The collinear two-electron atoms

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Abstract

Collinear configurations of the helium-like atomic systems, relevant e.g. for the quasifree mechanism of the double ionization of helium, are studied, parametrized by the single scalar parameter $-1 \leq \lambda \leq 1$. The particular case $\lambda = 0$ corresponds to the electron-nucleus coalescence, whereas $\lambda = 1$ corresponds to the electron-electron coalescence. In general, $\lambda > 0$ corresponds to the n-e-e configuration, and $\lambda < 0$ to the e-n-e configuration. Simple mathematical representations of the expectation values of the Dirac delta function relevant for the collinear configurations are derived and calculated from full three-body dynamics without approximations for the two-electron atoms/ions with nuclear charge $1 \leq Z \leq 5$. Simple formulas for calculating the expectation values of the kinetic and potential energy operators in collinear configurations are derived and their numerical results presented. Unusual physical properties of the n-e-e collinear configurations were found for certain ranges of the parameter $\lambda$. 

I. INTRODUCTION

There are many scientific publications with numerical results of expectation values of the Dirac delta \( \langle \delta(r_1) \rangle, \langle \delta(r_{12}) \rangle \equiv \langle \delta(r_1 - r_2) \rangle \) and \( \langle \delta(r_1)\delta(r_{12}) \rangle \) for the two-electron atom/ions, where \( r_1, r_2 \) are electron positions relative to the nucleus (see, e.g., [1–4] and references therein). Quantum-mechanical applications of these expectation values can be found, e.g., in [1, 5, 6]). The two-electron wave functions (WF) at the two-particle coalescences, \( \psi(0, r) \) and \( \psi(r, r) \), were also applied, for example, in the description of the quasifree mechanism of double photoionization of helium (see, e.g., [7–9]). The collinear case of \( \psi(r, -r) \) (\( \lambda = -1 \)), corresponding to the so called time-reversed double photoionization at specific kinematics, was studied in [10, 11].

However, we have not found published results for \( \langle \delta(r_1 + r_2) \rangle \) (corresponding to the boundary value \( \lambda = -1 \)), nor results for other values of \( \lambda \).

We have also found a rather small number of articles devoted to the particular case of the helium-like atomic systems in collinear configurations (see [12–15]). Moreover, to simplify the problem the authors considered a system of three particles constrained to move along a straight line and interacting via the Coulomb forces [12], or used the adiabatic approach [13, 14]. Semiclassical calculations using the Herman-Kluk initial value treatment were performed in Ref. [15] to determine energies of bound and resonance states of the collinear helium atom.

In contrast, in this work we employ the direct approach, calculating the non-relativistic WFs and the corresponding expectation values from a full three-body method for the particles interacting via the Coulomb potentials [16, 17], and also verifying them by the independent, so called, correlation function hyperspherical harmonic method [18, 19]. Using proper three-body calculations as well as certain properties of the Dirac-delta function enabled us to obtain interesting novel results.

II. EXPECTATION VALUES OF THE DIRAC DELTA

The atomic units system will be used throughout the paper.

Let \( \psi(r_1, r_2) \) represent the S-state solution of the Schrödinger equation

\[
(T + V - E) \psi(r_1, r_2) = 0,
\]
where $E$ denotes the non-relativistic electron energy of the two-electron atom/ion with infinitely massive nucleus of charge $Z$. The kinetic energy operator reads

$$T \equiv -\Delta/2,$$

where $\Delta$ is the Laplacian. The potential energy operator representing the interparticle Coulomb interactions is

$$V \equiv -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}},$$

where $r_1 = |\mathbf{r}_1|$, $r_2 = |\mathbf{r}_2|$ and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ are the interparticle distances.

The *collinear* arrangement of the particles (nucleus and two electrons) is defined by the relation

$$\mathbf{r}_1 = \lambda \mathbf{r}_2,$$

where $\lambda \in [-1, 1]$ is a scalar parameter (at least for S-states treated here). It is clear that $\lambda = 0$ corresponds to the case of the *electron-nucleus coalescence*, whereas $\lambda = 1$ describes the case of the *electron-electron coalescence*. The boundary value $\lambda = -1$ corresponds to the collinear e-n-e configuration with the same distances of both electrons from the nucleus. In general, $0 < \lambda \leq 1$ corresponds to the collinear arrangement of the form n-e-e (or equivalently e-e-n) where both electrons are on the same side of the nucleus. Accordingly, $-1 \leq \lambda < 0$ corresponds to the collinear arrangement of the form e-n-e where the electrons are on the opposite sides of the nucleus. The absolute value $|\lambda|$ measures the ratio of the distances of electrons from the nucleus.

