(say, $Z \geq 80$) in the present incident-energy range.[15]

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Low-Energy Electron Scattering in the Random-Phase Approximation

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A general formalism for the computation of low-energy inelastic and elastic electron scattering cross sections within the context of the particle-hole Bethe-Salpeter equation is presented and shown to reduce to the random-phase approximation (RPA) in lowest order. The theory is then applied to triplet elastic electron-He^+ scattering. A short discussion of the differences between the RPA for scattering processes and for low-lying bound states is given, and the numerical methods used to solve the equations are considered in some detail in an appendix.

I. INTRODUCTION

One of the major problems associated with low-energy elastic and inelastic electron scattering from atomic systems is the role of electron correlations. Straightforward application of the close-coupling formalism of Burke and Schey,[1–3] while quite successful in predicting scattering cross sections, requires a great deal of computational effort. Although a number of new numerical techniques adapted to handling large numbers of coupled differential equations,[4,5] or in some way circumventing their direct solution,[6] have reduced the time needed to obtain cross sections, there are still considerable difficulties when there are large numbers of exchange terms. One of the basic difficulties associated with low-energy electron scattering is the need to antisymmetrize the total scattering wave function. In configuration space this necessitates the inclusion of large numbers of nonlocal potentials in each scattering channel. An alternative to this procedure is to introduce creation and destruction operators as in field theory and utilize the formalism of modern many-body theory.[7,8] Such methods have been used quite successfully in nucleon scattering by systems of identical nucleons and, as we shall show, exhibit promise in electron scattering problems. In this article we present a discussion of inelastic and elastic scattering which in lowest approximation reduces to the solution of the eigenvalue problem of the random-phase approximation (RPA).[9–11] The for-

malism is then applied to triplet electron-He^+ elastic scattering, and the results are compared with other calculations in the literature. A discussion of the numerical techniques used to solve the equations is given in the Appendix.

II. THEORY

In order to facilitate the derivation which follows we introduce the following notation:

$$|\psi^{\pm}_{m,k}\rangle = \begin{Bmatrix}\text{incoming}\\ \text{outgoing}\end{Bmatrix} \text{ state of the full Hamiltonian,} \tag{1a}$$

$$|\phi_m\rangle = \text{exact target-state wave function of scatterer,} \tag{1b}$$

$$|\phi^0_{m,k}\rangle = \text{unperturbed-state wave function of our scattering system,} \tag{1c}$$

$$\begin{Bmatrix}\psi(r,t)\\ \psi^\dagger(r,t)\end{Bmatrix} = \text{electron} \begin{Bmatrix}\text{annihilation}\\ \text{creation}\end{Bmatrix} \text{ operator in the Heisenberg representation,} \tag{1d}$$

$$\begin{Bmatrix}\psi^{\text{in,out}}(r,t)\\ \psi^{\text{in,out}\dagger}(r,t)\end{Bmatrix} = \text{electron} \begin{Bmatrix}\text{annihilation}\\ \text{creation}\end{Bmatrix} \text{ operators satisfying (incoming, outgoing) boundary conditions,} \tag{1e}$$

i.e.,

$$\lim_{t\to\mp\infty} \psi^{\text{in,out}}(r,t) = \lim_{t\to\mp\infty} \psi^{\text{free}}(r,t)\,, \tag{1f}$$

where $\psi^{\text{free}}(r,t)$ is the annihilation operator of a free electron.

The quantity basic to the discussion of any scattering process is the so-called S matrix. The S matrix is the overlap integral between exact incoming and outgoing wave functions:

$$S_{mk,m'k'} = \langle \psi^-_{m,k} | \psi^+_{m',k'} \rangle\,, \tag{2}$$

where m is a channel index and k labels the momentum of the unperturbed beam. One can formally simplify the calculation using the LSZ[12] reduction formula in which adiabatic decoupling is applied to the field operators. Thus,

$$\lim_{t\to\mp\infty} \psi(r,t) = \lim_{t\to\mp\infty} \psi^{\text{in,out}}(r,t)\,, \tag{3}$$

where $\psi^{\text{in}}(r,t)$ and $\psi^{\text{out}}(r,t)$ are the asymptotic forms of $\psi(r,t)$ in the distant past and future. In the momentum representation our exact scattering state can be written as

$$|\psi^{\pm}_{m,k}\rangle = a^{\text{in,out}\dagger}_k |\phi_m\rangle\,, \tag{4a}$$

$$a^{\text{in,out}\dagger}_k = \lim_{t\to\mp\infty} a^\dagger_k(t)\,. \tag{4b}$$

Using the definitions above we have

$$\begin{aligned} S_{m'k',0k} &= \langle \psi^-_{m'k'} | \psi^+_{0,k} \rangle = \langle \phi_{m'} | a^{\text{out}}_{k'} a^{\text{in}\dagger}_k | \phi_0 \rangle \\ &= \lim_{\substack{t'\to\infty\\ t\to-\infty}} \langle \phi_{m'} | a_{k'}(t') a^\dagger_k(t) | \phi_0 \rangle \\ &= \lim_{\substack{t'\to\infty\\ t\to-\infty}} \langle \phi_{m'} | T(a_{k'}(t') a^\dagger_k(t)) | \phi_0 \rangle\,. \end{aligned} \tag{5}$$

Since the field operators $\psi(r,t)$, $\psi^*(r,t)$ may be expanded in any arbitrary basis, we also have

$$S_{m'k',0k} = \lim_{\substack{t'\to\infty\\ t\to-\infty}} \int dr_1\, dr_2\, \varphi^*_{k'}(r_2,t')\, \varphi_k(r_1,t) \times \chi_{0m'}(r_2 t', r_1 t)\,, \tag{6}$$

$$\chi_{0m}(rt, r't') = \langle \phi_m | T(\psi(r,t)\psi^\dagger(r't')) | \phi_0 \rangle\,. \tag{7}$$

