LETTER TO THE EDITOR

Accurate Hylleraas-*like* functions for the He atom with correct cusp conditions

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Abstract
In this letter, a set of ground state wavefunctions for the He atom is given.
The functions are constructed in terms of exponential and power series as
similar as possible to the Hylleraas functions of Chandrasekhar and Herzberg
(1955 *Phys. Rev.* **98** 1050). The accuracy of the calculated energies is found
to be about 10^{-4} au and all the cusp conditions at the Coulomb singularities
are satisfied. The nine-parameter functions proposed here are found to have
better local energy than those given by the 6 and 14 terms Hylleraas functions
of Chandrasekhar. The mean value of various functions evaluated with the
different proposals shows their good quality. These properties highly qualify
the function to be used as an alternative to the Chandrasekhar functions in
collisional problems. The whole set of functions given here can be considered
as an alternative to the proposals of Chandrasekhar (1955 *Phys. Rev.* **98** 1050),
Bonham and Kohl (1966 *J. Chem. Phys.* **45** 2471) and Le Sech (1997 *J. Phys.
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The determination of accurate wavefunctions for atoms with two electrons or two active
electrons is of importance for the study of variety of physical processes like the double
ionization of atoms by the impact of photons and electron, etc [1, 2]. Nowadays, a large
variety of methods can be applied to the determination of the wavefunctions and the energies
not only of the ground state of the system, but also of many excited states (see, e.g. [3]
and references therein). However, for the evaluation of cross sections it is important to have
not only accurate but also simple wavefunctions. Many collisional processes require the
inclusion of, e.g., two electron ground state functions in calculations that usually involve
many integrations over the coordinates and also over the momenta of the particles resulting
after the collision. Even when many authors have done contributions in this direction there is
still work to be done. This letter follows the steps initiated by Le Sech [4] and gives simple
and accurate wavefunctions to be used in further calculations involving the He atom [5].

   The papers of Hylleraas and Undheim [6, 7] initiated the process of generating highly
correlated wavefunctions for two-electron systems. In the 1950s, the work was continued by

Green *et al* [8] and Chandrasekhar *et al* [9, 10]. For a long time, the application of these functions to collisional problems was difficult due to the fact that they resulted in highly time demanding calculations. However, functions such as those given by Bonham and Kohl [11] and Byron and Joachain (see e.g. Bransden and Joachain [12]) were practical because their functional forms were simple enough for cross section calculations. With the development of new computers, calculations using Hylleraas functions became feasible, and they are nowadays used as an initial channel in different processes [1, 2, 13–15]. The quality of these functions can be improved by increasing the number of variational parameters. The functions given by Green *et al* [8] and Chandrasekhar *et al* [9, 10] involve up to 20 parameters and give a very accurate mean energy for the He atom. However, in some situations it is important to properly describe the configurational space at the coalescence point where the Coulomb potential diverges [1, 13, 14, 16–18]. In those cases the Hylleraas functions failed [17, 18]. Many different functions satisfying the cusp condition have been given (see e.g. [3]), but no simple alternatives to the functions of Green and Chandrasekhar. In this letter, we present a set of Hylleraas-*like* functions which are as simple as those of [8–10] but with correct description at the coalescence points. Some work in this direction has been done by Teng and Shakeshaft [17, 18] but here we developed functions with faster convergency rate similar to that observed on the functions given by Green *et al*, Chandrasekhar *et al* and Bonham and Kohl. We also give functions with the correct behaviour at the coalescence point which can be considered as alternatives to those given by Bonham and Kohl [11] and Le Sech [4].

The non-relativistic Schrödinger equation for the He atom is written in atomic units (used throughout this letter) and in terms of the relative coordinates of the particles as follows:

$$\left\{ -\left[\frac{1}{2}\nabla_1^2 + \frac{Z}{r_1} \right] - \left[\frac{1}{2}\nabla_2^2 + \frac{Z}{r_2} \right] - \left[\nabla_{12}^2 - \frac{1}{r_{12}} \right] - \nabla_1 \cdot \nabla_{12} - \nabla_2 \cdot \nabla_{12} - E \right\} \Phi = 0 \qquad (1)$$

