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Entanglement Entropies in the Ground States of Helium-Like Atoms

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Abstract We examine the entanglement in the ground states of helium and helium-like ions using an original Hylleraas expansion. The von Neumann and linear entropies of the reduced density matrix are accurately computed by performing the Schmidt decomposition of the S singlet spatial wavefunctions. The results presented are more accurate than currently available in published literature.

1 Introduction

In recent years there has been a lot of interest in entanglement properies of few-body systems. Besides an important role in quantum information technology, entanglement also attracts attention in view of the problem of quantifying the amount of correlations in the systems. Mainly, two-particle model systems confined by various potential have been studied in this respect [1–12]. The von Neumann entropy (vN) of the one-particle reduced-density matrix (RDM) is accepted as a reliable entanglement measure for systems of two indistinguishable particles [13]. At the same time, the vN entropy determines the strength of correlation in the system. The linear entropy, being the lower approximation of the vN entropy, is also used to this end, since it can be more easily calculated without knowing the spectrum of the RDM.

The quantum information content of two-electron atoms become also interesting for chemists. For example, Manzano et al. [5], Dehesa et al. [14] and Benenti et al. [15] have studied the entanglement properties of the ground and excited states of the helium atom. Lin et al. [16] explored entanglement in the ground and excited states of the helium atom and helium-like ions, using configuration interaction wave functions constructed with B-spline basis. Very recently, Lin et al. [17] studied entanglement in the ground states of helium and the hydrogen negative ion, establishing the values of linear entropies with relatively small uncertainties. In most of the studies mentioned above, only the linear entropy was used to quantify the amount of the entanglement. We are aware of only four papers [15,18,22,23], where the results for the von Neumann entropy were reported. However, there are large discrepancies between the results of those papers. This was our motivation for performing accurate calculations of entropies for the helium isoelectronic series. We calculated the vN and linear entropy, basing on the Schmidt decomposition of the two-particle wavefunction. In our calculations, we used an original correlated Hylleraas basis which allows determination of the wavefunction within a reasonable accuracy with relatively low computational cost.

This paper is organized as follows. In Sect. 2 we briefly discuss the procedure to analyze the entanglement properties of the singlet S-symmetry states. Section 3 outlines our results, and some concluding remarks are placed in Sect. 4.

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2 Methods

The Hamiltonian of atomic systems with two electrons and a nucleus of charge Ze is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \tag{1}$$

where atomic units are used. As mentioned before, we are interested in the singlet ground-state, the spatial wave-function of which depends only on the radial coordinates r_1, r_2 and the inter-electronic angle θ. The Schmidt decomposition of the wave-function has a form [20]

$$\psi(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi(r_1, r_2, \cos\theta) = \sum_{n,l=0}^{\infty} \sum_{m=-l}^{m=l} a_{nl} u^*_{nlm}(\mathbf{r}_1) u_{nlm}(\mathbf{r}_2), \tag{2}$$

with $u_{nlm}(\mathbf{r}) = \frac{v_{nl}(r)Y_{lm}(\theta,\varphi)}{r}$ and $a_{nl} = \frac{4\pi k_{nl}}{2l+1}$, where Y_{lm} are the spherical harmonics and l and n are the angular and principal quantum numbers, respectively. Both the radial orbitals $v_{nl}(r)$ and the coefficients k_{nl} are real and can be determined by the following integral equations [19]

$$\int_0^{\infty} f_l(r_1, r_2) v_{nl}(r_2) dr_2 = k_{nl} v_{nl}(r_1) \tag{3}$$

with

$$f_l(r_1, r_2) = r_1 r_2 \frac{2l+1}{2} \int_0^{\pi} \psi(r_1, r_2, \cos\theta) P_l(\cos\theta) \sin\theta d\theta, \tag{4}$$

where P_l are the Legendre polynomials. The natural orbitals $u_{nlm}(\mathbf{r})$ are the eigenvectors of the spatial RDM

$$\rho(\mathbf{r}, \mathbf{r}') = \int [\psi(\mathbf{r}, \mathbf{r}_1)]^* \psi(\mathbf{r}', \mathbf{r}_1) d\mathbf{r}_1,$$

