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Variational principles for inhomogeneous scattering equations

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As a generalization of the Schwinger variational principle (VP), the normalization-independent feature of the VP derived from inhomogeneous scattering equations is studied. An optimum form of the VP is derived which contains the "free" Green's function G_0. Quasipotentials are then introduced to improve the efficiency of the variational procedure. Various extensions are discussed to include the composite-system scattering, multichannel processes, and the exchange effect.

I. INTRODUCTION

Variational principles (VP) for scattering processes of the Kohn[1] and Hulthen[2] types are well known,[3] in which the non-Hermiticity of the Hamiltonian H in the space of scattering states is exploited to construct simple variational functionals. By contract, the Schwinger VP (Ref. 4) and the variational bound formulation[5] treat inhomogeneous (integral or differential) scattering equations with the distinct advantages that the trial functions can often be square integrable and the variational functionals are "normalization independent". That is, the overall normalization of the trial function is completely controlled by the "known" inhomogeneous terms, so that the functional can be written in a form which is independent of this normalization factor.

In this paper, we consider the general problem of formulating VP for the inhomogeneous scattering equations. The Schwinger VP is first generalized by projecting the Lippmann-Schwinger equation with an arbitrary operator W. Different choices for W are then considered, and some of the results obtained[6] are shown to follow from special choices of W.

The quasipotential formulation[7] is introduced in Sec. III to improve the efficiency of the VP. The formulas are compared with the result of Ref. 6 and also with the Sasakawa-Austern approach.[8,9] A variational treatment of the latter is formulated. Various extensions of the results of Secs. II and III are considered in Sec. IV, in particular, the composite-system scattering, multichannel processes, and the exchange effect. The main result of the VP is contained in Eqs. (2.10)–(2.12). The quasiparticle modifications (3.5) and (3.17) are also of interest. The simple form (4.12) is without G_0 but with the full exchange effect.

II. INHOMOGENEOUS SCATTERING EQUATIONS AND VARIATIONAL PRINCIPLES

We begin with the nonrelativistic potential scattering described by $H = H_0 + V$. Extensions of our result to composite-system scattering with full exchanges and multichannel complications will be considered in Sec. IV. The scattering function u with the standing-wave boundary conditions satisfies

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

or the integral equation

$$u=u_0+G_0Vu\ ,$$

i.e., (2.2)

$$(1-G_0V)u=u_0$$

with

$$(H_0-E)u_0=0,$$
$$(H_0-E)G_0=-1, \tag{2.3}$$

where G_0 satisfies again the standing-wave boundary condition. If we define

$$u\equiv u_0+\omega \quad (\omega\equiv G_0Vu) \tag{2.4}$$

then

$$(H-E)\omega=-Vu_0\equiv -B_0. \tag{2.5}$$

The scattering amplitude K (reactance matrix) is given by

$$K\equiv(u\mid V\mid u_0)=(u_0\mid V\mid u)$$
$$=K_0+K_c, \tag{2.6}$$

where

$$K_0=(u_0\mid V\mid u_0),$$
$$K_c=(u_0\mid V\mid \omega). \tag{2.7}$$

The scattering equations (2.2) and (2.5) are both *inhomogeneous* so that the overall magnitudes of u and ω, respectively, are completely determined by the inhomogeneous term with u_0.

Equation (2.2) is often treated by first projecting it from the left with an arbitrary weighting operator W, as

$$Au\equiv W(1-G_0V)u=Wu_0\equiv B \tag{2.8}$$

or

$$A\omega=WG_0Vu_0\equiv C. \tag{2.9}$$

In general, the operator A is not symmetric, so that its left inverse, for example, can be different from the right inverse. A bilinear spectral expansion of A and A^{-1} can be constructed using the eigenfunctions of A and A^+. In the following discussion, however, we will choose W such that A is always symmetric.

Variational treatment of (2.8) requires the construction of a functional (for a symmetric A)

$$J_t[u_t]=2(u_t\mid W\mid u_0)-(u_t\mid A\mid u_t), \tag{2.10}$$

and the variations

$$\delta J_t[u_t]/\delta u_t=0 \tag{2.11}$$

gives an estimate of J, where

$$J=(u\mid B)\sim J_t=\frac{(u_0\mid W\mid u_t)(u_t\mid W\mid u_0)}{(u_t\mid A\mid u_t)}. \tag{2.12}$$

If we set $u_t\equiv u+\delta u$, J_t obtained from (2.10) and (2.11) is such that

$$J_t-J=O((\delta u)^2); \tag{2.13}$$

that is, J_t is a *variational* estimate of J. The important characteristic of (2.12) is that J_t is normalization independent in the sense that the overall normalization of u_t is irrelevant in (2.12). This is of course the direct consequence of the inhomogeneity of the scattering equation (2.8).