In (6) φ_k are either plane waves or Coulomb waves depending on the charge of the target. The $\chi_{0m}(rt, r't')$ defined above is known in field theory as the Bethe-Salpeter amplitude.[13] In order to study electron–positive-ion scattering, which is the main purpose of this paper, we have to study the behavior of electron-hole pairs lying in the continuous spectrum of the system under consideration. Stated in another way, we annihilate a bound electron in the noninteracting ground state to create a zeroth-order state of the positive ion, create a free electron on this ionic target, and then adiabatically turn on the interaction until we reach the true scattering wave function. We may define our exact ionic target states as

$$|\psi^{\text{ion}}_n\rangle = c^{\text{in}}_n |\psi_0\rangle\,, \qquad c^{\text{in}}_n = \lim_{t\to-\infty} c_n(t)\,, \tag{8}$$

where $c^\dagger_n$ and c_n create or destroy Hartree-Fock electrons in the infinite past. Similarly, any ionic state existing in the infinite future can be written as

$$|\psi^{\text{ion}}_n\rangle = c^{\text{out}}_n |\psi_0\rangle\,, \quad c^{\text{out}}_n = \lim_{t\to+\infty} c_n(t)\,. \tag{9}$$

We may now write down the S matrix for the $(mk'\text{-}0k)$ transition:

$$S_{mk',0k} = \langle \psi^-_{m,k'} | \psi^+_{0,k} \rangle = \langle \psi^{\text{ion}}_m | a^{\text{out}}_{k'} a^{\text{in}\dagger}_k | \psi^{\text{ion}}_0 \rangle$$

$$= \lim_{\substack{t\to\infty \\ t'\to-\infty}} \langle \psi_m^{\text{ion}} | a_{k'}(t) a_k^\dagger(t') | \psi_0^{\text{ion}} \rangle$$

$$= \lim_{\substack{t\to\infty \\ t'\to-\infty}} \int dr dr' \, \langle \psi_m^{\text{ion}} | \psi(r,t) \psi^\dagger(r',t') | \psi_0^{\text{ion}} \rangle \times \varphi_{k'}^*(r,t) \; \varphi_k(r',t')$$

$$= \lim_{\substack{t\to\infty \\ t'\to-\infty}} \int dr dr' \, \langle \psi_0 | c_m^{\text{out}\dagger} \psi(r,t) \psi^\dagger(r',t') c_0^{\text{in}} | \psi_0 \rangle \times \varphi_{k'}^*(r,t) \, \varphi_k(r',t')$$

$$= \lim_{\substack{t_1 t_2 \to \infty \\ t_1' t_2' \to -\infty}} \int dr_1 \, dr_2 \, dr_1' \, dr_2' \, \varphi_{k'}^*(r_2, t_2) \times \varphi_k(r_1', t_1') \chi_m(r_1, t_1) \chi_0^*(r_{2'}, t_{2'}) \times \langle \psi_0 | \psi^\dagger(r_1, t_1) \psi(r_2, t_2) \; \psi^\dagger(r_1', t_1') \psi(r_2', t_2') | \psi_0 \rangle \, , \tag{10}$$

where φ_k are Coulomb waves and χ_m are Hartree-Fock one-particle states. In terms of the two-particle Green's function, [13–15]

$$S_{mk',0k} = \lim_{\substack{t_1 t_2 \to \infty \\ t_1' t_2' \to -\infty}} \int dr_1 \, dr_2 \, dr_1' \, dr_2' \, G_2(r_2 t_2 r_2' t_2', r_1' t_1' r_1 t_1) \times \varphi_{k'}^*(r_2 t_2) \, \varphi_k(r_1' t_1') \chi_m(r_1, t_1) \chi_0(r_2', t_2') \, , \tag{11}$$

where

$$G_2(12, 1'2') = (1/i^2) \langle \psi_0 | T(\psi(1) \psi(2) \psi^\dagger(2') \psi^\dagger(1')) | \psi_0 \rangle \, .$$

The S matrix may also be expressed in terms of a Bethe-Salpeter amplitude:

$$\chi_{0k}(1, 2) = \langle \psi_0 | T(\psi^\dagger(2) \psi(1)) | \psi_{0,k}^* \rangle$$

$$= \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' \, \langle \psi_0 | T(\psi^\dagger(2) \psi(1) \psi^\dagger(r_1' t_1') \psi(r_2', t_2')) | \psi_0 \rangle \times \varphi_k(r_1', t_1') \chi_0^*(r_2', t_2')$$

$$= \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' G_2(12', 1'2) \, \varphi_k(1') \chi_0^*(2') \tag{12}$$

and

$$S_{mk',0k} = \lim_{t_1 t_2 \to -\infty} \int dr_1 \, dr_2 \, \chi_{0k}(1, 2) \, \varphi_{k'}^*(1) \chi_m(2) \, . \tag{13}$$