the eigenvalues of which, λ_{nl}, are related to the expansion coefficients in (2) by $\lambda_{nl} = a_{nl}^2$. The natural orbitals $\{u_{nlm}(\mathbf{r})\}_{m=-l}^{m=l}$ correspond to the same occupation number λ_{nl}, which means that $2l+1$-fold degeneracy occurs and, therefore, the normalization condition gives $\sum_{nl}(2l+1)\lambda_{nl} = 1$. Using Eq. (2), the identity $[Y_{l,m}(\theta,\varphi)]^* = (-1)^m Y_{l,-m}(\theta,\varphi)$ and the spin singlet function representation $\chi_S = \frac{1}{\sqrt{2}}(\alpha(1)\beta(2) - \alpha(2)\beta(1))$, where $\alpha(\beta)$ denotes the up (down) spin, the Slater decomposition of the total two-electron singlet S-state wavefunction can be easily inferred, namely:

$$\Psi(\xi_1, \xi_2) = \sum_{\substack{n=0 \\ l=0}}^{\infty} a_{nl} SD[u_{nl0}\alpha, u_{nl0}\beta] + \sum_{\substack{i,j=\{\alpha,\beta\} \\ i\neq j}} \sum_{\substack{n=0 \\ l=1}}^{\infty} \sum_{m=1}^{l} \nu a_{nl} SD[u^*_{nlm} i, u_{nlm} j], \tag{5}$$

where $\nu = 1(-1)$ for $i = \alpha(\beta)$, and SD denotes a Slater determinant made out of two spin orbitals, $SD[\phi i, \varphi j] = 2^{-\frac{1}{2}} \begin{vmatrix} \phi(\mathbf{r}_1) i(1) & \varphi(\mathbf{r}_1) j(1) \\ \phi(\mathbf{r}_2) i(2) & \varphi(\mathbf{r}_2) j(2) \end{vmatrix}$.

Entanglement in pure states is usually quantified by the vN entropy of the RDM, which in the case of the singlet sates takes the form

$$\mathbf{S} = -\mathrm{Tr}[\rho \log_2 \rho], \tag{6}$$

or the linear entropy

$$\mathbf{L} = 1 - \mathrm{Tr}[\rho^2], \tag{7}$$

which both vanish when the corresponding total two-electron wavefunction can be expressed as a single determinant [21]. The linear entropy can be calculated without determining the occupation numbers, as the

spatial purity $\mathrm{Tr}[\rho^2]$ can be expressed by the twelve-dimensional integral (see for example [14]). With the help of (4) we derived an alternative representation of the purity by an infinite sum of eight-dimensional integrals

$$\mathrm{Tr}[\rho^2] = (2\pi)^4 \sum_{l=0}^{\infty} \int_0^{\infty} \ldots \int_0^{\infty} \int_0^{\pi} \ldots \int_0^{\pi} (rr' r_1 r_2)^2$$
$$\psi(r, r_1, \cos\theta)\psi(r', r_1, \cos\theta')\psi(r, r_2, \cos\theta'')\psi(r', r_2, \cos\theta''')$$
$$P_l(\cos\theta) P_l(\cos\theta') P_l(\cos\theta'') P_l(\cos\theta''') \sin\theta \sin\theta' \sin\theta''$$
$$\sin\theta''' dr_1 dr_2 dr dr' d\theta d\theta' d\theta'' d\theta''', \tag{8}$$

which may be useful when dealing with spherically symmetric two-particle systems. If most of the electrons' correlation is captured by the partial components with low l, the sum (8) may be more effective than the mentioned twelve-dimensional integral to calculate the purity.

The calculation of the vN entropy requires detemination of the Schmidt coefficients. For singlet S states, we have in terms of the occupation numbers $S = -\sum_{nl}(2l+1)\lambda_{nl}\log_2\lambda_{nl}$, $L = 1 - \sum_{nl}(2l+1)\lambda_{nl}^2$ [9]. To determine the coefficients $\lambda_{nl} = (\frac{4\pi k_{nl}}{2l+1})^2$ we solved Eq. (4) through a discretization technique. A set of approximations to the $n_m + 1$ coefficients k_{nl} can be thus obtained by diagonalizing the matrix $[M_{ij}^{(l)}]$, $M_{ij}^{(l)} = \triangle r f_l(\triangle r i, \triangle r j)$, $\triangle r = R/n_m$, $i, j = 0, \ldots, n_m$. [9], where R should be chosen as large as the side of a square in which the functions $f_l(r_1, r_2)$ are mainly confined. Having the coefficients k_{nl} determined in that way for l up to l_m, we obtain the approximate entropies $S = -\sum_{n=0}^{n_m}\sum_{l=0}^{l_m}(2l+1)\lambda_{nl}\log_2\lambda_{nl}$ and $L = 1 - \sum_{n=0}^{n_m}\sum_{l=0}^{l_m}(2l+1)\lambda_{nl}^2$. In order to obtain stable numerical values, the calculations have to be repeated for larger and larger R and n_m, l_m until the results converge to the desired accuracy.

