Self-consistent field theory of collisions I. Scattering channels

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Abstract. The conventional Hartree and Hartree-Fock approaches for treating many-electron bound systems have been extended recently to positive energy scattering problems, in which both the bound and continuum orbitals are determined by the requirement of full self-consistency. Serious consequences of such a theory are that the target orbitals become energy dependent and the asymptotic boundary conditions are satisfied only approximately, in lowest order. It is important therefore to test the theory for its convergence under configuration mixing. This self-consistent field (SCF) theory for scattering has been tested here for scattering from hydrogenic target as a model where the target function is determined dynamically. Penetration of the projectile inside the bound target orbital is manifest through the SCF for the bound state. Our results show that the theory converges to the correct amplitudes and to the exact boundary conditions as more configurations are added. The use of the amputated functions and the weak asymptotic condition (WAC) upon which the SCF theory is based, is justified as the WAC converges to the correct limit. It is then applied to the positron-helium and electron-helium scattering systems where the helium function is calculated simultaneously together with the scattering function. The resulting phase shifts and the SCF target functions are compared with those obtained with the pre-determined target functions in the conventional approaches.

1 Introduction

The interpretation of atomic spectra and applications of atomic spectroscopy to current problems in astrophysics, laser physics, and thermonuclear plasma require a precise knowledge of atomic structure and collision dynamics. Atomic systems to be analyzed are complex and many approximate methods have been developed in the past, among which the Hartree-Fock procedure [1] and its relativistic and multiconfiguration extensions have been most prominent. This self-consistent field (SCF) approach, however, has been limited to treating only fully bound state configurations. It is therefore worthwhile considering its extension to scattering problems. These methods have also been successfully applied to molecular systems as well as to some solid state and nuclear problems. With currently available computers, atomic and molecular structures are routinely calculated to very high accuracy [2–6]. Several efficient computer packages are available, and the wave functions generated by these programs are often sufficiently accurate for the evaluation of various transition matrix elements. The variational basis of the

HF approach, often with minimum bounds on the ground state energy eigenvalues, helps to obtain convergent results in many cases, both for the ground and low-lying exited states. In all cases, however, the atomic systems consist of bound, negative energy orbitals and the corresponding wave functions are square-integrable (L2). This L2 property is of course essential in deriving the SCF form of the theory.

In the past, numerous attempts to extend the approach to scattering problems involving continuum (positive-energy) orbitals have been made [7–10], but, no correspondingly satisfactory methods have been found until very recently [11,12]. The principal difficulties in extending the theory are well-known: (i) the non-normalizability of the continuum scattering function makes the SCF determination of the potentials inoperative, and (ii) the strong asymptotic boundary condition which requires exact target internal wave functions for all the open (allowed) channels. These target functions are required in formulating the scattering problem, prior to solving it. Various approaches have been tried to circumvent these difficulty (i); for example, the complex energy treatment [13] forces the scattering wave functions to decay asymptotically, and the final amplitudes are obtained by analytic continuation.

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The complex coordinate method [14] similarly adopts the decaying functions for the continuum orbitals. The condition (ii) can be satisfied only approximately [15,16] in practice.

A generalized Hartree-Fock (GHF) approach to collision systems was proposed [11] recently, in which the difficulties (i) and (ii) are removed and where all the orbitals are treated on an equal footing in so far as the SCF requirement is concerned. The non-integrability is removed by introducing the amputated wave functions (AWF) in place of the usual scattering functions. All the integrals involved are then well defined. However, it is important to distinguish this new approach from all the existing scattering theories in that the "exact" asymptotic boundary conditions are not specified; this condition is relaxed in the generalized SCF theory (GSCF) in terms of a weak asymptotic condition (WAC). Since the requirement (ii) cannot be met in practice, the question of how good these functions should be naturally arises. The usual accuracy criterion is that perhaps the bound cluster functions should be "much better" than the desired accuracy of the scattering amplitudes. By contrast, the GSCF approach considered here treats all the orbitals, including the asymptotic ones, self consistently simultaneously.

The new SCF theory was applied [11,12] earlier to the single channel elastic scattering of positrons by hydrogen below the positron pick-up threshold and electrons below the first excitation threshold. In both of these cases, the GSCF iterations converged well, and the solutions with the use of the WAC and AWF were found to be stable. Most encouragingly, in spite of the WAC, the GSCF phase shifts are found to be comparable to the well-known close coupling method [17], which has been widely applied to electron/positron-atom scattering [18–20].

The GSCF theory depends critically on the two ansatz, the AWF and WAC. In particular, their validity depends on the WAC, which is a serious modification of the original scattering problem. More precisely, the strong boundary condition of requiring the exact target function is relaxed by requiring instead a much weaker condition. This is of course a fundamental change in the scattering problem. To validate the GSCF theory, the two ansatz mentioned above must be tested by showing that the SCF approximate target wave function and the corresponding energy approach the exact ones as more configurations are added and also that the SCF phase shift approaches the exact value. We first critically examine this question in the cases of the well-known systems of electron-hydrogen and positron-hydrogen scattering, where the target function is known exactly and full scattering information is available for comparison. Of course the target functions calculated by the GSCF are different from the exact hydrogenic function and depend on the scattering energy.

Secondly, we apply the SCF theory for the first time to the positron-helium and electron-helium scattering systems where neither the exact asymptotic conditions in terms of the target functions nor the full scattering solutions are known. Both the helium target function and the scattering particle function are treated on equal footing as they are determined simultaneously in a fully self-

consistent way. Our results are then compared with several previous calculations in which various approximate forms of the helium target function were employed.

This is the first in a series of reports on the applications and extensions of the GSCF approach to collision problems. As an important next step, the theory will be extended to treat the ionization problem, where two or more continuum electrons co-exist. This is the first serious challenge of the new approach, where very few viable and systematic theories are actually available. As a result much current research activities are reported in recent years. As apparent from the contents of this paper, the GSCF theory is eminently suited for the ionization problem.

The outline of this paper is as follows. Section 2 contains a summary of the theoretical development of the generalized Hartree approximation (GHA)/generalized Hartree-Fock approximation (GHF) (in the presence of exchange) for atomic collisions. Sections 3 and 4 are devoted to testing the theory by applying it to the hydrogen target, scattering the incident projectile (positrons or electrons). Sections 5 and 6 contain the first application of the GHA and GHF theory to the helium atom in which the target ground eigenstate is not known exactly. Finally, we summarize the results and give concluding remarks.

It should be emphasized that the work reported here is to demonstrate that the GHF is, under configuration mixing, a valid theoretical approach to many-body scattering. It is *not* the purpose of this study to obtain the exact result which is already available. This applicability of the GHF will lead to cases which cannot readily be treated by the existing methods.

2 Generalization of the Hartree and Hartree-Fock methods to scattering

The conventional Hartree and Hartree-Fock approaches have been developed for bound state configurations of many electron ions, atoms, and molecules. For the ground states, the variational nature of the theory provides an important bound property, $E_g^{HF} \geq E_g$ where E_g is the ground state energy. The method has also been used in describing excited state configurations, although the bound property is not present. The wave function for an N electron system is written in the lowest order HF approximation as

$$\Psi \simeq \Psi_{HF} = A\Pi\psi_i \equiv A'\Psi_{-i}\psi_i \qquad (1)$$

for each orbital ψ_i and where Ψ_{-i} are the $(N-1)$-electron clusters without the ith electron which are assumed to be properly antisymmetrized within the clusters. A is the antisymmetrization operator, defined by $A = (1/\sqrt{N})\sum_{ij} P_{ij}$, where P_{ij} is the permutation operator for each electron pair ij, with the proper signs included. For notational convenience, we combine the electron and the orbital label. For example, ψ_i denotes a single-particle orbital for electron i in state i. For simplicity, we omit the complications which may arise from proper angular

and spin coupling, often requiring more than one determinant. The set of coupled nonlinear integro-differential equations for the individual orbitals $\{\psi_i\}$ is then given by

$$\langle \Psi_{-i}|H - E_{\mathrm{t}}|\Psi_{\mathrm{HF}}\rangle_{-i} = 0, \quad i = 1, 2, \ldots, N \qquad (2)$$

where $\langle \cdots \rangle_{-i} = \int dr_1 dr_2 \ldots dr_{i-1} dr_{i+1} \ldots dr_N$. The HF equations (2) determine the orbitals ψ_i. Another way of deriving the Hartree-Fock equations (2) is *via* the variational principle. Since all the orbitals involved are bound state functions, the $\{\psi_i\}$ are square-integrable. Consequently the integrations implied in equations (2) are finite. Thus, the HF single orbital equations (2) are mutually coupled, nonlinear, and contain the self-consistent mean field (SCF) for each bound electron i.

We now try to extend (2) to scattering problems in which one of the electrons (or positrons) occupies a continuum orbital. Rather than developing the continuum theory for complex atoms in a general way, we consider two simple examples of positron-hydrogen and electron-hydrogen scattering. This of course does not limit the applicability of the theory to more complex scattering systems. As will be clear below, the generalized SCF theory (GSCF) contains several new elements to make it conceptually different from all of the conventional theories. So, the simple example of positron-hydrogen scattering system brings out the essential aspects of the theory more clearly. The scattering energy is limited to the region below the first pickup threshold for positronium formation (no electron will be stripped off) and for the total angular momentum $L = 0$. It is then a single channel scattering problem, with no exchange effect. Since the hydrogen internal states are known exactly we are able to test the continuum theory.

The scattering wave function Ψ satisfies

$$(H - E)\Psi = 0, \quad H = T_{\mathbf{r}_2} + h(\mathbf{r}_1) + V \qquad (3)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ denote the electron and positron coordinates, respectively, $T_{\mathbf{r}_2}$ is the kinetic energy operator for the positron, and $h = T_{\mathbf{r}_1} + V_1$ is the target Hamiltonian, where V_1 is the attractive Coulomb potential between the electron and the proton. The interaction potential between the positron and the hydrogen target is $V = V_2 + V_{12}$, where $V_{12} < 0$ is attractive. The asymptotic boundary condition is required to fully specify the scattering problem posed by (3). We have asymptotically as $r_2 \to \infty$

$$\Psi \longrightarrow \psi_0(\mathbf{r}_1)u_0(\mathbf{r}_2) \quad \text{(strong asymptotic condition)} \quad (4)$$

where

$$h\psi_n(\mathbf{r}_1) = \varepsilon_n \psi_n(\mathbf{r}_1), \qquad (5)$$

$$u_0(\mathbf{r}_2) = s(\mathbf{r}_2) + c(\mathbf{r}_2) \to \frac{\sin(kr_2)}{r_2} + K_0 \frac{\cos(kr_2)}{r_2} \quad (6)$$

$$E = \varepsilon_0 + e_{\mathrm{c}} \qquad (7)$$

where ε_0 is the ground state energy of hydrogen, e_{c} is the kinetic energy of the incident particle defined as $e_{\mathrm{c}} = k^2$ in units of Rydberg where k is the continuum wave number, and K_0 is the reactance matrix defined as $K_0 = \tan \delta_0$ where δ_0 is the scattering phase shift. The scattering equation (3) with the boundary conditions (4–7) defines the problem. At $r_1 = r_2 = 0$, the boundary conditions are as usual $r_1 \psi_n(0) = 0$, and $r_2 u_n(0) = 0$, for all n. The form (4) with (5–7) will be called the strong asymptotic condition.

