Quantum entanglement in helium

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Abstract
We compute the entanglement of the ground state and several singlet and triplet excited states of the helium atom using high-quality, state-of-the-art wavefunctions. The behaviour of the entanglement of the helium eigenstates is similar to that observed in some exactly soluble two-electron systems. In particular, the amount of entanglement exhibited by the eigenstates tends to increase with energy.

1. Introduction

The exploration of the information-theoretic features exhibited by atomic systems has been the focus of a considerable research activity in recent years [1–24]. In this vein, several researchers have investigated the phenomenon of quantum entanglement in atomic physics [12–24]. Quantum entanglement is one of the most fundamental aspects of the quantum mechanical description of nature [25]. Besides its well-known role within new information technologies [26], quantum entanglement is beginning to be regarded as a basic ingredient in the characterization of the structural properties of composite quantum systems. In this sense, it is of great interest to analyse the entanglement properties of atoms. Most studies on entanglement in atoms have so far considered special model systems, or have been restricted to ground state computations. It is clearly desirable to extend these investigations to other scenarios, especially to the excited states of naturally occurring atomic systems. In this regard, the helium atom enjoys an important place, both from the conceptual and practical points of view. It constitutes one of the simplest non-trivial (real) composite quantum systems and it has played a distinguished role in the historical development of quantum theory [27, 28]. The purpose of the present effort is to calculate the amount of entanglement of the ground state and of the first few excited states of helium employing high-quality, state-of-the-art wavefunctions.

The paper is organized as follows. In section 2, we briefly review the concept of entanglement in systems consisting of identical fermions. The technical details of the calculations performed in this work are given in section 3. In section 4, we describe our main results. Finally, some conclusions are drawn in section 5.

2. Entanglement in systems of identical fermions

Quantum entanglement in systems consisting of N identical fermions has attracted considerable attention in recent years [29–37]. The entanglement features of a variety of systems constituted by identical fermions have been investigated. For example we can mention the entanglement in two-electron atomic models [12] and the entanglement between pairs of electrons in conducting bands [33], among many others.

A pure state of a system consisting of N identical fermions is separable (that is to say, non-entangled) if it can be written as a single Slater determinant det{$|1\rangle, |2\rangle, \ldots, |N\rangle$} constructed with N normalized and orthogonal single-particle states {$|i\rangle, i = 1, \ldots, N$}. N-fermion states that can be represented in this way are said to have a Slater rank equal to 1. Pure states of N identical fermions that do not admit such a representation are entangled. This means that the minimum correlations between the particles imposed by the antisymmetry of the fermionic state do not contribute to the state's amount of entanglement. Therefore, the entanglement exhibited by an N-fermion state corresponds to the quantum correlations that the state has on top of those minimum ones. There are profound physical reasons behind this notion of fermionic entanglement (see [29, 30]).

Let $|\Phi\rangle$ be a pure state of N identical fermions. The single-particle reduced density matrix obtained after taking the trace over $N-1$ particles is $\rho_1 = \text{Tr}_{2,3,\ldots,N}(|\Phi\rangle\langle\Phi|)$. The linear entropy of ρ_1, given by $S_L(\rho_1) = 1 - \text{Tr}(\rho_1^2)$, leads to a practical quantitative measure $\xi[|\Phi\rangle]$ for the amount of entanglement of the state $|\Phi\rangle$, namely

$$\xi[|\Phi\rangle] = N\left[S_L(\rho_1) - \left(\frac{N-1}{N}\right)\right]. \quad (1)$$

The entanglement measure (1) is a non-negative quantity that vanishes if and only if the state $|\Phi\rangle$ has Slater rank 1 and is therefore separable. The constant term appearing within the square brackets in (1) takes into account the fact that even for separable (pure) states (represented by a Slater determinant), the linear entropy of the single-particle density matrix does not vanish and is equal to $\frac{N-1}{N}$. The overall multiplicative factor N normalizes the entanglement measure to the range $[0, 1]$. In the spacial case of systems of two identical fermions ($N = 2$), the measure (1) can be related to the Schmidt decomposition. The measure (1) has been applied to several problems, particularly in connection with two-fermion systems (a recent discussion on the theoretical foundations of the measure (1) can be found in [37]).