Alternatively, for (2.9) we have, with $C=WG_0Vu_0$,

$$(\omega\mid WG_0V\mid u_0)\sim\frac{(C\mid\omega_t)(\omega_t\mid C)}{(\omega_t\mid A\mid\omega_t)} \tag{2.14a}$$

and also for (2.5),

$$(\omega\mid V\mid u_0)\sim\frac{(u_0\mid V\mid\omega_t)(\omega_t\mid V\mid u_0)}{(\omega_t\mid E-H\mid\omega_t)}. \tag{2.14b}$$

It is important to note that the variational estimates on the right-hand sides of (2.14) and (2.12) are only for the quantities on the left-hand side of the equations. The wave functions ω_t or u_t thus determined may nevertheless be used in the evaluation of other integrals, in which case the error is no longer of the $(\delta u)^2$ order. In this case, the resulting integrals are not variational estimates.

Now, we consider several specific choices for the operator W, with the requirement that the resulting A be symmetric: (This is not necessary but convenient for our discussions below.)

A. $W=V$

This choice gives

$$A=V-VG_0V,$$
$$B=Vu_0=B_0, \tag{2.15a}$$

and thus, from (2.12),

$$J_t^a=\frac{(B_0\mid u_t)(u_t\mid B_0)}{(u_t\mid V-VG_0V\mid u_t)}, \tag{2.15b}$$

which is the Schwinger variational principle (VP). As is well known, only the short-range behavior of u_t is relevant in (2.15b). However, the asymptotic boundary conditions on u and u_t are *already incorporated* in (2.15b) and (2.2) when G_0 and u_0 are constructed. Therefore, it is not entirely correct to assert that the asymptotic boundary conditions are not involved in the Schwinger VP. Secondly, the explicit evaluation of G_0 is not trivial in general except in a simple potential scattering. Thirdly, the exchange effect, which has been neglected thus far, can seriously complicate the problem, as will be discussed in Sec. IV. An expansion of u_t,

$$u_t=\sum_{n=1}^{N}a_n\phi_n^a,$$

gives

$$J_t^{(a)}=\sum_{n,m}^{N}(B_0\mid\phi_n^a)\left[\frac{1}{(\phi_i^a\mid V-VG_0V\mid\phi_j^a)}\right]_{nm}\times(\phi_m^a\mid B_0), \tag{2.16}$$

where the large parentheses indicate that it is the inverse of a matrix with elements given by the i,j

indices. Obviously, (2.16) is an approximation

$$J_t^{(a)} \sim J^{(a)} = (u \mid V \mid u_0) = K. \qquad (2.17)$$

B. $W = VG_0V$

This makes A symmetric, as

$$A = VG_0V - VG_0VG_0V,$$
$$B = VG_0Vu_0, \qquad (2.18)$$

and (2.12) becomes, with $\omega_t = G_0Vu_t = \sum_n^N b_n \phi_n^b$,

$$J_t^{(b)} = \sum_{n,m}^{N} (B_0 \mid \phi_n^b) \left[\frac{1}{(\phi_i^b \mid E-H \mid \phi_j^b)} \right]_{nm} \times (\phi_m^b \mid B_0). \qquad (2.19)$$

(With ω_t, $E-H$ is Hermitian.) Of course (2.19) is also obtained from (2.5) directly, and has been studied recently[6] as a variant of the Schwinger VP. The important feature of (2.19) is that G_0 no longer appears. However, the asymptotic boundary conditions on ϕ_n^b and ω_t are now important. We have

$$j_t^{(b)} \sim J^{(b)} = (\omega \mid V \mid u_0) = K_c. \qquad (2.20)$$

Incidentally, we also note that the choice

$$W = G_0^{-1} = E - H_0 \qquad (2.21)$$

in (2.14) gives $A = E - H$ and thus (2.19).

