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Quantum entanglement in $(d-1)$ -spherium

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Abstract

There are very few systems of interacting particles (with continuous variables) for which the entanglement of the concomitant eigenfunctions can be computed in an exact, analytical way. Here we present analytical calculations of the amount of entanglement exhibited by s -states of *spherium*. This is a system of two particles (electrons) interacting via a Coulomb potential and confined to a $(d-1)$ -sphere (that is, to the surface of a d -dimensional ball). We investigate the dependence of entanglement on the radius R of the system, on the spatial dimensionality d , and on energy. We find that entanglement increases monotonically with R , decreases with d , and also tends to increase with the energy of the eigenstates. These trends are discussed and compared with those observed in other two-electron atomic-like models where entanglement has been investigated.

Keywords: quantum entanglement, two-electron models, spherium, quasi-soluble models

(Some figures may appear in colour only in the online journal)

1. Introduction

It has been recently shown by Loos and Gill [1, 2] that ‘spherium’, a system consisting of two electrons trapped on the surface of a sphere and interacting through a Coulomb potential, belongs to the family of quasi-exactly solvable quantum mechanical models. These are models whose Schrödinger eigenvalue equation admits an explicit analytical solution for a finite portion of the energy spectrum. This kind of models are of considerable interest both for illuminating the properties of more complex or realistic systems and for testing and

developing approximate treatments, such as those related to density functional theory. Indeed, spherium has found interesting applications in the study of correlated quantum systems (see [1] and references therein). Spherium is related to another widely studied semi-solvable two-body model, the Hooke atom, which consists of a pair of electrons repelling Coulombically and confined by a harmonic external potential (this system has direct experimental relevance as a model of a two-electron quantum dot with parabolic confinement). Here we are going to consider a $(d-1)$ -dimensional version of spherium, where the two electrons are trapped on a $(d-1)$ -sphere of radius R . By a $(d-1)$ -sphere we mean the surface of a d -dimensional ball.

Exactly solvable and semi-solvable systems provide a valuable arena for the exploration of the entanglement properties of quantum systems of interacting particles. In particular, they provide useful insights for illuminating the entanglement-related features of natural and artificial atomic systems. Unfortunately, there are few such systems where entanglement measures can be evaluated analytically. In point of fact, to the best of our knowledge, the only system of two interacting particles with continuous variables where entanglement has been calculated in an exact analytical way is the Moshinsky model [3, 4]. Even for the Hooke atom, entanglement calculations are based upon the numerical evaluation of rather complex multi-dimensional integrals [5].

In the present contribution we show that spherium is a highly exceptional model, where the amount of entanglement exhibited by some of its eigenstates can be determined in an exact and fully analytical way. As far as we know, spherium is the only two-body system with Coulomb interaction where this goal has been achieved.

Entanglement is nowadays regarded as one of the most fundamental phenomena in quantum physics [6–8]. Entangled states of multipartite quantum systems are endowed with non-classical correlations that give rise to a variegated family of physical phenomena of both fundamental and technological significance. Quantum entanglement can be viewed in two complementary ways. On the one hand, entanglement constitutes a valuable resource. The controlled manipulation of entangled states is central to several quantum information technologies. On the other hand, entanglement can be regarded as a fundamental ingredient for the physical characterization of natural quantum systems such as, for instance, atoms and molecules. These two points of view are closely related to each other, although the latter is somehow less developed than the former. Concerning the second of the approaches mentioned above, several researchers have investigated in recent years the phenomenon of entanglement in two-electron atomic models and related systems [3–5, 8–30]. Most works dealing with entanglement in two-electron systems have been restricted to the associated ground state wavefunctions. However, the entanglement properties of excited states of two-electron atomic models have also been investigated [3, 5]. The most detailed results concerning the entanglement of excited states have been obtained from analytical investigations of exactly soluble models, in particular the Moshinsky one [3].

