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Generalization of the Hartree-Fock approach to collision processes

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The conventional Hartree and Hartree-Fock approaches for bound states are generalized to treat atomic collision processes. All the single-particle orbitals, for both bound and scattering states, are determined simultaneously by requiring full self-consistency. This generalization is achieved by introducing two *Ansätze*: (a) the weak asymptotic boundary condition, which maintains the correct scattering energy and target orbitals with correct number of nodes, and (b) square integrable amputated scattering functions to generate self-consistent field (SCF) potentials for the target orbitals. The exact initial target and final-state asymptotic wave functions are not required and thus need not be specified *a priori*, as they are determined simultaneously by the SCF iterations. To check the asymptotic behavior of the solution, the theory is applied to elastic electron-hydrogen scattering at low energies. The solution is found to be stable and the weak asymptotic condition is sufficient to produce the correct scattering amplitudes. The SCF potential for the target orbital shows the strong penetration by the projectile electron during the collision, but the exchange term tends to restore the original form. Potential applicabilities of this extension are discussed, including the treatment of ionization and shake-off processes. [S1050-2947(97)03806-7]

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I. INTRODUCTION

Many-particle bound systems are often treated by a self-consistent field (SCF) approach, where the wave function for a complex interacting system is represented by products of single-particle orbitals and the interactions are given by the SCFs of all the other particles. Thus the Hartree [1] and Hartree-Fock (HF) [2] approaches to atomic bound-state problems involving many electrons have been employed extensively and various extensions and refinements, including multiconfiguration mixing, the random-phase approximation, and relativistic theories for high- Z ions, have been successfully applied to many ionic and molecular as well as solid-state problems. The theory has also been applied to treating multiply excited states where the configuration energies may lie above the first ionization threshold. With currently available computers, atomic and molecular structures are routinely calculated [3–7]. The wave functions thus generated are often sufficiently accurate for evaluation of various transition matrix elements. In all cases, however, the individual orbital energies are negative and the corresponding wave functions are square integrable.

Previous attempts to extend the approach to scattering problems involving continuum orbitals have met with various conceptual and technical complications. The principal difficulties in extending the theory are well known: (i) the non-normalizability of the continuum scattering function makes the SCF averaging of the potentials using the continuum orbitals inoperative and (ii) the strong asymptotic boundary condition requires exact target internal functions prior to solving the scattering problem. Most textbooks on the HF theory do not even mention these difficulties. Nevertheless, some attempts have been made over the years to extend the theory to collision problems, with little success. An early study separated [8] the open channel space from the rest in the determinantal set of scattering equations, estimated [9] the accuracy requirement of the target function to approximately satisfy the necessary boundary condition, or introduced complex collision energy [10], complex coordinates [11], etc. Of course, there are many other approaches to scattering problems, which are fully developed and commonly used [12,13] but are not SCF theories.

The Hartree and Hartree-Fock approaches are generalized here to atomic scattering problems, in which the difficulties (i) and (ii) are removed simultaneously in a self-consistent way and all the orbitals are treated on an equal footing. Full self-consistency can be imposed [14], exactly as in the bound-state case, without wave-packet construction and box normalization with periodic boundary conditions. In the generalized HF (GHF) theory, to be discussed in Sec. II, the bound and continuum orbitals can be systematically improved by incorporating configuration interactions. To test the present approach, the GHF theory was applied [14,15] earlier to the simplest scattering systems of positron-hydrogen scattering below the first pickup threshold and to electron-hydrogen scattering without exchanges, below the $n=2$ excitation threshold. The preliminary result is very encouraging and the calculation is extended here to include the exchange effect.