The elastic scattering function in the generalized Hartree approximation (GHA) in its lowest approximation is chosen as a product form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) \simeq \Psi_{\mathrm{GHA}} = \psi(\mathbf{r}_1)u(\mathbf{r}_2) \qquad (8)$$

where u asymptotically behaves as in equation (6). We obviously note that

$$\langle \Psi|\Psi\rangle = \langle u|u\rangle \longrightarrow \infty. \qquad (9)$$

Hence, any attempt to construct the set of equations (2) is not possible. One is then forced to pre-determine the ψ since the ψ equation contains the difficulty (9). Furthermore, the strong asymptotic condition (Eq. (4)) with equation (6) requires that the exact cluster function ψ_0 must be known before solving equation (3). Of course this can only be done exactly in the case of the hydrogen atom. Hence, the question of how good these cluster functions should be in general cases and how they affect the scattering amplitudes arises. In fact, the sensitivity of the scattering amplitudes to the accuracy of the cluster functions has been discussed [21]. Accuracy of the cluster function ψ_i in (4) must be at least an order of magnitude greater than the scattering function u. Precise criteria for this arbitrariness are not known.

The standard procedure for deriving a set of SCF Hartree equations is

$$\langle \psi|H - E_{\mathrm{t}}|\Psi_{\mathrm{GHA}}\rangle_{\mathbf{r}_1} = 0 \qquad (10)$$

$$\langle u|H - E_{\mathrm{t}}|\Psi_{\mathrm{GHA}}\rangle_{\mathbf{r}_2} = 0, \qquad (11)$$

where $\langle \cdots \rangle_{\mathbf{r}} = \int \ldots d\mathbf{r}$. It is evident from (9) that the second equation (11) is ill-defined. In addition the solution of equation (11) will give an approximate bound state function with approximate energy $\varepsilon_{\mathrm{bt}}$. Since the total energy E is pre-fixed, this in turn makes the corresponding incident energy e_{c} vary, as $e_{\mathrm{c}} \simeq E - \varepsilon_{\mathrm{bt}}$. Therefore, the strong asymptotic condition cannot be imposed exactly in a SCF approach.

In order to resolve these difficulties we first write u as

$$u = s + gV^{\mathrm{S}}u \equiv s + gX, \qquad (12)$$

where

$$[T_{\mathbf{r}_2} - e_{\mathrm{c}}]s = 0, \qquad (13)$$

$$[T_{\mathbf{r}_2} - e_{\mathrm{c}}]g = -\delta(\mathbf{r}_2 - \mathbf{r}_2'), \qquad (14)$$

and

$$X(\mathbf{r}_2) \equiv (e_{\mathrm{c}} - T_{\mathbf{r}2})u = V^{\mathrm{S}}u \quad \text{(AWF)}, \qquad (15)$$

where V^S is the SCF potential function for the continuum orbital and in the present example V^S is short ranged. This implies that X is a decaying function, hence it is square integrable: $\langle X|X\rangle_{\mathbf{r}_2} < \infty$.

The GHA is formulated by introducing two ansatz: (a) the amputated function X is to replace u in equation (11). This replacement is based on the fact that the essential dynamical information carried by the scattering function u is in X and not in the oscillatory tail part represented by the asymptotic form of u. On the other hand, the tail gives rise to the non-normalizability difficulty. There may be other ways of constructing a square integrable function, but the AWF cleanly gets rid of the troublesome part and yet retains the essential physical information. The choice (15) also allows to maintain the (hermiticity) symmetry of the resulting set of coupled equations. The new set of equations may then be written as

$$\langle\psi|H - E|\Psi_{\text{GHA}}\rangle_{\mathbf{r}_1} = 0, \tag{16}$$

$$\langle X|H - E|\Psi_{\text{GHA}}\rangle_{\mathbf{r}2} = 0. \tag{17}$$

The coupled equations (16, 17) may be reduced to the following explicit forms

$$\left[T_{\mathbf{r}2} - e_c + V^S + \langle h - \varepsilon_{\text{bt}}\rangle_{\mathbf{r}_1}\right] u(\mathbf{r}_2) = 0 \tag{18}$$

$$\left[h + V_X - \varepsilon_{\text{bt}} - \langle X|X\rangle_{\mathbf{r}_2}\right]\psi(\mathbf{r}_1) = 0 \tag{19}$$

with

$$V^S(r_2) \equiv \frac{\langle\psi|V|\psi\rangle_{\mathbf{r}_1}}{\langle\psi|\psi\rangle_{\mathbf{r}_1}}, \tag{20}$$

$$\langle h - \varepsilon_{\text{bt}}\rangle_{\mathbf{r}_1} = \frac{\langle\psi|h - \varepsilon_{\text{bt}}|\psi\rangle_{\mathbf{r}_1}}{\langle\psi|\psi\rangle_{\mathbf{r}_1}}, \tag{21}$$

$$V_X(r_1) \equiv \frac{\langle X|V|u\rangle_{\mathbf{r}_2}}{\langle X|u\rangle_{\mathbf{r}_2}}, \tag{22}$$

and

$$\langle X|X\rangle_{\mathbf{r}_2} = \frac{\langle X|e_c - T_{\mathbf{r}_2}|u\rangle_{\mathbf{r}_2}}{\langle X|u\rangle_{\mathbf{r}_2}} \equiv E_{XX}. \tag{23}$$

Note that

$$V_X \to E_X = \langle X|V_2|u\rangle_{\mathbf{r}_2} \quad \text{as } r_1 \to \infty. \tag{24}$$

We also set $E = e_c + \varepsilon_{\text{bt}}$ in equations (18, 19), and $\varepsilon_{\text{bt}} + E_{XX} - E_X \equiv \varepsilon_{\text{dt}}$ which is the eigenvalue of (19). The e_c dependence of ε_{bt} arises through this relationship.

Furthermore, equation (18) contains a constant $\langle h - \varepsilon_{\text{bt}}\rangle_{\mathbf{r}_1}$ which modifies the asymptotic energy e_c. This is of course undesirable and we require that

$$\langle h - \varepsilon_{\text{bt}}\rangle_{\mathbf{r}_1} = 0, \quad \text{weak asymptotic condition (WAC).} \tag{25}$$

As we will show below, this is not an arbitrary condition imposed on the wave function ψ, but is a consequence of the full SCF theory. This weak asymptotic condition (WAC) allows us to maintain the pre-set energy e_c. It is roughly equivalent to a simple "node counting" ψ, as in the usual HF procedure.

The GHA coupled equations can then be written as

$$\left[T_{\mathbf{r}_2} + V^S - e_c\right] u = 0 \tag{26}$$

$$\left[T_{\mathbf{r}_1} + V^B - \varepsilon_{\text{dt}}\right]\psi = 0 \tag{27}$$

with

$$V^B = (V_X - E_X) + V_1 \tag{28}$$

and

$$\varepsilon_{\text{bt}} + E_{XX} - E_X \equiv \varepsilon_{\text{dt}} \tag{29}$$

where ε_{dt} is the eigenvalue of (19).

It is important to point out that ψ satisfies (27) with a very strong potential $V^B \ll V_1$ and a pseudo-binding energy ε_{dt}. The actual energy of ψ is, however, shifted by (29) in such a way that ε_{bt} is expected to be quite close to the actual energy of the hydrogen $1s$ electron, $\varepsilon_{1s} = -1Ry$.

The coupled set (26, 27) gives a self-consistent treatment of the scattering problem, where both the bound and the scattering state orbitals are treated on an equal footing and calculated self-consistently. V^S and V^B are the self-consistent field potentials for u and ψ, respectively. Evidently, V^B has never been derived before, because of the difficulty (9).

For the electron scattering, the exchange effect is incorporated without difficulty. The actual form of the equations is similar to equations (26–28). We illustrate the SCF theory in the presence of exchange by considering the simple example of single-channel elastic electron-hydrogen scattering for the case of zero total angular momentum, $L = 0$, and scattering energy, e_c, below the first excitation threshold, $i.e.$, the total energy E: $-1.0Ry < E < -0.25Ry$. The elastic scattering function in the generalized Hartree Fock approximation (GHF) in its lowest order is chosen as

$$\Psi_t = \frac{\psi(1)u(2) \pm \psi(2)u(1)}{\sqrt{2}} \tag{30}$$

where $\pm$ correspond to the spin eigenstates ($S = 0$ or 1). The coupled set is given by

$$\left[T_2 + V^S - e_c\right] u(2) = \pm K_u(2) \tag{31}$$

$$\left[T_1 + V^B - \varepsilon_{\text{dt}}\right]\psi(1) = \pm K_\psi(1) \tag{32}$$

where the exchange terms K_u and K_ψ are written as

$$K_u(2) = \psi(2)\int\psi^*(1)[H - E]u(1)\text{d}1, \tag{33}$$

$$K_\psi(1) = \frac{u(1)\int X^*(2)[H - E]\psi(2)\text{d}2}{\int X^*(2)u(2)\text{d}2}, \tag{34}$$

$$\varepsilon_{\text{dt}} \equiv \varepsilon_{\text{bt}} - E_{XX} - E_X, \tag{35}$$

and where the amputation of u results in the form

$$X = g^{-1}u = V^S u \mp K_u. \tag{36}$$

Aside from the fact that X now carries one extra term, K_u, the formalism remains the same as in the generalized Hartree case. In general we can write the Generalized Hartree Fock (GHF) equations as follows

$$\langle \Psi_{-i} | H - E_t | \Psi_t \rangle_{-i} = 0 \quad \text{for} \quad i = \text{continuum orbital} \tag{37}$$

$$\langle X_{-j} | H - E | \Psi_t \rangle_{-j} = 0 \quad \text{for} \quad j \neq i \tag{38}$$

and where $X_{-j} = (e_c - T_i)\Psi_{-j}$. In this notation the Ψ_{-i} do not contain the continuum orbital i, while all the Ψ_{-j} with $j \neq i$ contain the continuum orbital i explicitly (this form is only symbolic, because the amputation must be done on the orbital i, but of the exchanged coordinates).

We emphasize that the self consistent field (SCF) formulation given above, that is the GHA (without exchange) and the GHF, are valid if the two ansatz, AWF and WAC, can provide the correct amplitudes when more configurations are added. The convergence of the asymptotic boundary condition is therefore the critical test of the theory. This is demonstrated in the next two chapters by adding more than one (closed channel) term to Ψ_t as well as a mixture of other bound state configurations.

3 Positron-hydrogen scattering by GHA

The main purpose of this and the next section is to test the GSCF theory by adding configurations.

We first solved the set of coupled equations with the GHA wave function of the scattering system, $\Psi(1\tilde{s})$, chosen in its lowest approximation

$$\Psi(1\tilde{s}) \simeq \tilde{\psi}_{1s}(r_1)\tilde{u}_{1s}(r_2). \tag{39}$$

The $1\tilde{s}$ denotes the target state evaluated within the GHA and is different from the exact $1s$ function, where $\tilde{\psi}_{1s}$ and $\tilde{u}_{1s}$ are calculated by the GHA. We name it configuration $1\tilde{s}$.

The iterative procedure proceeded as follows: to start the iteration, we arbitrarily choose $\tilde{\psi}_{1s} = \psi_{1s}$ where ψ_{1s} is the ground state wave function of the hydrogen atom.