The main entanglement-related features exhibited by these models share some common trends. First, one observes that entanglement increases with the strength of the interaction between the particles. Alternatively, for a constant interaction strength, entanglement decreases with the strength of the confining potential (this behavior has also been verified in numerical studies of entanglement in Helium-like atoms with increasing nuclear charge). These effects are clearly two sides of the same coin, and can usually be described jointly in terms of the dependence of entanglement on an appropriate dimensionless parameter corresponding to the relative strengths of the interaction and the confining potentials. In the case of atomic-like models with an external harmonic confining potential, such as the Moshinsky and the Hooke ones, it is also observed that entanglement tends to increase with energy. This last property holds for the majority of states. However there are a few entanglement ‘level-

crossings' where a state has more entanglement than another state of higher energy [3]. Aside from these rare exceptions, the general monotonically increasing behavior of entanglement with energy has been observed in harmonically confined models endowed with different types of particle interaction (i.e., harmonic interaction in the Moshinsky system, Coulomb interaction in the Hooke atom; and a r^{-2} -interaction potential in the Crandall model). Another trend exhibited by two-electron models with harmonic confinement (which also holds for different interaction laws between the constituent particles) is that the amount of entanglement associated with excited states does not always vanish in the limit of a vanishing interaction [22].

The goal of the present paper is to calculate analytically the amount of entanglement of the ground state of $(d-1)$ -spherium. The paper is organized as follows. In section 2, we briefly review the concept of entanglement in systems consisting of identical fermions. In section 3, we show the technical details of the calculations performed in this work. In section 4, we describe our main results. Finally, some conclusions are drawn in section 5.

2. Entanglement in systems of identical fermions

There is a natural and physically meaningful measure of entanglement for pure states of systems consisting of two identical fermions. It is based on the Schmidt decomposition for fermions [31, 32], which reads

$$|\Psi\rangle = \sum_i \sqrt{\frac{\lambda_i}{2}} (|2i\rangle|2i+1\rangle - |2i+1\rangle|2i\rangle), \quad (1)$$

where $\{|i\rangle, i = 0, 1, \dots\}$ is an appropriate orthonormal basis of the single-particle Hilbert space, and $0 \leq \lambda_i \leq 1$ with $\sum_i \lambda_i = 1$. The entanglement of the pure state $|\Psi\rangle$ can then be expressed in terms of the above fermionic Schmidt coefficients, as

$$\xi[|\Psi\rangle] = 1 - \sum_i \lambda_i^2 = 1 - 2 \operatorname{Tr}(\rho_1^2), \quad (2)$$

where $\rho_1 = \operatorname{Tr}_2 |\Psi\rangle\langle\Psi|$ is the single-particle reduced density matrix obtained from the global, two-particle density matrix $\rho = |\Psi\rangle\langle\Psi|$. The Schmidt coefficients λ_i are the eigenvalues (each one two-fold degenerate) of ρ_1 . The entanglement measure (2) is (up to appropriate additive and multiplicative constants) basically given by the linear entropy $S_L(\rho_1) = 1 - \operatorname{Tr}(\rho_1^2)$ of the single-particle density matrix ρ_1 . Alternatively, one could consider an entanglement measure based upon the von Neumann entropy of the density matrix ρ_1 , given by $S_{\text{vN}}(\rho_1) = -\operatorname{Tr} \rho_1 \ln \rho_1$. This last measure is extremely difficult to evaluate analytically for systems with continuous variables. Even in the case of the Moshinsky model, which is the atomic model where entanglement has been studied more systematically [3, 4], the entanglement measure based on the von Neumann entropy has been determined in an exact analytical way only for the ground state [9, 14]. It is highly unlikely that in systems with Coulomb interactions the entanglement measure based on the von Neumann entropy can be calculated analytically. In these cases the (exact) analytical approach seems basically intractable. Entanglement measures based on the linear entropy have many computational advantages, both from the analytical and the numerical points of view. In particular, and in contrast with measures based on the von Neumann entropy, measures based on the linear entropy can be evaluated directly from ρ_1 , without the need of first determining ρ_1 's eigenvalues. They constitute a practical tool for assessing the amount of entanglement that has been applied to the study of a variety of systems (see [3–5, 31] and references therein).

An important property of the entanglement measure (2) is that correlations between the two particles that are solely due to the antisymmetry of the fermionic state do not contribute to the state's entanglement. In fact, the amount of entanglement exhibited by a two-fermion state is given, basically, by the quantum correlations that the state has beyond the minimum correlations required by the antisymmetric constraint on the fermionic wavefunction [31–38]. Consequently, the entanglement of a pure state of two identical fermions that can be written as a single Slater determinant is zero.