It is important to distinguish the present approach from all the existing scattering theories in which the asymptotic boundary conditions must be specified ‘‘exactly’’ in order to properly define the scattering problem. This condition is relaxed in the GHF approach, however. Thus, for example, we consider the R-matrix method, which is perhaps the most accurate procedure available for low-energy scattering. First of all, in the R-matrix approach, the exact asymptotic cluster functions (such as oxygen atom in its ground and some excited states in the e^{-}O scattering) have to be prepared to specify the asymptotic conditions. Since this cannot be done in practice when the bound clusters involved in the asymptotic region have more than one electron, naturally the question of how good these functions should be arises. (We are not talking here about the distortion inside the matching radius.) The usual recipe is that the bound cluster functions should be ‘‘much better’’ than the desired accuracy of the scattering amplitudes. The GHF approach answers this questions automatically, where all the orbitals, including the asymptotic ones, are calculated self-consistently at the same time. Second, the most profound difference between the GHF theory and all other collision theories is that the asymptotic conditions are never assumed to be imposed exactly in the GHF approach, even in the hydrogen case, as the example in this paper will show. Third, the division of the space into the inner and outer regions and subsequent matching are not present in the GHF approach. This also has the advantage when high Rydberg states with long wave-function tails are treated by the same amputation.

The SCF approach presented below seems to work. The examples considered are for the purpose of showing the convergence to the correct asymptotic values rather than getting the exact phase shifts. These will come later with multiconfiguration mixing, especially for complex targets.

II. THEORY OF THE GHF APPROACH

In order to discuss the main elements of the theory of the GHF approach, we concentrate on the two-electron systems, such as He and e^-H, without loss of essential aspects of the theory. The total Hamiltonian is written as $H=K_1+K_2+V_1+V_2+V_{12}$, in obvious notation. In a single-configuration approximation, the HF wave function for the bound system is written as $\Psi_{\mathrm{HF}}=]\psi_a(1)\psi_b(2)+\varepsilon\psi_a(2)\psi_b(1)]/\sqrt{2}$, where $\varepsilon=+1$ or -1 for $S=0$ or 1, respectively, and $(\psi_\alpha,\psi_\beta)=\delta_{\alpha gb}$ for $\alpha,\beta=$ a or b. The bound-state Hartree-Fock equations are obtained by the projections, as

$$(\psi_\alpha,[H-E_t]\Psi_{\mathrm{HF}})=0. \tag{1}$$

Here the normalizability $(\psi_\alpha,\psi_\beta)=\delta_{\alpha,\beta}$ is essential. The HF equations (1) can also be derived by a variational principle. When all the orbitals involved are of the bound-state type, then the $\psi_\alpha$are square integrable and the integrations implied in Eq. (1) are well defined. Thus the HF orbital equations (1) are mutually coupled, nonlinear, and contain the self-consistent mean fields for each bound electron $i=1$ or 2.

We now try to extend Eq. (1) to scattering problems in which one of the electrons occupies a continuum orbital $c=(e_c,l_c)$ with collision energy e_c and the orbital angular momentum l_c. The simple single-configuration wave function may be given in the form $\Psi_{\mathrm{GHF}}=\psi(1)u(2)+\varepsilon\psi(2)u(1)$, where ψ denotes the bound-state orbital and u the continuum orbital. To make the problem simpler, we limit the scattering energy to the single-channel elastic region $0\leqslant e_c<0.75$ Ry, i.e., the total E in the range -1 Ry $\leqslant E<-0.25$ Ry, where $E=e_c+E_b$. The asymptotic boundary condition for the direct channel is given by $(l_c=0)$

$$\Psi_{\mathrm{GHF}}\rightarrow\psi_{b1}(\vec{r}_1)u_c(\vec{r}_2), \tag{2}$$

where

$$(K_1+V_1)\psi_{bn}=E_{bn}\psi_{bn}(\vec{r}_1), \tag{3a}$$

$$u_c(r)=s(r)+c(r)\rightarrow[\sin(p_cr)+R_0\cos(p_cr)]/(p_cr), \tag{3b}$$

and R_0 is the reactance matrix ($R_0=\tan\delta_0$). The exact target function $\psi_{b1}=\psi_{1s}$ is required in Eq. (2) for the asymptotic boundary condition and this function must be supplied beforehand in order to fully define the scattering problem to be solved. For target atoms with more than one electron, this is in general not possible and the question of how accurate such functions should be arises.

