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Test of the Pluvinage wave function for the helium ground state

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The accuracy of the Pluvinage wave function for the ground state of helium is investigated by considering a number of different physical processes including double ionization by photoabsorption, Compton scattering, and electron impact. In the high-energy limit of these processes, the accuracy of the initial ground state can be ascertained without reference to the final double-continuum state. In this limit, we find that a Hylleraas description is superior to the Pluvinage one. For intermediate energies, final-state correlation becomes important, so we employ a 3C description of the final state (the 3C wave function is the double-continuum analog of the Pluvinage wave function). In this case, however, better agreement with experiment is obtained with the Pluvinage initial state. A possible explanation for this seemingly paradoxical result is suggested.

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I. INTRODUCTION

Continuum distorted wave (CDW) approximations offer a relatively simple way of treating the few-body problem. For N interacting charged particles, the idea is to diagonalize the Hamiltonian H in the $N(N-1)/2$ two-body interactions by constructing a product of $N(N-1)/2$ exact two-body eigenfunctions. The primary advantage of this simple model is that it is realistic enough to provide considerable insight into few-body reactions. The primary disadvantage is, of course, that the part of H that is neglected in constructing the CDW, dubbed the "nonorthogonal kinetic energy" by Crothers [1], is not always negligible.

CDW methods have been successful in describing ion-atom collisions for intermediate and higher energies since the mid 1960s [1–7] and, more recently, electronic [8–10] and photonic [11–13] collisions with atoms. A CDW wave function, ψ_{CDW}, shares a number of important properties with the exact wave function ψ: (a) for three-body problems, it reduces to an exact eigenfunction of the two-body problem if any one of the three particles is removed; (b) it diagonalizes H in all two-body interactions; (c) $H\psi_{\mathrm{CDW}}$, like $H\psi$, has no singularities; (d) it satisfies the cusp conditions of Kato [14] at all two-body coalescence points; and (e) it satisfies correct asymptotic boundary conditions.

The Pluvinage [15] approximation for the ground state of two-electron atoms or ions may be considered a CDW. It is the product of (i) a hydrogenic 1s wave function for one electron in the field of the nucleus of charge Z; (ii) the same for the other electron; and (iii) a continuum Coulomb wave for the electron-electron subsystem. The well-known 3C CDW [16] is the double-continuum analog of the Pluvinage wave function.

Some interesting results have recently been obtained with a 3C description of the helium final state for double ionization by electron impact [10] and photoabsorption [13]. It was found that the 3C calculations are in better agreement with absolute measurements when the Pluvinage wave function is used for the initial state (as opposed to a wave function of the Hylleraas [17] type). On the other hand, when a nonperturbative "convergent close-coupling" (CCC) approach is employed for the the final state [18], the use of the Pluvinage function for the initial state yields much poorer results than a Hylleraas function. Here, we suggest a possible explanation for these conflicting results.

One argument pertinent to the Pluvinage wave function for two-electron processes is that these are processes that can occur even in the limit where the nucleus charge Z vanishes. Then, the Pluvinage initial state with the 3C final state exactly treats the transfer of energy between atomic electrons in processes where two electrons are ejected by photoabsorption, Compton scattering, or electron impact in the Born approximation. Of course, an expression that is exact in the limit $Z\to 0$ does not ensure that it will be accurate for $Z \neq 0$; however, it shows that the double-scattering component requires consistency of initial and final states.

The double-scattering component is known to be important for double-electron ejection by Compton scattering at intermediate energies [19]. Alternatively, the high-energy limit of these processes depends only on the initial-state correlation [20]. We will show that in this limit the Pluvinage wave function is unreliable, but the limit values improve when corrections are introduced.