We apply now the above measure to a pure state of a two-electron system. In order to analyze the entanglement of the eigenstates of spherium we have to consider states described by wavefunctions of the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2)\chi(\sigma_1, \sigma_2), \quad (3)$$

with the total wavefunction factorized as the product of a coordinate wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2)$ and a spin wavefunction $\chi(\sigma_1, \sigma_2)$. Here \mathbf{r}_1 and \mathbf{r}_2 stand for the vector positions of the two electrons. The density matrix corresponding to a wavefunction of the form (3) is given by

$$\rho = \rho^{(\text{coord.})} \otimes \rho^{(\text{spin})} \quad (4)$$

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

$$\langle \mathbf{r}'_1, \mathbf{r}'_2 | \rho^{(\text{coord.})} | \mathbf{r}_1, \mathbf{r}_2 \rangle = \psi(\mathbf{r}'_1, \mathbf{r}'_2)\psi^*(\mathbf{r}_1, \mathbf{r}_2). \quad (5)$$

Even if we are going to investigate the entanglement features only of pure states of spherium, it is conceptually convenient to consider the corresponding density matrix (projector) (4) in order to obtain from it the single-particle reduced density matrix, in terms of which the entanglement measure to be used can be clearly formulated. For a state with a wavefunction of the form (3) (and a density matrix of the form (4)) the entanglement measure (2) reads

$$\begin{aligned} \xi[|\Psi\rangle] &= 1 - 2 \text{Tr} \left[\rho_1^2 \right] \\ &= 1 - 2 \text{Tr} \left[\left(\rho_1^{(\text{coord.})} \right)^2 \right] \text{Tr} \left[\left(\rho_1^{(\text{spin})} \right)^2 \right], \end{aligned} \quad (6)$$

where $\rho_1 = \rho_1^{(\text{coord.})} \otimes \rho_1^{(\text{spin})}$ is the single-particle reduced density matrix, and $\rho_1^{(\text{coord.})}$ and $\rho_1^{(\text{spin})}$ are, respectively, the marginal density matrices obtained after tracing 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 electrons described by (3) involves both the translational and the spin degrees of freedom of electrons.

To calculate the entanglement measure (6), it is necessary to consider separately the cases of a spin wavefunction corresponding to parallel spins or antiparallel spins. When spins are parallel (that is, when the coordinate wavefunction is antisymmetric and the spin wavefunction is either χ_{++} or χ_{--}), one has $\text{Tr}[(\rho^{(\text{spin})})^2] = 1$, and the entanglement measure (6) of a two-electron state of the form (3) is

$$\xi[|\Psi\rangle] = 1 - 2 \int \left| \langle \mathbf{r}'_1 | \rho_1^{(\text{coord.})} | \mathbf{r}_1 \rangle \right|^2 d\mathbf{r}'_1 d\mathbf{r}_1. \quad (7)$$

On the other hand, when the spins are anti-parallel (when the coordinate wavefunction is symmetric and the spin wavefunction is $\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})$, or alternatively, when the coordinate wavefunction is antisymmetric and the spin wavefunction is $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+})$), one has $\text{Tr}[(\rho^{(\text{spin})})^2] = \frac{1}{2}$, and the entanglement is

$$\xi[|\Psi\rangle] = 1 - \int \left| \langle \mathbf{r}'_1 | \rho_1^{(\text{coord.})} | \mathbf{r}_1 \rangle \right|^2 d\mathbf{r}'_1 d\mathbf{r}_1 \quad (8)$$

In equations (7) and (8) we have

$$\langle \mathbf{r}'_1 | \rho_1^{(\text{coord.})} | \mathbf{r}_1 \rangle = \int \psi(\mathbf{r}'_1, \mathbf{r}_2) \psi^*(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2 \quad (9)$$

for the matrix elements of the *coordinate* marginal matrix density.