Now we derive a set of SCF equations analogous to Eq. (1) for the scattering problem posed above. Due to the fact that $(u,u)=\infty$, however, it is not possible to project the Schrödinger equation using the orbital u for the function ψ, as in Eq. (1). Furthermore, if the requirement on the target function ψ is relaxed, so that ψ is no longer exact, then the scattering energy $e_{ct}=E-E_{bt}\neq e_c$ and this will change the scattering function u. These two points are directly related to the difficulties (i) and (ii) discussed above. To resolve these difficulties, we introduce two simple operational *Ansätze.* First, for the purpose of projections of the form (1), we introduce the amputated wave function (AWF) in place of u, as

$$X(2)\equiv(e_c-K_2)u(2)\quad(\mathrm{AWF}). \tag{4}$$

Evidently, X is a square-integrable function, with $\langle X|X\rangle_{\vec{r}}<\infty$. This function then can be used in the projection of the equation for the ψ orbital. The introduction of the AWF is based on the observation that the essential dynamical information carried by u is in X and not in the long-range tail represented by the asymptotic part of u. On the other hand, the tail gives rise to the non-normalizability difficulty. There may be other ways of constructing a square-integral function for the projection purpose, but the AWF cleanly gets rid of this troublesome part. The equation for the target function ψ is then given by

$$\langle X(2)|H-E_t|\Psi_{\mathrm{GHF}}(1,2)\rangle_{\vec{r}_2}=0, \tag{5}$$

Now we proceed to deriving the equation for the u orbital. This can be done immediately using the ψ to project the scattering equation. The only problem is that now, due to the approximate nature of the ψ function itself, the scattering energy is no longer e_c. To remedy this situation, we introduce the second *Ansätz*, by requiring that

$$\langle\psi(1)|[E_{bt}-K_1-V_1]|\psi(1)\rangle_{\vec{r}_1}\rightarrow0\quad(\mathrm{WAC}). \tag{6}$$

which defines E_{bt} for given ψ obtained from Eq. (5). The weak asymptotic condition (WAC) (6) allows us not only to retain the exact scattering energy e_c throughout the SCF iteration cycles, but also places a constraint on ψ to satisfy approximately the condition (2). However, it is not at all clear *a priori* whether Eq. (6) is strong enough to lead to the correct solution of the original problem of the elastic scattering. This is tested in the example given below. Now we have

$$\langle\psi(1)|H-E_t|\Psi_{\mathrm{GHF}}(1,2)>_{\vec{r}_1}=0 \tag{7}$$

with the *Ansatz* (6). The coupled equations (5) and (7) are reduced to the form

$$[K_2+U_c(2)-e_c]u(\vec{r}_2)=-\varepsilon Y_c(\vec{r}_2), \tag{8a}$$

$$[K_1+U_b-E_{bX}]\psi(\vec{r}_1)=-\varepsilon Y_b(\vec{r}_1), \tag{8b}$$

where

$$U_c(2)\equiv\langle\psi|V_{12}+V_2|\psi\rangle_{\vec{r}_1}/\langle\psi|\psi\rangle_{\vec{r}_1}, \tag{9a}$$

$$E_{bX}=E_{bt}-E_{X1}-E_{X2}=E_{bt}-E_X, \tag{9b}$$

$$V_X(1)\equiv\langle X|V_{12}+V_1|u_{\vec{r}_2}>/\langle X|u\rangle_{\vec{r}_2}$$
$$\equiv E_{X1}+U_b(1)\rightarrow E_{X1} \quad \text{as} \quad r_1\rightarrow\infty, \tag{9c}$$

which defines both E_{X1} and U_b, and

$$E_{X2}=\langle X(2)|K_2-e_c|u(2)\rangle_{\vec{r}_2}/\langle X|u\rangle_{\vec{r}_2}. \tag{9d}$$

The exchange terms are defined by

$$Y_c(2)=\langle\psi(1)|H-E_t|u(1)\rangle_1\psi(2)/\langle\psi|\psi\rangle, \tag{10a}$$

$$Y_b(1)=\langle X(2)|H-E_t|\psi(2)\rangle_2 u(1)/\langle X|u\rangle. \tag{10b}$$

In Y_b, the term proportional to $u(1)$ is dropped to ensure ‘‘approximate orthogonality’’ between X and ψ. More explicitly, the term $\langle X|K_2+V_2-E_{bt}|\psi\rangle$in Y_b is dropped to ensure that the spurious long-range contribution to Y_b is absent. This term is generally small and should approach zero as the target function ψ improves with the multiconfiguration interaction. Furthermore, this term represents the overlap between the two amputated functions X and $\chi_b=(K_2+V_2-E_{bt})\psi$ and thus, if nonzero, must be eliminated using a Lagrangian multiplier, in complete analogy with the bound-state HF case. We also note that Y_b turned out to be very small, as compared with U_b and V_1. Reasons for this unexpected but desirable feature of the theory are not yet clear.