1. The potential $V_{1s,1s}^S(r)$ is evaluated. In the zeroth iteration this simply gives the static potential denoted as V^{st} for the scattering function $\tilde{u}_{1s}$.
2. We then solve for $\tilde{u}_{1s}$ and the corresponding phase shift δ^{GHA} is evaluated in accordance with (6), for the scattering energy $e_c = k^2$ in units of Ry.
3. The amputated function, X, is then evaluated:

$$X_{1s}(r) = \left(-T(r) + k^2\right)\tilde{u}_{1s}(r) = V_{1s,1s}^S(r)\tilde{u}_{1s}(r)$$

4. The effective potential $V_{1s,1s}^B$ is evaluated and an estimate of the eigenvalue ε_{dt} is obtained.
5. Equation (19) is solved for $\tilde{\psi}_{1s}$ and ε_{dt}. The GHA binding energy of the target hydrogen, ε_{bt}, is then evaluated *via* equation (29).
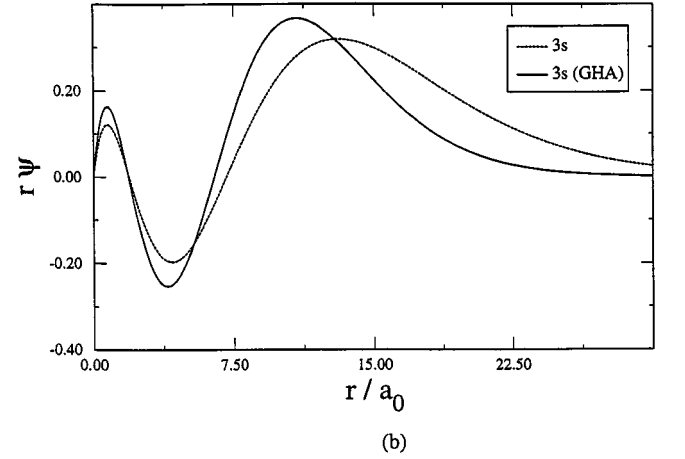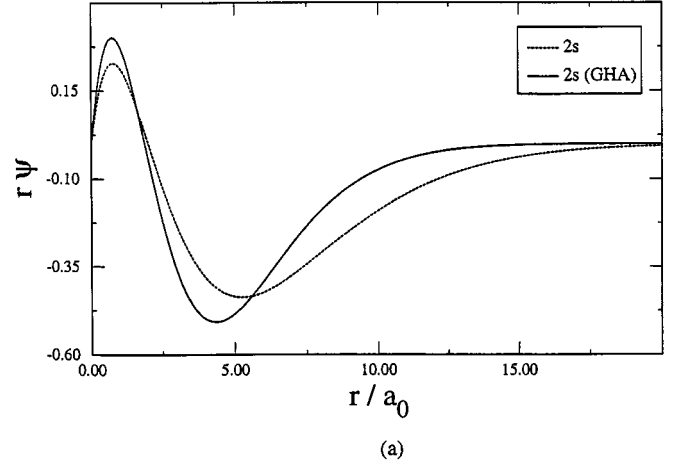

Fig. 1. (a) Comparison of the bound state function in the present GHA (solid line) with the undistorted $2s$ wave function (dotted line). (b) Comparison of the bound state function in the present GHA (solid line) with the undistorted $3s$ wave function (dotted line).

6. The phase shift δ^{GHA} and ε_{bt} are then compared with the values obtained in the previous iterations. If the changes are larger than a preset limit, we return to step 1 of the iteration cycle and repeat the procedure until the method converges. In all cases treated, at most five iterations are required to obtain a convergence of one part in ten thousand.

We also calculated the excited state scattering using the same GHA code by simply guessing the approximate initial energy values for the $2s$ and $3s$. The solutions automatically converged to the specified asymptotic values as long as the initial choice was close to one particular energy. The converged energies for the bound electron are close to one of the $-(1/n^2)Ry$, (-0.2246 and -0.0994 in Rydberg for $2s$ and $3s$ target respectively) and the corresponding wave functions have the correct number of nodes associated with the particular n. This is shown in Figures 1a and 1b. None of these functions are exact, however, as they are determined by self-consistency. The only way
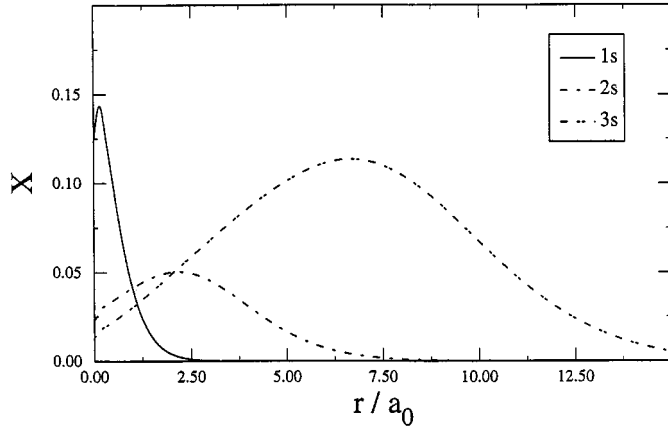
Fig. 2. Plot of the amputated function, X, for the $1s$ (solid line), $2s$ (dashed-dotted line), and $3s$ (dashed-dot-dotted line) configuration.

Table 1. We display the phase shift values in radians for the hydrogen-positron scattering case calculated with the GHA formalism, δ^{GHA}, with various configuration mixing and the corresponding energies $\varepsilon_{\mathrm{bt}}$, in units of Rydberg. Also displayed are phase shifts calculated in the close coupling approximation δ^{CCA}, phase shifts obtained by including all the virtual s excited states, δ^s, and the phase shifts given by [22] which are considered to be "exact" δ^{ex} at $ka_0 = 0.2$ and 0.4, where ka_0 is the continuum wave number.

(a) $k_c a_0 = 0.2$	δ^{CCA}	δ^{GHA}	$\varepsilon_{\mathrm{bt}}(Ry)$
$1s$	-0.1145	-0.0648	-0.9724
$1s + 2s$	-0.1109	-0.1021	-1.049
$1s + 2s + 3s$	-0.0426	-0.1030	-1.043
$1s + 2s + 3s + 4s$		-0.1035	-1.036
$1s + 2\tilde{s}$		-0.0847	-1.005
all s	-0.1051		(-1.0000)
$1s + 2p$	-0.0458	-0.0337	-1.011
$1s + 2p + 3p$		-0.0291	-1.009
$1s + 2p + 3p + 4p$		-0.0282	-1.006
$1s + \bar{p}$		0.0458	-1.017
exact	$+0.188$		

(a) $k_c a_0 = 0.4$	δ^{CCA}	δ^{GHA}	$\varepsilon_{\mathrm{bt}}(Ry)$
$1s$	-0.2181	-0.1246	-0.9723
$1s + 2s$	-0.2110	-0.1769	-1.034
$1s + 2s + 3s$	-0.2095	-0.1845	-1.031
$1s + 2s + 3s + 4s$		-0.1871	-1.029
$1s + 2\tilde{s}$		-0.1637	-1.017
all s	-0.2000		(-1.0000)
$1s + 2p$	-0.1531	-0.1103	-1.023
$1s + 2p + 3p$		-0.0963	-1.012
$1s + 2p + 3p + 4p$		-0.0938	-1.009
$1s + \bar{p}$		-0.0324	-1.011
exact	$+0.120$		

to confirm that the calculated wave function corresponds to that of the desired channel is to count the number of nodes of the wave functions. This is in fact the same 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. The amputated functions corresponding to $1s$, $2s$, and $3s$ configurations are plotted in Figure 2 showing that they extend further as the target orbital principal quantum number increases. We do not pursue this interesting aspect of the GHA approach any further here because, for excited target scattering we have to include all the open channels with channel binding energies greater than that particular excited state, and this requires a further generalization of the GHA theory.

Next, we add the closed channel configurations $\sum_{n=2}^{n_{\max}} nl$ where $n_{\max} = 2$ to 4, $2\tilde{s}$, or $\bar{p}$ to configuration $1\tilde{s}$. In configuration nl, we use the exact wave function of the hydrogen atom in quantum state nl, and in configuration $\bar{p}$ we use a pseudo-state wave function for the hydrogen atom of the form $r\psi_{\bar{p}} \sim r^2(1 + r/2)\exp(-r)$.

During the iteration cycle, we force orthogonality between $\tilde{\psi}_{1s}$ and ψ_{ns} to ensure that no spurious tails remain asymptotically. As a test for our numerical code we set $\tilde{\psi}_l = \psi_l$, for which we recovered the exact numerical results of the close coupling approximation (CCA) [19]. We dropped constant terms of the form $\langle X_{1s}|h_2 - k_n^2|u_n\rangle$ for $n \neq 1$, which appear on the right hand side of the ψ equation to ensure that no spurious tails are retained asymptotically. These constant terms are small. These terms represent the overlap between the two amputated wave functions X_{1s} and $X_n = (h_2 - k_n^2)u_n$. To cleanly eliminate them a Lagrange multiplier must be used, in analogy with the bound-state HF.

Calculated phase shifts and the corresponding energies of the GHA approximate target function of the present theory in different multiconfiguration approximations are presented in Table 1. Also presented for comparison are the phase shift results of the close coupling approximation, the phase shifts obtained by including all of the vir-

tual s excited states, δ_s, and the phase shifts obtained by Schwartz [22], δ_{ex}. His results are considered to be the best existing values of s-wave elastic scattering phase shifts. In his approach he used an extensive variational method with many parameters in the trial function.

In Figure 3a, we show a plot of the GHA effective potential, V^{S}, seen by the continuum state function in configuration $1\tilde{s}$ and the static potential V^{st} *versus* Bohr radius at $ka_0 = 0.5$, where ka_0 is the continuum wave number. This figure shows that potential V^{S} is deeper but of shorter range than the static potential. This may explain why the GHA phase shifts are higher than those of the static case (one term kept in the expansion).
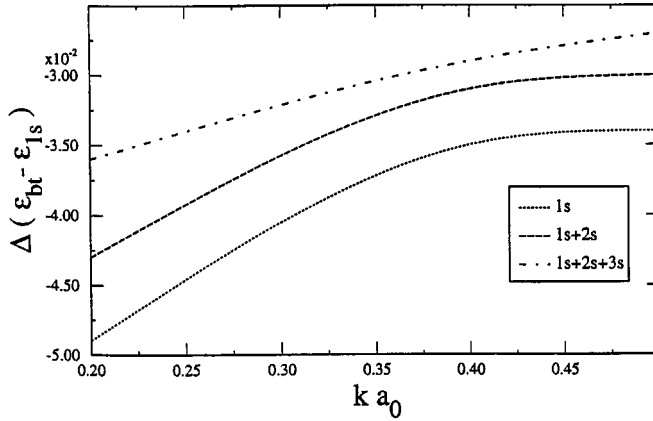
The deviation in the target binding energy $\Delta\varepsilon$ is plotted *versus* ka_0 in Figure 3b, where $\Delta\varepsilon = \varepsilon_{\mathrm{bt}} - \varepsilon_b$ with $\varepsilon_b = -1.0Ry$. The smallness of $\Delta\varepsilon$ shows that the weak asymptotic condition (WAC) still places strong enough
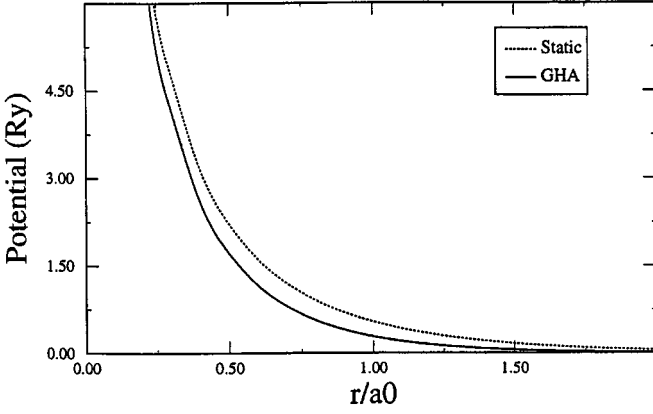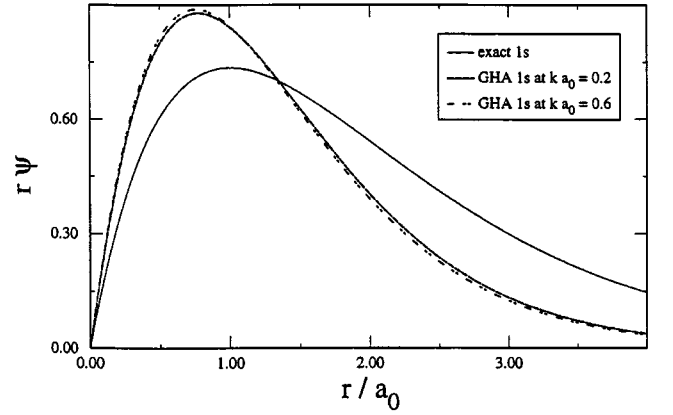
(a)
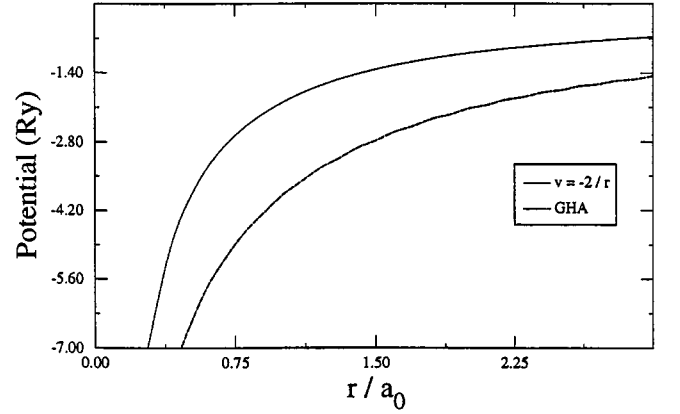
(a)