In the above discussion we have considered two-electron states that are separable with respect to the spin and spatial degrees of freedom. Moreover, among these states we only considered states where the spin parts of the wavefunction correspond to the standard singlet and triplet states. When studying two-electron systems with a Hamiltonian not depending on spin, and energy levels with no degeneracy arising from the spatial part of the Hamiltonian, it is standard and natural to focus on eigenstates of the above described forms. However, even in these cases the spin-independence of the Hamiltonian leads to degeneracy of the energy spectra, and to the existence of eigenstates with the spin part of the wavefunction different from the ones just mentioned. For instance, one can have as spin wavefunction a linear combination of the triplet states. The corresponding (global) eigenstate would have an amount of entanglement different from the ones given by equations (7) and (8). But the difference would be due solely to the spin part, and would not correspond to any specific feature of the particular two-electron system under consideration. If the Hamiltonian includes spin-orbit interaction terms, coupling the spin and the spatial degrees of freedom, the situation becomes much more complex. The eigenstates would not, in general, have the spin and the spatial parts disentangled. In such cases both types of degrees of freedom need to be considered jointly in order to evaluate the entanglement between the two electrons constituting the system. These situations are outside the scope of the present work. The spherium Hamiltonian does not depend on spin, and we shall consider only *s*-states, where the spatial part of the wavefunction is symmetric, and the spin part is given by the singlet state.

3. (*d*−1)-spherium: description

As already mentioned, spherium consists of two identical particles ('electrons') interacting via a Coulomb potential and confined to the surface of a (*d*−1)-sphere of radius *R*. The corresponding Hamiltonian, expressed in atomic units, reads

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + \frac{1}{r_{12}}, \quad (10)$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the interelectronic distance (a brief review of some basic aspects of the spherium Hamiltonian is given in appendix A). ¹S states (*s*-states) have a wavefunction $\Psi(r_{12})$ that depends only on the inter-electronic distance. The corresponding Schrödinger equation can be cast in the form

$$\left[\frac{u^2}{4R^2} - 1 \right] \frac{d^2\Psi}{du^2} + \left[\frac{u(2d-3)}{4R^2} - \frac{d}{u} \right] \frac{d\Psi}{du} + \frac{\Psi}{u} = E\Psi, \quad (11)$$

where $u = r_{12}$. As was recently proved by Loos and Gill in [1], equation (11) admits closed analytical solutions for particular, discrete values of the radius $R = R_{n,m}$. These exact eigenfunctions of the spherium system have a polynomial form,

Table 1. Ground state for $n = 1$ of $(d-1)$ -spherium.

State	(n, m)	Configuration	$\chi(\Omega_1, \Omega_2)$	δ	γ
1S	(1,0)	s^2	1	$2(d-1) - 1$	$\frac{1}{(d-1)-1}$

$$\Psi_{n,m}(r_{12}) = \sum_{k=0}^n s_{k,m} r_{12}^k, \tag{12}$$

where the coefficients $s_{k,m} \equiv s_{k,m}(d)$ are determined by the recurrence relation

$$s_{k+2,m} = \frac{s_{k+1,m} + \left[k(k + 2(d-1) - 2) \frac{1}{4R_{n,m}^2} - E_{n,m} \right] s_{k,m}}{(k+2)(k+(d-1))}, \tag{13}$$

with the starting values $s_{0,m} = 1$ and $s_{1,m} = \frac{1}{(d-1)-1} \equiv \gamma$. The integer parameter n has values $n = 1, 2, \dots$ and m is the number of roots that the polynomial (12) has in the range $[0, 2R]$. That is, the wavefunction (12) corresponds to the m th excited s -state.

For a given n , the energies are obtained by finding the roots of the equation $s_{n+1,m} = 0$, which is a polynomial in E , of degree $(n+1)/2$. The corresponding radius $R_{n,m}$ is found through the relation

$$R_{n,m}^2 E_{n,m} = \frac{n}{2} \left(\frac{n}{2} + (d-1) - 1 \right). \tag{14}$$

We see that the special R -values for which the s -states of spherium can be obtained in a closely analytical way arise from an expansion of the wavefunction in powers of r_{12} that, for the mentioned R -values, becomes a finite polynomial (for a full discussion see [1, 2] and references therein). Of course, the spherium system is well defined for any value of R , and the corresponding Schrödinger equation can be solved numerically, leading to results that interpolate between those corresponding to the special R -values yielding analytical solutions.

The (un-normalized) wavefunction, radius and energy for the ground state ($m = 0$) and $n = 1$ are given by

$$\Psi_{1,0}(r_{12}) = s_0 + s_1 r_{12}, \quad R_{1,0}^2 = \frac{\delta}{4\gamma}, \quad E_{1,0} = \gamma, \tag{15}$$

where from now on we have denoted $s_{k,0} \equiv s_k$. The parameters δ and γ are tabulated in table 1.