3 Numerical Results

In our ground-state calculations we employ the Hylleraas variational wave function

$$\psi(r_1, r_2, \cos\theta) = \sum_{nmp} c_{nmp} e^{-\mu s} s^n t^m u^p, \tag{9}$$

with $0 \le n+m+p \le \omega$ (m-even), where $s = r_1 + r_2$, $t = r_1 - r_2$, $u = r_{12} = |\mathbf{r}_2 - \mathbf{r}_1| = (r_1^2 + r_2^2 - 2r_1 r_2\cos\theta)^{\frac{1}{2}}$ and μ is a non-linear variational parameter.

The ground state energy E and the corresponding linear parameters c_{nmp} are determined by the solution of a generalized eigenvalue problem

$$\sum_{nmp}(H_{n'm'p',nmp} - E S_{n'm'p',nmp})c_{nmp} = 0 \tag{10}$$

where $S_{n'm'p',nmp} = \langle n'm'p'|nmp\rangle$ and $H_{n'm'p',nmp} = \langle n'm'p'|H|nmp\rangle$, whereas, the non-linear parameter μ is iteratively optimized so as to minimize the approximate energy $\partial E^{(\omega)}/\partial\mu = 0$.

For demonstration purpose, the ω-order ground state energies obtained as described above are shown in Table 1, where the underlines represent the digits that agree with the very accurate results of Nakashima and Nakatsuji [24].

Calculating entanglement entropies, we first determine the Schmidt coefficients by solving Eq. (3) numerically. We found that for the Hylleras expansion, the integrals (4) can be carried out analytically: Substitution of an explicit representation $P_l(\cos\theta) = 2^l \sum_{k=0}^{l}(\cos\theta)^k \binom{l}{k}\binom{\frac{l+k-1}{2}}{l}$, and the Hylleras expansion (9) expressed in r_1, r_2 and θ into (4) yields

$$f_l(r_1, r_2) = C 2^{l-1}(2l+1) r_1 r_2 e^{-\mu(r_1+r_2)} \sum_{k=0}^{l}\sum_{nmp} c_{nmp}\binom{l}{k}\binom{\frac{l+k-1}{2}}{l}(r_2 - r_1)^m (r_1 + r_2)^n I(k, p) \tag{11}$$

Table 1 Ground state energies determined variationally as discussed in the text

ω	$Z=1$	$Z=2$	$Z=3$	$Z=4$	$Z=5$
6	−0.5277432488	−2.903723702	−7.279912718	−13.65556549	−22.03097079
8	−0.5277500643	−2.903724305	−7.279913342	−13.65556616	−22.03097150
10	−0.5277508656	−2.903724366	−7.279913402		
12	−0.5277509860	−2.903724375			
14	−0.5277510091				

Table 2 The stable numerical results for the linear entropy L obtained at different R with different expansion lengths $\omega = 6, 10, 14$ corresponding to number of terms 50, 161, 372, respectively

	$R=7$	$R=9$	$R=10$
$\omega=6$	0.0159173	0.0159162	0.0159162
$\omega=10$	0.0159172	0.0159157	0.0159157
$\omega=14$	0.0159172	0.0159157	0.0159157

Table 3 The linear entropy L computed at $R=10$ with an expansion given by a 372-term wavefunction ($\omega=14$) as a function of l_m, for $n_m = 300, 600, 1200$ corresponding to $\triangle r = 30^{-1}, 60^{-1}, 120^{-1}$, respectively

	$n_m=300$	$n_m=600$	$n_m=1{,}200$
$l_m=0$	0.0159242	0.0159207	0.0159205
$l_m=1$	0.0159194	0.0159159	0.0159157
$l_m=2$	0.0159194	0.0159159	0.0159157

where C is the normalization constant and $I(k,p)$ are given by the following integrals

$$I(k,p) = \int_0^\pi \sin\theta(\cos\theta)^k (r_1^2+r_2^2-2r_1r_2\cos\theta)^{\frac{p}{2}} d\theta = \frac{1}{r_1^2+r_2^2}\Gamma(1+k)$$
$$\left(\frac{(-1)^k(r_1+r_2)^{2+p}}{\Gamma(2+k)}\,{}_2F_1\left(1,2+k+\frac{p}{2},2+k,-\frac{2r_1r_2}{r_1^2+r_2^2}\right)\right.$$
$$\left.+\frac{(r_1-r_2)^{2+p}}{\Gamma(2+k)}\,{}_2F_1\left(1,2+k+\frac{p}{2},2+k,\frac{2r_1r_2}{r_1^2+r_2^2}\right)\right). \quad (12)$$

In some cases it is computationally less demanding to treat Eq. (4) numerically for discretized values of r_1 and r_2, especially when a large number of terms is included in the Hylleras expansion. The above analytical expressions of Eq. (4) are however useful when testing the accuracies of numerical integrations.