(b)

(b)

Fig. 3. (a) Plot of the GHA potential (dashed line) and the static potential (solid line) for the continuum function at $ka_0 = 0.5$. (b) Plot of the strong energy dependence of $\Delta(\varepsilon_{bt} - \varepsilon_{1s})$. For details see text.

Fig. 4. (a) Comparison of the Coulombic potential (solid line) and the GHA potential (dashed line) for the bound electron at $ka_0 = 0.5$. (b) Comparison of the exact (solid line) and the GHA hydrogen $1s$ wave function at $ka_0 = 0.2$ (dashed line) and 0.6 (dashed-dotted line).

constraint on the solution to eventually lead to the correct boundary condition.

In Figure 4a, we show a plot of the GHA effective potential, V^B, seen by the bound state function in configuration $1\tilde{s}$ with the pure Coulombic potential V_1 given by $V_1 = -2/r_1$ at $ka_0 = 0.5$. Figure 4a shows that for $r > 3a_0$, V^B is almost twice the Coulombic potential V_1. This is the most striking feature of the SCF theory. This SCF potential for the target electron during a collision has only recently been displayed [11,12]. This can be understood from the fact that when the electron is far away from the proton core, which means that the positron has penetrated into the inner region of the electron orbit, the target electron feels the Coulomb field of two positive charges. As a result, the GHA approximate target wave function is pulled in by comparison to the hydrogen target function. Moreover, the amount of distortion caused by the scattering positron is energy dependent. This is shown in Figure 4b at $ka_0 = 0.2$ and 0.6. Nevertheless, the final binding energy ε_{bt} of the GHA target function and the

corresponding wave function $\tilde{\psi}_{1s}$ do not differ greatly from those of the ground state hydrogen.

Table 1 shows that as we add the ns configurations to the total scattering function, such as $2s$, $3s$, $4s$ states, the binding energy of the GHA approximate target function approaches $1Ry$. Moreover the scattering function and the corresponding phase shift approach the exact value of the all-s virtual exited states as expected. We plot, in Figure 5, the difference between the converged GHA target wave function, $\tilde{\psi}_{1s}^{(i)}$, where $(i) = 1\tilde{s}$, $1\tilde{s} + 2s$, $1\tilde{s} + 2s + 3s$, $1\tilde{s} + 2s + 3s + 4s$ and the exact hydrogen wave function ψ_{1s} *versus* r, where r is in units of Bohr radii. One can see that as we add the $2s$, $3s$, $4s$ states the $\tilde{\psi}_{1s}$ target wave function approaches that of hydrogen ψ_{1s}. The phase shift for the $1\tilde{s}$ configuration, as shown in Table 1, was a bit high, but the added channels systematically brought it to all the virtual s excited states, δ_s, as more ns configurations are added to the scattering wave function Ψ of the scattering system. The convergence rate toward the
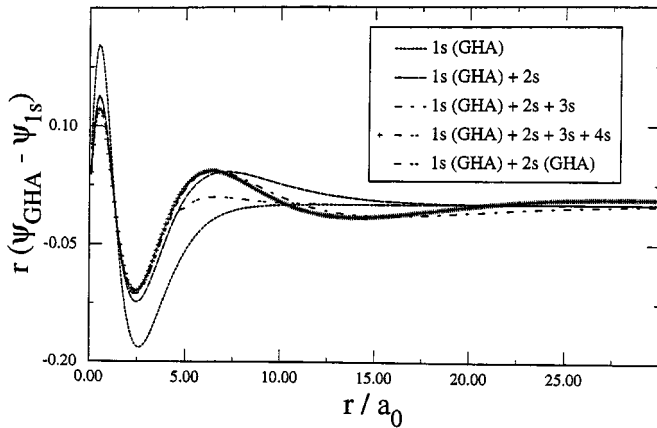
Fig. 5. Plot of the difference between the exact wave function and successively converged ones by configuration mixings in the GHA: $1s$ (GHA) + $2s$ (dashed line), $1s$ (GHA) + $2s + 3s$ (dashed-dotted line), $1s$ (GHA) + $2s + 3s + 4s$ (plus-dash-dotdotted line), and $1s$ (GHA) + $2s$ (GHA) (dashed-dot-dotted line).

exact phase shift values was rather slow and is also shared by the CCA method. We then let the $2s$ hydrogen wave function relax in the SCF calculation. The converged GHA phase shift as well as the corresponding binding energies are shown in Table 1, indicating that the GHA binding energy converges much faster to the correct value than that of the previous added ns configurations. Also, as shown in Figure 5, $\tilde{\psi}_{1s}^{(1\tilde{s}+2\tilde{s})}$, approaches ψ_{1s} faster than the previous cases. This is not surprising since $2\tilde{s}$ is equivalent to adding a large number of ns terms to configuration $1\tilde{s}$. The converged GHA results, when np configurations are added to configuration $1\tilde{s}$, are also presented in Table 1. These results also show as in previous configurations that the present theory converges to the correct value as more np configurations are added. When the pseudo-state $\bar{p}$ was added to $1\tilde{s}$, we recovered most of the long range effects as in the case of the close coupling approximation.

The above results further demonstrate that the use of the weak asymptotic condition and the use of amputated functions are, in this case, valid and effective.

4 Electron-hydrogen scattering by GHF

We have demonstrated the validity of the GHA formulation (without exchange) in the case of positron-hydrogen scattering by showing its convergence by including many configurations. We now turn to explore electron-hydrogen scattering and the effects of exchange on such a system as more configurations are added. This system has been studied extensively using varying approaches [19–23]. In the case of CCA, the singlet state recovers somewhere between 80% and 90% of the polarization effect using only the static approximation. To account for the rest of the polarization, one presumably must include higher angular momentum states. In the case of the triplet state, the static approximation gives a value within 1 to 2% of the exact value.

In this work, we do not concentrate on pursuing the full polarization effects in the singlet case. Our goal is to investigate how well this theory can explain the physics of such a system without violating the asymptotic condition. The electron-hydrogen system is a rich and robust system and provides an excellent starting point for testing the new theory.

We first solved the set of coupled equations with the GHF wave function of the scattering system, $\Psi(1\tilde{s})$, chosen in its lowest approximation:

$$\Psi(1\tilde{s}) \simeq \tilde{\psi}_{1s}(r_1)\tilde{u}_{1s}(r_2) \pm \tilde{\psi}_{1s}(r_2)\tilde{u}_{1s}(r_1). \qquad (40)$$

The $1\tilde{s}$ denotes the target state evaluated within the GHF approximation. We name it configuration $1\tilde{s}$.

The term

$$\int r'^2 dr' X(r') \left(+T(r') - \frac{2}{r'} - \varepsilon_{\text{bt}} \right) \tilde{\psi}_{1s}(r') \qquad (41)$$

is dropped to ensure orthogonality between X and $\tilde{\psi}$. This way the spurious long range contribution to the inhomogeneous term of equation (32) is not present. This term is checked at the end of each iteration cycle. It is of the order of 0.1 in the $1\tilde{s}$ configuration and approaches zero as more configurations are added (of the order of 10^{-4}). To completely remove it, however, a Lagrange multiplier must be used as in the Hartree-Fock case for bound state type systems.

For the $1\tilde{s}$ configuration the iterative procedure proceeded as follows.

1. First we arbitrarily choose $\tilde{\psi}_{1s} = \psi_{1s}$ and $\varepsilon_{\text{bt}} = -1Ry$. The potential $V_{1s,1s}^{\text{S}}$ is evaluated. Next, we solve for the scattering function $\tilde{u}_{1s}$ by adopting a variety of techniques which will be discussed below. This gives the phase shift δ^{GHF}.
2. The amputated function X (r_2) is evaluated using the scattering function $\tilde{u}_{1s}$ calculated above (in 1.).
3. The effective potential V^{B} and an initial estimate of ε_{dt} as well as the exchange term are then evaluated. Next we solve for $\tilde{\psi}_{1s}$ and the corresponding energy self-consistently. The correct binding energy is then calculated $\varepsilon_{\text{bt}} = \varepsilon_{\text{dt}} - E_x$.
4. The full iteration cycle is then completed. If the resulting energy and the phase shift δ from $\tilde{u}$ are not within the small allowed change from the previous iteration values, then we go back to step 1. and repeat the cycle again until self-consistency is reached within some preset tolerance. This way, both the target wave function $\tilde{\psi}_{1s}$ with its binding energy ε_{bt} and the scattering function $\tilde{u}_{1s}$ with the phase shift δ^{GHF} are simultaneously determined.

In the presence of exchange, the mathematical problem involves the solution of a system of coupled integro-differential equations. Since the exchange potential is not separable, non-iterative procedures are not possible. For the scattering functions, we adopt a straightforward iteration procedure using the Born iterative scheme where the

free Green's functions are used. This method fails to converge for $k \lesssim 0.3$ in the symmetric case and $k \gtrsim 0.6$ in the antisymmetric case.

To overcome this divergence, we developed a new approach which we intend to publish in the future. In this method, the exchange term is decomposed into an infinite number of separable terms using the method of singular value decomposition (SVD). Hence, we are able to diminish the effect of the exchange term by subtracting from it a larger number of terms contained in the SVD. We then iterate over the remaining part of the kernel using the non-free Green's function scheme.