Let us now apply the above measure to the particular case of a system consisting of two spin-$\frac{1}{2}$ fermions (that is, we have $N = 2$). In the present context, it will be sufficient to consider states described by wavefunctions of the type

$$\Phi = \Psi(\vec{r}_1, \vec{r}_2)\,\chi(\sigma_1, \sigma_2), \quad (2)$$

where the global wavefunction Φ is factorized as the product of a coordinate wavefunction $\Psi(\vec{r}_1, \vec{r}_2)$ and a spin wavefunction $\chi(\sigma_1, \sigma_2)$, where $\vec{r}_1$ and $\vec{r}_2$ denote the vector positions of the two electrons. The density matrix associated with a wavefunction of the type (2) is given by

$$\rho = \rho^{(\text{coord.})} \otimes \rho^{(\text{spin})}, \quad (3)$$

where the matrix elements of $\rho^{(\text{coord.})}$ are

$$\langle \vec{r}_1{}', \vec{r}_2{}' | \rho^{(\text{coord.})} | \vec{r}_1, \vec{r}_2 \rangle = \Psi(\vec{r}_1{}', \vec{r}_2{}')\Psi^*(\vec{r}_1, \vec{r}_2). \quad (4)$$

When evaluating the entanglement measure (1) on a state described by the wavefunction (2) (or the density matrix (3)), one obtains

$$\xi[|\Phi\rangle] = 1 - 2\,\text{Tr}\left[\left(\rho_1^{(\text{coord.})}\right)^2\right]\text{Tr}\left[\left(\rho_1^{(\text{spin})}\right)^2\right], \quad (5)$$

where $\rho_1^{(\text{coord.})}$ and $\rho_1^{(\text{spin})}$ denote the marginal density matrices respectively obtained after computing the partial traces of the matrices $\rho^{(\text{coord.})}$ and $\rho^{(\text{spin})}$ over the degrees of freedom of one of the two particles. It is clear that the entanglement between the two fermions (electrons) given by (5) involves both the translational and spin degrees of freedom of the electrons. To evaluate the entanglement measure (5), it is convenient to discuss separately the cases of a spin wavefunction describing parallel spins or antiparallel spins. When the spins are parallel (that is, the coordinate wavefunction is antisymmetric and the spin wavefunction is either χ_{++} or χ_{--}), we have $\text{Tr}\left[\left(\rho_1^{(\text{spin})}\right)^2\right] = 1$. In this case, the measure (1) reduces to

$$\xi[|\Phi\rangle] = 1 - 2\int |\langle \vec{r}_1{}'|\rho_1^{(\text{coord.})}|\vec{r}_1\rangle|^2\,\mathrm{d}\vec{r}_1{}'\,\mathrm{d}\vec{r}_1. \quad (6)$$

In the case of anti-parallel spins we have two alternative situations. On one hand, we have a symmetric coordinate wavefunction and the spin wavefunction $\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})$. Alternatively, the coordinate wavefunction is antisymmetric and the spin wavefunction is $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+})$. In either case we have $\text{Tr}\left[\left(\rho_1^{(\text{spin})}\right)^2\right] = \frac{1}{2}$, and the amount of entanglement is given by

$$\xi[|\Phi\rangle] = 1 - \int |\langle \vec{r}_1{}'|\rho_1^{(\text{coord.})}|\vec{r}_1\rangle|^2\,\mathrm{d}\vec{r}_1{}'\,\mathrm{d}\vec{r}_1. \quad (7)$$

In equations (6) and (7), we have

$$\langle \vec{r}_1{}'|\rho_1^{(\text{coord.})}|\vec{r}_1\rangle = \int_{-\infty}^{\infty} \Psi(\vec{r}_1{}', \vec{r}_2)\Psi^*(\vec{r}_1, \vec{r}_2)\,\mathrm{d}\vec{r}_2. \quad (8)$$

It is worth stressing that a two-electron state with a wavefunction of the form

$$\frac{1}{\sqrt{2}}\left[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_2(\vec{r}_1)\psi_1(\vec{r}_2)\right]\chi_{kk},\, k = \pm, \quad (9)$$

with $\psi_1(\vec{r})$ and $\psi_2(\vec{r})$ being orthogonal, normalized single-particle (coordinate) wavefunctions (corresponding a Slater determinant), has no entanglement (that is, it describes a separable fermion state). This example illustrates an essential point already mentioned: the correlations between two fermions that are entirely due to the anti-symmetry requirement on the fermionic state do not contribute to the entanglement of the state.