The (un-normalized) ground state wavefunctions for $n = 2, 3$ are the following,

$$\Psi_{2,0}(r_{12}) = s_0 + s_1 r_{12} + s_2 r_{12}^2, \tag{16}$$

$$\Psi_{3,0}(r_{12}) = s_0 + s_1 r_{12} + s_2 r_{12}^2 + s_3 r_{12}^3, \tag{17}$$

where the coefficients $s_k \equiv s_{k,0}(d)$, obtained through the recurrence relation (13), are analytically given in appendix A for $k = 1, 2, 3$ and numerically shown in table 2 for $d = 3-6$.

In order to compute the entanglement of the spherium's eigenstates (with $m = 0$) we are going to work with appropriately normalized eigenfunctions

$$\psi_{n,0} = \frac{\Psi_{n,0}}{R^{d-1} N_n^{1/2}}, \tag{18}$$

where $N_n = \int |\Psi_{n,0}|^2 d\Omega_1 d\Omega_2$. The wavefunctions $\psi_{n,0}$ are now normalized to one over the surface of a hyper-sphere of radius R : $\int |\psi_{n,0}|^2 R^{2(d-1)} d\Omega_1 d\Omega_2 = 1$. The analytical values of the constant N_n are determined in the next section.

Table 2. Numerical values of the expansion coefficients $s_k \equiv s_{k,0}$ for $d = 3, 4, 5, 6$ and $n = 1, 2, 3$.

d	s_0	s_1	s_2	s_3
3	1	1	0.178571	0.012946
4	1	0.5	0.053030	0.002703
5	1	0.333333	0.025	0.000968
6	1	0.25	0.014474	0.000449

4. Entanglement in $(d-1)$ -spherium

Let us now evaluate in an analytical way the entanglement for the wavefunctions $\psi_{n,0}(r_{12})$ of the $(d-1)$ -spherium as described in the two previous sections. For this purpose we need to calculate first the constant $N_n = \int |\Psi_{n,0}|^2 d\Omega_1 d\Omega_2$, and then the trace $\text{Tr} \left[\left(\rho_1^{(\text{coord.})} \right)^2 \right]$ which is given by the following multidimensional definite integral

$$\text{Tr} \left[\left(\rho_1^{(\text{coord.})} \right)^2 \right] = \int_{\mathbb{R}^{4(d-1)}} \psi_{n,0}(\mathbf{r}'_1, \mathbf{r}_2) \psi_{n,0}^*(\mathbf{r}_1, \mathbf{r}_2) \psi_{n,0}^*(\mathbf{r}'_1, \mathbf{r}'_2) \psi_{n,0}(\mathbf{r}_1, \mathbf{r}'_2) \times R^{4(d-1)} d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2, \quad (19)$$

where $R^{d-1} d\Omega_k$, $k = 1, 2$ are area elements on the surface of a $(d-1)$ -hypersphere, and $d\Omega_k$ are elements of hyper-spherical angle, given by

$$d\Omega_k = \left(\prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(k)} \right) d\phi^{(k)}. \quad (20)$$

In terms of the hyperspherical angular coordinates of the two particles $\{\theta_1^{(k)}, \dots, \theta_{d-2}^{(k)}, \phi^{(k)}\}$, with $0 \leq \theta_j^{(k)} \leq \pi$ for $j = 1, \dots, d-2$, and $0 \leq \phi^{(k)} \leq 2\pi$. Atomic units will be used throughout the rest of the paper.

Here a comment concerning coordinates is in order. In section 2, when discussing general aspects of entanglement, the integrals involved in the calculation of entanglement were expressed in cartesian coordinates. However, in the particular case of spherium, it is clear that the most natural coordinates to employ are the hyper-spherical ones. Hence, as already indicated by the elements $d\Omega_i$ appearing in (19), in the present work we are going to formulate all the relevant integrals first in terms of hyper-spherical coordinates on the $(d-1)$ -sphere where the two electrons are confined. For technical reasons we are also going to define a new set of angular variables in order to actually compute the aforementioned integrals.