Having recognized the connection between the Bethe-Salpeter amplitude and the scattering matrix, it is now possible to use many-body theory to derive useful approximations. The basic equation needed is the integral equation for the linear response function[15,16]

$$R(12, 1'2') = G(1, 2') G(2, 1') + \int d3 d3' d4 d4' \, G(1, 3) \times G(3', 1') \, \Delta(33' | 44') R(42, 4'2') \, , \tag{14}$$

where $G(1, 1')$ is an exact one-particle Green's function,

$$\frac{\delta \Sigma(1, 2)}{\delta G(3, 4)} = \Delta(12 | 34) \, ,$$

and

$$G_2(12, 1'2') = G(1, 1') G(2, 2') - R(12, 1'2') \, . \tag{15}$$

An integral equation for the Bethe-Salpeter amplitude is obtained by inserting (15) in (12) and multiplying both sides by the kernel appearing under the integral sign in (14):

$$\int dx \, dx' d1 d2 \, G(a, x) G(x', b) \, \Delta(xx' | 12) \chi_{0k}(1, 2)$$

$$= - \lim_{t_1' t_2' \to -\infty} \int dx \, dx' d1 d2 \, dr_1' dr_2' G(a, x) G(x', b) \, \Delta(xx' | 12) G_2(12', 21') \, \varphi_k(1') \chi_0^*(2')$$

$$= - \lim_{t_1' t_2' \to -\infty} \int dx \, dx' d1 d2 dr_1' dr_2' G(a, x') G(x', b) \, \Delta(xx' | 12) \, [G(1, 2) G(2', 1') - R(12', 21')] \, \varphi_k(1') \chi_0^*(2')$$

$$= \lim_{t_1' t_2' \to -\infty} \int dx \, dx' d1 d2 dr_1' dr_2' G(a, x) G(x', b) \, \Delta(xx' | 12) R(12'21') \, \varphi_k(1') \chi_0^*(2')$$

$$= \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' \, [R(a2', b1') - G(a, 1') G(2', b)] \, \varphi_k(1') \chi_0^*(2')$$

$$= \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' [G(a,b)G(2',1') - G(a,1')G(2',b) - G_2(a2',b1')] \varphi_k(1') \chi_0^*(2')$$

$$= - \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' \, \varphi_k(1') \chi_{0k}^*(2') G_2(a2',b1') - \chi_{0k}^0(a,b) = \chi_{0k}(a,b) - \chi_{0k}^0(a,b) , \quad (16)$$

or

$$\chi_{0k}(a,b) = \chi_{0k}^0(a,b) + \int dx dx' d1 d2 G(a,x) G(x',b) \times \Delta(xx'|12) \chi_{0k}(1,2) , \quad (17)$$

where

$$\chi_{0k}^0(1,2) = \lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' \, \varphi_k(r_1', t_1') \chi_0^*(r_2', t_2') \times G(1, r_1' t_1') G(r_2' t_2', 2) .$$

In deriving (17) we have made use of the following relation:

$$\lim_{t_1' t_2' \to -\infty} \int dr_1' dr_2' G(1',2') \varphi_k(1') \chi_0^*(2') = 0 .$$

In order to solve (17), a fundamental noncomputational approximation for $\Delta(12|1'2')$, the irreducible vertex part, must be made. In earlier work[15,16] it was shown that the lowest approximation for $\Delta(12|1'2')$ leads to the so-called RPA. In Sec. III we will examine the RPA from another, more familiar, point of view and elaborate further on the approximation for a two-electron system.

III. RANDOM-PHASE APPROXIMATION

The more usual derivations of the RPA start from the equation of motion for the excitation operator $O^\dagger$,[17,18] where

$$O^\dagger |G\rangle = |N\rangle = N\text{th-excited-state wave function}, \quad |G\rangle = \text{exact ground-state wave function}. \quad (18)$$

Substitution into the Schrödinger equation gives

$$[\mathcal{H}, O^\dagger] |G\rangle = \omega_n O^\dagger |G\rangle , \quad (19a)$$

$$\omega_n = E_n - E_G . \quad (19b)$$

The basic approximations inherent in the RPA are to restrict $O^\dagger$ to be a linear combination of particle-hole operators

$$O^\dagger = \sum_{mi} (y_{mi} c_{mi}^\dagger - z_{mi} c_{mi}) \quad (20)$$

and to "linearize" somehow the commutator in (19) to a sum of particle-hole terms. This procedure has the advantage of simplicity and is easily extended to include a larger operator space. On the other hand, the justification for "linearization"[17] is often quite difficult. The eigenvalue spectrum of the operator $O^\dagger$ has, of course, a continuous as well as a discrete portion. The continuous spectrum represents scattering from the positive ion if the ground state is neutral and it is possible to extract the phase shifts directly from the solution of the RPA eigenvalue problem. This procedure is exactly equivalent to the solution of the Bethe-Salpeter equation for continuum particle-hole pairs in lowest approximation. The RPA has been used quite successfully to describe the properties of the low-lying excited states of atomic and molecular systems.[10,16] There are important physical differences between the low-lying excited states of atomic system and the scattering states. These differences are a direct consequence of the boundary conditions for a scattering state and become important when choosing the correct single-particle basis for the expansion of $O^\dagger$. One can argue with some justification that the ground-state Hartree-Fock basis should be pretty good for describing the core electrons in low-lying bound excited states. The change in the core electrons in going from the ground to the excited state in such cases is a "small" effect. Thus the expectation value of the number operator for a given core electron in the ground and excited states is about the same. The situation is quite different for a scattering state. The average electron density at any point in space for a continuum electron is zero. Consequently, the difference in the average potential seen by a given core electron in ground and excited states can be quite large. Thus, if one uses the ground-state Hartree-Fock orbitals for a description of the core electrons in the ion, one scatters off the wrong electrons. At infinity the state consists of a free electron and an ionic target with the target electrons frozen in their ground-state configuration. For a small atom this can be disastrous. A better description of the scattering event is given in terms of the Hartree-Fock orbitals of the ion. The numerical calculations on electron-He^+ scattering that we have performed show that this is indeed the case. The RPA eigenvalue equations for an arbitrary one-particle basis take the form[16]