3. Kinoshita wavefunctions: description

In this paper, we use the Kinoshita-type wavefunctions described in [38]. The wavefunctions have the form

$$\Psi_N(s, u, t) = \exp(-\zeta s)\sum_{i=1}^{N} c_i\, s^{l_i/2}\left(\frac{t}{u}\right)^{m_i}\left(\frac{u}{s}\right)^{n_i/2}, \quad (10)$$

where (s, u, t) are the Hylleraas coordinates [39]

$$
\begin{aligned}
s &= \|\vec{r}_1\| + \|\vec{r}_2\|, & s &\in [0, +\infty[\\
u &= \|\vec{r}_1 - \vec{r}_2\|, & u &\in [0, s] \\
t &= \|\vec{r}_1\| - \|\vec{r}_2\|, & t &\in [-u, u],
\end{aligned}
\quad (11)
$$

and the exponents (l_i, m_i, n_i) are non-negative integers. In the determination of the wavefunction, for fixed N, optimization with respect to the exponents (l_i, m_i, n_i), the expansion coefficients c_i and the exponential exponents ζ is performed. The use of half-integer exponents in the Kinoshita expansion, instead of integer exponents, was found to dramatically improve the quality of the Kinoshita wavefunctions for two-electron atoms. The detailed comparisons were given in [38]. It is also described in [38] how the optimizations of exponents were performed.

In the evaluation of the corresponding integrals, we have taken into account that the corresponding volume element for this coordinate system is $\mathrm{d}v = \pi^2 u(s^2 - t^2)\mathrm{d}u\,\mathrm{d}s\,\mathrm{d}t$, being the

normalization of the wavefunction

$$d^2 = \int_0^\infty ds \int_0^s du \int_{-u}^{+u} dt \, (\Psi_N(s,u,t))^2$$

$$= \pi^2 \sum_{i,j=1}^N c_i c_j \zeta^{-6-\frac{l_i+l_j}{2}} 2^{-4-\frac{l_i+l_j}{2}}$$

$$\times \frac{(1+(-1)^{m_i+m_j})(12+2m_i+2m_j+n_i+n_j)\Gamma\left(\frac{12+l_i+l_j}{2}\right)}{(1+m_i+m_j)(3+m_i+m_j)(6+n_i+n_j)(10+n_i+n_j)}. \tag{12}$$
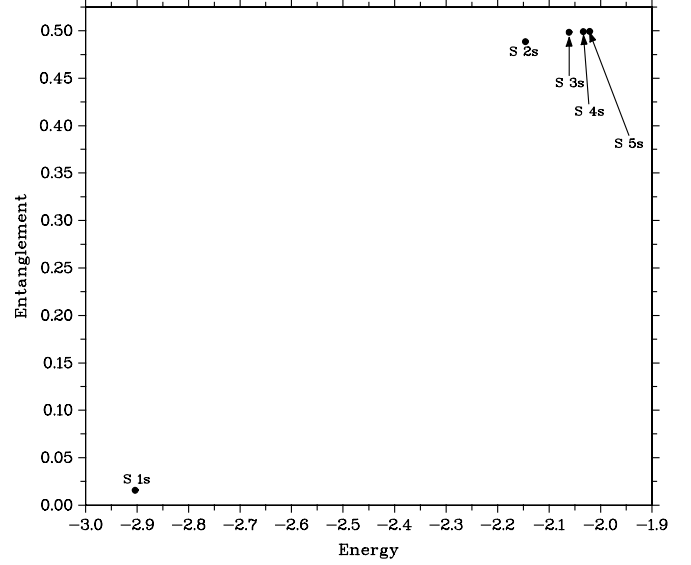
4. Entanglement in helium