$\mathbf{r}_{1,2}$ is the relative electron-nucleus (e–N) vector and $\mathbf{r}_{12}$ is the relative vector between the electrons. The S states of the He atom require zero total angular momentum $\mathbf{L}$; in this case the Schrödinger equation considerably simplifies

$$\left\{ -\left[\frac{1}{2}\left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} \right) + \frac{Z}{r_1} + E_1 \right] - \left[\frac{1}{2}\left(\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} \right) + \frac{Z}{r_2} + E_2 \right] \right.$$
$$- \left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} - \frac{1}{r_{12}} + E_{12} \right] - \frac{1}{2}\frac{\mathbf{r}_{12} \cdot \mathbf{r}_1}{r_{12}r_1}\frac{\partial^2}{\partial r_{12}\partial r_1}$$
$$\left. - \frac{1}{2}\frac{\mathbf{r}_{12} \cdot \mathbf{r}_2}{r_{12}r_2}\frac{\partial^2}{\partial r_{12}\partial r_2} \right\} \Phi(r_1, r_2, r_{12}) = 0. \qquad (2)$$

Here we write the total energy $E = E_1 + E_2 + E_{12}$ as the sum of three partial energies. The domain of the coordinates r_1, r_2 and r_{12} are $r_1 \in [0, \infty)$, $r_2 \in [0, \infty)$ and $|r_1 - r_2| \leqslant r_{12} \leqslant r_1 + r_2$, respectively. The first three terms of equation (2) do not couple the coordinates, they are three independent two-body Coulomb problems. The cross derivatives couple the two-body subsystems and lead to a non-separable equation. For the case of a heavy nucleus and two light particles, we deal with the coupling between the electron–electron (e–e) subsystem and each e–N separately. The structure of the equation suggests a possible structure for the wavefunction; it might be possible to write it as the product of two factors one exactly solving the first three terms, and the other taking into account the coupling between them. This idea was originally proposed by Pluvinage [19] using a set of coordinates different from the Hylleraas coordinates that we are using. The wavefunction proposed in his pseudo-separable method solved exactly the first three terms of equation (2). The energy E_{12} was variationally obtained by minimizing the cross derivatives. E_1 and E_2 resulted from enforcing an exponentially

decreasing behaviour of the functions on r_1 and r_2, respectively. By exactly solving the first three terms of equation (2), the Coulomb interactions are included in the wavefunctions and the Kato cusp conditions [21]

$$\left[\frac{\partial\overline{\Phi}}{\partial r_1}\right]_{r_1\longrightarrow 0} = -Z\Phi(0, r_2, r_{12}), \qquad \left[\frac{\partial\overline{\Phi}}{\partial r_2}\right]_{r_2\longrightarrow 0} = -Z\Phi(r_1, 0, r_{12}) \quad (3)$$

$$\left[\frac{\partial\overline{\Phi}}{\partial r_{12}}\right]_{r_{12}\longrightarrow 0} = \frac{1}{2}\Phi(r, r, 0), \qquad r = \frac{1}{2}|\mathbf{r}_1 + \mathbf{r}_2| \qquad (4)$$

are satisfied. In this equation $\overline{\Phi}$ means the average of Φ, e.g. in the first term of equation (3), over a small sphere of radius r_2 (respectively, r_2 or r_{12}) keeping the other values fixed. The idea of pseudo-separability was later followed by other authors [4, 22, 23]. Moumeni and co-workers [22] modified the Pluvinage proposal by multiplying it by a screening function which resulted from approximately solving the cross derivatives and the terms coming from their action over the separable part of the solution. Later Siebbeles and co-workers [23] continued the work of Moumeni and also showed that it is not necessary to fully diagonalize the e–e Coulomb interaction; describing appropriately the region close to the coalescence, it is enough to fulfil the cusp conditions. These authors replaced, in the Pluvinage proposal, the continuum wavefunction representing the e–e interaction by a simpler function which was equally efficient but gave the function a simpler functional form. Le Sech in 1997 [4] modified the screening term and also generalized the idea to other atomic systems [24, 25]. Following these ideas we propose as approximated solution for equation (2) the function

$$\Phi(r_1, r_2, r_{12}) = \phi(r_1, r_2, r_{12}) \sum_{i,j,k\neq 1} c_{i,j,k} r_1^i r_2^j r_{12}^k \qquad (5)$$

where

$$\phi(r_1, r_2, r_{12}) = \varphi_{n_1}(Z, r_1)\varphi_{n_2}(Z, r_2)[2\beta + 1 - e^{-\beta r_{12}}]/2\beta. \qquad (6)$$