This paper is organized as follows. In Sec. II, we discuss the Pluvinage and Hylleraas wave functions for the ground state of two-electron atoms, and construct a two-parameter wave function that is the sum of $(1s,1s)$ and $(1s,2s)$ Pluvinage wave functions. Local energies for the Pluvinage, two-parameter, and Hylleraas wave functions are also presented and discussed. Next, we investigate various physical processes using these wave functions. In Sec. III, we study the high-energy limit of double ionization and "excitation-ionization" (single ionization of the target atom with simul-

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taneous excitation of the residual target ion) of He (and H$^-$) by photoabsorption. In Sec. IV, we do the same for Compton scattering. In Sec. V, we consider 5.6-keV electron-impact double ionization of helium within the first Born approximation, using the 3C wave function for the final double-continuum state of the atom. Our conclusions are summarized in Sec. VI.

Atomic units (a.u.) are used throughout, except where specified otherwise, and we denote by $\mathbf{r}_1$ and $\mathbf{r}_2$ the coordinates of two electrons relative to an infinitely massive nucleus of charge Z. The interelectronic coordinate is denoted by $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$.

II. GROUND STATE

For a two-electron atom in an S state (zero total angular momentum), the Hamiltonian may be written in interparticle coordinates (r_1,r_2,r_{12}) as

$$H = h_1 + h_2 + h_{12} + h_x. \tag{1}$$

Here, h_1, h_2, and h_{12} are the Hamiltonians for each of the three two-body subsystems acting independently:

$$h_i = -\frac{1}{2}\left[\frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i}\right] - \frac{Z}{r_i}, \quad i=1,2, \tag{2}$$

and

$$h_{12} = -\left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right] + \frac{1}{r_{12}}. \tag{3}$$

The cross terms for this nonorthogonal coordinate system are contained in

$$h_x = -\left[\frac{r_1^2 + r_{12}^2 - r_2^2}{2r_1r_{12}}\frac{\partial}{\partial r_1} + \frac{r_2^2 + r_{12}^2 - r_1^2}{2r_2r_{12}}\frac{\partial}{\partial r_2}\right]\frac{\partial}{\partial r_{12}}, \tag{4}$$

and represent the nonorthogonal kinetic energy.

The Pluvinage approximation for the ground state is given by [15]

$$\psi_{\mathrm{P}}(r_1,r_2,r_{12}) = N\psi_{1,1,k}, \tag{5}$$

where N is a normalization constant and

$$\psi_{n_1,n_2,k} \equiv \phi_{n_1s}(r_1)\phi_{n_2s}(r_2)g_k(r_{12}). \tag{6}$$

Here

$$\phi_{ns}(r) = \sqrt{\frac{Z^3}{n^3\pi}}e^{-Zr/n}{}_1F_1\left(1-n,2;\frac{2Zr}{n}\right) \tag{7}$$

is the ns eigenfunction for one electron in the field of the nucleus of charge Z, and

$$g_k(r_{12}) = e^{-ikr_{12}}{}_1F_1(1-i\eta,2;2ikr_{12}) \tag{8}$$

is an (unnormalized) eigenfunction of h_{12}, i.e., a continuum Coulomb wave for the electron-electron subsystem. Here, $\eta=1/(2k)$ is the Sommerfeld parameter and k is the wave number, which can be varied to minimize the energy. Although it is not obvious, g_k (8) is a real function of the complex variable ik.

The Pluvinage approximation is simplistic in that only 1s orbitals are considered for the electron-nucleus subsystems. It also has only a single variational parameter, the wave number k of the Coulomb wave for the electron-electron subsystem. To approximate the exact solution to high accuracy would require a complete set of orbitals, including the continuum. In an attempt to improve upon the original single-parameter Pluvinage wave function ψ_{P}, while keeping the desirable properties (a)–(e) (cf. the Introduction) intact, we include a $(1s,2s)$ Pluvinage configuration in a two-parameter wave function

$$\psi^{(2)} = N[\psi_{1,1,k} + A(\psi_{1,2,k} + \psi_{2,1,k})]. \tag{9}$$

The parameters k and A were chosen to minimize the energy

$$E = \langle\psi^{(2)}|H|\psi^{(2)}\rangle. \tag{10}$$

$\psi_{n_1,n_2,k}$ (6) is an eigenfunction of $h_1+h_2+h_{12}$, with eigenvalue $k^2-Z^2[(1/n_1^2)+(1/n_2^2)]/2$, which makes it easy to derive