C. $W = E - H_0 + V$

Equation (2.8) becomes

$$(E - H_0 - VG_0V)u = Vu_0, \qquad (2.22)$$

which obviously is a combination of (2.1) and (2.15a). Equation (2.12) then assumes the form

$$J_t^{(c)} = \frac{(u_0 \mid V \mid u_t)(u_t \mid V \mid u_0)}{(u_t \mid E - H_0 - VG_0V \mid u_t)} \sim J^{(c)} = (u \mid V \mid u_0) = K. \qquad (2.23)$$

(With u_t, $E-H_0$ is not Hermitian.) Since u_t is needed in the interaction region for $(u_t|V|u_0)$, the expression $J_t^{(c)}$ is not expected to be sensitive to the asymptotic behavior of u_t, just as in the case of the Schwinger VP (2.15b). On the other hand, the explicit appearance of $E-H_0$ in the denominator provides a stronger constraint on u_t in the interaction region than (2.15b). Finally, (2.22) can be approximated by first setting, in the interaction region,

$$G_0 \approx G_{0t} = \mid \phi_t) \frac{1}{E - E_{0t}} (\phi_t \mid,$$
$$(\phi_t \mid \phi_t) = 1, \quad (\phi_t \mid H_0 \mid \phi_t) = E_{0t}, \qquad (2.24)$$

which gives in turn

$$E - H_0 \approx \mid \phi_t)(E - E_{0t})(\phi_t \mid. \qquad (2.25)$$

Equations (2.24) and (2.25) can be generalized by including additional ϕ_t's generated by the diagonalization of H_0 with a set of square-integrable bases functions. Substitution of (2.24) and (2.25) into (2.23) provides an approximation to $J_t^{(c)}$ and thus to $J^{(c)} = K$.

Similarly, the present choice for W gives (2.9) in the form (Hermitian)

$$(E - H_0 - VG_0V)\omega = (V + VG_0V)u_0 \equiv \widetilde{C}, \qquad (2.26a)$$

and (2.14) becomes, with $\omega_t = \sum_n b_n \phi_n^b$,

$$J_t^{(d)} = \sum_{n,m}^{N} (\widetilde{C} \mid \phi_n^b) \times \left[\frac{1}{(\phi_i^b \mid E - H_0 - VG_0V \mid \phi_j^b)} \right]_{nm} (\phi_n^b \mid \widetilde{C}). \qquad (2.26b)$$

Once it is assumed that an explicit G_0 *is* available, then (2.26) are presumably more sensible to use than (2.23) and (2.15). Of course, (2.19) does not require G_0, but then $J_t^{(b)}$ can be more sensitive to the asymptotic boundary conditions. $J_t^{(d)}$ is an estimate for $J^{(d)}$, where

$$J^{(d)} = (\omega \mid C) = 2K_c - K_1, \qquad (2.27)$$

where $K_c = (\omega \mid V|u_0)$ and $K_1 = (u_0|VG_0V|u_0)$, thus stressing the K_c part of the calculation. Thus, without G_0 we have (2.5) and (2.19), while with G_0 we have (2.16), (2.23), and (2.26), among which (2.26) may be the most efficient in estimating the amplitude K.

III. QUASIPOTENTIALS AND VARIATIONAL PRINCIPLES

Since the scattering problem with separable potentials can be treated exactly, many different procedures have been developed in the past to facilitate the solution using such quasipotentials. We study in this section the possibility of improving the variational formulation of Sec. II by introducing the quasipotential of the form[7]

$$V_s=\sum_\alpha |\zeta_\alpha)(\xi_\alpha| \,. \tag{3.1}$$

In (3.1), ζ_α and ξ_α are so far arbitrary, but square-integrable functions. Then, (2.5) for example can be modified to a form

$$(H-E-V_s)z=-Vu_0\equiv -B_0, \tag{3.2}$$

where z satisfies the same boundary conditions as ω and G_0. For $\alpha=1$ and $\zeta_\alpha = B_0 = Vu_0$, we have the simple case

$$z=a\omega, \tag{3.3}$$

where

$$a=1-(\xi\,|\,z)=\frac{1}{1+(\xi\,|\,\omega)}. \tag{3.4}$$

The main advantages of introducing V_s are twofold: Firstly, the operator $(E-H+V_s)^{-1}$ in $z=(E-H+V_s)^{-1}\,Vu_0 = a\omega$ is sufficiently modified such that a perturbative treatment of (3.2) may be possible. The effect of the driving term Vu_0 is magnified by a^{-1}. Secondly, possible spurious singularities in an approximation to $(E-H)^{-1}$ may be avoided by V_s as it shifts the position of the singularities for a fixed E.