The function $\phi(r_1, r_2, r_{12})$ is given by the product of two hydrogenic functions $\varphi_{n_i}(Z, r_i)$, with $i = 1, 2$, times the factor $[2\beta + 1 - e^{-\beta r_{12}}]/2\beta$ to represent the e–e dynamics. $\phi(r_1, r_2, r_{12})$ satisfies all the cusp conditions given by equations (3) and (4). Thus, the power series of equation (5) must be restricted and should not include first power on the coordinates, otherwise the Kato cusp conditions are not satisfied. The factor in the bracket of equation (6) can be replaced by $[e^{-z_c r_{12}} + C_0 e^{-\beta r_{12}}]$ with C_0, β and z_c all related and restricted by the e–e cusp condition [5]. The parameter z_c can be included to have a full exponentially decaying function of r_{12}. Taking β as a minimization parameter and z_c fixed and small (usually 0.001), it is possible to obtain a function which does not require any integration factor at the moment of using it on the evaluation of cross sections [5].

For the ground state, $\Phi(r_1, r_2, r_{12})$ of equation (5) has to be spatial symmetric under the exchange of the electron coordinates, i.e. $c_{i,j,k} = c_{j,i,k}$, and multiplied by the antisymmetric spin function $[\alpha(1)\beta(2) - \alpha(2)\beta(1)]$. To fulfil with that symmetry the series on equation (5) has to include terms up to the same values of the indices i and j.

The linear parameters $c_{i,j,k}$ and the nonlinear parameter β are determined by minimizing the mean energy

$$E = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle}. \qquad (7)$$

A *numerical exact* value for the $^1S_0$ ground state of the He atom has been given by Drake [26] and corresponds to $E_{\text{exact}} = -2.903\,724$ au. For the ground state of the system n_1 and

n_2 on equation (6) have to be set equal to 1 and this reduces $\varphi_{n_1}(Z, r_1)\varphi_{n_2}(Z, r_2)$ to $e^{-Z(r_1+r_2)}$. The function $\phi(r_1, r_2, r_{12})$ diagonalizes the e–N interactions completely and solves the e–e problem exactly at the origin. The power series of equation (5) solves the two-body subsystem coupling produced by the cross derivatives and the part of the e–e interaction not included in $\phi(r_1, r_2, r_{12})$.

In table 1, we present the results obtained minimizing the mean energy of equation (7) for the ground state of the He atom. We discuss functions having up to nine parameters. The function GR1 of table 1 was used to minimize the mean energy and only one parameter is involved. This function is the counterpart of the Pluvinage proposal where the e–e part is replaced by $[2\beta + 1 - e^{-\beta r_{12}}]/2\beta$. We found that this factor is as *flexible* as that used by Le Sech, but has a simpler structure and make it well adapted to further calculations. As can be seen in table 1 the mean energy obtained with $\phi(r_1, r_2, r_{12})$ is similar to that given by Pluvinage ($E_P = -2.8780$) [19]. GR2 with one nonlinear and one linear parameters added the simplest radial correlation and is the counterpart of the function number 8 of Bonham and Kohl [11] with three parameters. The value $\beta = 0.45$ was optimal in this case. We found that β remains almost constant when the number of linear parameters is increased. Thus once these are determined, only the linear parameters $c_{i,j,k}$ remain to be obtained. This considerably simplifies the calculations because minimizing the mean energy of equation (7) requires to solve an $N \times N$ determinant. GR3 and GR4 in table 1 were determined using $\beta = 0.45$ and minimizing the mean energy with two and three linear parameters. An accuracy of 6×10^{-4} au was obtained in this case. The energy obtained is similar to that given by function numbers 9 and 10 of Bonham and Kohl [11] and also to those proposed by Moumeni *et al* [22], Siebbeles *et al* [23] and Le Sech [4]. These are alternative proposals to those of Le Sech and co-workers, and an improvement with respect to the Bonham and Kohl functions, which do not satisfy the Kato cusp conditions. Further improvements to the mean energy are obtained with GR5 which gives accurate values for the energies within 3.2×10^{-4} au. The best of the functions presented in this letter is GR9 of table 1 and gives an energy with an accuracy of 1.6×10^{-4} au. GR5 and GR9 are our alternative proposals to the Hylleraas functions of 6, 10 and 14 terms [6, 9, 10].