$$H\psi^{(2)} = N[E_{1,1,k}\psi_{1,1,k} + A(E_{1,2,k}\psi_{1,2,k} + E_{2,1,k}\psi_{2,1,k})], \tag{11}$$

where

$$E_{n_1,n_2,k} \equiv k^2 - \frac{Z^2}{2}\left(\frac{1}{n_1^2}+\frac{1}{n_2^2}\right) + Z\left[\left(\frac{1}{2}+ik\right)\frac{{}_1F_1(2-i\eta,3;2ikr_{12})}{{}_1F_1(1-i\eta,2;2ikr_{12})} - ik\right]\left[\left\{\frac{1}{n_1} + \left(1-\frac{1}{n_1}\right)\frac{{}_1F_1\left(2-n_1,3;\frac{2Zr_1}{n_1}\right)}{{}_1F_1\left(1-n_1,2;\frac{2Zr_1}{n_1}\right)}\right\}\frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}} + \left\{\frac{1}{n_2} + \left(1-\frac{1}{n_2}\right)\frac{{}_1F_1\left(2-n_2,3;\frac{2Zr_2}{n_2}\right)}{{}_1F_1\left(1-n_2,2;\frac{2Zr_2}{n_2}\right)}\right\}\frac{r_2^2+r_{12}^2-r_1^2}{2r_2r_{12}}\right]. \tag{12}$$

We calculated the energy (10) using three-dimensional numerical (Gauss-Legendre) quadrature. The optimal values of k and A are listed in Table I, along with the corresponding normalization constant and the energy. The usual single-parameter Pluvinage wave function is also summarized in Table I. (It should be noted that Pluvinage [15] did not

TABLE I. A summary of the variational parameters k and A, the normalization constant N, and the mean ground-state energy E for the two-parameter wave function $\psi^{(2)}$. The exact energy (to three significant digits) is given in parentheses in the bottom row. For comparison, k, N, and E are also given for the usual single-parameter Pluvinage wave function ψ_{P} (previously given for He by Pluvinage [15]).

	H$^-$		He	
	ψ_{P}	$\psi^{(2)}$	ψ_{P}	$\psi^{(2)}$
k	0.12	0.42	0.41	0.70
A		−0.27		−0.11
N	0.332 16	0.312 92	0.603 37	0.637 70
E	−0.498	−0.523	−2.88	−2.89
	(−0.528)		(−2.90)	

present results for H$^-$, so even our one-parameter wave function ψ_{P} is new in this case.) It is interesting that including a $(1s,2s)$ configuration increases the optimal wave number by more than a factor of 3 for H$^-$ and by almost a factor of 2 for He.

The effect of the $(1s,2s)$ configuration is much larger for the negative hydrogen ion (H$^-$) than for helium (He). The usual single-parameter Pluvinage wave function fails to predict binding for H$^-$ (it yields a ground-state energy of −0.498 a.u., which is higher than the energy of a hydrogen atom). Including the $(1s,2s)$ configuration not only leads to binding, but to a substantially lower energy, −0.523 a.u.

We also investigated Hylleraas wave functions of the form

$$\psi_H(s,t,u) = Ne^{-\lambda s}\sum_{a,b,c} C_{a,b,c}s^a t^b u^c, \tag{13}$$

where $s=r_1+r_2$, $t=r_1-r_2$, and $u=r_{12}$ are elliptic coordinates (see Ref. [21] for the specific values of the parameters in the case of the 20-parameter wave function). In these coordinates, the Hamiltonian is written

$$H = -\frac{\partial^2}{\partial s^2} - \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial u^2} - \frac{1}{s^2-t^2}\left[4s\frac{\partial}{\partial s} - 4t\frac{\partial}{\partial t} + \frac{2}{u}\left\{s(u^2-t^2)\frac{\partial}{\partial s} - t(u^2-s^2)\frac{\partial}{\partial t}\right\}\frac{\partial}{\partial u}\right] - \frac{2}{u}\frac{\partial}{\partial u} - \frac{4Zs}{s^2-t^2} + \frac{1}{u}. \tag{14}$$

