hermitian R (whether approximate or exact) auto-

matically satisfy the conservation and time-reversal requirements.⁴ Using these ideas, Seaton proposed a calculational scheme (his method II) in which the conservation and symmetry requirements are fully satisfied even if the conservation laws are violated in the initial approximation.⁵ For electron-atom scattering, this scheme has been applied many times.⁶⁻¹⁹ It has also been much applied for other quantum-mechanical scattering problems.²⁰⁻²⁷ For inelastic scattering, Seaton's method requires approximate calculations not only of the inelastic scattering amplitudes, but also of the elastic scattering amplitudes in at least the initial and final channels. We consider here two similar methods for making the scattering calculation satisfy all the conservation requirements for an inelastic process without calculating the elastic scattering. They are alternatives to Seaton's method which may be considered as approximations of it. They are, however, different ap-