Denoting for simplicity $\delta^3(\mathbf{r}) \equiv \delta(\mathbf{r})$, and using the well-known properties of the Dirac-delta function one obtains

$$\langle \delta(\mathbf{r}_1 - \lambda \mathbf{r}_2) \rangle \equiv \frac{1}{N} \int d^3\mathbf{r}_2 \int d^3\mathbf{r}_1 \delta(\mathbf{r}_1 - \lambda \mathbf{r}_2)\psi^2(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{N} \int d^3\mathbf{r}_2 \psi^2(\lambda \mathbf{r}_2, \mathbf{r}_2),$$

where the normalization integral is

$$N = \int d^3\mathbf{r}_2 \int d^3\mathbf{r}_1 \psi^2(\mathbf{r}_1, \mathbf{r}_2).$$

Clearly $\psi(\lambda \mathbf{r}_2, \mathbf{r}_2)$ represents the WF describing the *collinear arrangement* of the particles.

Taking into account the relationship

$$\langle \delta(\mathbf{r}_1)\delta(\mathbf{r}_2) \rangle \equiv \frac{1}{N} \int d^3\mathbf{r}_2 \int d^3\mathbf{r}_1 \delta(\mathbf{r}_1)\delta(\mathbf{r}_2)\psi^2(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{N} \psi^2(\mathbf{0}, \mathbf{0}),$$

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we can rewrite Eq.(5) in the form
\[ \langle \delta(r_1 - \lambda r_2) \rangle = \langle \delta(r_1) \delta(r_2) \rangle \int d^3r_2 \tilde{\psi}^2(\lambda r_2, r_2), \] (8)
where \( \tilde{\psi}(\lambda r_2, r_2) = \psi(\lambda r_2, r_2)/\psi(0, 0) \) is the collinear WF normalized such that \( \tilde{\psi}(0, 0) = 1 \).

It is well-known that for the S-states the two-electron wave function \( \psi(r_1, r_2) \) reduces to the function of only three internal coordinates (see, e.g., [20]). The simplest and most natural choice for these coordinates is the set of the interparticle distances \( r_1, r_2 \) and \( r_{12} \).

This reduces the solution \( \psi(r_1, r_2) \) of the Schrödinger equation (1) to the form \( \Phi(r_1, r_2, r_{12}) \).

However, for our consideration it is more convenient to use the coordinate system \( \{r_1, r_2, \theta\} \), where \( \theta \) is the angle between the radius-vectors \( r_1 \) and \( r_2 \) of the electrons. Let’s denote the corresponding S-state WF as \( \Psi(r_1, r_2, \theta) \) (\( \equiv \Phi(r_1, r_2, r_{12}) \)). The volume element in the \( \{r_1, r_2, \theta\} \) coordinates is
\[ d^3r_2 d^3r_1 = 8\pi^2 r_1^2 r_2^2 dr_1 dr_2 \sin \theta d\theta, \quad \theta \in [0, \pi]. \] (9)

It can be shown that the Dirac delta for the \( \{r_1, r_2, \theta\} \) coordinate system is similar to the one in the spherical coordinates with azimuthal symmetry, whence
\[ \delta(r_1 - \lambda r_2) = \frac{1}{2\pi r_1^2 \sin \theta_1} \delta(r_1 - |\lambda| r_2) \delta(\theta_1 - \theta_2), \quad \theta_2 = 0, \pi. \] (10)

Inserting representations (9) and (10) into the RHS of Eq.(5), one obtains
\[ \langle \delta(r_1 - \lambda r_2) \rangle = \frac{4\pi}{N} \int_0^\infty \Psi^2(|\lambda| r_2, r_2, \theta_2) r_2^2 dr_2 = \frac{4\pi}{N} \int_0^\infty \Phi^2(|\lambda| r_2, r_2, (1 - \lambda) r_2) r_2^2 dr_2, \] (11)
where the angle \( \theta_2 = 0 \) corresponds to the collinear configuration \( n-e-e \) (\( \lambda > 0 \)), whereas \( \theta_2 = \pi \) corresponds to the collinear configuration \( e-n-e \) (\( \lambda < 0 \)).