The local energy for the Hylleraas wave function (13) is given by

$$\frac{H\psi_H}{\psi_H} = \frac{\sum_{a,b,c} \epsilon_{a,b,c}(s,t,u)C_{a,b,c}s^a t^b u^c}{\sum_{a,b,c} C_{a,b,c}s^a t^b u^c}, \tag{15}$$

where

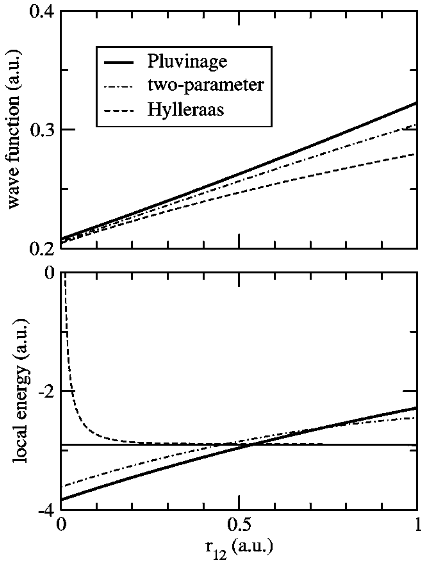

FIG. 1. A representative slice $(r_1=r_2=0.5\text{ a.u.})$ of the wave function (top panel) and the local energy (bottom panel) for the Pluvinage wave function [15], the two-parameter wave function, and the 20-parameter Hylleraas wave function [21] for the ground state of helium. The two-parameter wave function is the energy-optimized sum of $(1s,1s)$ and $(1s,2s)$ Pluvinage wave functions. The horizontal solid line is the local energy for the exact solution.

$$\epsilon_{a,b,c}(s,t,u) \equiv \frac{H(s^a t^b u^c e^{-\lambda s})}{s^a t^b u^c e^{-\lambda s}}, \tag{16}$$

and is given explicitly by

$$\epsilon_{a,b,c} = \frac{1}{u} - \lambda^2 - \frac{a(a-2\lambda s-1)}{s^2} - \frac{b(b-1)}{t^2} - \frac{c(c+1)}{u^2} - 4\frac{a+(Z-\lambda)s-b}{s^2-t^2} - 2c\frac{(a-\lambda s)(u^2-t^2)-b(u^2-s^2)}{(s^2-t^2)u^2}. \tag{17}$$

A representative slice $(r_1=r_2=0.5\text{ a.u.})$ of the local energy is shown in the bottom panel of Fig. 1 for the Pluvinage wave function ψ_{P} [15], the two-parameter wave function $\psi^{(2)}$, the 20-parameter Hylleraas wave function $\psi_{\mathrm{H}}^{(20)}$ [21], and the exact wave function for the ground state of helium. The local energy for the exact wave function is, of course, known to high precision—it is constant and equal to the exact ground-state energy, which (to six significant digits) is −2.903 72 a.u. [22]. The local energy provides a better test of the structural quality of a wave function than the mean energy, since the latter is just the expectation value of the former.