To evaluate the entanglement for the helium wavefunction, we need to compute $\mathrm{Tr}[(\rho_1^{(\text{coord.})})^2]$, which is tantamount to the evaluation of the 12-dimensional definite integral,

$$\mathrm{Tr}\left[\left(\rho_1^{(\text{coord.})}\right)^2\right]$$

$$= \int_{\mathbb{R}^6} \left|\rho_1^{(\text{coord.})}(\vec{r_1}', \vec{r_1})\right|^2 d\vec{r_1}' d\vec{r_1}$$

$$= \int_{\mathbb{R}^6} \left|\int_{\mathbb{R}^3} \Psi(\vec{r_1}', \vec{r_2})\Psi^*(\vec{r_1}, \vec{r_2}) d\vec{r_2}\right|^2 d\vec{r_1}' d\vec{r_1}$$

$$= \int_{\mathbb{R}^{12}} \Psi(\vec{r_1}', \vec{r_2})\Psi^*(\vec{r_1}, \vec{r_2})\Psi^*(\vec{r_1}', \vec{r_2}')\Psi(\vec{r_1}, \vec{r_2}')$$

$$\times d\vec{r_1}' d\vec{r_1} d\vec{r_2}' d\vec{r_2}. \tag{13}$$

To perform this computation, we have used the Vegas routine in the CUBA library [40, 41], version 2.1 [42], for Monte Carlo multidimensional numerical integration. It uses importance sampling for variance reduction [43].

The results obtained for the amount of entanglement exhibited by the available helium ground and excited states, both singlet and triplet, are summarized in table 1 and in figures 1–3. In the concomitant calculations, we used Kinoshita wavefunctions with $N = 100$ terms, keeping an accuracy which was shown to be high enough to determine accurate entanglement values (more on this below). In our study, we stop at the 5s excited state because to obtain Kinoshita wavefunctions becomes computationally too demanding as we go to higher excited states. In table 1, we provide the amounts of entanglement and the energies corresponding to several singlet and triplet states of helium. In figure 1, we depict the amount of entanglement against the energy of the singlet states considered in this work. A similar plot is given in figure 2 for the case of triplet states.

As already mentioned, we have performed our computations employing Kinoshita-type wavefunctions with $N = 100$ terms, because they are the highest quality helium eigenfunctions available to date. To illustrate the fact that this number of terms is large enough to compute appropriately the entanglement of the helium wavefunctions, we provide in table 2 the entanglement ξ of the ground state of helium, computed via Monte Carlo integration using Kinoshita wavefunctions with different numbers of terms. Note that, from $N = 20$ terms on, the numerically computed entanglement (estimated error included) stays basically constant.

Figure 1. Entanglement against energy for singlet states of helium. Energy is given in hartrees and entanglement is a dimensionless quantity.
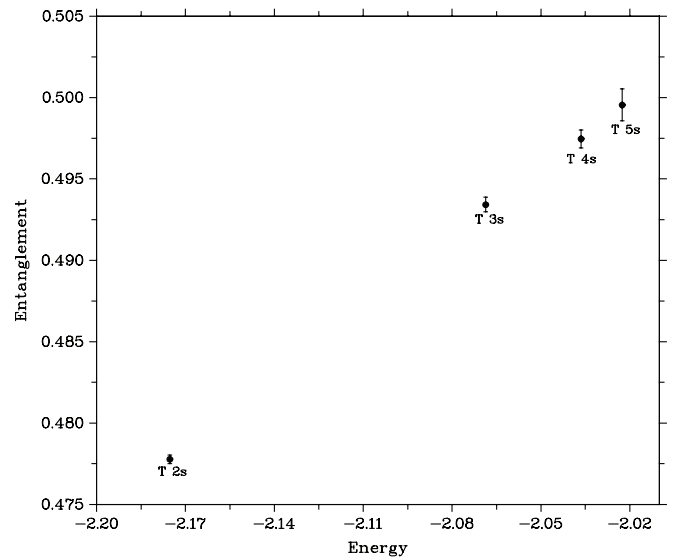
Figure 2. Entanglement against energy for triplet states of helium. Energy is given in hartrees and entanglement is a dimensionless quantity. The triplet states represented correspond to the $S_z = 0$ case with anti-parallel spins.
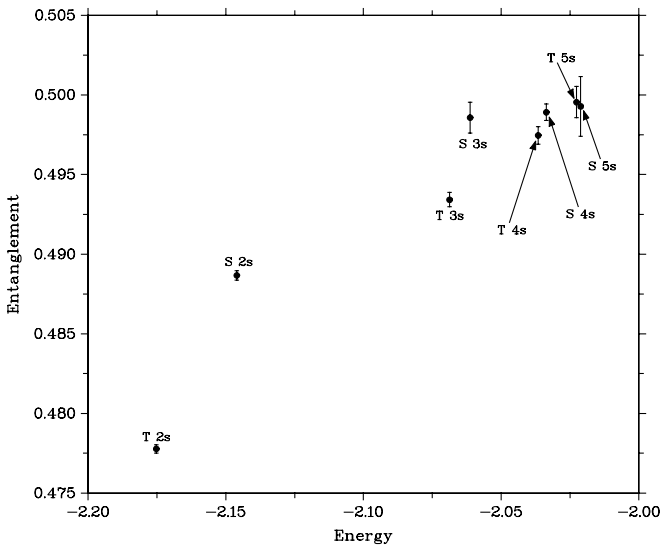
The entanglement of the singlet and triplet states of helium is depicted against energy in figures 1 and 2, respectively. A similar plot representing both singlet and triplet states together is given in figure 3. It can be observed in figures 1–3 that the amount of entanglement associated with helium eigenstates tends to increase with energy. That is, higher excited states tend to exhibit more entanglement. This trend is compatible with the entanglement behaviour observed in exactly soluble two-fermion models such as the Moshinsky one [18]. Although the results depicted in figure 2 seem compatible with an approximate linear relation between entanglement and energy for triplet states, one must bear in mind that the data available correspond only to a limited