It is simple to convert u to X and vice versa, as from Eq. (8a) $u=s+gU_cu+\varepsilon gY_c$, where $g=(e_c-K_2)^{-1}$, or $X=g^{-1}u=U_cu+\varepsilon Y_c$ since $g^{-1}s=0$. All the integrals in expression (8) are finite, thus the difficulty (i) is eliminated. The set (8), with Eqs. (4) and (6), is the desired set of SCF equations for the GHF approach, in its lower-order approximation without the configuration interaction. It is important to maintain the mathematical consistency of Eq. (9b) with Eq. (9a) plus Eq. (7).

We emphasize that the formulation given above will be valid if the two *Ansätze*, the AWF and the WAC, can deliver the correct amplitudes that satisfy the original boundary conditions. The convergence of the asymptotic boundary condition is therefore the critical test of the theory. This is not *a priori* apparent. The example given in Sec. III is to demonstrate this point (and not so much to calculate the correct phase shift) within the simple static and static-exchange approximations. The full demonstration of the problem requires the multiconfiguration interaction, which we plan to report on in the future.

III. HERMITICITY OF THE GHF EQUATIONS

A comment on the projection procedure is in order. The usual coupled-channel method proceeds with the expansion of the type Ψ_{HF} or Ψ_{GHF} and the projection is carried out using the same basis set involved in the total wave function. In fact, it is not necessary that we have to project in this way. Apparently, this is not the case with Eq. (5), where the amputated function X was used instead. In general [15] we may introduce weighting functions W during the projection and let

$$\langle\psi_i|W_i[H-E]|\Psi_t\rangle=0, \tag{11}$$

where different W_i may be associated with each ψ_i. All the integrals in Eq. (11) are then well defined. Therefore, in the case of the GHF approach, the amputation of u may be viewed as a special example of the weighted projection, with the weight function $W\simeq U_c$, or $Wu\simeq U_cu+\varepsilon Y_c$. Such a procedure can be effective if a judicious choice of the weight function W is made. Further generalizing this aspect of the approach, the weighted projection method in the context of the coupled-channel theory has been discussed in detail in Ref. [15], where proper construction of W to optimize the coupled-channel equations was illustrated.

We simply note that the procedure (11) is related to the variational principle with a trial function $GV\Psi$ and making a closure approximation on the Green’s function G such that $GV\Psi\rightarrow(E-\overline{E})^{-1}V\Psi=\alpha_tV\Psi$ a new trial function, with α_t as a constant variational parameter. Here the weight function was the interaction potential V. This form was previously used effectively in deriving the nucleon-nucleus potential [16].

A more serious problem with the use of the weighting function in the projection procedure is the fact that often the resulting set of coupled equations is not apparently ‘‘symmetric’’ with respect to the initial- and final-state exchanges. That is, due to the noncommutativity of W with H, in general, the projected operators are not Hermitian. We had similar situations with the usual sturmian function expansion of the total wave function, where the normalization of the basis set is defined in terms of the weighting potential; the scattering equations are projected onto different basis function subspaces with the weighting potentials, resulting in a set of coupled equations with the operators that are not Hermitian. The non-Hermiticity can violate unitarity. (For a slightly different reason, the Faddeev equations also give an asymmetric set of operators that couple different rearrangement channels; this is only in appearance, and the resulting amplitudes are quite symmetric.)