The local energy for the Hylleraas wave function is poor (becomes infinite) for $r_{12}\to 0$, as expected, corresponding to the singularity in the electron-electron Coulomb interaction. For r_{12} greater than about 0.2 a.u., however, it is nearly constant and very close to the exact energy. In addition, the mean energy [21] for the Hylleraas wave function is the same as the exact value to six significant digits. Thus, the

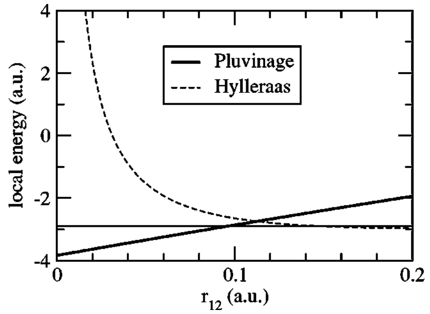

FIG. 2. A slice ($r_1=r_2=0.1$ a.u.) of the local energy for the Pluvinage [15] and 20-parameter Hylleraas [21] wave functions for the ground state of helium. The horizontal solid line is the exact local energy.

positive and negative singularities in the local energy cancel each other to high precision when the mean is taken.

In contrast, the local energy $E_{1,1,k}$ for the Pluvinage wave function [Eq. (12), with $n_1=n_2=1$ and $k=0.41$ a.u.] remains bounded for $r_{12}\to 0$. However, away from $r_{12}=0$ it is not nearly as close as the Hylleraas local energy to the exact energy. The local energy for the two-parameter wave function $\psi^{(2)}$ is also shown in Fig. 1. It is obtained by dividing $H\psi^{(2)}$, given in Eq. (11), by $\psi^{(2)}$, given in Eq. (9). It is similar to the Pluvinage local energy but is overall slightly closer to the Hylleraas local energy. Importantly, the local energy for the Pluvinage and the two-parameter wave function is *not flat*. The Pluvinage local energy has a nearly constant (non-negligible) slope over the whole range of r_{12}. The local energy for the two-parameter wave function is only slightly flatter. We may therefore conclude that neither the Pluvinage wave function ψ_{P} nor the two-parameter wave function $\psi^{(2)}$ is very close to the exact solution.

The top panel of Fig. 1 compares the wave functions for $r_1=r_2=0.5$ a.u. It is clear that $\psi^{(2)}$ is closer to $\psi_{\mathrm{H}}^{(20)}$ than ψ_{P}, and that a very small difference in the wave function for $r_{12}\to 0$ can produce an infinite change in the local energy. Thus, while examining the local energy is extremely useful, an infinite local energy *does not* imply [23] a large error in the wave function.

The local energy for the Pluvinage wave function is closer to the exact energy than the Hylleraas local energy when all three particles are close together (separations smaller than about 0.1 a.u.; see Fig. 2).

Since the large deviations of the Hylleraas local energy in Figs. 1 and 2 are confined to such small regions, it seems unlikely they imply a large error for the wave function in these regions. Moreover, even a relatively large error for the wave function in such a small region should not significantly affect the high-energy limit of the two-electron processes investigated below, since $H\psi_{\mathrm{H}}\approx E\psi_{\mathrm{H}}$ (where E is the exact energy) over *most* of the region that contributes to these processes.

III. PHOTOABSORPTION

In 1960, Dalgarno and Stewart [24] derived a simple formula for the ratio R_A of double to total (single plus double) ionization cross sections of helium-like atoms or ions by photoabsorption in the limit of infinite incoming-photon energy:

$$R_A = 1 - \sum_{nlm} \frac{\left| \int d^3 r_2 \phi^*_{nlm}(\mathbf{r}_2)\psi_i(\mathbf{0},\mathbf{r}_2)\right|^2}{\int d^3 r_2 |\psi_i(\mathbf{0},\mathbf{r}_2)|^2}. \qquad (18)$$

Here, $\psi_i(\mathbf{r}_1,\mathbf{r}_2)$ is the wave function for the initial state of the two-electron system. Each term in the sum of Eq. (18) represents the probability for ionization of one electron while the other remains bound in an eigenstate ϕ_{nlm} of the residual ion or atom with principal n, orbital l, and azimuthal m quantum numbers (i.e., the probability for excitation-ionization). Here, our interest is when the initial state ψ_i is the ground state.