We adopt the same energy matching scheme as in the positron-hydrogen case when solving for the bound state functions and their corresponding eigenvalues. An alternative approach that we adopt when convergence is not achievable, is to expand $\tilde{\psi}$ in some known basis set that satisfies the same boundary conditions as $\tilde{\psi}$. In the electron case, we naturally use the Laguerre polynomials as the suitable basis set. As a result the integro-differential equation of $\tilde{\psi}$ is transformed into a set of algebraic equations. Retaining up to ten Laguerre polynomials, in this case, is sufficient to produce an accurate $\tilde{\psi}$ and its corresponding energy $\varepsilon_{\rm bt}$.

As in positron-hydrogen scattering, we force orthogonality between $\tilde{\psi}_{1s}$ and ψ_{ns} to ensure that no spurious tails remain asymptotically and also dropped constant terms of the form $\langle X_{1s}|h_2 - k_n^2|u_n \rangle$ for $n \neq 1$, which appear on the right hand side of the ψ equation to ensure that no spurious tails are retained asymptotically. These constant terms are small as in the $e + \rm H$ case.

The converged phase shifts of configuration $1\tilde{s}$ calculated without the effect of exchange, $\delta^{\rm GHA}$, together with the static approximation (without exchange), $\delta^{\rm ST}$, are presented in Table 2. In this case the GHF formalism is equivalent to that of GHA. Table 2 shows that again, as in the positron-hydrogen scattering case, the GHA phase shifts are quite high. The converged GHF phase shifts for the singlet and triplet states in electron-hydrogen scattering, $\delta^{\rm GHF}$, are also presented in Table 2, together with the static (with exchange), $\delta^{\rm CCA}$, values both for singlet ($S = 0$) and triplet case ($S = 1$). Table 2 shows that when the exchange terms are kept in the $\tilde{u}$ equation the enhancement in $\delta^{\rm GHA}$ is completely gone. This may be understood from the symmetry (or antisymmetry) of the wave functions. When the projectile penetrates the bound orbital it becomes the new "inner core" electron because of the indistinguishability of their wave functions and hence does not change any of the physics. The GHF phase shifts and those of the static with exchange are comparable. This is, of course, a very encouraging result.

The binding energies of the GHF approximate target function are presented in Table 2. They are very close to the exact values. This small variation in the energy indicates that the WAC places a strong constraint on the solution to eventually lead to the correct boundary condition. The effective potential for the bound orbitals is nearly one half of the Coulomb potential, for $r > 3a_0$. This large deviation is apparently caused by the penetra-

Table 2. We display the phase shift values δ in radians for the hydrogen-electron scattering case calculated in the various approximations for the singlet and triplet states. ST = phase shifts obtained in the static case without exchange (only the ground state of hydrogen is kept in the expansion). GHA = phase shift obtained with the present theory without exchange. CCA = close coupling approximation where the exact hydrogen functions are used. GHF = phase shift obtained in the GHF approximation, where both the target function and the scattering function are calculated simultaneously in a self-consistent way. EX = the exact phase shifts obtained by Schwartz [22]. All s = phase shifts obtained by including all the virtual s excited states. The GHF values are very close to that of CCA, both in $S = 0$ and $S = 1$. $\varepsilon_{\rm bt}$ is the binding energy of the approximate GHF target function and ka_0 is the continuum wave number.

$ka_0 = 0.2$					
$S = 0$	$\delta^{\rm ST}$	$\delta^{\rm GHA}$	$\delta^{\rm CCA}$	$\delta^{\rm GHF}$	$\varepsilon_{\rm bt}(Ry)$
$1s$	0.9725	1.609	1.871	1.868	-0.973
$1s + 2s$			1.878	1.877	-1.002
$1s + 2s + 3s$				1.878	-1.001
all s			1.897		
exact			2.067		(-1.000)
$S = 1$					
$1s$			2679	2.677	-0.993
$1s + 2s$			2.680	2.678	-1.011
$1s + 2s + 3s$				2.678	-1.009
all s			2.679		
exact			2.717		

$ka_0 = 0.4$					
$S = 0$	$\delta^{\rm ST}$	$\delta^{\rm GHA}$	$\delta^{\rm CCA}$	$\delta^{\rm GHF}$	$\varepsilon_{\rm bt}(Ry)$
$1s$	1.058	1.371	1.239	1.236	-1.043
$1s + 2s$			1.257	1.256	-1.013
$1s + 2s + 3s$				1.257	-1.008
all s			1.270		
exact			1.415		(-1.000)
$S = 1$					
$1s$			2.257	2.256	-1.022
$1s + 2s$			2.258	2.257	-1.017
$1s + 2s + 3s$				2.257	-1.009
all s			2.258		
exact			2.294		

tion into the target cloud by the projectile electron. This is illustrated in Figure 6a. The GHF approximate target wave function $\tilde{\psi}_{1s}$ turns out to be close to the exact one. It is slightly pushed out, however, by comparison to the ground state of hydrogen ψ_{1s}. This can be understood from the increase in the range of the effective self consistent potential as seen by the target electron. This effect is only attainable with this theory and is due mainly to its self-consistent nature. These types of effects have never been observed before and are being presented here for the first time. This effect is illustrated in Figure 6b.
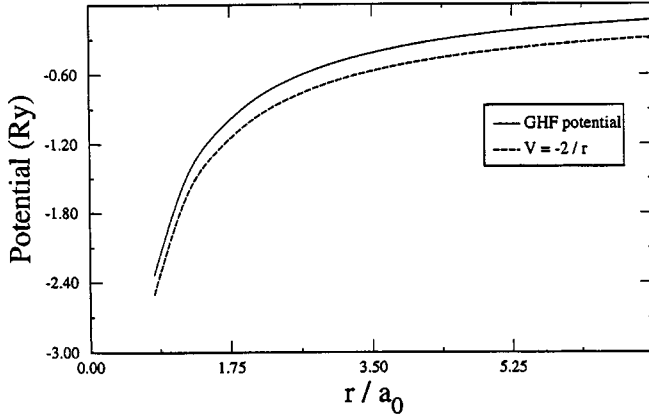
(a)
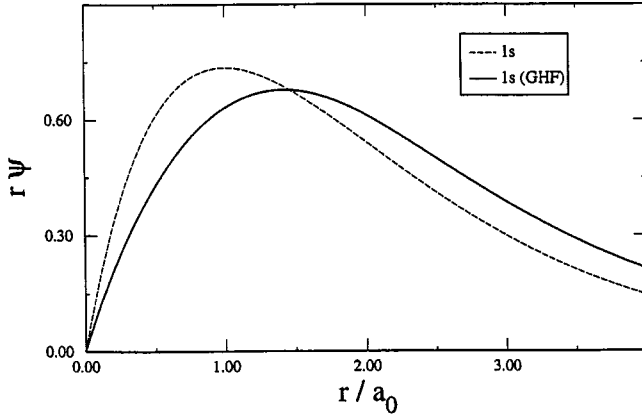
(b)

Fig. 6. (a) Comparison of the Coulombic potential (dashed line) and the GHF potential (solid line) for the bound electron at $ka_0 = 0.4$. (b) Comparison of the exact (dashed line) and the GHF (solid line) for the hydrogen $1s$ wave function at $ka_0 = 0.4$.

Fig. 7. Plot of the difference between the exact wave function and successively converged ones by configuration mixings in the GHF: $1s$ (GHF) (solid line), $1s$ (GHF) $+ 2s$ (dashed line), and $1s$ (GHF) $+ 2s + 3s$ (dashed-dotted line).

Fig. 8. Comparison of the singlet exact phase shift (long dashed), and all s (solid) with those calculated with successive GHF approximations as a function of ka_0: $1s$ (static) (dashed-dotted line), $1s$ (GHF) (dotted line), $1s$ (GHF) $+ 2s$ (dashed-dotted-line), and $1s$ (GHF) $+ 2s + 3s$ (dashed-dot-dotted line).

Table 2 shows that as we add the ns configurations to the total scattering function, such as $2s$ and $3s$ states, the binding energy of the GHF approximate target function approaches $-1Ry$. Moreover the scattering function and the corresponding phase shift approach the exact value of the all-s virtual exited states as expected. We plot, in Figure 7, the difference between the converged GHF target wave function, $\tilde{\psi}_{1s}^{(i)}$, where $(i) = 1\tilde{s}, 1\tilde{s}+2s$, and $1\tilde{s}+2s+3s$ and the exact hydrogen wave function ψ_{1s} versus r, where r is in units of Bohr radii. One can see that as we add the $2s$ and $3s$ states the $\tilde{\psi}_{1s}$ target wave function approaches that of hydrogen ψ_{1s}. The phase shift for the $1\tilde{s}$ configuration, as shown in Figure 8, converges monotonically toward the exact value of all virtual s excited states.

Based on the above results and those of the positron-hydrogen scattering, we conclude that the new self-consistent approach to scattering system is proven to converge to the correct asymptotic values as more terms are added and is effective as well. Hence, the use of ampu-
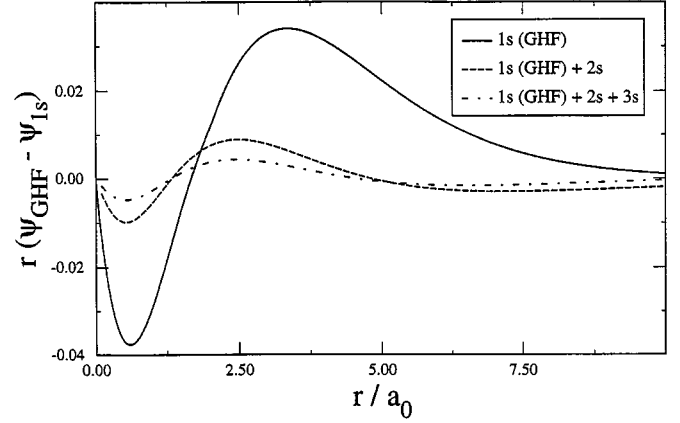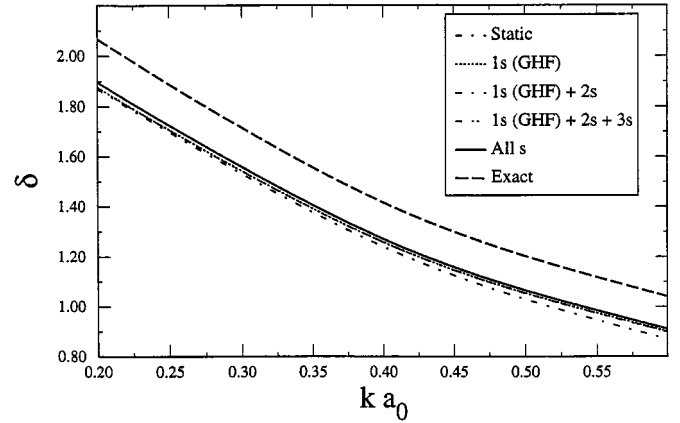
tated functions along with the weak asymptotic condition are justified. So, knowing the exact asymptotic boundary condition is no longer necessary in the present formalism. Moreover, the scattering and the bound parts of a scattering system are no longer separated, as they are treated here on equal footing in a fully self consistent way. Thus, the question of how good the cluster functions have to be for composite targets in order to specify the asymptotic boundary condition may no longer be raised. Most importantly, in this formalism the scattering problem is well defined unlike in the other approaches where the asymptotic boundary conditions have to be satisfied exactly. Of course, in practice this is only possible for the hydrogen atom.