Therefore, in order to avoid possible spurious properties, it is useful to check the Hermiticity of the equations involved in the GHF approach. As is shown below, in fact, the Hermiticity is preserved in an asymmetric projection (11). The Hermiticity of the coupled set of equations for u and ψ may be demonstrated by showing that the particular choice of the weighting function W in the amputation is such that $[H,W]=0$. This property should be useful in guaranteeing the unitarity of the scattering amplitude, especially when multichannel scattering is involved, and in securing the real bound-state energies. First, the u equation (7) is obtained with the weighting function $W=1$, so that the resulting operator after the ψ projection from the both sides is Hermitian. Therefore, we concentrate on Eq. (5), in which, due to the use of the left weight W in the function X, the resulting operator for ψ may not be Hermitian. However, we recall the special form of the amputation (4), which can be combined with Eq. (8a), as

$$X(2)=[U_c(2)+\varepsilon I_c]u, \tag{4'}$$

where I is the exchange integral operator, and the commutativity within I also follows in the same way. Evidently, $I_c u = Y_c$. In Eq. (5) the K_2-dependent term is symmetric when Eq. (4) is used for X, as the two K_2 operators involved are the same. On the other hand, the rest of the terms in Eq. (5) may be made Hermitian by using Eq. (4′). This completes the proof. Note that the Hemiticity of the operators in the coupled SCF equations is guaranteed here by the very special choice of the amputating operator. In some sense, this suggests that the choice of W in amputating u adopted here may be unique.

IV. CALCULATION OF ELECTRON AND POSITRON SCATTERING FROM HYDROGEN

This section attempts to show that the GHF theory formulated in Sec. II with two principal *Ansätze* works in the sense that the overall solution satisfies approximately the correct asymptotic boundary conditions (ABC). Since the requirement on the ABC is changed to an approximate one in the GHF theory, it is not automatically satisfied. Although in the present case where the ABC can be specified exactly in terms of the hydrogenic function, the GHF theory takes the SCF value, as will be clear below.

The simple set of equations derived above is applied to the single-channel electron-hydrogen scattering, with $L=0$, the scattering energy e_c below the excitation threshold, i.e., $e_c<0.75$ Ry, and the total energy $E<-0.25$ Ry. Recently, we applied the generalized Hartree approximation (GHA) to the positron-hydrogen and electron-hydrogen scatterings without exchanges [14]. They are perhaps the simplest examples in which the theory may be tested. The fact that the exact target states are available provides a convenient basis to examine the validity of the theory without getting involved in the complicated numerical analysis. The physics involved in the collision are clearly brought out by this mean-field picture.

The solution of Eq. (8) involves the following iteration steps for self-consistency.

(a) First, we arbitrarily choose $\psi\simeq\psi_{1s}$ and $E_{bt}\simeq-1$Ry. The potential $U_c=\langle\psi|V_{12}+V_2|\psi\rangle_{\vec{r}_1}$ is evaluated; let $Y_c=0$ for the first iteration, with $\langle\psi|\psi\rangle_{\vec{r}}=1$.

(b) Equation (8a) is numerically solved for u and the phase shift δ_{GHF} evaluated in accordance with Eq. (5b), for the scattering energies $e_c=(p_c a_0)^2$ Ry. This gives the phase shift δ_{STT}, corresponding to the static approximation without exchange. The resulting u is used to evaluate the exchange term Y_c. Repeat the $u$calculation until a self-consistency is reached with the exchange term.

(c) The amputated function $X=(e_c-K_2)u=U_c u+\varepsilon Y_c$ is evaluated using the scattering function u calculated in (b) above.

(d) Evaluate the effective potential U_b and the constants E_{X1} and E_{X2}, as well as the exchange term Y_b. Solve Eq. (8b) for ψ and the energy E_{bX}. The correct binding energy E_{bt} is then calculated by $E_{bt}=E_{bX}+E_X$ from (9b).