It is seen that according to Eq. (5) in the general case, and according to Eq. (11) for the S-state, the expectation value \( \langle \delta(r_1 - \lambda r_2) \rangle \) reduces to the expectation value over the collinear WF.

Using the Pekeris-like three-body method [16, 17] we have calculated the expectation value \( h(\lambda, Z) \equiv \langle \delta(r_1 - \lambda r_2) \rangle \) for the ground states of the two-electron atom/ions with \( 1 \leq Z \leq 5 \). Making use of the normalization parameter over \( \lambda \), defined as
\[ M(Z) = \int_{-1}^1 h(\lambda, Z) d\lambda, \] (12)
enables us to present the plots of $h(\lambda, Z)/M(Z)$ for all considered $Z$ on a single plot (Fig. 1).

It is seen that the derivative $dh(\lambda, Z)/d\lambda$ is singular at $\lambda = 0$. In particular, for helium atom we obtain $\lim_{\lambda \to 0^+} dh(\lambda, 2)/d\lambda \simeq -7.92$, whereas $\lim_{\lambda \to 0^-} dh(\lambda, 2)/d\lambda \simeq 6.96$.

In Table I we have presented the values of $h(\lambda, Z)$ at the boundary points $\lambda = -1, 0, 1$, as well as at some intermediate points; the physical meaning of the latter will be clarified in the next section. The values of normalization $M(Z)$ are presented as well. To estimate the accuracy of our calculations, we have presented the ground state energies $E$ calculated by our Pekeris like method [17]. For comparison, the corresponding values of the energies $\tilde{E}$ obtained by the more accurate calculations [1–4] are presented in the last line of Table I.

III. EXPECTATION VALUES OF THE PRODUCT OF DIRAC DELTA AND HAMILTONIAN

Let us multiply the Schrödinger equation (1) on the left by $\delta (r_1 - \lambda r_2) \psi(r_1, r_2)$ and integrate both sides over the whole space. This yields

$$\int d^3r_2 \int d^3r_1 \delta (r_1 - \lambda r_2) \psi(r_1, r_2)(T + V)\psi(r_1, r_2) = E \int d^3r_2 \int d^3r_1 \delta (r_1 - \lambda r_2) \psi^2(r_1, r_2).$$

(13)

Dividing both sides of Eq. (13) by the RHS integral and simplifying, one obtains the relation

$$\langle \delta T \rangle + \langle \delta V \rangle = E,$$

(14)

where the term associated with expectation value of the kinetic energy operator in the $1S$ collinear configuration is

$$\langle \delta T \rangle = -\frac{2\pi}{N h(\lambda, Z)} \int_0^\infty \Psi (|\lambda| r_2, r_2, \theta_2) [\Delta(r_1, r_2, \theta_2) \psi (r_1, r_2, \theta_1) |_{r_1=|\lambda| r_2} r_2^2 dr_2, (15)$$

and $h(\lambda, Z)$ is given by Eq. (11). Here $\theta_2 = 0$ for $\lambda > 0$, and $\theta_2 = \pi$ for $\lambda < 0$. In the derivation of Eq. (15) we used representations (9) and (10). In the $\{r_1, r_2, \theta\}$ coordinate system the Laplacian is of the form (see, e.g., [21])

$$\Delta(r_1, r_2, \theta) = r_1^{-2} \frac{\partial}{\partial r_1} r_1^2 \frac{\partial}{\partial r_1} + r_2^{-2} \frac{\partial}{\partial r_2} r_2^2 \frac{\partial}{\partial r_2} + \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) (\sin \theta)^{-1} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}.$$ 

(16)

For the term associated with the expectation value of the potential energy operator in the $1S$ collinear configuration, we easily obtain:

$$\langle \delta V \rangle = \frac{4\pi}{N h(\lambda, Z)} \left( -Z - \frac{Z}{\lambda} + \frac{1}{1 - \lambda} \right) \int_0^\infty \Psi^2 (|\lambda| r_2, r_2, \theta_2) r_2 dr_2.$$