In order to gain insight into the effectiveness of the method described in previous section, we first determine the occupation numbers of the ground state helium atom and assess their accuracy by comparing the linear entropy with the data available in literature. Our numerical values obtained for $L = 1 - \sum_{nl}(2l+1)\lambda_{nl}^2$ at different R with different expansion lengths ω are listed in Table 2. The numerical stability was achieved by increasing n_m and l_m until the results stay fixed to the quoted accuracy. It can be seen that already at $R=9$ and $\omega=10$ the results start to match with the benchmark value for the linear entropy 0.0159156 ± 0.000001 established with relative small estimated uncertainty in Ref. [17], which proves the effectiveness of the method we are using here for determining the occupation numbers. Tables 3 and 4 show how the values of the linear and von Neumann entropies, respectively, converge as the cut-offs l_m and n_m are increased. Performing calculations at larger R and ω, we have verified that the value of the vN entropy 0.0848999 faithfully reproduces the true value with to at least 7 significant digits. It is worth stressing at this point that the convergence with increasing l_m appears monotonic (from above for the linear entropy and from below for the vN entropy).

In Table 5 our results for the entropies of the helium atom are compared with those obtained by other workers in different ways. For example, in Refs. [15] and [18] the authors calculated the vN and linear entropies using configuration interaction method with basis wave functions constructed by Slater-type orbitals (STO) and by B-spline basis with one-electron momentum states up to $l=3$ and up to $l=5$, respectively. From the comparison, we conclude that our value for the vN entropy is the best so far determined for the helium atom.

Table 4 Same as in Table 3, but for the von Neumann entropy S

	$n_m = 300$	$n_m = 600$	$n_m = 1{,}200$
$l_m = 0$	0.0428655	0.0428631	0.0428630
$l_m = 1$	0.0814955	0.0814931	0.0814930
$l_m = 2$	0.0842412	0.0842388	0.0842387
$l_m = 3$	0.0847083	0.0847058	0.0847057
$l_m = 4$	0.0848295	0.0848271	0.0848269
$l_m = 5$	0.0848702	0.0848678	0.0848676
$l_m = 10$	0.0849006	0.0848982	0.0848980
$l_m = 14$	0.0849022	0.0848997	0.0848996
$l_m = 18$	0.0849025	0.0849001	0.0848999
$l_m = 20$	0.0849025	0.0849001	0.0848999

Table 5 Comparison of the vN and linear entropies calculated for the helium atom ground state with the results published in literature

	L	S
This work	0.0159157	0.0848999
Dehesa et al. [14]	0.015914 ± 0.000044	
Benetti et al. [15]	0.01606	0.0785
Lin et al. [16]	0.015943 ± 0.00004	
Lin et al. [17]	0.0159156 ± 0.000001	
Lin et al. [18]	0.015943	0.085022
Huang et al. [22]		0.0675

Table 6 Linear entropy (L) and the vN entropy (S) calculated for the ground state of helium-like ions compared with the best literature results

	$Z = 1$	$Z = 2$	$Z = 3$	$Z = 4$	$Z = 5$
L	0.106153	0.0159157	0.006539	0.003558	0.002235
[16]		0.015943	0.006549	0.003562	0.002237
[17]	0.106153	0.0159156			
S	0.380012	0.0848999	0.039496	0.023146	0.015324
[18]		0.085022			

We also computed the entanglement entropies for the ground states of the two-electron atoms with different values of Z. Our results for the linear entropy and the vN entropy are listed in the table 6, where a comparison with the literature [16,17] is also made. It is worth stressing that in each case considered here, the stability of the results up to at least six decimal places was achieved already at $l_m = 1$, similarly as for the helium atom. Our value of the linear entropy of the hydrogen negative ion ($Z = 1$) coincides with the recently obtained value 0.106153 of Ref. [17]. In all the remaining cases, our values are more accurate being slightly lower than the results of the recent calculations [16]. The only accurate value reported in the literature is that for the helium atom [18] which compares well with our result. The vN entropy for other values of Z was calculated only in Ref. [23], where the convergence of correlated Gaussian basis sets has been tested. However, the results for helium-like ions reported in supplementary material to this work differ widely depending on the type of Gaussian basis used. Despite of using large basis sets, the results for the linear and vN entropies of helium-like ions obtained in Ref. [23] are of low accuracy and were presented only graphically in the article. We would like to stress that using the Hylleraas basis set (9) provides much better convergence properties, which enabled us to determine the vN entropy to 6 digits accuracy.