$$(\epsilon_m - \epsilon_i) y_{mi} + \sum_n \bar{\gamma}_{mn} y_{ni} - \sum_j \bar{\gamma}_{ij} y_{mj} + \sum_{nj} (\tilde{v}_{in,mj} y_{nj} + \tilde{v}_{ij,mn} z_{nj}) = \omega y_{mi} , \quad (21a)$$

$$(\epsilon_m - \epsilon_i) z_{mi} + \sum_n \bar{\gamma}_{mn} z_{ni} - \sum_j \bar{\gamma}_{ij} z_{mj}$$

$$+\sum_{nj}(\tilde{v}_{ij,mn}y_{nj}+\tilde{v}_{in,mj}z_{nj})=-\omega z_{mi}\ , \quad (21b)$$

where (i,j,k) are hole indices, (m,n,o) particle indices, and we define

$$\bar{\gamma}_{\alpha\beta}=\sum_i \tilde{v}_{\alpha i,\beta i}-U_{\alpha\beta}\ ,$$

$U(r)$ = arbitrary one-particle potential,

$$h_{\alpha\beta}+U_{\alpha\beta}=\epsilon_\alpha\delta_{\alpha,\beta}\ ,$$

$$\tilde{v}_{\alpha\beta,\gamma\delta}=\langle\alpha\beta|g_{12}|\gamma\delta\rangle-\langle\alpha\beta|g_{12}|\delta\gamma\rangle\ .$$

For the scattering problem considered below, we choose the one-particle potential to be zero. It proves to be convenient to rewrite these in configuration space. This is done quite simply once it is realized that (21a) and (21b) are merely matrix representatives of the following pair of coupled differential equations:

$$\begin{aligned}&[h(r)-\epsilon_i+\bar{\gamma}(r)]\,y_i(r)-\sum_j\bar{\gamma}_{ij}y_j(r)\\&\quad+\sum_j[\varphi_i(r)\langle\varphi_j|g|y_j\rangle-y_j(r)\langle\varphi_i|g|\varphi_j\rangle\\&\quad+\varphi_i(r)\langle\varphi_j|g|z_j\rangle-\varphi_j(r)\langle\varphi_i|g|z_j\rangle]=\omega y_i(r)\ ,\end{aligned} \quad (22a)$$

$$\begin{aligned}&[h(r)-\epsilon_i+\bar{\gamma}(r)]z_i(r)-\sum_j\bar{\gamma}_{ij}z_j(r)\\&\quad+\sum_j[\varphi_i(r)\langle\varphi_j|g|z_j\rangle-z_j(r)\langle\varphi_i|g|\varphi_j\rangle\\&\quad+\varphi_i(r)\langle\varphi_j|g|y_j\rangle-\varphi_j(r)\langle\varphi_i|g|y_j\rangle]=-\omega z_i(r)\ ,\end{aligned} \quad (22b)$$

with

$$h(r)=-\tfrac{1}{2}\nabla^2-z/r+U(r)\ ,$$

subject to orthogonality of $y_i(r)$ and $z_i(r)$ to the occupied orbitals. In the case of a two-electron system, Eqs. (22a) and (22b) reduce to

$$\begin{aligned}&[h(r)-\epsilon_{He^+}-\omega-J_{He^+,He^+}+\langle\varphi_{He^+}|g|\varphi_{He^+}\rangle]\,y_{He^+}(r)\\&\quad\pm[\langle\varphi_{He^+}|g|y_{He^+}\rangle+\langle\varphi_{He^+}|g|z_{He^+}\rangle\\&\quad-2\langle\varphi_{He^+}\varphi_{He^+}|g|\varphi_{He^+}y_{He^+}\rangle\\&\quad-\langle\varphi_{He^+}\varphi_{He^+}|g|\varphi_{He^+}z_{He^+}\rangle]\varphi_{He^+}(r)=0\ ,\end{aligned} \quad (23a)$$

$$\begin{aligned}&[h(r)-\epsilon_{He^+}+\omega-J_{He^+,He^+}+\langle\varphi_{He^+}|g|\varphi_{He^+}\rangle]\,z_{He^+}(r)\\&\quad\pm[\langle\varphi_{He^+}|g|z_{He^+}\rangle+\langle\varphi_{He^+}|g|y_{He^+}\rangle\\&\quad-2\langle\varphi_{He^+}\varphi_{He^+}|g|\varphi_{He^+}z_{He^+}\rangle\\&\quad-\langle\varphi_{He^+}\varphi_{He^+}|g|\varphi_{He^+}y_{He^+}\rangle]\varphi_{He^+}(r)=0\ ,\end{aligned} \quad (23b)$$

and

$$J_{He^+,He^+}=\langle\varphi_{He^+}\varphi_{He^+}|g|\varphi_{He^+}\varphi_{He^+}\rangle\ .$$

The plus sign refers to the singlet while the minus sign is for the triplet. This pair of equations will represent scattering from an He^+ ion when

$$\omega>|\epsilon_{He^+}|-J_{He^+,He^+}\ .$$

In the particle-hole picture of scattering given by the Bethe-Salpeter equation, only elastic scattering is possible for a two-electron system. In order to describe inelastic scattering in a two-electron system, one would have to allow excitations which were products of particle-hole operators. In larger systems the present formalism is capable of giving elastic and specific inelastic scattering amplitudes that can be achieved by adiabatic coupling from a particle-hole zeroth-order model.