5 Positron scattering from helium by GHA

The scattering of low energy positron by helium is the subject of continuing interest, both theoretically and experimentally [24–27]. In general the major difficulty associated with the scattering by atoms other than hydrogen is that the asymptotic boundary condition requires the exact target functions which are very difficult to evaluate. Such bound state functions are either not available in many cases, except in very crude forms, or too cumbersome to use. Naturally the question arises as to what extent such approximate cluster functions affect the scattering amplitudes. This is not well understood because the scattering parameters, such as the phase shift, depend on the cluster functions in a very complicated way.

The most successful method in treating many-particle systems is the close coupling approximation (CCA). Even though it produces some of the most accurate scattering amplitudes, it suffers from the same problem that afflicts most present theories. Namely, one is faced with the problem of generating, *a priori* in an accurate form, the internal cluster wave functions. The close coupling method was first used by Wardle [28] to investigate positron-helium scattering below the positronium formulation threshold. She has performed the calculation with and without the effect of virtual positronium formation. In both models, she used two approximate (the Hylleraas and Hartree-Fock) helium ground state wave functions. In the static-virtual positronium formation, the calculated scattering phase shifts differ qualitatively with different approximate helium target wave functions. As of now, there are no criteria which determine the effects of the inaccuracies inherent in collisions involving all atoms except hydrogen.

Hahn [10] critically examined this problem by parametrizing the ground state of the hydrogen atom in a nonlinear way. This model wave function of hydrogen was then used in the case of single channel elastic scattering of electrons by a hydrogen atom. The phase shifts in the case of the static approximation depend strongly on the static potential and exchange kernel. These potentials were found to be very sensitive to the target function. His test results showed that the static phase shift deviated from its correct value as the ground state of the hydrogen atom was slowly modified. This suggests that in order to obtain reliable scattering amplitudes, the target functions have to be improved in the case of target atoms that contain more than one electron, to an accuracy at least an order of magnitude better than that desired for the scattering function.

In the present GHA formalism, the asymptotic conditions that require the exact knowledge of the target function are not assumed to be strictly imposed, even in the hydrogen case. Since it has been tested and shown to be effective in the positron/electron-hydrogen scattering, we attempt to apply it for the first time to the single channel positron-helium scattering. Both the scattering wave function and the helium wave function are treated in a fully self-consistent way. The resulting wave functions and the corresponding scattering phase shifts are then uniquely determined, and can be improved simultaneously by multiconfiguration mixing.

In atomic units, the Schrödinger equation for a helium atom and one free positron can be written as

$$\left[- \left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2 \right) - \frac{4}{r_1} - \frac{4}{r_2} + \frac{4}{r_3} \right.$$
$$\left. + \frac{2}{r_{12}} - \frac{2}{r_{13}} - \frac{2}{r_{23}} - E \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0, \quad (42)$$

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|, \quad (43)$$

where E is the total energy of the system in units of Rydberg. r_1, r_2 and r_3 are the coordinates of the two atomic electrons and the incident positron, respectively.

We apply the GHA to positron He elastic scattering with $L = 0$. Only one single channel is considered, limiting the scattering energy to be less than 15 eV, for energies below the pickup threshold. The wave function of the scattering system can then be written in GHA lowest approximation as

$$\Psi^{L=0,S=1/2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \simeq \tilde{\psi}(r_1)\tilde{\psi}(r_2)\tilde{u}(r_3) \quad (44)$$

where α and β are the spin up and spin down states. For this case the WAC to be satisfied for this case is

$$\left\langle \tilde{\psi}(r_1)\tilde{\psi}(r_2) \right| - \left(\nabla_1^2 + \nabla_2^2 \right) - \frac{4}{r_1} - \frac{4}{r_2}$$
$$+ \frac{2}{r_{12}} - \varepsilon_{\rm bt} \left| \tilde{\psi}(r_1)\tilde{\psi}(r_2) \right\rangle_{12} = 0. \quad (45)$$

where

$$\langle \cdots \rangle_{12} = \iint {\rm d}r_1 {\rm d}r_2 \ldots$$

The radial differential equation for $\tilde{u}$ is obtained by multiplying equation (42) by $\tilde{\psi}(r_1)\tilde{\psi}(r_2)$ then integrating over the radial coordinates r_1 and r_2 and all the angles. The $\tilde{u}$ equation is given as

$$\left[T(r_3) + k^2 - V^{\rm S}(r_3) \right] \tilde{u}(r_3) = 0 \quad (46)$$

where

$$V^{\rm S}(r_3) = \frac{4}{r_3} - \frac{4}{r_3} \int_0^{r_3} r'^2 {\rm d}r' \tilde{\psi}(r')\tilde{\psi}(r')$$
$$- \int_{r_3}^{\infty} r'^2 {\rm d}r' \tilde{\psi}(r')\frac{4}{r'}\tilde{\psi}(r'). \quad (47)$$

Similarly, the radial differential equation for $\tilde{\psi}$ is obtained by multiplying equation (42) by $\tilde{\psi}(r_2)X(r_3)$ then integrating over the radial coordinates r_2 and r_3 and all the angles. The $\tilde{\psi}$ equation is given by

$$\left[T(r_1) + \varepsilon_{\rm dt} - V^{\rm B}(r_1) \right] \tilde{\psi}(r_1) = 0 \quad (48)$$

where

$$V^{\mathrm{B}}(r_1) = \frac{-4}{r_1} - \frac{V_{X\tilde{u}}(r_1) + \Delta(X,\tilde{u})V_{\tilde{\psi}\tilde{\psi}}(r_1)}{\Delta(X,\tilde{u})}, \qquad (49)$$

where

$$\Delta(X,\tilde{u}) = \int_0^\infty r'^2 \mathrm{d}r' X(r')\tilde{u}(r'), \qquad (50)$$

$$V_{X\tilde{u}}(r_1) = \frac{4}{r_1}\int_0^{r_1} r'^2 \mathrm{d}r' X(r')\tilde{u}(r')$$
$$+ \int_{r_1}^\infty r'^2 \mathrm{d}r' X(r')\frac{4}{r'}\tilde{u}(r'), \qquad (51)$$

$$V_{\tilde{\psi}\tilde{\psi}}(r_1) = \frac{2}{r_1}\int_0^{r_1} r'^2 \mathrm{d}r' \tilde{\psi}(r')\tilde{\psi}(r')$$
$$+ \int_{r_1}^\infty r'^2 \mathrm{d}r' \tilde{\psi}(r')\frac{2}{r'}\tilde{\psi}(r'), \qquad (52)$$

$$X(r_3) = \left(T(r_3) + k^2\right)\tilde{u}(r_3) \qquad (53)$$
$$= V^{\mathrm{S}}(r_3)\tilde{u}(r_3) \qquad (54)$$

and

$$\varepsilon_{\mathrm{dt}} = \varepsilon_{\mathrm{bt}} + \frac{\Delta(X,X) - \Delta\left(X,\frac{2}{r'}\tilde{u}\right) + c_1}{\Delta(X,\tilde{u})} - c_2. \qquad (55)$$

where

$$c_1 = \int r_2^2 \mathrm{d}r_2 r_3^2 \mathrm{d}r_3 \tilde{\psi}^2(r_2)\frac{1}{r_{23}}X(r_3)\tilde{u}(r_3) \qquad (56)$$

and

$$c_2 = \int_0^\infty r'^2 \mathrm{d}r' \tilde{\psi}(r')\left(+T(r') - \frac{4}{r'}\right)\tilde{\psi}(r'). \qquad (57)$$

It has been difficult to show the conditions under which methods for treating scattering problems will provide bounds on the phase shift. The Kohn and Hulthen [29] variational methods do not guarantee phase shift bounds at positive nonzero energies. The lack of a bound property has been demonstrated by Schwartz [22] by performing extensive calculations of the scattering of electrons and positrons from hydrogen. Percival [18] considered this problem from another point of view based on the famous Rayleigh-Ritz method that has been very successful in providing upper energy bounds for the bound states. His results were suggestive but incomplete. The proof of the rigorous bound was given in a new formulation later [30,31]. The phase shift bound is a very desirable feature which one would like to have in a computational method, providing a criterion for determining the accuracy of the phase shift calculated. To accomplish these goals, the open channels must be treated "exactly" by continuous variation of functions, while the closed channels are treated by variation of the coefficients. Such a method was introduced earlier [32–34].

The close coupling approximation (CCA) has the property of providing phase shift bounds, but its convergence

Table 3. We display the phase shift values in radians for the helium-positron scattering case calculated from the GHA theory δ^{GHA} and the corresponding energies $\varepsilon_{\mathrm{bt}}$, in units of Rydberg, of the target helium function. Also displayed are phase shifts calculated with various approximate forms for the He function: (a) $\delta^{Z_{\mathrm{eff}}}$ where the helium target function is hydrogenic with effective $Z_{\mathrm{eff}} = 2 - 5/16$; (b) δ^{HF}, where the helium target function is of Hartree-Fock form [28]. The phase shift given by McEachran *et al.* [36] is denoted by δ^{po} where they have performed polarized orbital calculations.

ka_0	$\delta^{Z_{\mathrm{eff}}}$	δ^{HF}	δ^{GHA}	$\varepsilon_{\mathrm{bt}}$	δ^{po}
0.1	-0.0381	-0.0424	-0.0300	-5.699	0.0428
0.2	-0.0759	-0.0842	-0.0596	-5.699	0.0584
0.3	-0.1131	-0.1252	-0.0890	-5.698	0.0536
0.4	-0.1493	-0.1649	-0.1174	-5.698	0.0350
0.5	-0.1843	-0.2030	-0.1448	-5.698	0.0076
0.6	-0.2179	-0.2392	-0.1710	-5.697	-0.0248
0.7	-0.2500	-0.2735	-0.1958	-5.697	-0.05974

has turned out to be poor at low energy scattering because of its inability to account for atomic distortion. This is due to the fact that computationally only a finite number of target eigenstates may be included. The inclusion of all $l = 0$ target states, for example in the case of positron-hydrogen scattering, results in a phase shift only slightly better than the static approximation (retaining only the $1s$ state). An alternative method was devised to improve the convergence of the CCA. It carries the name of pseudo-state expansion [32]. This method is based on expansion in target states but some of them are chosen for best convergence rather than restricted to the target eigenstates. It has also been shown [30,31] that this method produces lower bounds on phase shifts.

We adopt the above method to account for atomic distortion in the present case. A pseudo-state of the form $r\psi_{\bar{p}} \sim r^2(1 + r/2)\exp(-\lambda r)$ is employed [35]. When the nonlinear parameter λ is varied, a quasi-bound property is observed. It is not a rigorous-bound property because the helium target function is known only approximately.

In Table 3 we present the phase shift values calculated from the GHA theory and the corresponding energies of the target helium function. These are compared with several previous calculations in which various approximate forms for the He function were used. As Table 3 shows, the calculated phase shifts using different approximate forms of the He function vary considerably. This is not surprising, since it has been shown [10] that the scattering phase shifts depend critically on the approximate form used for the target helium function. The present theory, however, gives better results than that of effective Z and HF. As in the $e + \mathrm{H}$ and $e - \mathrm{H}$ case, the GHA proves to be effective in converging to the correct value.