To solve some of the integrals appearing in the study of entanglement in spherium we shall apply the methodology recently developed by Ruiz [39] to deal with atomic-related integrals. Let us first calculate the normalization constant N_1 of the ground state wavefunction $\Psi_{1,0}(r_{12})$ given by equation (15); that is

$$N_1 = \int |\Psi_{1,0}|^2 d\Omega_1 d\Omega_2 = J_0 + 2\gamma J_1 + \gamma^2 J_2, \quad (21)$$

where the symbols J_k , $k = 0, 1, 2$, denote the integral functions

$$J_k \equiv \int r_{12}^k d\Omega_1 d\Omega_2, \quad k = 0, 1, 2. \quad (22)$$

To evaluate these integrals we begin by doing a change of variables. Consider the triangle formed by the vectors \mathbf{r}_1 , \mathbf{r}_2 , and \mathbf{r}_{12} , where the last one stands for the relative vector position

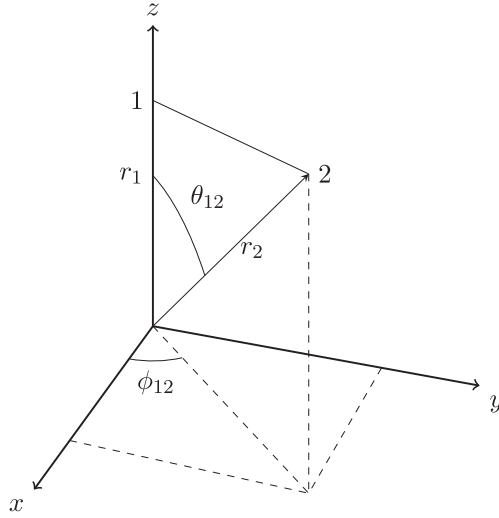


Figure 1. Definition of the electron’s coordinates used for the evaluation of entanglement-related integrals.

of particle 2 with respect to particle 1 (see figure 1). Following an idea originally advanced by Calais and Löwdin [40], we rotate the coordinate frame used to define the angular spherical coordinates of the vector \mathbf{r}_2 . The z axis of the new frame is the line joining the origin (which is the same as in the original frame) with particle 1, with the positive direction towards particle 1. The angular coordinates of \mathbf{r}_2 in the new frame are now denoted $\{\theta_1^{(12)}, \dots, \theta_{d-2}^{(12)}, \phi^{(12)}\}$ (see figure 1 for a three-dimensional illustration of this change of reference frame). The integration variables concerning particle 2 are then transformed as: $\theta_i^{(2)} \rightarrow \theta_i^{(12)}$, and $\phi^{(2)} \rightarrow \phi^{(12)}$. The volume element associated to electron 2 can then be re-cast as

$$d\Omega_2 = \left(\prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(2)} \right) d\phi^{(2)} = \left(\prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(12)} \right) d\phi^{(12)} = d\Omega_{12}. \quad (23)$$

Moreover, we use the Cohl representation [41] for r_{12}^p in terms of the orthogonal Gegenbauer polynomials $C_n^\alpha(x)$:

$$\begin{aligned} r_{12}^p &= \sum_{n=0}^{\infty} \frac{(d + 2n - 2) 2^{d+p-3} \Gamma\left(\frac{d-2}{2}\right) \left(-\frac{1}{2}\right)_n R^p}{\sqrt{\pi} \Gamma\left(d + n + \frac{p}{2} - 1\right)} \\ &\quad \times \Gamma\left(\frac{1}{2}(d + p - 1)\right) C_n^{d/2-1}(\cos \theta_{12}) \\ &= \sum_{n=0}^{\infty} - \frac{\pi^{\frac{d}{2}-1} 2^{d+p-2} \Gamma\left(n - \frac{1}{2}\right) R^p \Gamma\left(\frac{1}{2}(d + p - 1)\right)}{\Gamma\left(d + n + \frac{p}{2} - 1\right)} \\ &\quad \times \sum_{\{\mu\}} \mathcal{Y}_{n,\{\mu\}}^*(\Omega_2) \mathcal{Y}_{n,\{\mu\}}(\Omega_1), \quad p = 1, 2, \dots, \end{aligned} \quad (24)$$