(17)
To derive the latter equation we used the relation \( r_{12} = r_2 (1 - \lambda) \) corresponding to the *collinear* configuration. The factor in parentheses enables us to conclude that the term \( \langle \delta V \rangle \) becomes negligible when the parameter \( \lambda \) takes the value

\[
\lambda_{v0} = \frac{\sqrt{1 + 4Z^2} - 1}{2Z}.
\]  

(18)

Using the Pekeris-like method [16, 17] we have calculated the expectation values \( \langle \delta V \rangle \) and \( \langle \delta T \rangle \) for the ground state of the helium-like atom/ions with \( 1 \leq Z \leq 5 \). The dependencies of the expectation values (10) upon the *collinear* parameter \( \lambda \) are displayed in Fig. 2 for the ground state of helium. The plots for the two-electron ions are similar. It is seen that the plots in Fig.2 possess some characteristic points (peculiarities). One of them is defined by Eq.(18). The others are as follows:

1) the point \( \lambda_{t0} > 0 \) at which \( \langle \delta T \rangle = 0 \);

2) the point \( \lambda_2 > 0 \) at which \( \langle \delta V \rangle / \langle \delta T \rangle = -2 \), corresponding to the virial theorem for the Coulomb interactions;

3) the point \( \lambda_{cr} > 0 \) of crossing when \( \langle \delta V \rangle = \langle \delta T \rangle \);

4) the point \( \lambda_{v2} > 0 \) at which \( d^2 \langle \delta V \rangle / d\lambda^2 = 0 \) (inflection point);

5) the point \( \lambda_{t2} > 0 \) at which \( d^2 \langle \delta T \rangle / d\lambda^2 = 0 \) (inflection point);

6) the boundary point \( \lambda = -1 \).

The above peculiarities are listed in Table II for the helium-like atomic systems under consideration. We would like to highlight the following specific points:

i) the most important and interesting features of the expectation values \( \langle \delta V \rangle \) and \( \langle \delta T \rangle \) as functions of the parameter \( \lambda \) are related to the collinear configuration (n-e-e) corresponding to \( \lambda > 0 \);

ii) the inflection points \( \lambda_{v2} \) and \( \lambda_{t2} \) for the curves \( \langle \delta V \rangle \) and \( \langle \delta V \rangle \) as functions of the *collinear* parameter \( \lambda \) are coincident (at least to the accuracy of four significant digits) for the given atom/ion;
ii) interpreting \( h(\lambda, Z)/M(Z) \) as a function characterizing the probability of formation of the collinear configuration with given \( \lambda \) among all possible \( \lambda \in [-1, 1] \), we obtain that \( h(\lambda_2, Z)/M(Z) \) gives the maximum value for \( Z = 2 \). In other words, the probability of the \( \lambda_2 \) collinear configuration (when \( \langle \delta V \rangle / \langle \delta T \rangle = -2 \), corresponding to the virial theorem) for the helium atom is higher than for the two-electron ions (both negative and positive); 

iv) for every two-electron atom/ion there are points \( \lambda_v > 0 \) and \( \lambda_t > 0 \) at which the curves \( \langle \delta V \rangle \) and \( \langle \delta T \rangle \) as functions of \( \lambda \) change sign. In other words, \( \langle \delta V \rangle = 0 \) for \( \lambda = \lambda_v \), and \( \langle \delta T \rangle = 0 \) for \( \lambda = \lambda_t \). Most importantly, \( \lambda_t < \lambda_v \), and the derivative \( d \langle \delta T \rangle /d\lambda < 0 \) at \( \lambda = \lambda_t \), whereas \( d \langle \delta V \rangle /d\lambda > 0 \) at \( \lambda = \lambda_v \). Under these conditions, for each two-electron atom/ion there exists a region \( \lambda_t < \lambda < \lambda_v \) in which both \( \langle \delta V \rangle \) and \( \langle \delta T \rangle \) are negative. Clearly, the point \( \lambda_{cr} \) is inside this region (see Fig.2).