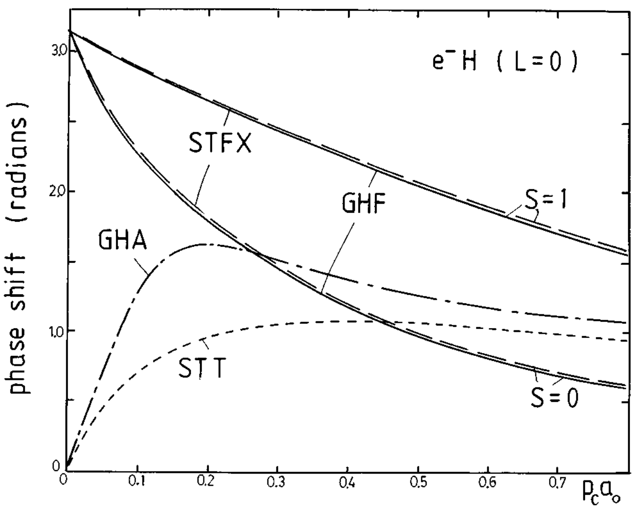

FIG. 1. Phase shifts for the elastic electron-hydrogen scattering are calculated in the various approximations for both the singlet and triplet states; STT denotes the static approximation without exchange and STFX the static approximation with exchange effects included. In STT and STFX, the exact target function ψ_{1s} is used for comparison. GHA denotes the Hartree approximation with $\psi \neq \psi_{1s}$ and without the exchanges. GHF denotes the phase shift obtained in the GHF approximation, where both the target function and the scattering function are simultaneously determined self-consistently. The GHF values (solid curves) are very close to that of STFX (dashed lines) for both $S=0$ and 1.

(e) This completes the full iteration cycle. If the resulting energy E_{bt} and the phase shift δ from u are not within the small allowed change from the previous iteration values, then we go back and repeat the first four steps above, until the self-consistency is attained. This way, both the target function ψ with its orbital energy E_{bt} and the scattering function u with the phase shift δ are simultaneously determined.

The converged phase shifts for the singlet and triplet states in the electron-hydrogen elastic scattering are presented in Fig. 1, together with the static without exchanges (STT) and the static exchange (STFX) approximations for comparison. Here both the STT and STFX approximations are determined with the exact ψ_{1s}. The GHA is equivalent to the STT approximation and the ψ calculated from Eq. (8b) without the exchange term Y_b. The GHF approach with one configuration in Ψ_{GHF} gives phase shifts that are very close to the STFX values, for both $S=0$ and 1. This is surprising because the apparent enhancement in $\delta_{\mathrm{GHA}}$is wiped out when the exchange term is added in the u equation. This may be understood from the symmetry (or antisymmetry) of the wave functions; when the projectile penetrates the bound orbital, we can assign the penetrated electron as the new ‘‘inner core’’ electron without changing the physics. In this sense, the GHF theory describes a quite different physics from the GHA. The approximate target function ψ calculated with Eq. (8b) also turned out to be very close to that of the exact value. Nevertheless, the GHF binding energy E_{bt} deviates slightly from -1 Ry. This variation in the binding energy is given in Fig. 2, where $\Delta E_{bt}=E_{bt}-E_{1s}$is plotted for $S=0$ and 1. The smallness of ΔE_{bt} shows that the weak asymptotic condition (6), which replaces the exact one in Eq.

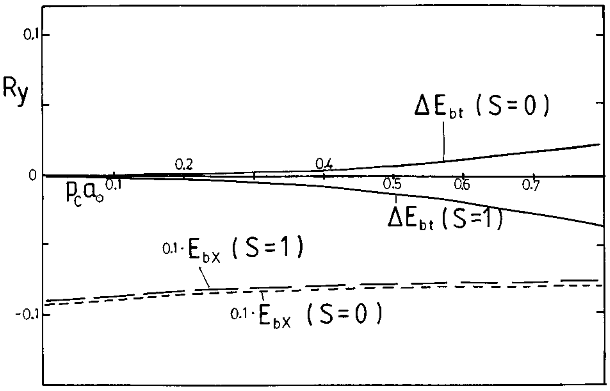

FIG. 2. The apparent binding energy E_{bX} as determined by Eq. (9b) and the actual binding energy E_{bt} are shown for the singlet and triplet spin states. Although the potential U_b is quite distinct from the Coulombic V_1, E_{bt} is very close to the exact value of -1 Ry. The energy shift is $E_X = E_{X1} + E_{X2} = E_{bt} - E_{bX}$. We present $\Delta E_{bt} = E_{bt} - E_{1s}$, showing the strong energy dependence. e_c(Ry) $= (p_c a_0)^2$. The effective binding energy in the potential U_b is also given $E_{bX}|10$ for both $S=0$ and 1.