where $\Omega_k = (\theta_1^{(k)}, \theta_2^{(k)}, \dots, \theta_{d-2}^{(k)}, \theta_{d-1}^{(k)} \equiv \phi^{(k)})$, and $\mathcal{Y}_{n,\{\mu\}}$ denote the known hyperspherical harmonics, which have the following expression [42–44]

$$\begin{aligned} \mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1}) &= A_{l,\{\mu\}} e^{im\phi} \prod_{j=1}^{d-2} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}} \\ &= \frac{1}{\sqrt{2\pi}} e^{im\phi} \prod_{j=1}^{d-2} \tilde{C}_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos \theta_j) (\sin \theta_j)^{\mu_{j+1}}, \end{aligned} \quad (25)$$

with $\alpha_j = (d - j - 1)/2$, and the normalization constant is

$$\begin{aligned} |A_{l,\{\mu\}}|^2 &= \frac{1}{2\pi} \prod_{j=1}^{d-2} \frac{(\alpha_j + \mu_j)(\mu_j - \mu_{j+1})! \left[\Gamma(\alpha_j + \mu_{j+1}) \right]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}} \Gamma(2\alpha_j + \mu_j + \mu_{j+1})} \\ &\equiv \frac{1}{2\pi} \prod_{j=1}^{d-2} A_{\mu_j, \mu_{j+1}}^{(j)}. \end{aligned} \quad (26)$$

The symbols $C_m^\alpha(x)$ and $\tilde{C}_m^\alpha(x)$ denote the orthogonal and orthonormal Gegenbauer polynomials [45] of degree m and parameter α with respect to the weight function $\omega_\alpha^* = (1 - x^2)^{\alpha-\frac{1}{2}}$ on the interval $[-1, +1]$, respectively, so that

$$\tilde{C}_m^\alpha(x) = \left(\frac{m!(m + \alpha)\Gamma^2(\alpha)}{\pi 2^{1-2\alpha}\Gamma(2\alpha + m)} \right)^{\frac{1}{2}} C_m^\alpha(x). \quad (27)$$

Then, by using the expressions (22) and (24) as explained in detail in appendix B, we obtain that the integrals J_k , $k = 0-2$, are given by

$$J_0 = \left(\frac{2\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)} \right)^2, \quad (28)$$

$$J_1 = \frac{2^{d+1}\pi^{d-\frac{1}{2}}}{\Gamma\left(d - \frac{1}{2}\right)} R \quad (29)$$

and

$$J_2 = \frac{8\pi^d}{\Gamma\left(\frac{d}{2}\right)^2} R^2 \quad (30)$$

respectively. Finally, these values together with equation (21) allows us to write the normalization constant as

$$N_1 = 4\pi^d \left(\frac{1 + 2\gamma^2 R^2}{\Gamma\left(\frac{d}{2}\right)^2} + \frac{2^d \gamma}{\sqrt{\pi} \Gamma\left(d - \frac{1}{2}\right)} R \right). \quad (31)$$

Replacing the analytical expressions for the spherium state $\psi_{1,0}(r_{12})$, into the general expression for $\text{Tr}[(\rho_1^{(\text{coord.})})^2]$ one gets

$$\begin{aligned}
\text{Tr}\left[\left(\rho_1^{(\text{coord.})}\right)^2\right] &= R^{2d-2} \int \left|\rho_1^{(\text{coord.})}(\mathbf{r}'_1, \mathbf{r}_1)\right|^2 d\Omega'_1 d\Omega_1 \\
&= R^{4d-4} \int \psi_{1,0}(\mathbf{r}'_1, \mathbf{r}_2) \psi_{1,0}^*(\mathbf{r}_1, \mathbf{r}_2) \psi_{1,0}^*(\mathbf{r}'_1, \mathbf{r}'_2) \\
&\quad \times \psi_{1,0}(\mathbf{r}_1, \mathbf{r}'_2) d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2 \\
&= N_1^{-2} \int_{\mathbb{S}^{d-1}} (1 + \gamma r_{12})(1 + \gamma r_{12}') \\
&\quad \times (1 + \gamma r_{1'2})(1 + \gamma r_{1'2}') d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2 \\
&= N_1^{-2} \int \left[1 + \gamma(r_{12} + r_{12}' + r_{1'2} + r_{1'2}') \right. \\
&\quad + \gamma^2(r_{12}r_{12}' + r_{12}r_{1'2} + r_{12}'r_{1'2} + r_{12}r_{1'2}') \\
&\quad + r_{12}'r_{1'2}' + r_{1'2}r_{1'2}') \\
&\quad + \gamma^3(r_{12}r_{12}'r_{1'2} + r_{12}r_{12}'r_{1'2}') + r_{12}r_{1'2}r_{1'2}') \\
&\quad \left. + r_{12}'r_{1'2}r_{1'2}') + \gamma^4 r_{12}r_{12}'r_{1'2}r_{1'2}') \right] \\
&\quad \times d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2 \tag{32}
\end{aligned}$$