On the other hand, (3.2) may be efficiently treated variationally

$$J_t^{(z)}=\sum_{n,m}^{N}(B_0\,|\,\phi_n^b)\times\left[\frac{1}{(\phi_i^b\,|\,E-H+V_s\,|\,\phi_j^b)}\right]_{nm}(\phi_m^b\,|\,B_0). \tag{3.5}$$

Of course $J_t^{(z)}$ is an approximation to $(z|V|u_0)$ to order $O(\delta z^2)$, but not necessarily to that order for $(\omega|V|u_0)$. We have

$$J_t^{(z)}\sim(z\,|\,V\,|\,u_0)=\frac{(\omega\,|\,V\,|\,u_0)}{1+(\xi\,|\,\omega)}=(\omega\,|\,V\,|\,u_0)[1-(\xi\,|\,z)]. \tag{3.6}$$

So far the form of ξ is left arbitrary, and may be adjusted to shift the *spurious zeros* of the denominator in (3.5), thus avoiding the usual stabilization problem associated with the Kohn and Hulthen variational principles.

In a recent paper,[7] we have considered an iteration procedure formulated with V_s^u given by

$$V_s^u=V\,|\,u)\frac{1}{(\xi\,|\,V\,|\,u)}(\xi\,|\,V, \tag{3.7a}$$

and the exact relation

$$(H_0-E+V_s^u)u=0. \tag{3.7b}$$

(Obviously, the solution of (3.7b) requires an iterative procedure.[7]) A similar procedure may be devised for ω, as

$$V_s^\omega=V\,|\,\omega)\frac{1}{(\xi\,|\,V\,|\,\omega)}(\xi\,|\,V, \tag{3.8a}$$

in the differential equation (2.5)

$$(E-H_0-V_s^\omega)\omega=Vu_0. \tag{3.8b}$$

However, the variational principle (3.5) may be as effective when a sufficient number of terms are included in (3.1).

Instead of the differential equation (2.5), we now consider the integral equation (2.2) for u and introduce a separable form,[8,9] as

$$u=u_0+[\,|\,\omega_q)(\phi_q\,|+\mathcal{G}_{0q}]Vu, \tag{3.9}$$

where ω_q and ϕ_q are arbitrary but known functions and

$$\mathcal{G}_{0q}\equiv G_0-\,|\,\omega_q)(\phi_q\,|\,. \tag{3.10}$$

Equation (3.9) can be written as

$$(1-\mathcal{G}_{0q}V)u=u_0+\omega_q C_q, \tag{3.11}$$

where $C_q = (\phi_q|V|u)$, which is of course unknown. If we solve, for given ω_q and ϕ_q,

$$X=\frac{1}{1-\mathcal{G}_{0q}V}u_0,\qquad Y=\frac{1}{1-\mathcal{G}_{0q}V}\omega_q, \tag{3.12}$$

then

$$u=X+YC_q=X+Y\frac{(\phi_q\,|\,V\,|\,X)}{1-(\phi_q\,|\,V\,|\,Y)}, \tag{3.13}$$

and

$$K=(u\,|\,V\,|\,u_0)=(u_0\,|\,V\,|\,u)=(u_0\,|\,V\,|\,X)+\frac{(u_0\,|\,V\,|\,Y)(\phi_q\,|\,V\,|\,X)}{1-(\phi_q\,|\,V\,|\,Y)}. \tag{3.14}$$