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Table 1. Entanglement and energies of helium eigenstates. Entanglement is dimensionless and energy is given in hartrees.

State	Energy	Entanglement
Singlet 1s	−2.903 724 377	0.015 914 ± 0.000 044
Singlet 2s	−2.145 974 046	0.488 66 ± 0.000 30
Singlet 3s	−2.061 271 954	0.498 57 ± 0.000 97
Singlet 4s	−2.033 586 653	0.498 92 ± 0.000 52
Singlet 5s	−2.021 176 531	0.4993 ± 0.0019
Triplet 2s	−2.175 229 378	0.477 78 ± 0.000 27
Triplet 3s	−2.068 689 045	0.493 42 ± 0.000 45
Triplet 4s	−2.036 512 038	0.497 46 ± 0.000 55
Triplet 5s	−2.022 618 670	0.499 55 ± 0.000 98

Table 2. Entanglement and energy of the ground state of helium computed with Kinoshita wavefunctions having different numbers N of terms. Entanglement is dimensionless and energy is given in hartrees.

N	Energy	Entanglement
5	−2.903 569 904	0.016 295 ± 0.000 068
10	−2.903 721 712	0.015 956 ± 0.000 075
20	−2.903 724 228	0.015 915 ± 0.000 044
30	−2.903 724 361	0.015 915 ± 0.000 044
50	−2.903 724 376	0.015 914 ± 0.000 044
100	−2.903 724 377	0.015 914 ± 0.000 044

Figure 3. Entanglement against energy for both singlet and triplet states of helium. Energy is given in hartrees and entanglement is a dimensionless quantity.

number of states and the errors of the entanglement values make them also compatible with a more general, nonlinear relation with energy.

The present results concerning the entanglement properties of helium have some similarities with the entanglement-related features of some exactly soluble models such as the Moshinsky, Crandall and Hooke models [18, 19]. These models comprise two interacting spin-$\frac{1}{2}$ fermions in an external confining potential. In the alluded exactly soluble models the confining potential is harmonic, while

in helium the confining potential is given by the Coulomb electrostatic potential due to the atomic nucleus. In the Moshinsky model the interaction between the particles is harmonic; in the Crandall model, the interaction is given by a $-1/r^2$ potential function, while in the Hooke atom the interaction is the standard $-1/r$ Coulomb interaction. It is remarkable that, in spite of the great differences between these models, their entanglement-related features have some qualitative similarities that are also shared by helium. Two of the main trends observed in these models are the following.