Table 2 displays mean values of several radial quantities strongly dependent on the shape of the wavefunction, involved in various calculations of physical quantities such as dipole polarizabilities or magnetic susceptibilities. The mean value of the hyperspherical radius $R = \left(r_1^2 + r_2^2\right)^{1/2}$, which is representative of the size of the system, is given in column 8. Angular correlation calculations related to the values of $\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle$ are reported, showing a good agreement with other accurate results. As we can see from table 2, with the nine-parameter functions we obtain better results for different quantities of the He atom than those obtained with the Le Sech and the 6 and 14 terms of the Hylleraas functions which we shall call Hy6 and Hy14, respectively, in comparison with the 'numerical exact' values given by Pekeris [27]. We do not include the calculations with the ten-parameter Hylleraas functions [9] because it leads to results that lie between Hy6 and Hy14. Already our five-parameter function GR5 shows a general better agreement with the precise values of Pekeris than those obtained with the Hy14 parameters. The same behaviour is found when comparing our GR3 to the Hy6. Our GR3 has a similar form to the Le Sech function [4] and as can be expected gives similar results for the different mean values of table 2.

Further analysis on the properties of our proposal of equation (5) can be done studying the local energy introduced by Bartlett *et al* [28]

$$E_l(r_1, r_2, r_{12}) = \frac{1}{\psi(r_1, r_2, r_{12})} H\psi(r_1, r_2, r_{12}). \tag{8}$$

Table 1. Normalization constants, minimization parameters and mean energies for the different GR wavefunctions for the ground state of He.

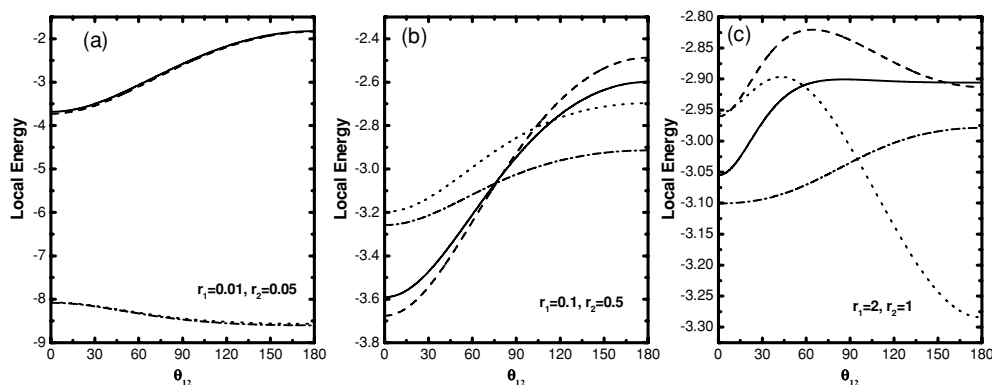| GR	N	β	c_{200}	c_{002}	c_{300}	c_{220}	c_{202}	c_{320}	c_{302}	c_{402}	E (au)
1	1.621 03	0.001									−2.877 3
2	1.399 1	0.45	0.156 426								−2.901 272
3	1.405 01	0.45	0.134 4							0.005 74	−2.901 96
4	1.415 38	0.45	0.109 085	0.000 218 94	0.024 017 5						−2.9020
5	1.396 57	0.45	0.127 498	0.000 487 771	0.023 723	−0.020 958 9					−2.902 79
7	1.379 815	0.45	0.169 579	−0.007 811 4	0.005 453 05	−0.066 821 8	0.002 5641	0.009 998 05			−2.903 099
9	1.388 945	0.45	0.165 300	−0.022 629	0.009 517	−0.087 765	0.018 344	0.013 773	−0.009 148	0.001 274	−2.903 255

Figure 1. Local energy as a function of θ_{12}, with different values for r_1 and r_2. Dot-dashed line: 14-parameter Hylleraas, dotted line: 6-parameter Hylleraas, solid line: GR9, dashed line: Le Sech [4].

Table 2. Calculated expectation values of various functions (in atomic units) for the ground state of the helium, compared to available extended calculations and exact values.