For $\phi_q = u_0$, we have

$$K=\frac{(u_0\mid V\mid X)}{1-(u_0\mid V\mid Y)}. \tag{3.15}$$

The convergence of the series expansion of $(1-\mathscr{G}_{0t}V)^{-1}$ has been studied in detail by Coester.[10] Austern[9] formulated an iteration procedure for X and Y with the choice $\omega_q = G_0 V u/C_q$ and $\phi_q = u_0$. Such procedure is found to be much better than the simple Born series obtained by $(1-G_0V)^{-1}$, but requires modifications[7] when V gets too large. In the present discussion, we consider a variational treatment of (3.12). As in Sec. II, we may set

$$W(1-\mathscr{G}_{0q}V)X=Wu_0,$$
$$W(1-\mathscr{G}_{0q}V)Y=W\omega_q, \tag{3.16}$$

and construct the functionals for a symmetric $W(1-\mathscr{G}_{0q}V)$:

$$J_t^{(X)}=-(X_t\mid W(1-\mathscr{G}_{0q}V)\mid X_t)+2(X_t\mid W\mid u_0),$$
$$(3.17)$$
$$J_t^{(Y)}=-(Y_t\mid W(1-\mathscr{G}_{0q}V)\mid Y_t)+2(Y_t\mid W\mid \omega_q).$$

Different choices for W are now possible, such as $W=V$ and $W=V\mathscr{G}_{0q}V$, etc. Instead, we first derive differential equations equivalent to (3.16) by inverting $\mathscr{G}_{0q}$; that is,

$$\mathscr{G}_{0q}^{-1}=G_0^{-1}-G_0^{-1}\mid\omega_q)\frac{1}{1+(\phi_q\mid G_0^{-1}\mid\omega_q)}(\phi_q\mid G_0^{-1}$$
$$\equiv E-\mathscr{H}_{0q}. \tag{3.18}$$

Define

$$\mathscr{H}_q\equiv\mathscr{H}_{0q}+V,$$
$$X\equiv u_0+x, \tag{3.19}$$
$$Y\equiv\omega_q+y,$$

then,

$$(E-\mathscr{H}_q)x=Vu_0, \tag{3.20a}$$

$$(E-\mathscr{H}_q)y=V\omega_q, \tag{3.20b}$$

which are equivalent to (2.5) with the quasipotential and are identical in structure to (3.8). Incidentally we note in (3.15) that for $\phi_q = u_0$, $(y|V|u_0) = (\omega_q|V|x)$ so that an approximation to x will be enough to evaluate the amplitude K. But such estimate will not be variational. A slightly simpler procedure may be to combine the two equations in (3.20). With $u\equiv u_0+\omega$ as before, we can get

$$(E-\mathscr{H}_q)\omega=Vu_0+(E-\mathscr{H}_{0q})\omega_q C_q\equiv B_q, \tag{3.21}$$

where $C_q = (\phi_q|V|u)$, and the right-hand side is known except for the C_q. When $\omega_q = G_0Vu_0$, we have

$$(E-\mathscr{H}_{0q})\omega_q=V\mid u_0)\frac{1}{1+(\phi_q\mid V\mid u_0)}, \tag{3.22}$$

and the right-hand side of (3.21) simplifies to

$$(E-\mathscr{H}_q)\omega=V\mid u_0)\widetilde{C}_q, \tag{3.23}$$

where

$$\widetilde{C}_q=\frac{1-(\phi_q\mid V\mid\omega)}{1+(\phi_q\mid V\mid u_0)}, \tag{3.24}$$

which is consistent with (3.2), (3.3), and (3.4), $(\phi_q\rightarrow\xi)$.

We have thus shown that (3.2) has the same structure as (3.8) and (3.20a). In particular, the variational treatment of the Sasakawa-Austern procedure is similar to the approach of Ref. 6 considered recently.

IV. MULTICHANNEL SCATTERING AND EXCHANGE EFFECTS

The results of Secs. II and III for the potential scattering may be extended to composite-system scattering with or without the full exchange effect and also to multichannel scattering. Our discussion will be brief, as most of these extensions are straightforward except for the exchange effect.

A. Composite-system scattering—single-channel process

When the antisymmetrization between the incoming electron and target electrons is neglected, the Hamiltonian of the system can be written as

$$H=T+H_A+V\equiv H_0+V, \tag{4.1}$$

where T is the kinetic energy of the projectile electron, H_A is the internal Hamiltonian of the target atom (or ion), and V is the projectile-target interaction. As will be considered later, this separation of H into the H_0 and V parts is *not* possible if the exchange effect is to be included. H_0 can include the central part of the long-range Coulomb interaction in case of ionic targets. The full scattering function Ψ may be written as