TABLE II. Ratios (in %) of single to total ionization for photoabsorption by H$^-$ and He, leaving the residual atom or ion in the *ns* state indicated and the ratio R_A (%) of double to total ionization in the limit of infinite incoming photon energy. The results using the 20-parameter Hylleraas wave function of Hart and Herzberg [21], labeled $\psi_{\mathrm{H}}^{(20)}$, are from Dalgarno and Sadeghpour [25]. The present results employ the Pluvinage function ψ_{P} and the two-parameter function $\psi^{(2)}$.

	H$^-$			He		
n	$\psi_{\mathrm{H}}^{(20)}$	ψ_{P}	$\psi^{(2)}$	$\psi_{\mathrm{H}}^{(20)}$	ψ_{P}	$\psi^{(2)}$
1	59.10	85.98	60.42	92.94	96.75	94.19
2	38.85	8.28	38.45	4.45	1.46	4.67
3	0.31	1.17	0.56	0.55	0.27	0.28
4	0.11	0.40	0.04	0.18	0.10	0.07
5	0.05	0.18	0.01	0.08	0.05	0.03
R_A	1.51	3.65	0.51	1.68	1.29	0.71

In Table II, we present the relative percentages of single and double to total ionization, calculated from Eq. (18) using three-dimensional numerical quadrature. We see that the probabilities are very sensitive to the description of the ground state. Including a $(1s,2s)$ correction to the Pluvinage wave function leads to large changes and brings the results into overall better agreement with the benchmark calculations of Dalgarno and Sadeghpour [25], which employed the 20-parameter Hylleraas wave function $\psi_{\mathrm{H}}^{(20)}$ of Hart and Herzberg [21]. In particular, the $(1s,2s)$ configuration has a very large effect on the $2s$ excitation-ionization cross section, especially for the negative hydrogen ion, leading to much improved agreement with the calculations of Dalgarno and Sadeghpour [25]. On the other hand, results for single ionization with simultaneous excitation to higher states, as well as double ionization, are not in good agreement, especially for helium (in the case of double ionization of helium, there is experimental evidence [26] that the ratio R_A predicted by the Hylleraas wave function is accurate). We believe that this indicates that the contribution from continuum (as well as higher bound-state) orbitals is important. Thus, our two-

TABLE III. Ratios (in %) of single to total ionization for Compton scattering of a photon off H$^-$ and He, leaving the residual atom or ion in the *nl* state indicated and the ratio R_C (%) of double to total ionization in the limit of infinite incoming photon energy. The results using the 20-parameter Hylleraas wave function of Hart and Herzberg [21], labeled $\psi_{\mathrm{H}}^{(20)}$, are from Surić *et al.* [20]. The present results employ the Pluvinage function ψ_{P} and the two-parameter function $\psi^{(2)}$.

	H$^-$			He		
nl	$\psi_{\mathrm{H}}^{(20)}$	ψ_{P}	$\psi^{(2)}$	$\psi_{\mathrm{H}}^{(20)}$	ψ_{P}	$\psi^{(2)}$
1*s*	79.68	88.02	78.71	96.00	97.15	96.20
2*s*	18.53	4.06	18.73	2.49	0.78	2.78
2*p*	0.75	3.00	0.93	0.16	0.51	0.12
3*s*	0.06	0.55	0.26	0.28	0.14	0.14
3*p*	0.09	0.47	0.33	0.03	0.10	0.06
4*s*	0.03	0.18	0.02	0.09	0.05	0.03
4*p*	0.03	0.16	0.10	0.01	0.04	0.02
R_C	0.69	3.10	0.80	0.80	1.12	0.58

parameter wave function $\psi^{(2)}$ is still inferior to the Hylleraas wave function, which implicitly includes such contributions.