	$\langle r_i \rangle$	$\langle r_i^2 \rangle$	$\langle 1/r_i \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$	$\langle 1/r_{12} \rangle$	$\langle R \rangle$	$\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle$	**virial**
Hylleraas (14-terms)	0.922 741	1.177 3	1.708 5	1.413 63	2.478 98	0.950 613	1.411 73	−0.062 1897	−1.966 11
Hylleraas (6-terms)	0.897 648	1.103 91	1.737 65	1.359 37	2.279 39	0.980 671	1.371 34	−0.035 7839	−1.944 16
Le Sech	0.931 211	1.198 77	1.681 09	1.423 94	2.530 3	0.946 55	1.423 94	−0.066 3753	−2.050 17
GR3	0.932 364	1.200 01	1.679 1	1.421 88	2.521 88	0.948 405	1.422 33	−0.061 1123	−2.012 54
GR4	0.931 667	1.196 52	1.681 27	1.420 88	2.515 63	0.948 894	1.421 21	−0.061 2947	−2.009 68
GR5	0.929 266	1.191 21	1.686 46	1.419 85	2.502 54	0.946 291	1.420 06	−0.060 0585	−2.002 09
GR7	0.929 552	1.193 22	1.686 73	1.421 33	2.513 72	0.945 824	1.420 71	−0.063 6402	−2.001 76
GR9	0.929 301	1.192 51	1.688 04	1.421 34	2.514 17	0.946 537	1.420 31	−0.064 572	−2.000 32
Exact	0.929 47[a]	1.193 48[a]	1.688 31[a]	1.422 07[a]	2.516 43[a]	0.945 81[a]	–	−0.064 736[a]	−2

[a] Taken from [26].

Solely for the exact solution, this local energy will be constant throughout the entire configuration space, i.e., an eigenvalue of equation (2), and hence equal to the mean energy (this is the case, e.g., for the hydrogenic ions of nuclear charge Z, for which the local and mean energies are equal to $E = -\frac{Z^2}{2n^2}$ (au)). For any other trial wavefunction, the local energy will not necessarily be constant; the averaging over the whole space smooths out the variations of $E_l(r_1, r_2, r_{12})$ and provides the finite constant value given by the mean energy of equation (7). For the study of collisional problems involving helium atoms, it is necessary to have not only a good wavefunction but also a good mean energy. Obtaining a good mean energy is not a sufficient criterion to state that a trial wavefunction is good. Having a local energy as smooth as possible and close to the exact energy value is much stronger as a quality test.

For illustrational purposes, we plot the local energy $E_l(r_1, r_2, r_{12})$ on figures 1 and 2. In these figures we chose in the three-dimensional space (r_1, r_2, r_{12}) the following situations: r_1 and r_2 fixed but with different values, and the local energy plotted versus their mutual angle, $\theta_{12} = \cos^{-1}\left[(r_1^2 + r_2^2 - r_{12}^2)/(2r_1r_2)\right]$, with $\theta_{12} \in [0, \pi]$.

From figures 1(a)–(c) we can see that E_l as given by GR9, see table 1, and the Le Sech function of [4] are near the exact value −2.903 72 au in the whole range of θ_{12}. On the other
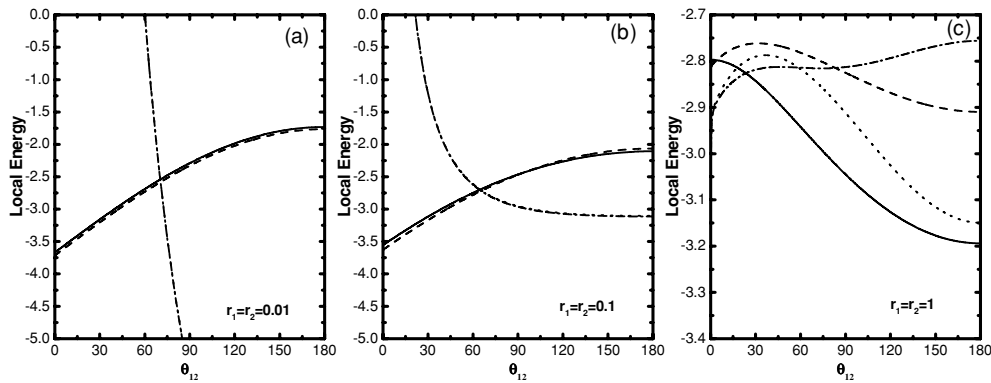
Figure 2. Local energy as a function of θ_{12}, with $r_1 = r_2$. Dot-dashed line: 14-parameter Hylleraas, dotted line: 6-parameter Hylleraas, solid line: GR9, dashed line: Le Sech [4].