The accurate results allow us to study the relation between the linear entropy and the vN entropy of the RDM for the helium-like ions as a function of Z. This is an important issue since the linear entropy is frequently used to measure entanglement in the system. The linear entropy is much easier to calculate than the vN entropy since it is directly calculable from the integral representation and does not require diagonalization of the RDM.

Comparing the dependence on Z of the linear and vN entropies, we noted that from $Z = 2$ to $Z = 5$ they are almost linearly related. This is demonstrated in Fig. 1, where the vN entropy is shown together with the rescaled linear entropy $6.856L$, where the factor 6.856 is obtained as the proportionality constant between S and L at $Z = 5$. The departure from the linear realtionship occurs in the vicinity of $Z = 1$. This may be caused by the proximity to the critical point Z_c below which there are no bound states in the system. It has been shown in Ref. [25] that the ionization point at which the helium-like system has a bound state with zero

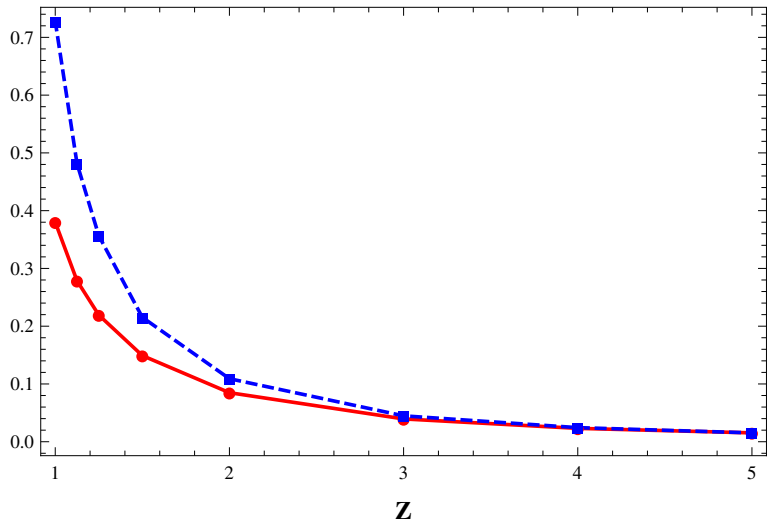

Fig. 1 Comparison of the vN entropy (*full line*) and the rescaled linear entropy $6.856L$ (*dashed line*) as functions of Z

binding energy is at $Z_c \approx 0.911$. Our calculation show that in the vicinity of the critical point, where the system is highly correlated, the behavior of the linear and vN entropies is different.

Our results may be compared with the discussion of entanglement in the spherical helium-like model in Ref. [26]. The spherical model is an approximation to the atom obtained by replacing the Coulombic repulsion between the electrons by its spherical average. The approximate model has been shown to exhibit a similar near-threshold behavior as the two-electron atom [27]. In Ref. [26], the scaling properties of the von Neumann entropy have been studied for the ground state of the spherical helium-like model and its singular behavior was demonstrated at $Z_c^{sph} \approx 0.949$. This value appears really close to the critical point of the helium-like atom ($Z_c \approx 0.911$).

4 Conclusions

In conclusion, we have performed accurate calculations of the linear and vN entropy of the ground states of the helium atom and helium-like ions, basing on the Schmidt decomposition of the two-particle spatial wavefunctions. The accurate wvefunctions were obtained, employing expansions in terms of original Hylleraas-type basis functions. Using a discretization technique, we determined the natural occupation numbers λ_{nl} up to very large l and n for a series of values of the nuclear charge from $Z = 1$ to $Z = 5$, which enabled high-precision determination of the corresponding entropies. In particular, the vN entropies of the helium-like ions have been calculated for the first time and that of the helium atom has been determined with much better accuracy than earlier calculations. Furthermore, our results revealed that relationship between the vN and linear entropies is almost linear for $Z \geq 2$. However with Z decreasing to the critical value, the increase of the vN entropy gets much faster than that of the linear entropy. This may give a warning that using the linear entropy instead of the vN entropy to measure entanglement not always is justified.

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