(i) The entanglement of the eigenstates tends to increase when the interaction strength becomes more important compared with the strength of the confining potential. That is, entanglement increases with the interaction strength, for a given strength of the confining potential or, alternatively, entanglement decreases with the strength of the confining potential, for a given strength of the interaction.

(ii) Entanglement tends to increase with the energy of the system's eigenstates.

Due to the great differences between helium and the models previously mentioned, a quantitative comparison between the entanglement features of helium and those exhibited by the exactly soluble models is not feasible. However, a qualitative comparison between these systems is indeed quite illuminating.

Let us first consider the first one of the trends listed above. In the case of helium, the strength of the interaction, corresponding to the electrostatic repulsion between the electrons, is fixed. However, it is of interest to consider helium-like atoms with different values of the nuclear charge Z. Larger values of Z correspond to situations where the interaction strength becomes weaker as compared with the confining potential. On the basis of the behaviour of Moshinsky's and other models, one should expect entanglement in helium-like atomic systems to decrease with Z. This is precisely what was observed in [19], where the entanglement of the ground state of helium-like atoms was computed for different values of the nuclear charge Z.

Concerning the second trend (ii), the results reported in this work indicate that helium does indeed behave in the same qualitative way as the exactly soluble models studied previously: entanglement tends to increase with energy. Helium, however, exhibits some interesting peculiarities. In the case of the models of Moshinsky and Crandall, as well as in the case of the Hooke atom, the entanglement measure $\xi[|\Phi\rangle]$ of the system's eigenstates $|\Phi\rangle$ (given by equation (1)) approaches its maximum possible value $\xi = 1$ as one considers eigenstates of increasing energy. In this respect helium is different: the entanglement of the eigenstates of helium (for both the singlet and the triplet states) seems to saturate at $\xi = 1/2$. This difference may be due to the form of the confining potential: all of the two-fermion models mentioned have a harmonic confining potential, while the confining potential in helium is the Coulomb potential proportional to $-1/r$. The excited states of helium studied here can be approximately described as consisting of two electrons in a hydrogen-like

Coulomb potential (with an appropriate nuclear charge). One of the electrons is in the corresponding hydrogenic ground state, while the other is in an excited s-state with principal quantum number $n > 1$. Now, the higher the excitation of the helium state considered, the better is this independent-particle description. This approximate description improves because the average distance between the electrons becomes larger and, consequently, the Coulomb interaction between them becomes less important. Therefore, higher excited states approach the form

$$\frac{1}{\sqrt{2}}[\Psi_{100}(\mathbf{r_1})\Psi_{n00}(\mathbf{r_2}) \pm \Psi_{n00}(\mathbf{r_1})\Psi_{100}(\mathbf{r_2})]\frac{1}{\sqrt{2}}[\chi_{+-} \mp \chi_{-+}], \tag{14}$$

where $\Psi_{nlm}(\mathbf{r})$ are the standard hydrogenic eigenfunctions and $\frac{1}{\sqrt{2}}[\chi_{+-} \mp \chi_{-+}]$ are (in self-explanatory notation) the spin wavefunctions. The upper signs in (14) correspond to the singlet states and the lower signs to the triplet states (the triplet states represented in figures 2 and 3 correspond to the $S_z = 0$ case with anti-parallel spins). In summary, as one considers higher excited states their entanglement tends to the entanglement of the states (14), which is $\xi = \frac{1}{2}$. In previously studied models like the Moshinsky atom, with a harmonic confining potential, the situation is different because this potential is much more 'confining' than the Coulomb one, and the interaction term does not become negligible as one considers states of higher energy.

5. Conclusions

We have computed the amount of entanglement exhibited by the ground state and several singlet and triplet excited states of the helium atom using high-quality, state-of-the-art wavefunctions of the Kinoshita type. We found that the behaviour of the entanglement of the eigenstates of helium is consistent with that observed in the case of previously studied exactly soluble two-electron systems such as the Moshinsky model, the Crandall system and the Hooke atom. In particular, the amount of entanglement exhibited by the eigenstates tends to increase with energy. The present calculations therefore provide further evidence suggesting that this behaviour is universal in two-electron systems. It would be interesting to extend this investigation to atoms with more than two electrons. Any further results along these lines will be very welcome.

Acknowledgments

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