IV. NUMERICAL RESULTS

The solution of the set of coupled equations (23a) and (23b) may be achieved in a variety of ways. We have chosen the integral-equation method of Sams and Kouri[5] for the following reason: Equation (23b) represents a closed channel to the scattering amplitude of (23a) and must, therefore, decay exponentially at infinity. The integral-equation technique incorporates this boundary condition directly and allows a straightforward integration out from the origin to the desired wave function. If one were to try to solve these equations by applying a Numerov technique directly to the differential equations, one would have to integrate both inward and outward and match the functions and slopes at some intermediate point. Alternatively, one could integrate outward N times until the correct ratio of slopes (y'/z') at the origin is achieved to give an exponentially decaying solution at infinity. Either of these two methods is more tedious than the integral-equation technique. In order to set up the problem, the following definitions are needed:

$$\epsilon_k=\tfrac{1}{2}k^2=\epsilon_{He^+}+\omega+J_{He^+,He^+}>0\ , \quad (24a)$$

$$\epsilon_\kappa=-\tfrac{1}{2}\kappa^2=\epsilon_{He^+}-\omega+J_{He^+,He^+}<0\ , \quad (24b)$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}+k^2\right)\begin{pmatrix}F_k(r)\\G_k(r)\end{pmatrix}=0\ , \quad (24c)$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}-\kappa^2\right)\begin{pmatrix}M_\kappa(r)\\W_\kappa(r)\end{pmatrix}=0\ , \quad (24d)$$

$$F_k(0)=0,\quad G_k(0)=\left(\frac{e^{2\pi\gamma}-1}{2\pi\gamma}\right)^{1/2},\quad \gamma=-1/k \quad (24e)$$

$$\lim_{r\to\infty}F_k(r)=\sin[kr+(1/k)\ln 2kr+\sigma]\ ,$$

$$\sigma=\arg\Gamma(1-i/k), \quad (24f)$$

$$\lim_{r\to\infty}G_k(r)=\cos[kr+(1/k)\ln 2kr+\sigma]\ ,$$

$$M_\kappa(0)=0, \quad W_\kappa(0)=1 , \tag{24g}$$

$$\lim_{r\to\infty} M_\kappa(r)=(c_\kappa r^{-1/\kappa}e^{\kappa r}+d_\kappa r^{1/\kappa}e^{-\kappa r}) ,$$

$$\lim_{r\to\infty} W_\kappa(r)=a_\kappa r^{1/\kappa}e^{-\kappa r} . \tag{24h}$$

These definitions correspond fairly closely to the standard ones for free and bound Coulomb waves.[19] We construct the two Green's functions[20] $G_k(r\,|\,r')$ and $G_\kappa(r\,|\,r')$ as

$$G_k(r\,|\,r')=F_k(r)G_k(r')/R_k, \quad r<r'$$

$$=F_k(r')G_k(r)/R_k, \quad r>r' \tag{25a}$$

$$G_\kappa(r\,|\,r')=M_\kappa(r)W_\kappa(r')/R_\kappa, \quad r<r'$$

$$=M_\kappa(r')W_\kappa(r)/R_\kappa, \quad r>r' \tag{25b}$$

where R_k and R_κ are the Wronskians of the two solutions defined as

$$R_k=F_k(r)\frac{dG_k(r)}{dr}-G_k(r)\frac{dF_k(r)}{dr} , \tag{26a}$$

$$R_\kappa=M_\kappa(r)\frac{dW_\kappa(r)}{dr}-W_\kappa(r)\frac{dM_\kappa(r)}{dr} . \tag{26b}$$

Using the definitions given above, we may now rewrite (23a) and (23b) as follows:

$$y_{\mathrm{He}^+}(r)=F_k(r)+\int_0^\infty dr'\,G_k(r\,|\,r')[v_l(r')y_{\mathrm{He}^+}(r')$$

$$+v_{nl}(r')y_{\mathrm{He}^+}(r')+v_{nl}(r')z_{\mathrm{He}^+}(r')+\gamma_1\varphi_{\mathrm{He}^+}(r')], \tag{27a}$$

$$z_{\mathrm{He}^+}(r)=\int_0^\infty dr'\,G_\kappa(r\,|\,r')[v_l(r')z_{\mathrm{He}^+}(r')$$

$$+v_{nl}(r')z_{\mathrm{He}^+}(r')+v_{nl}(r')y_{\mathrm{He}^+}(r')+\gamma_2\varphi_{\mathrm{He}^+}(r')], \tag{27b}$$

where we define

$$v_l(r)=2[\langle\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}\rangle-1/r],$$

$$v_{nl}(r)\psi(r)=\pm 2\langle\varphi_{\mathrm{He}^+}|g\,|\psi\rangle\,\varphi_{\mathrm{He}^+}(r) ,$$

$$\gamma_1=\mp 2[2\langle\varphi_{\mathrm{He}^+}\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}y_{\mathrm{He}^+}\rangle$$

$$+\langle\varphi_{\mathrm{He}^+}\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}z_{\mathrm{He}^+}\rangle] ,$$

$$\gamma_2=\mp 2[2\langle\varphi_{\mathrm{He}^+}\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}z_{\mathrm{He}^+}\rangle$$

$$+\langle\varphi_{\mathrm{He}^+}\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}y_{\mathrm{He}^+}\rangle] ,$$

and we have explicitly recognized the fact that we are dealing with only S-wave scattering. The numerical details associated with the solution of this pair of coupled equations is presented in the Appendix. It should be mentioned that there are certain problems associated with the singlet equation which are non-numerical in origin. The difficulty can best be appreciated by examining the equation for y_{He^+} in the limit of zero coupling:

$$[h(r)-\epsilon_k+\langle\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}\rangle]\,y^0_{\mathrm{He}^+}(r)+[\langle\varphi_{\mathrm{He}^+}|g\,|y^0_{\mathrm{He}^+}\rangle$$

$$-2\langle\varphi_{\mathrm{He}^+}\varphi_{\mathrm{He}^+}|g\,|\,\varphi_{\mathrm{He}^+}y^0_{\mathrm{He}^+}\rangle]\,\varphi_{\mathrm{He}^+}(r)=0 . \tag{28}$$