We are currently studying the applications of our results to the time-reversed double photoionization \( (\lambda = -1) \) as well as examining possible applications of the unusual behavior \( \langle \delta V \rangle = 0, \langle \delta T \rangle = 0 \) in the \( \lambda_0 < \lambda < \lambda_v \) interval. We have reason to presume that a collinear configuration of the two-electron atomic systems corresponding to the described region of the collinear parameter \( \lambda \) has especial physical significance.

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TABLE I: Expectation values $\langle \delta (r_1 - \lambda r_2) \rangle$ for the two-electron atom/ions (with nuclear charge $Z$) in the ground state. The WFs are calculated by the Pekeris-like method [16, 17] with the number of shells equal to $\Omega = 25$. The ground state energies $E$ calculated by our Pekeris-like method are presented in the line before the last. The last line contains the corresponding energies $\tilde{E}$ by the more accurate calculations [1–4].

| $\lambda$ | $Z$ | 1         | 2         | 3         | 4         | 5         |
|-----------|-----|-----------|-----------|-----------|-----------|-----------|
| -1        | 0   | 0.009126180 | 0.1827953 | 0.7571888 | 1.9716346 | 4.0649090 |
| 0         | 0.1645526(8) | 1.8104292(3) | 6.8520098(4) | 17.198176(3) | 34.75874369(6) |
| 1         | 0.00273804(0) | 0.1063455(4) | 0.5337224(5) | 1.5228955(4) | 3.3124417(21) |

$\lambda_v^2$ 0.018649 0.34767 1.4281 3.6692 7.4792
$\lambda_2$ 0.01210173 0.2141994 0.8548817 2.175692 4.415435
$\lambda_{00}$ 0.009520788 0.1837904 0.7597262 1.9766583 4.073548
$\lambda_{cr}$ 0.008659116 0.1739671 0.7302144 1.915920 3.970376
$\lambda_{v0}$ 0.007979059 0.1664143 0.7074943 1.869972 3.892486

| $M(Z)$ | 0.0659991408 | 1.0994792 | 4.5084853 | 11.728245 | 24.191315 |
| $-E$ | 0.52775101652 | 2.903724377033 | 7.279913412668 | 13.6555662384231 | 22.0309715802421 |
| $-\tilde{E}$ | 0.52775101654 | 2.903724377034 | 7.279913412669 | 13.6555662384235 | 22.0309715802428 |

TABLE II: The characteristic points and other peculiarities of the expectation values $\langle \delta V \rangle$ and $\langle \delta T \rangle$ for the ground state of the two-electron atom/ions with nuclear charge $Z$ as functions of the colinear parameter $\lambda$.

| $Z \setminus \lambda$ | $\lambda_v^0$ | $\lambda_{00}$ | $\lambda_2$ | $\lambda_{cr}$ | $\lambda_{v2}$ | $\langle \delta V \rangle / \langle \delta T \rangle (\lambda = -1)$ |
|------------------------|----------------|----------------|--------------|----------------|----------------|----------------------------------|
| 1                      | 0.6181         | 0.5659         | 0.4992       | 0.5936         | 0.3896         | -1.3941                           |
| 2                      | 0.7811         | 0.7362         | 0.6701       | 0.7607         | 0.4801         | -1.3473                           |
| 3                      | 0.8472         | 0.8106         | 0.7520       | 0.8308         | 0.5207         | -1.3406                           |
| 4                      | 0.8828         | 0.8524         | 0.8012       | 0.8694         | 0.5481         | -1.3381                           |
| 5                      | 0.9050         | 0.8791         | 0.8342       | 0.8937         | 0.5674         | -1.3369                           |
FIG. 1: Normalized expectation values $\langle \delta (r_1 - \lambda r_2) \rangle$ as functions of the collinear parameter $\lambda$ for the two-electron atom/ions considered.
FIG. 2: Helium atom in the collinear 1S state. Expectation values of $T = -\Delta/2$ (red circles), and of $V = r^{-1} [-Z - Z/\lambda + 1/(1 - \lambda)]$ (blue triangles). $r$ is the distance between the nucleus and one of the electrons, $|\lambda|r$ is the distance between the nucleus and the other electron. The (e-n-e) configuration corresponds to $\lambda < 0$, the (n-e-e) configuration to $\lambda > 0$. 