$$\Psi=\Phi+G_0V\Psi, \tag{4.2}$$

with

$$(H_0-E)\Phi=0 \text{ and } (H_0-E)G_0=-\delta.$$

In terms of the target functions ψ_n generated by H_A, we have $\Phi = \psi_0 u_0^{(o)}$, where $u_0^{(o)}$ is the "free" wave function (including the static long-range scattering part.) Except for the fact that the trial functions now carry all the coordinates of the electrons involved, the formalisms for the composite particle scattering are identical to the potential scattering case, with the replacements $u_0 \to \Phi$, $u \to \Psi$, and $H_0 = T + H_A$. Thus, for example, (2.26b) becomes

$$J_t^{(d)} = \sum_{n,m}^{N} (\widetilde{C} \mid \phi_n^b) \times \left[\frac{1}{(\phi_i^b \mid E - H_0 - VG_0V \mid \phi_j^b)} \right]_{nm} (\phi_n^b \mid \widetilde{C}), \quad (4.3)$$

where

$$\widetilde{C} = (V + VG_0V)\Phi,$$

and the basis functions ϕ_n^b are introduced through an expansion

$$\Omega \equiv G_0 V \Psi = \sum_n^N a_n \phi_n^b.$$

Alternatively, for (3.23), we have

$$(E - \mathscr{H}_q)\Omega = V\Phi\widetilde{C}_q, \quad (4.4)$$

where

$$\widetilde{C}_q = \frac{1-(\phi_q \mid V \mid \Omega)}{1+(\phi_q \mid V \mid \Phi)},$$

and

$$\mathscr{H}_q = H - (H_0 - E) \mid \omega_q) \times \frac{1}{1+(\phi_q \mid E - H_0 \mid \omega_q)} (\phi_q \mid H_0 - E).$$

B. Multichannel scattering

Neglecting again the exchange effect and the ionization channels,[11] we can formulate the multichannel case in a trivial way by generalizing $\{\phi_i\}$, Φ, Ψ, and G_0 to multicomponent forms in which all the open channels are included.[3] Thus, for example, $J_t^{(d)}$ of (4.3) becomes

$$J_t^{(d)} = \sum_{\alpha\beta} \sum_{\alpha'\beta'} \sum_{nm} (\Phi_\alpha \mid \widetilde{V} \mid \phi_{\alpha' n}) \left[\frac{1}{(\phi_{\alpha'' i} \mid (E - H_0)\delta_{\alpha''\beta''} - VG_{0\alpha''\beta''}V \mid \phi_{\beta' j})} \right]_{\substack{\alpha'\beta' \\ nm}} (\phi_{\beta' m} \mid \widetilde{V} \mid \Phi_\beta), \quad (4.5)$$

where

$$\widetilde{V}_{\alpha\beta} = (V + VG_0V)_{\alpha\beta} \equiv \left[V + \sum_{\alpha'} V(G_0)_{\alpha'\alpha'} V \right]_{\alpha\beta}.$$

In (4.5), α and β are the channel labels. Similar generalizations can also be made for (3.21).

C. Exchange effect

For scattering of electrons by atomic (or ionic) targets, the total scattering wave function of the system should be completely antisymmetric under the exchange of any pairs of electrons. This in turn requires that all the operators we have dealt with in our discussion thus far should be symmetric under the electron pair exchanges. Obviously, H is completely symmetric, but as soon as we write $H = H_0 + V$ where $H_0 = T + H_A$, H_0 and V are not separately symmetric any more, even though the target electrons are still treated symmetrically. Thus, the exchange effect between the projectile and target electrons has been neglected in the Schwinger VP and all the other formulations above. Since a symmetric V is not readily available, modification of the formulas derived in Secs. II and III to incorporate this effect is *not trivial.*

Before modifying (2.5) and (2.8), we first consider a way to construct the symmetric V. For a specific choice of the projectile electron, we have for example,

$$H_0 \equiv T(\vec{r}_0) + H_A(\vec{r}_1\vec{r}_2 \cdots \vec{r}_A),$$

and

$$(H_0 - E)(\psi_0(\vec{r}_1\vec{r}_2 \cdots \vec{r}_A)u_0^{(0)}(\vec{r}_0)) = 0. \quad (4.6)$$