If we believe that this limiting case should be the one-state approximation, the cause of the difficulty is immediately apparent: The RPA forces the scattering function to be orthogonal to the φ_{He^+} orbital. This is a constraint on the scattering amplitude which does not appear in the one-state approximation. The additional node in the scattering function introduced by this constraint proves to be fatal to the accuracy of the numerical results. This constraint can be removed but the details lie outside the scope of the present work and will be presented in a later publication. Perhaps it is worthwhile to mention that quantum chemists have faced similar difficulties in the treatment of excited states of bound atomic systems having two open shells of the same symmetry. The spatial orbitals of the two shells need not satisfy the same effective one-particle Hamiltonian and there is no reason for them to be orthogonal. For the triplet state these orbitals are automatically orthogonal and consequently there is no problem. The results for the phase shift in the triplet case are presented in Table I. We also include the results of other calculations, including the semiempirical quantum defect method. The agreement with the best calculation in the literature is excellent and suggests that applications to other larger systems should be initiated in the future.

TABLE I. Zero-order phase shifts for triplet electron-He^+ scattering calculated by different methods.

K (a.u.)	Static exchange (Ref. 21)	Exchange adiabatic (Ref. 21)	Polarized orbital (Ref. 21)	$1s$-$2s$-$2p$ close coupling (Ref. 22)	Quantum defect (Ref. 23)	RPA
0	0.920	0.945	0.942	···	0.932	···
0.05	···	···	···	···	···	0.938
0.1	···	···	···	···	···	0.937
0.2	···	···	···	···	···	0.933
0.3	···	···	···	···	···	0.927
0.491	0.893	0.918	0.915	0.909	0.903	0.910
0.779	0.855	0.879	0.875	0.865	0.861	0.870
1.076	0.802	0.827	0.832	0.808	0.803	0.816
1.353	0.748	0.772	0.775	0.752	0.740	0.759

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APPENDIX

To facilitate a noniterative solution to Eqs. (27a) and (27b) we separate the nonlocal potential $v_{nl}(r)$ as follows:

$$v_{nl}(r)\,[y_{\mathrm{He}^+}(r)+z_{\mathrm{He}^+}(r)]$$

$$=\pm 2\left(\frac{1}{r}\int_0^r dr'\,\varphi_{\mathrm{He}^+}(r')\,[y_{\mathrm{He}^+}(r')+z_{\mathrm{He}^+}(r')]\right.$$

$$-\int_0^r dr'\,\varphi_{\mathrm{He}^+}(r')\,\frac{z_{\mathrm{He}^+}(r')+y_{\mathrm{He}^+}(r')}{r'}$$

$$\left.+\int_0^\infty dr'\,\varphi_{\mathrm{He}^+}(r')\,\frac{y_{\mathrm{He}^+}(r')+z_{\mathrm{He}^+}(r')}{r'}\right)\varphi_{\mathrm{He}^+}(r)$$

$$=v_{nl}^0(r)\,[y_{\mathrm{He}^+}(r)+z_{\mathrm{He}^+}(r)]+\beta\,\varphi_{\mathrm{He}^+}(r)\,,$$

$$\beta=\pm 2\int_0^\infty dr\,\varphi_{\mathrm{He}^+}(r)\,\frac{y_{\mathrm{He}^+}(r)+z_{\mathrm{He}^+}(r)}{r}\,. \tag{A1}$$

In writing out (A1) we have recognized the S-wave nature of our scattering function. Using (A1), Eqs. (27a) and (27b) may be rewritten as

$$y_{\mathrm{He}^+}(r)=F_k(r)+\int_0^\infty dr'\,G_k(r|r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')]$$

$$+(\gamma_1+\beta)\int_0^\infty dr'\,G_k(r|r')\,\varphi_{\mathrm{He}^+}(r')\,, \tag{A2a}$$

$$z_{\mathrm{He}^+}(r)=\int_0^\infty dr'\,G_\kappa(r|r')\,[v_l(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')]$$

$$+(\gamma_2+\beta)\int_0^\infty dr\,G_\kappa(r|r')\,\varphi_{\mathrm{He}^+}(r')\,, \tag{A2b}$$

and

$$y_{\mathrm{He}^+}(r)=F_k(r)+\frac{G_k(r)}{R_k}\int_0^r dr'\,F_k(r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')]$$

$$-\frac{F_k(r)}{R_k}\int_0^r dr'\,G_k(r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')]$$

$$+\frac{F_k(r)}{R_k}\int_0^\infty dr\,G_k(r)\,[v_l(r)\,y_{\mathrm{He}^+}(r)+v_{nl}^0(r)\,y_{\mathrm{He}^+}(r)+v_{nl}^0(r)\,z_{\mathrm{He}^+}(r)]+(\gamma_1+\beta)\int_0^\infty dr'\,G_k(r|r')\,\varphi_{\mathrm{He}^+}(r')$$

$$=F_k(r)+\frac{G_k(r)}{R_k}\int_0^r dr'\,F_k(r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')]$$

$$-\frac{F_k(r)}{R_k}\int_0^r dr'\,G_k(r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')]+\alpha_1 F_k(r)+\epsilon_1 I_k(r)\,, \tag{A3a}$$