The GHA phase shifts in the single configuration approximation, δ^{GHA} are plotted in Figure 9 *versus* ka_0. They are then compared with the phase shifts obtained by using the helium function in the Z_{eff} approximation, $\delta^{Z_{\mathrm{eff}}}$, and in HF approximation, δ^{HF}, and the phase shift given by McEachran *et al.* [36], δ^{po}, which included a polarized
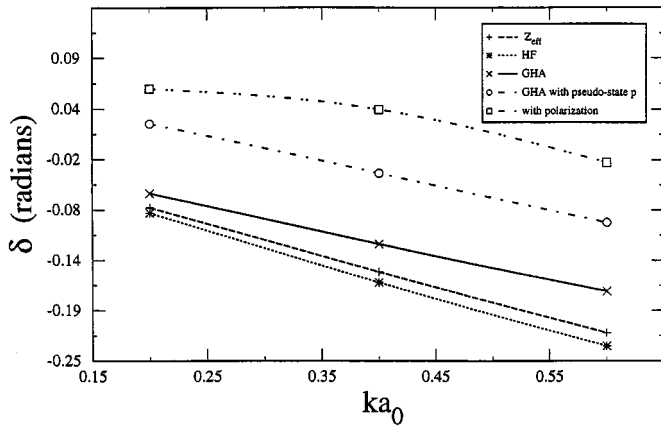
Fig. 9. The positron-helium elastic scattering phase shift calculated with the GHA (solid line) plotted as a function ka_0. This is compared with those obtained with the helium function in the HF approximation (dotted line) and in the $Z_{\rm eff}$ approximation (dashed line). The phase shift obtained with a pseudo-state function corresponding to the target polarization with the nonlinear parameter $\lambda = 1$ is shown (dashed-dotted line). Also shown is the phase shift obtained with the nonlinear parameter $\lambda = 1.62$ at $ka_0 = 0.6$ (square symbol), which agrees with the result of reference [36].
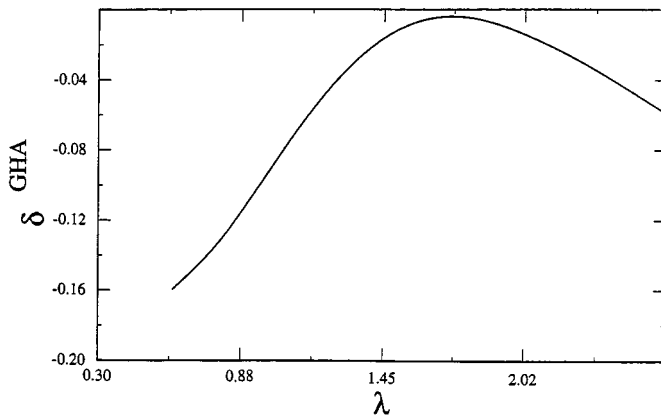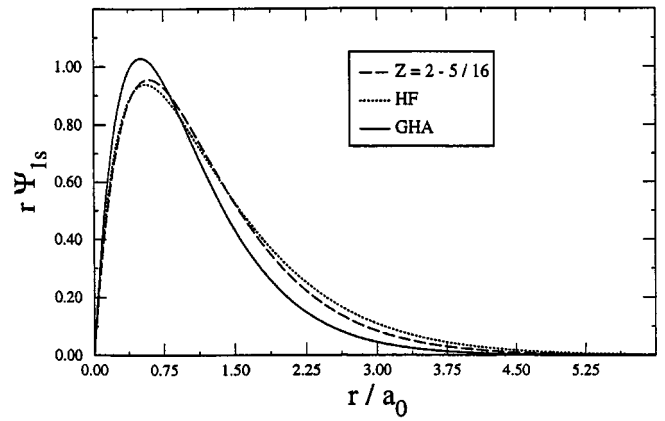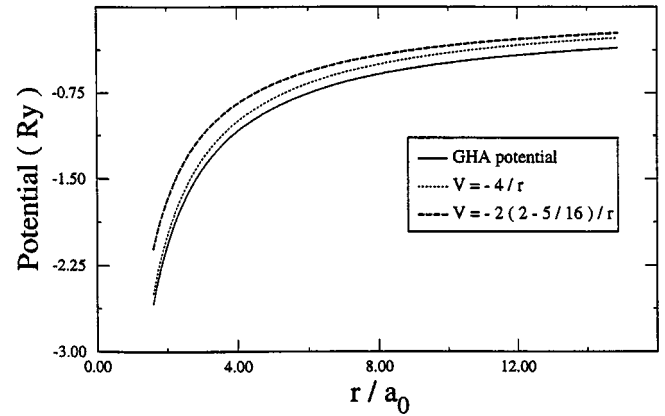

Fig. 10. The phase shift obtained with a pseudo-state function plotted as a function of the non-linear parameter λ for the case of $ka_0 = 0.6$.

(a)

(b)

Fig. 11. (a) The GHA helium orbital (solid line) compared with that of HF (dotted line) and with $Z_{\rm eff}$ (dashed line). (b) The effective SCF potential for the helium bound electron (solid line) in the positron-helium scattering plotted at $ka_0 = 0.6$. This is compared with the proton-electron Coulomb potentials with $Z = 2$ (dotted line) and $Z = Z_{\rm eff}$ (dashed line).

orbital. In their study, they evaluated the full adiabatic polarization potential using a perturbative approach. The GHA phase shift results obtained with pseudo-state function, $\psi_{\bar p}$, is shown, corresponding to the target polarization with the nonlinear parameter $\lambda = 1$. This figure shows that with the inclusion of one pseudo-state, a little more than half of the polarization effects are recovered. This again demonstrates its effectiveness as it converges toward the value of McEachran *et al.* In order to show that this theory obeys the quasi-bound property, we varied λ. Figure 10 shows the dependence of the phase shift on λ. Note that the optimal phase shift, which occurs for $\lambda \simeq 1.62$, closely approaches the value given by McEachran *et al.* Although the target function is not exact, a potentially important quasi-bound property [21] is observed.

The principal conclusion, as illustrated by the above results, is that the present theory with the two key ansatz works and produces reliable results when applied to collision problems with targets that involve more than one electron. The GHA in principle changes the original scattering problem in the sense that the asymptotic boundary conditions no longer need to be specified. At present we can not pin-point reasons for the effectiveness of the present formalism.

Interesting features are found with the use of the present theory in this positron-helium case.

(1) In Figure 11a, the GHA He target function, the Hartree-Fock wave function, and that of $Z_{\rm eff}$ are plotted for comparison. The GHA orbital function is close to that of isolated helium, that is, the wave function for the He orbital looks almost exactly like a hydrogenic function. Apparently, this is due to the cancellation between the static screening and an attractive contribution from the amputated wave function term.

The bound state of the He orbital is however different from that of Z_{eff} and He HF result because the GHA He orbital is pulled in considerably, due to the penetration of the positron inside the helium cloud. This is in qualitative agreement with the $e + \text{H}$ case.

(2) The SCF potential given in Figure 11b which generates the He orbital is different from the conventional one, *i.e.*, asymptotically the SCF potential is a Coulomb field of charge $+2.2e$, not the charge $2e$ of the helium core. This is again due to the penetration of the positron.

More accurate forms of the helium function may give more improved phase shift. In practice, this is done in an arbitrary way by first deciding on the desired accuracy of the scattering amplitudes. Then the target function used has to be better than the desired accuracy of the scattering amplitudes. In addition, at low energy more terms have to be retained in the expansion to account for polarization in order to improve the scattering part. Thus in the conventional theories, the target part and the scattering part are treated separately. In the present formalism, however, this arbitrariness is lifted, and both the scattering wave function and the helium wave function are treated on equal footing as they are determined in a fully self-consistent way.

Summarizing the positron-helium elastic scattering phase shift calculated with the GHA (solid line) is plotted as a function of ka_0 in Figure 9. This is compared with those obtained with the helium function in the HF approximation (dotted line) and in the Z_{eff} approximation (dashed line). The phase shift obtained with a pseudo-state function corresponding to the target polarization with the nonlinear parameter $\lambda = 1$ is shown (dashed-dotted line). Also shown is the phase shift obtained with the nonlinear parameter $\lambda = 1.62$ at $ka_0 = 0.6$.

6 Electron scattering from helium by GHF

The scattering of low energy electrons from a helium atom requires the solution of a three electron problem. Theoretically there are three sources of complications: firstly, the Pauli exclusion principle due to the indistinguishability of the electrons must be imposed. Next, the target function of helium is needed to satisfy the asymptotic boundary conditions, as was the case with the positron projectile, as explained in Section 5. Finally, the necessity to account for the distortion of the targets as represented primarily by polarization effects. The GHF approach considered here, with the full exchange effect, self-consistently and simultaneously calculates the target and scattering function.

In atomic units, the Schrödinger equation for a helium atom and one free electron can be written as

$$
\begin{aligned}
\Bigg[-\left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2\right) - \frac{4}{r_1} - \frac{4}{r_2} - \frac{4}{r_3} \\
+ \frac{2}{r_{12}} + \frac{2}{r_{13}} + \frac{2}{r_{23}} - E \Bigg] \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0, \quad (58)
\end{aligned}
$$

Table 4. We display the phase shift values in radians for the helium-electron scattering case calculated from the GHF theory, δ^{GHF}, and the corresponding energies, ε_{bt} in units of Rydberg, of the target helium function at $ka_0 = 0.2$, 0.4, 0.6 and 1. where ka_0 is the continuum wave number. Also displayed are phase shifts calculated with various approximate forms for the He function: (a) $\delta^{Z_{\text{eff}}}$ where the helium target function is hydrogenic with effective $Z_{\text{eff}} = 2 - 5/16$; (b) δ^{HF} where the helium target function is of Hartree-Fock form. The phase shift given by Pu [38] is denoted by δ^{po} where they have performed polarized orbital calculations.

ka_0	$\delta^{Z_{\text{eff}}}$	δ^{HF}	δ^{GHF}	δ^{po}	ε_{dt}
0.4	2.553	2.559	2.563	2.606	-5.831
0.6	2.281	2.298	2.310	2.355	-5.823
0.8	2.026	2.085	2.107	2.133	-5.702
1.0	1.800	1.902	1.920	1.941	-5.689

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and where E is the total energy of the scattering system.

The Pauli exclusion principle requires that the total wave function for the system be antisymmetric in the interchange of any two electrons. Since the target configuration forms a singlet spin state, only one orientation of the scattering electron spin need to be considered. Furthermore, since exchange is explicitly included, the atomic orbitals must be properly paired with the wave function for the scattering electron. From these considerations the total wave function with total angular momentum $L = 0$ and total spin $S = 1/2$ quantum numbers describing the scattering electron by a helium atom is written as

$$
\begin{aligned}
\Psi^{L=0,S=1/2}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \simeq \frac{1}{\sqrt{3}} \Big[&\Phi(1,2)\tilde{u}(3)S(1,2)\alpha(3) \\
+ &\Phi(1,3)\tilde{u}(2)S(1,3)\alpha(2) \\
+ &\Phi(2,3)\tilde{u}(1)S(2,3)\alpha(1) \Big] \quad (59)
\end{aligned}
$$

where S is the singlet spin function

$$
S(i,j) = \frac{1}{\sqrt{2}}\big(\alpha(i)\beta(j) - \alpha(j)\beta(i)\big). \quad (60)
$$

α and β are single electron spinors with projections $m_s = 1/2$ and $m_s = -1/2$ respectively, $\tilde{u}$ is the wave function of the scattering electron and $\Phi^{(n)}(i,j)$ is the wave function of the helium atom. First we consider the helium atom in its ground state, *i.e.*,

$$
\Phi(i,j) = \tilde{\psi}(i)\tilde{\psi}(j). \quad (61)
$$

The radial differential equation for $\tilde{u}$ is obtained by multiplying equation (58) by $S(1,2)\tilde{\psi}(r_1)\tilde{\psi}(r_2)$, then integrating over the radial coordinates r_1 and r_2 and all angles. The radial differential equation for $\tilde{\psi}$ is similarly derived by multiplying (58) by $S(1,2)\tilde{\psi}(r_2)X(r_3)$ then integrating over the radial coordinates r_2 and r_3 and all the angles. The $\tilde{u}$ and $\tilde{\psi}$ equations are presented elsewhere [37].