Now define the antisymmetrized function[12]

$$\Phi(\vec{r}_0\vec{r}_1 \cdots \vec{r}_A) = \mathscr{A}(\psi_0(\vec{r}_1 \cdots \vec{r}_A)u_0^{(0)}(\vec{r}_0)) \quad (4.7)$$

and construct implicitly a new H_0^A such that Φ is a solution,

$$(H_0^A - E)\Phi = 0. \quad (4.8)$$

In general, H_0^A is a complicated operator but is symmetric under the exchange of any electron pairs. Thus the desired V^A is

$$V^A \equiv H - H_0^A \quad \text{and} \quad H_0^A = H - V^A. \tag{4.9}$$

A more direct way is to combine (4.8) and (4.9) and write

$$V^A = (H-E)\Phi/\Phi \equiv D\Phi/\Phi, \quad D \equiv H - E. \tag{4.10}$$

The expression (4.10) for V^A *can* be evaluated for a given form of Φ, (4.7), and thus the formulas derived in Secs. II, III, and IV above can be retained with V replaced by V^A of (4.10). At least, formally, $H_0^A = H - V^A$ and $G_0 = (E - H_0^A)^{-1}$.

From a practical point, it is more desirable if a particular formula is rewritten in terms of Φ and H alone, without ever introducing V and H_0 explicitly.

1. Schwinger VP (2.15b). The right-hand side of (2.15b) can be written as $B_0 = V\Phi = D\Phi$. On the other hand, the denominator $(\Psi_t | V - VG_0V | \Psi_t)$ cannot be transformed to an expression with only D. Thus, we need V^A and H_0^A explicitly in accordance with (4.10) and (4.9). For (2.15a), we have

$$J_t^{(a)} = \frac{(\Phi | V^A | \Psi_t)(\Psi_t | V^A | \Phi)}{(\Psi_t | V^A - V^A G_0^A V^A | \Psi_t)}. \tag{4.11}$$

This is probably too complex to be of practical use, and the situation is similar with $J_t^{(c)}$ of (2.23) and $J_t^{(d)}$ of (2.26b).

2. Equation (2.19). $J_t^{(b)}$ can be written without explicitly evaluating V^A and H_0^A, as

$$J_t^{(b)} = \sum_{n,m}^{N} (\Phi | \overleftarrow{\mathrm{D}} | \phi_n^b) \times \left[\frac{1}{(\phi_i^b | E - H | \phi_j^b)} \right]_{nm} (\phi_m^b | \overrightarrow{\mathrm{D}} | \Phi), \tag{4.12}$$

where $\overleftarrow{\mathrm{D}}$ implies the operator D to act on functions to its left. For square-integrable basis functions ϕ_n^b, however, this restriction is not necessary.

3. Equation (3.20a). The equation for $\mathcal{X} = X - \Phi$ is

$$(E - \mathscr{H}_q)\mathcal{X} = V\Phi = D\Phi, \tag{3.20'}$$

where

$$\mathscr{H}_q = H - E + G_0^{-1} | \omega_q) \frac{1}{1 + (\phi_q | G_0^{-1} | \omega_q)} (\phi_q | G_0^{-1}. \tag{3.18'}$$

For specific choice of $\omega_q = G_0 D\Phi$, (3.18′) becomes

$$\mathscr{H}_q = D + D | \phi) \frac{1}{1 + (\phi_q | D | \phi)} (\phi_q | G_0^{-1}. \tag{4.13}$$

Noting that G_0^{-1} is not Hermitian if ϕ_q is not square integrable, we have to have H_0^A for the last $(\phi_q | G_0^{-1}$ factor in (4.13). On the other hand, (3.20b) cannot be transformed into a form independent of H_0^A and V^A. The situation is similar for (3.9) and (3.11).

An alternative approach for the exchange scattering is to regard the exchange channels as special rearrangement channels and to extend the scattering function space to a multicomponent matrix space.[13,14] The structure of the theory then becomes formally identical to that of the potential theory of Secs. II and III. With proper identifications of the V's and D's, explicit variational principles can be formulated.

V. DISCUSSION

A unified variational treatment of the inhomogeneous scattering equations has been presented which clarifies the relationship between the various formulations considered previously. In particular, the results of Refs. 6, 7, 8, and 9 are shown to be closely related through the quasipotential approach of Sec. III. The general approach adopted here in terms of the W operator suggests many other possible forms of VP, specially of the asymmetric A of (2.8). Possibilities of bound principles[5] and the inclusion of the ionization channel[11] within the present formalism have not been discussed here, and will be treated extensively elsewhere.

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