$$z_{\mathrm{He}^+}(r)=\int_0^\infty dr'\,G_\kappa(r|r')\,[v_l(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')]+(\gamma_2+\beta)\int_0^\infty dr'\,G_\kappa(r|r')\,\varphi_{\mathrm{He}^+}(r')$$

$$=\int_0^\infty dr'\,G_\kappa(r|r')\,[v_l(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,z_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')]+\epsilon_2 I_\kappa(r)\,, \tag{A3b}$$

where

$$\epsilon_1=\gamma_1+\beta\,,\quad \epsilon_2=\gamma_2+\beta\,,$$

$$\alpha_1=\frac{1}{R_k}\int_0^\infty dr\,G_k(r)\,[v_l(r)\,y_{\mathrm{He}^+}(r)+v_{nl}^0(r)\,y_{\mathrm{He}^+}(l)$$

$$+v_{nl}^0(r)\,z_{\mathrm{He}^+}(r)]\,,$$

$$\alpha_2=\frac{1}{R_\kappa}\int_0^\infty dr\,W_\kappa(r)\,[v_l(r)\,z_{\mathrm{He}^+}(r)+v_{nl}^0(r)\,z_{\mathrm{He}^+}(r)$$

$$+v_{nl}^0(r)\,y_{\mathrm{He}^+}(r)]\,,$$

$$I_k(r)=\int_0^\infty dr'\,G_k(r|r')\,\varphi_{\mathrm{He}^+}(r')\,,$$

$$I_\kappa(r)=\int_0^\infty dr'\,G_\kappa(r|r')\,\varphi_{\mathrm{He}^+}(r')\,.$$

Further manipulations are considerably simplified by introducing the following matrix notation:

$$\mathfrak{L}_k^0(r)\,y_{\mathrm{He}^+}(r)$$

$$=\frac{G_k(r)}{R_k}\int_0^r dr'\,F_k(r')\,[v_l(r')\,y_{\mathrm{He}^+}(r')+v_{nl}^0(r')\,y_{\mathrm{He}^+}(r')]$$

$$-\frac{F_k(r)}{R_k}\int_0^r dr'\, G_k(r')\,[v_l(r')\,y_{He^+}(r')+v_{nl}^0(r')\,y_{He^+}(r')]\,, \tag{A4a}$$

$$U_k^0(r)\,z_{He^+}(r)=\frac{G_k(r)}{R_k}\int_0^r dr'\, F_k(r')\,v_{nl}^0(r')\,z_{He^+}(r')$$

$$-\frac{F_k(r)}{R_k}\int_0^r dr'\, G_k(r')\,v_{nl}^0(r')\,z_{He^+}(r'), \tag{A4b}$$

$$\mathcal{L}_\kappa(r)\,z_{He^+}(r)=\frac{W_\kappa(r)}{R_\kappa}\int_0^r dr'\, M_\kappa(r')$$

$$\times[v_l(r')\,z_{He^+}(r')+v_{nl}^0(r')\,z_{He^+}(r')]$$

$$+\frac{M_\kappa(r)}{R_\kappa}\int_r^\infty dr'\, W_\kappa(r')$$

$$\times[v_l(r')\,z_{He^+}(r')+v_{nl}^0(r')\,z_{He^+}(r')]\,, \tag{A4c}$$

$$U_\kappa(r)\,y_{He^+}(r)=\frac{W_\kappa(r)}{R_\kappa}\int_0^r dr'\, M_\kappa(r')\,v_{nl}^0(r')\,y_{He^+}(r')$$

$$+\frac{M_\kappa(r)}{R_\kappa}\int_r^\infty dr'\, W_\kappa(r')\,v_{nl}^0(r')\,y_{He^+}(r')\,. \tag{A4d}$$

The coupled equations can now be written in the following form:

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa & I-\mathcal{L}_\kappa \end{pmatrix}\begin{pmatrix} y_{He^+} \\ z_{He^+}\end{pmatrix}=\begin{pmatrix} 1+\alpha_1 & 0 \\ 0 & 0\end{pmatrix}\begin{pmatrix} F_k \\ M_\kappa\end{pmatrix}$$

$$+\begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2\end{pmatrix}\begin{pmatrix} I_k \\ I_\kappa\end{pmatrix}. \tag{A5}$$

The solution to this set of equations is

$$\begin{pmatrix} y_{He^+} \\ z_{He^+}\end{pmatrix}=(1+\alpha_1)\begin{pmatrix} y_{He^+}^0 \\ z_{He^+}^0\end{pmatrix}+\epsilon_1\begin{pmatrix} y_{He^+}^1 \\ z_{He^+}^1\end{pmatrix}+\epsilon_2\begin{pmatrix} y_{He^+}^2 \\ z_{He^+}^2\end{pmatrix}, \tag{A6}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa & I-\mathcal{L}_\kappa\end{pmatrix}\begin{pmatrix} y_{He^+}^0 \\ z_{He^+}^0\end{pmatrix}=\begin{pmatrix} F_k \\ 0\end{pmatrix}, \tag{A7a}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa & I-\mathcal{L}_\kappa\end{pmatrix}\begin{pmatrix} y_{He^+}^1 \\ z_{He^+}^1\end{pmatrix}=\begin{pmatrix} I_k \\ 0\end{pmatrix}, \tag{A7b}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa & I-\mathcal{L}_\kappa\end{pmatrix}\begin{pmatrix} y_{He^+}^2 \\ z_{He^+}^2\end{pmatrix}=\begin{pmatrix} 0 \\ I_k\end{pmatrix}. \tag{A7c}$$