(3a), still places a strong enough constraint on the solution to lead eventually to the correct boundary condition. Also shown in Fig. 2 is the actual energy E_{bX} obtained from Eq. (8b). The final E_{bt} is obtained from this by adding the shift E_X.

Incidentally, we also calculated the excited-state scattering using the same GHF code by simply setting the approximate energy values for the $2s$, $3s$, etc., states. The solutions automatically converged to the specific asymptotic values as long as the initial choice was close to one particular energy E_{bnt}. The converged energies for the bound electron are close to $-1/n^2$Ry and the corresponding wave functions have the correct numbers of nodes associated with the particular n. However, none of these functions are exact, as they are determined by the self-consistency. This is also the case with the $1s$ scattering, where the exact wave function is known, but the GHF approach instead approximately determines it by the SCF. The only way to confirm whether the calculated wave function corresponds to that of the desired channel is to ''count nodes'' of the wave function. This is in fact precisely the behavior we encounter in the bound-state calculation by the conventional HF procedure; a bad initial guess at the binding energy allows drift in the calculated values to some other n states of the same symmetry. On the other hand, the scattering energy e_c remains the same throughout the iterations. We do not pursue this interesting aspect of the GHF approach further here because for excited target scattering we have to include all the open channels with channel binding energies larger than that particular excited state, and this requires automatically the generalization of the GHF computation described in Sec. V.

Another unexpected result of this calculation is that the effective potential U_b for the bound orbitals is nearly one-half of the direct potential V_1, for $r > 3a_0$. This large deviation found in U_b from V_1 is apparently caused by the penetration of the target cloud by the projectile electron. This time this penetration effect is explicitly demonstrated using the SCF picture. As a result, the corresponding energy shift

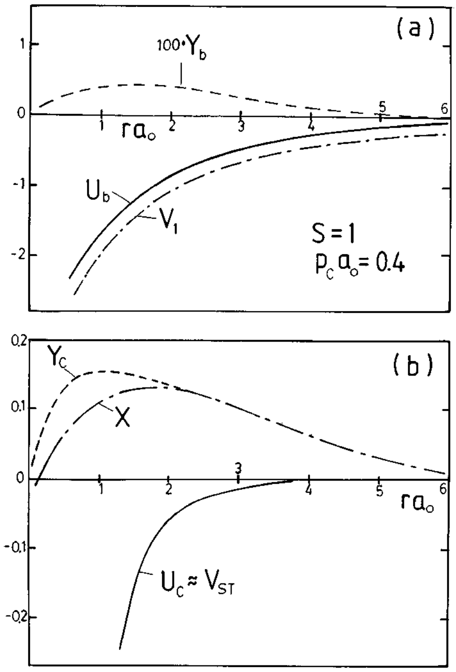

FIG. 3. (a) The SCF iteration-converged potential U_b and the exchange term Y_b are given for $p_c a_0 = 0.4$ and $S=1$. The direct potential is compared with the pure Coulombic potential V_1. Note the drastic change in U_b from V_1. (b) The effective direct potential U_c and the exchange term Y_c are shown for $p_c a_0 = 0.4$ and $S=1$. U_c is compared with the static potential $V_{\rm st}(\psi_{1s})$. The amputated wave function X merges into Y_c at large r. Clearly, $(X,X) < \infty$.

$E_{X1} + E_{X2}$ is also large. The direct potential U_b and the exchange potential Y_b for the bound orbital are given in Fig. 3(a) for the triplet state and $p_c a_0 = 0.4$. Figure 3(b) contains the direct potential U_c and the exchange term Y_c for the continuum orbital u. Overall, the solutions with the *Ansätze* (4) and (6) are found to be very stable. For comparison, we note that, in the positron-hydrogen and in the electron-hydrogen scattering without exchanges, the penetration effect was found [14,15] to be significant.

One important and desirable consequence of fixing the continuum energy e_c is that in a multichannel scattering all the asymptotic energies must be specified and held fixed throughout the calculation, and this is independent of how accurately the asymptotic cluster functions are determined.