In Table 4 and Figure 12 we have presented the calculated phase shift values obtained from the present formalism. Also presented for comparison are several previous
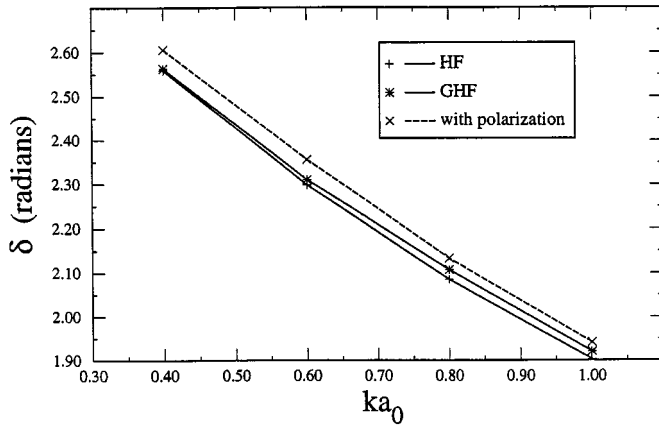
Fig. 12. The electron-helium elastic scattering phase shift calculated with the GHF (solid line) plotted as a function of the continuum wave number ka_0. This is compared with those obtained with the helium function in the HF approximation (dashed line) and in the Z_{eff} approximation (dotted line).

calculations in which various approximate forms for the He function were used.

In Figure 13a, we compare the GHF He target function with the Hartree-Fock wave function. Unlike the $e + \mathrm{He}$ case, the He function seems to be identical to the HF values. This may be understood from the exchange in the role of the inner and the outer electrons as the incoming electron penetrates the He core. A similar phenomenon was also seen in the $e - \mathrm{H}$ case, although, the function is somewhat pushed out. In Figure 13b, the GHF effective potential seen by the bound state function is shown at $ka_0 = 0.6$. It is then compared with that obtained in Z_{eff} and HF approximations. We note that this effective potential is mildly energy dependent.

As Table 4 shows, only small differences ($< 5\%$) are found between the computed phase shifts in the Z_{eff} approximation, $\delta^{Z_{\mathrm{eff}}}$, in HF approximation, δ^{HF}, and the GHF phase shifts δ^{GHF}. This indicates that the calculated phase shifts are rather insensitive to the choice of the target state wave function. Nevertheless, the GHF results are closer to those of Pu *et al.* [38], where the polarized orbital method was used to account for the full polarization induced in the target. This is illustrated in Figure 13a and indicates that the GHF helium function already contains a sizeable polarization effect.

In conclusion, we have demonstrated that the present formalism GHF proves to be effective. This clearly indicates that the WAC is strong enough to lead to the correct boundary condition even in this case. The amputated wave function carries much of the relevant physics information that is contained in the scattering function u. More precisely, the dynamics carried by the u is in the amputated function and not so much in the long range tail of u. Thus, we have shown for the first time that a self-consistent field approach can be employed in treating scattering systems other than hydrogen.
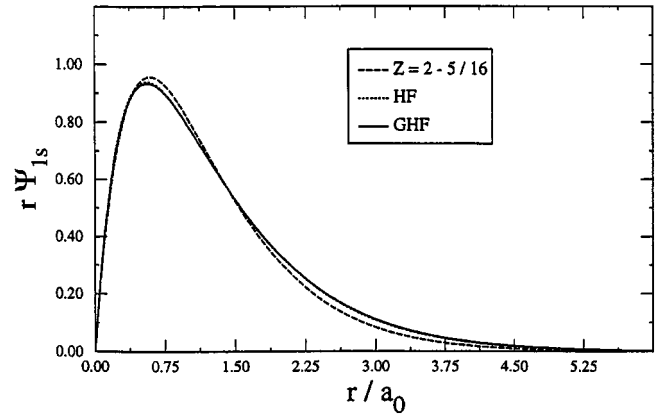
(a)
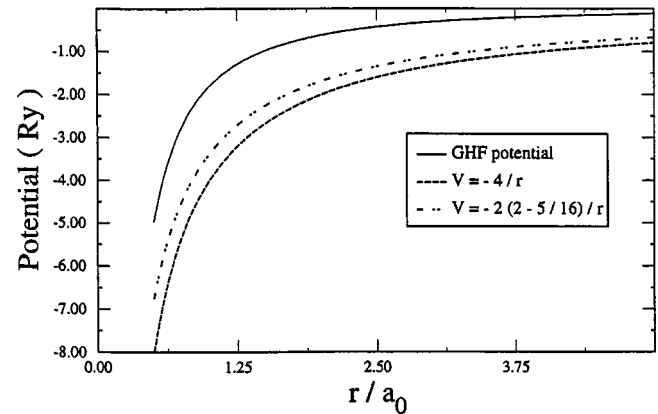
(b)

Fig. 13. (a) The $1s$ orbital of the helium obtained with GHF (solid line) at $ka_0 = 0.6$ compared with that of the HF (dotted line) and with the simple Z_{eff} (dashed line). (b) The effective SCF potential for the helium bound electron (solid line) in the electron-helium scattering plotted at $ka_0 = 0.6$. This is compared with the proton-electron Coulomb potentials with $Z = 2$ (dotted line) and $Z = Z_{\mathrm{eff}}$ (dashed line).

7 Conclusion

The generalized SCF theory introduced in this work puts forth two critical ansatz which required validation. These two key ansatz are the weak asymptotic condition (WAC) which replaces the usual strong asymptotic condition and the amputated wave function (AWF), allowing a fully self consistent approach for the first time. The strong asymptotic condition requires a knowledge of the exact target wave function which is known exactly in the case of the hydrogen atom. For target systems with more than one electron, this can only be met in an approximate form. This introduces a certain amount of arbitrariness in calculating the phase shifts, because the calculation of the target state is decoupled from the scattering problem and is treated on completely different footing. The phase shift can be sensitive to the choice of the target wave function and its accuracy criteria are not known. The WAC

together with AWF removes this arbitrariness by relaxing the asymptotic condition in such a way that an SCF approach is possible in which both the target and scattering wave function are treated on equal footing. This theory must be validated, however, since it relies heavily on these two ansatz which fundamentally change the usual way of dealing with scattering systems.

In validating the theory carried out in the present work, we chose the simplest possible non-trivial system for which exact data are available for comparisons. We study the single channel elastic scattering of positrons by hydrogen target below the positron pick-up threshold and electron below the first excitation threshold. In both these cases, it has been shown that the ansatz are valid and effective. Convergence to the strong asymptotic condition was attained. In the case of positron-hydrogen scattering, the GHA (without exchange) approximate target function contained information which has never been seen before due to the emergence of a self-consistent potential for the target. The GHA potential, as seen by the electron, is roughly twice the Coulomb potential. This is due to the fact that when the positron penetrates into the inner region of the electron orbit, the target electron sees the Coulomb field of two positive charged particles. The manifestation of this effect is that approximate target wave function was shifted to small r region, and this shift was energy dependent. The approximate target wave function and corresponding energy were close to that of hydrogen, indicating that the WAC, although not directly used in the determination of the target orbitals, still put sufficient constraint on the system to lead to the correct answer. In addition, phase shifts from the present theory were much improved in comparison to those obtained by including all the s virtual excited states. We have further shown that, as more configurations are added, the approximate target wave functions and corresponding energies and phase shifts approach those of all s values and the exact hydrogen atom. This is the main results of this paper. We accounted for polarization by using the method of pseudo-states and recovered most of the long range effects. This demonstrated the validity of the ansatz for this case.

The physics in the case of electron-hydrogen scattering is qualitatively different. Unlike the positron-hydrogen case, the GHF approximate target function was very close to the exact one but was slightly pushed or shifted to large r region. This phenomenon is due to the exchange effects where the role of the core and scattering electrons are interchanged as the scattering electron penetrates the core orbit. The results on the phase shift are comparable to the CCA when multiconfiguration mixing was applied. This is again a good indication that the ansatz are sound. In the triplet case, the effect of polarization is negligible, but in the singlet case, we were able to account for about 80% of the polarization, by retaining three terms in the wave function expansion. We did not further pursue this point since our objective was to demonstrate the validity of the ansatz in this theory. Improving upon the phase shifts can be realized by performing a more extensive multiconfiguration calculation, as in the bound case.

The satisfactory results generated from the positron-hydrogen and electron-hydrogen scattering problems provided the basis to extend the study more complex systems. We examined low energy positron and electron scattering from helium. Unlike other theories where the exact asymptotic condition cannot be imposed and some arbitrary accuracy are needed, the asymptotic conditions in this theory are determined in a self-consistent way. We treat the helium and the scattering wave function in a fully self-consistent fashion as was done in the positron-hydrogen and electron-hydrogen case.

We have found some interesting qualitative as well as quantitative features in the case of positron-helium scattering. The SCF potential which generates the He orbital is different from the conventional one. Asymptotically, the SCF potential is a Coulomb field of charge $+2.2e$, not the charge $2e$ of the helium core. Unlike the positron-hydrogen case, there is a partial screening due to the two electrons when the positron penetrates the helium core region. Nevertheless, the GHA orbital function is close to that of isolated helium. Apparently, this is due to the cancellation between the static screening and an attractive contribution from the amputated wave function term. The bound state of the helium orbital is however different from that of Z_{eff} and the helium wave function of HF result because the GHA helium orbital is pulled in considerably, due to the penetration of the positron inside the helium cloud. This is in qualitative agreement with the positron-hydrogen case.

Another important feature that has emerged from this work is that of the quasi-bound property for composite target as in the CCA. By varying a non-linear parameter in a pseudo-state, we have observed that the quasi-bound property [23] holds for this system. This further indicates potential applicability of the theory.

In the case of electron-helium scattering, where the target function occupies a singlet state, our results did not show a substantial improvement when compared to HF and that of Z-effective. This shows that the calculated phase shifts are rather insensitive to the choice of the target state wave function. The GHF results are closer to the result of Pu *et al.* [38], where the full polarization effects were included *via* an extensive perturbative adiabatic approach. We have shown that the GHF helium function is almost identical to the HF wave function of the isolated helium. Unlike the positron-helium scattering case, the exchange seems to reduce the polarization effect on the target atom. This is in agreement with other previous calculations [28]. The GHF helium target wave function is slightly pushed out. In addition, the GHF effective potential seen by the bound state function is mildly energy dependent, resulting in the kinetic energy-dependent binding energies.

Based on the above discussion, we have demonstrated that the two key ansatz, WAC and AWF, produce valid results. The amputated wave function seems to carry all of the relevant physics information that is contained in the scattering function. More precisely, the dynamics carried by the scattering function is in the amputated function and not in the long range tail of the scattering function.

The result of the analysis presented in this paper will be the foundation on which the next extension of the GSCF theory to ionization will be based. Thus the effectiveness of the WAC and the convergence of the theory under multi-configuration mixing as described here are essential in such extensions. As originally envisaged, the GSCF approach can not only combine the conventional HF procedures for the bound configurations to scattering, but also treat the ionization problem in a natural way in terms of the AWF; we can introduce as many AWF's as the number of continuum electrons present.

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