In order to solve (A7a)–(A7c) noniteratively, we must go one step further. We define the two operators $\mathcal{L}_\kappa^0$ and U_κ^0 as

$$\mathcal{L}_\kappa^0(r)\,z_{He^+}^i(r)=\frac{W_\kappa(r)}{R_\kappa}\int_0^r dr'\, M_\kappa(r')$$

$$\times[v_l(r')z_{He^+}^i(r')+v_{nl}^0(r')\,z_{He^+}^i(r')]$$

$$-\frac{M_\kappa(r)}{R_\kappa}\int_0^r dr'\, W_\kappa(r')$$

$$\times[v_l(r')\,z_{He^+}^i(r')+v_{nl}^0(r')\,z_{He^+}^i(r')]\,, \tag{A8a}$$

$$U_\kappa^0(r)\,y_{He^+}^i(r)=\frac{W_\kappa(r)}{R_\kappa}\int_0^r dr'\, M_\kappa(r')\,[v_{nl}^0(r')\,y_{He^+}^i(r')]$$

$$-\frac{M_\kappa(r)}{R_\kappa}\int_0^r dr'\, W_\kappa(r')\,v_{nl}^0(r')\,y_{He}^i(r')\,. \tag{A8b}$$

Using these definitions gives

$$\begin{pmatrix} y_{He^+}^0 \\ z_{He^+}^0\end{pmatrix}=c_1\begin{pmatrix} y_{He^+}^{00} \\ z_{He^+}^{00}\end{pmatrix}+\begin{pmatrix} y_{He^+}^{01} \\ z_{He^+}^{01}\end{pmatrix}, \tag{A9a}$$

$$c_1=\frac{1}{R_\kappa}\int_0^\infty dr\, W_\kappa(r)\,[v_l(r)\,z_{He^+}^0(r)+v_{nl}^0(r)\,z_{He^+}^0(r)$$

$$+v_{nl}^0(r)\,y_{He^+}^0(r)]\,, \tag{A9b}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa^0 & I-\mathcal{L}_\kappa^0\end{pmatrix}\begin{pmatrix} y_{He^+}^{00} \\ z_{He^+}^{00}\end{pmatrix}=\begin{pmatrix} 0 \\ M_\kappa\end{pmatrix}, \tag{A9c}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa^0 & I-\mathcal{L}_\kappa^0\end{pmatrix}\begin{pmatrix} y_{He^+}^{01} \\ z_{He^+}^{01}\end{pmatrix}=\begin{pmatrix} F_k \\ 0\end{pmatrix}, \tag{A9d}$$

$$\begin{pmatrix} y_{He^+}^1 \\ z_{He^+}^1\end{pmatrix}=c_2\begin{pmatrix} y_{He^+}^{00} \\ z_{He^+}^{00}\end{pmatrix}+\begin{pmatrix} y_{He^+}^{11} \\ z_{He^+}^{11}\end{pmatrix}, \tag{A10a}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa^0 & I-\mathcal{L}_\kappa^0\end{pmatrix}\begin{pmatrix} y_{He^+}^{11} \\ z_{He^+}^{11}\end{pmatrix}=\begin{pmatrix} I_k \\ 0\end{pmatrix}, \tag{A10b}$$

$$c_2=\frac{1}{R_\kappa}\int_0^\infty dr\, W_\kappa(r)\,[v_l(r)\,z_{He^+}^1(r)+v_{nl}^0(r)\,z_{He^+}^1(r)$$

$$+v_{nl}^0(r)\,y_{He^+}^1(r)]\,, \tag{A10c}$$

and

$$\begin{pmatrix} y_{He^+}^2 \\ z_{He^+}^2\end{pmatrix}=c_3\begin{pmatrix} y_{He^+}^{00} \\ z_{He^+}^{00}\end{pmatrix}+\begin{pmatrix} y_{He^+}^{21} \\ z_{He^+}^{21}\end{pmatrix}, \tag{A11a}$$

$$\begin{pmatrix} I-\mathcal{L}_k^0 & -U_k^0 \\ -U_\kappa^0 & I-\mathcal{L}_\kappa^0\end{pmatrix}\begin{pmatrix} y_{He^+}^{21} \\ z_{He^+}^{21}\end{pmatrix}=\begin{pmatrix} 0 \\ I_\kappa\end{pmatrix}, \tag{A11b}$$

$$c_3 = \frac{1}{R_\kappa}\int_0^\infty dr\, W_\kappa(r)\,[v_l(r)\, z^2_{\mathrm{He}^+}(r) + v^0_{nl}(r)\, z^2_{\mathrm{He}^+}(r) + v^0_{nl}(r)\, y^2_{\mathrm{He}^+}(r)]\,. \quad \text{(A11c)}$$

All of the "basic" solutions (A9c), (A9d), (A10b), and (A11b) can be computed noniteratively. The "intermediate" solutions (A9a), (A10a), and (A11a) can be computed from the "basic" solutions by solving a simple algebraic equation. The "final" coupled pair is then constructed from the intermediate solutions by solving a set of three coupled algebraic equations for α_1, ϵ_1, and ϵ_2. From the solution $y_{\mathrm{He}^+}(r)$, the phase shift is extracted as

$$\tan\delta = \frac{1}{R_k}\int dr\, F_k(r)\,[v_l(r)\, y_{\mathrm{He}^+}(r) + v_{nl}(r)\, y_{\mathrm{He}^+}(r) + v_{nl}(r)\, z_{\mathrm{He}^+}(r) + \gamma_1\, \varphi_{\mathrm{He}^+}(r)]\,.$$

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