IV. COMPTON SCATTERING

Surić *et al.* [20] derived a formula for Compton (inelastic photon) scattering analogous to (18)

$$R_C = 1 - \sum_{nlm} \int d^3r_1 \left| \int d^3r_2 \phi^*_{nlm}(\mathbf{r}_2)\psi_i(\mathbf{r}_1,\mathbf{r}_2) \right|^2 . \qquad (19)$$

In Table III, we present the relative percentages of single and double to total ionization, calculated from Eq. (19) using six-dimensional numerical quadrature. We again see that the probabilities are quite sensitive to the description of the ground state. Including a $(1s,2s)$ correction to the Pluvinage wave function leads to large changes and brings the results into better agreement with the benchmark calculations of Surić *et al.* [20], which employed the 20-parameter Hylleraas wave function [21]. As for photoabsorption, the improvement is largest for 2*s* excitation-ionization and larger for H$^-$ than for He. It is also clear that our calculations using the two-parameter wave function $\psi^{(2)}$ are in better agreement with Hylleraas results for Compton scattering than for photoabsorption.

V. ELECTRON IMPACT

In this section, we consider electron-impact double ionization of helium at high incident-electron energy and small momentum transfer, with a very large difference in energy between the projectile and either ejected electron. Under these conditions, the use of the first Born approximation (FBA) is justified.

The motivation for the present work was provided by a recent Letter [10], where a “3C-Pluvinage” model for electron-impact double ionization of helium within the FBA was introduced. In this model, the final double-continuum state of the atom is given by the 3C wave function and the initial ground state is given by the Pluvinage function.

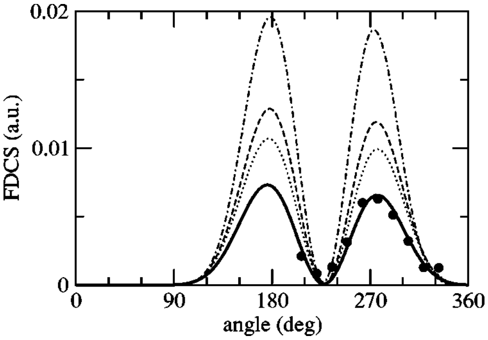

FIG. 3. Fully differential cross section (FDCS) in the scattering plane for 5.6-keV electron-impact double ionization of the ground state of helium. The incident electron is scattered 0.45° and the ejected electrons have equal energies (10 eV). One of the ejected electrons is observed at the fixed observation angle of 41° and the FDCS is presented as a function of the ejection angle of the other atomic electron (all angles are measured in the same sense relative to the forward beam direction). The absolute measurements (solid circles) are from Lahmam-Bennani *et al.* [27]. The calculations were performed in first Born approximation using the 3C wave function for the final double-continuum state of the atom and different initial ground states as follows. Thick solid line: Pluvinage wave function ψ_{P}. Dot-dashed line: two-parameter wave function $\psi^{(2)}$, which includes a $(1s,2s)$ correction to the Pluvinage wave function. Dashed line: 20-parameter Hylleraas wave function $\psi_{\mathrm{H}}^{(20)}$. Dotted line: three-parameter Hylleraas-type wave function $\psi_{\mathrm{H}}^{(3)}$.

It was shown that the use of the Pluvinage wave function for the ground state leads to improved agreement with the overall magnitude of absolute measurements [27] as compared to a three-parameter Hylleraas-type function $\psi_{\mathrm{H}}^{(3)}$, which leads to cross sections about 65% too large. It can be seen from Fig. 3 that the 20-parameter Hylleraas wave function $\psi_{\mathrm{H}}^{(20)}$ of Hart and Herzberg [21] leads to results not very different from the three-parameter ones. It can also be seen that adding a $(1s,2s)$ configuration to the original Pluvinage wave function raises the overall magnitude of the cross section significantly, leading to strong disagreement with observation. Note that including a $(1s,2s)$ correction to the Pluvinage wave function means that the nonorthogonal kinetic energy is no longer being neglected in the formation of the initial state. Since it *is* neglected in the 3C final state, it seems possible that the transition amplitude could be contaminated by spurious contributions from using an inconsistent treatment of the initial and final states of the helium atom [29].