hand, the Hylleraas functions Hy6 and Hy14 of [6, 10] show that for small r_1 and r_2 there is a great departure from the exact value. This is due to the fact that the Hylleraas functions do not satisfy the e–N cusp conditions. In the situation plotted in figure 1(b) all the functions show similar behaviours. While for the situation of figure 1(c) Hy14 again shows a departure from the correct value.

In figure 2, we plot the situation where the electrons are at the same distance from the nucleus ($r_2 = r_1$). In all the cases plotted in figures 2(a)–(c), the local energy given by the function of Le Sech and GR9 is plotted as a function of the angle but it remains smooth and close to the exact energy value. For the Hy6 and Hy14 local energy is quite different; a singularity appears in E_l for $\theta_{12} \to 0$, i.e. when $r_{12} \to 0$, which corresponds to the failure in satisfying the e–e Kato cusp condition.

The divergencies observed in the figures 1 and 2 are those predicted by Bartlett *et al* [28]. These authors showed that Hylleraas wavefunctions provide local energies ranging from $-\infty$ to ∞. Infinite local energies can come from two sources:(i) the wavefunction has nodes and $H\psi \neq 0$; (ii) one or several of the singularities of the potential terms in H_1, H_2 and H_{12} are not compensated by the corresponding kinetic terms. In the case of the functions given by [6, 9, 10] the situation (ii) occurs.

Even though it is not the objective of this letter to apply the wavefunctions presented here to evaluate cross sections for different collisional processes, it is interesting to mention what is found in the work published by Kheifets and Bray [1]. In connection with the accuracy as well as the simplicity of the He ground state functions, these authors showed that the agreement between gauges in the double photo ionization of He within their convergent close-coupling approach is obtained when the quality of the wavefunction is improved by the use of Hylleraas functions of 6-, 10- and 14-parameters. This agreement is based upon the improvement of the quality of the functions in different parts of the configuration space as tested by the different gauges (length, velocity and acceleration) discussed by the authors. They said that a considerable effort has to be done to use Hylleraas functions with a large number of parameters. The mean values of different physical quantities of the He atom listed in table 2 show that the functions proposed here introduce an improvement in different parts of the configurations' space when compared with, e.g., the 14-parameter Hylleraas functions even using a smaller number of parameters. Thus, a faster convergence of the mentioned cross section is expected and also a less time demanding calculation will probably be needed due to the lesser number of terms required.

In conclusion, we have introduced a set of wavefunctions for the ground state of the He atom satisfying the cusp condition at the two-body coalescence. We have shown that accurate values for the energies up to 1.6×10^{-4} au can be obtained using nine-parameter wavefunctions. Improvements to this value can be easily obtained by adding more terms in accordance with equation (5). As the nonlinear parameter β remains constant almost independently of the number of linear parameters, further improvements of the function require basically to solve an $N \times N$ determinant. Functions simpler than GR9 as well as their normalization constants were given. They can be considered as an alternative to the Le Sech and Bonham and Kohl functions. Aside from the mean energy, the three- and five-parameter functions GR3 and GR5 already show better description of the different physical properties of the He atom as given by the mean values of table 2 than the 6- and 14-parameter Hylleraas functions, respectively. For those calculations requiring a good description of different physical properties of the atom, the GR3 and GR5 become simpler alternatives to the 6- and 14-parameter functions of Chandrasekhar [6, 10]. The functions of table 1 are mostly proposed, with the spirit of Le Sech, as useful functions to be applied in practical calculation of transition amplitudes as an alternative to the function given by Green *et al* [8], Chandrasekhar *et al* [6, 10] and Bonham and Kohl [11] which are now being used for various authors [1, 13, 14, 30–32] and which do not satisfy the cusp conditions. The set of functions given in this letter were developed trying to keep their form as similar as possible to the functions that are now being used in collisional problems.

Acknowledgments

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