The calculation presented here shows that the two *Ansätze* we introduced in Sec. II in the formulation of the GHF approach seem to be effective in producing the correct (approximate) asymptotic boundary condition. It is not the purpose here to demonstrate the effectiveness of the GHF approach in generating the accurate phase shift. This will come with multiconfiguration mixing, just as in the bound-state case.

V. EXTENSIONS OF THE THEORY

The theory developed above for a simple three-body, single-channel scattering system may be extended to more general systems. Of course, these require extensive numerical computations, the results of which will be reported elsewhere. We simply list some of the major potentiality of the approach as it is developed here.

(i) More than one (closed-channel) term may be added to Ψ_t as well as a mixture of other bound-state configurations. This is the same as the configuration interaction in the usual HF approach, and we expect that this will make ψ approach ψ_{1s}. This is the most pressing task in proving the validity of the GHF theory with one- and two-electron targets. The validity of the basic *Ansätze* (4) and (6) in providing the correct converged amplitudes must be tested in full by including other configurations.

(ii) More than one (open) scattering channel may be included for inelastic and rearrangement scatterings. Since the continuum orbitals are treated here the same way as the bound orbitals, except for the amputation, this problem is equivalent to that of (i) above and the purely bound-state HF procedures. It is of theoretical interest as to how the rearrangement channels are handled in practice, where the ''orthogonality'' among the channels are much more difficult to treat.

(iii) Scattering systems with more than one particle in the continuum, as in collisional ionization, may be treated by additional amputations. We may then have a consistent way to evaluate the Auger amplitudes that involve both the bound and continuum orbitals determined by the SCF procedure. More importantly, we may be able to treat the ionization channels, as well as the multiparticle cluster channels, as the positronium formation in the poistron-atom scattering.

(iv) The GHF theory may also be adopted to treat the loosely bound states that are spatially extended to large distances and thus cumbersome to be treated together with tightly bound orbitals in a SCF calculation. This is a welcome improvement of the conventional HF procedure, where the large spatial orbitals are not readily treated with the same kind of accuracy with the more compact orbitals within the same configurations. The amputated function provides a more compact description of such states, and this is somewhat equivalent to the quantum-defect procedure [17].

(v) In view of the strong penetration of the bound orbits by the projectile particles, especially in the nonexchange cases, it is of special interest to examine whether the shake-off processes during a collision process may be better treated by the GHF approach. The usual procedure of estimating the shake-off probabilities by the overlap of wave functions in the initial- and final-state configurations can be extended in a natural way using the wave functions generated by the GHF approach.

VI. CONCLUSION

Summarizing, we have presented a simple generalization of the SCF theory to scattering problems, in which the principal obstacles in the HF approach have been removed in terms of the amputated scattering functions and weak asymptotic conditions. The rigid requirement for the exact target wave functions is also relaxed.

To illustrate the approach, the theory has been applied to elastic electron-hydrogen scattering in the lowest Hartree-Fock approximation, with full exchange. The theory treats both the bound and continuum orbitals on an equal footing and the solution can be systematically improved by configuration interaction. The SCF iterations converged well and the solution with Eqs. (4) and (6) was found stable. It is not yet clear whether the two *Ansätze* (4) and (6) provide the optimum way to generalize the HF procedure to collision problems, but they seem to work well thus far, with a limited set of cases tested. This generalization would eventually be incorporated into all the bound-state multiconfiguration HF codes for extended versatility. The fact that we obtained the result very close to the STFX values with the single-configuration GHF wave function we have used is most encouraging.

We reemphasize that the GHF presented here is fundamentally different in its basic approach from all the previous collision theories in that the asymptotic boundary conditions are relaxed in a controlled way. This could in principle change the original scattering problem altogether. However, the sample calculation in Sec. III showed that in fact the calculation seems to converge to the corret asymptotic conditions, albeit weakly. The WAC (6) is sufficient; it is simlar to a node counting in the usual HF calculation. As such, the example given here should not be taken as a test of the power of the theory in producing the accurate phase shift. This can be accomplished with multiconfiguration mixing. The real potential of the GHF approach should become apparent as soon as we start to apply it to treat the collision problems with targets that involve more than one electron.

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