The above explanation is based on experience with earlier calculations [10,13]; however, there are more basic reasons for maintaining consistency between initial and final states when computing transition probabilities. First, it is usually true that the error in transition probabilities computed using approximate wave functions is of first order in the error of the wave functions. With special procedures to maintain consistency between initial and final states, it is sometimes possible to obtain transition probabilities that are of second order in the error of the wave functions [30,31]. In this case, an inferior initial state could nonetheless give more accurate transition probabilities.

VI. CONCLUSION

We constructed a two-parameter wave function for the ground state of helium that is the sum of the original $(1s,1s)$ and a $(1s,2s)$ Pluvinage wave function. The purpose of this was to test the accuracy of the original Pluvinage wave function. Although our primary interest is the helium atom, we also considered the negative hydrogen ion to gain a more general perspective.

We compared local energies for the Pluvinage wave function, the two-parameter wave function, the 20-parameter Hylleraas wave function, and the exact wave function for the ground state of helium. This (purely theoretical) comparison immediately suggested that the Hylleraas wave function is generally closer to the exact solution than the Pluvinage wave function.

We considered the high-energy limit of double ionization (and single ionization with excitation) by both photoabsorption and Compton scattering. In this limit, only initial-state correlation is important and the quality of the two-electron atomic ground state can be ascertained without reference to the final double-continuum state. At infinite incoming-photon energies, the Pluvinage and 20-parameter Hylleraas wave functions yield very different results, especially for single ionization with simultaneous $2s$ excitation of the residual ion. When a $(1s,2s)$ correction to the Pluvinage wave function is included, however, the results for $2s$ excitation-ionization for both photoabsorption and Compton scattering in both H^- and He become quite close to the Hylleraas values. It should also be noted that we observed a small overall improvement in the local energy and that the wave function itself moved closer to the Hylleraas function. In the case of photoabsorption, experiments have confirmed that the Hylleraas wave function yields an accurate asymptotic ratio for double-to-single ionization of helium. Both the Pluvinage and two-parameter wave functions fail to predict the correct ratio. These observations provide additional evidence that the Hylleraas function is generally closer to the exact solution than the Pluvinage function.

Nevertheless, at intermediate energies, if the final double-continuum state is approximated by the 3C wave function (the analog of the Pluvinage wave function), then the use of the Pluvinage function for the initial state evidently leads to more accurate transition probabilities (see Fig. 3, and Refs. [10,13]). The 3C wave function approximates the three-body final state as a product of three two-body states. For intermediate and lower energies, the part of the Hamiltonian that is neglected in constructing the 3C wave function is not negligible, which means that the model of the helium atom for which the 3C wave function is an exact solution differs significantly from the "full" model. One possible explanation for the conflicting results is that the use of the Hylleraas (or even the exact) ground-state wave function leads to spurious contributions, since different models are used for the atom initially and finally.

If this conjecture is true, then it also helps explain the poor results obtained in Ref. [18] when the Pluvinage wave function is used for the initial state, since the Pluvinage initial state is obtained by neglecting the cross terms of the kinetic-energy operator expressed in interparticle coordinates (the nonorthogonal kinetic energy), while the CCC final state is obtained from the full Hamiltonian. Combining the CCC final state with the 20-parameter Hylleraas initial state should provide a consistent treatment of the two-electron transition. Nevertheless, CCC-Hylleraas results [18] are not in agreement with the overall magnitude of the absolute measurements [27] for electron-impact double ionization of helium. (They are, however, in agreement with absolute photoabsorption measurements; see Ref. [28].) Thus, further experimental and/or theoretical work is needed to resolve these issues.

In light of these findings, we would modify conclusion (ii) in the abstract of Jones and Madison [10] by replacing "poor" with "inconsistent," since a Hylleraas description is not poor *per se*, but evidently leads to poor transition probabilities when combined with a 3C description of the final state. As noted in the Introduction, poor transition probabilities with inconsistent initial and final states are particularly pertinent for two-electron processes since these can occur even in the limit $Z \rightarrow 0$.

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