For convenience and taking into account the symmetries of the integrand of (32), we rewrite this expression as

$$\text{Tr}\left[\left(\rho_1^{(\text{coord.})}\right)^2\right] = N_1^{-2}(I_0 + 4\gamma I_1 + 6\gamma^2 I_2 + 4\gamma^3 I_3 + \gamma^4 I_4), \tag{33}$$

where the symbols I_i , $i = 1 - 4$, denote the following integral functions:

$$I_0 \equiv \int d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2, \tag{34}$$

$$I_1 \equiv \int r_{12} d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2, \tag{35}$$

$$I_2 \equiv \int r_{12} r_{12}' d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2, \tag{36}$$

$$I_3 \equiv \int r_{12} r_{12}' r_{1'2} d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2, \tag{37}$$

$$I_4 \equiv \int r_{12} r_{12}' r_{1'2} r_{1'2}' d\Omega_1 d\Omega_2 d\Omega'_1 d\Omega'_2. \tag{38}$$

These integrals have been analytically evaluated by means of the methodology described in appendix B, obtaining the following values:

$$I_0 = \left(\frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}\right)^4, \tag{39}$$

$$I_1 = \frac{2^{d+3}\pi^{2d-\frac{1}{2}}}{\Gamma\left(d-\frac{1}{2}\right)\Gamma\left(\frac{d}{2}\right)^2} R, \tag{40}$$

$$I_2 = \frac{4^{d+1}\pi^{2d-1}}{\Gamma\left(d-\frac{1}{2}\right)^2} R^2, \tag{41}$$

$$I_3 = \frac{2^{3d+1}\pi^{2d-\frac{3}{2}}\Gamma\left(\frac{d}{2}\right)^2}{\Gamma\left(d-\frac{1}{2}\right)^3}R^3, \tag{42}$$

$$I_4 = 2^{4d-3}\pi^{2d-2}\left[\frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d+\frac{1}{2}\right)}\right]^4 R^4 \\ \times \left[{}_5F_4\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, d-1; d+\frac{1}{2}, d+\frac{1}{2}, d+\frac{1}{2}, d+\frac{1}{2}; 1\right) + 8\left(d-\frac{1}{2}\right)^4 \right. \\ \left. \times {}_5F_4\left(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, d-2; d-\frac{1}{2}, d-\frac{1}{2}, d-\frac{1}{2}, d-\frac{1}{2}; 1\right) \right]. \tag{43}$$

Then, taking into account (8) and (33) we obtain that the entanglement measure for the spherium state $\psi_{1,0}(r_{12})$ is given by

$$\xi\left[|\psi_{1,0}\rangle\right] = 1 - \text{Tr}\left[\left(\rho_1^{\text{(coord.)}}\right)^2\right] \\ = 1 - N_1^{-2}(I_0 + 4\gamma I_1 + 6\gamma^2 I_2 + 4\gamma^3 I_3 + \gamma^4 I_4). \tag{44}$$

The calculations required for evaluating the normalization constants N_n and the integrals I_i , $i = 1 - 4$ involved in the determination of the amount of entanglement of the spherium s -eigenstates $\psi_{n,0}(r_{12})$ with $n \geq 2$ are similar to those for the state $\psi_{1,0}(r_{12})$, following the lines indicated in appendix B. In particular, the above explained analytical techniques can be readily applied to the $n = 2$ and $n = 3$ s -states, with the wavefunctions given by equations (16), (17) and table 2.

The results obtained for the amount of entanglement exhibited by the $(d-1)$ -spherium (singlet) ground state are summarized in table 3 and in figures 3–6. In table 3 we provide the amounts of entanglement and the energies corresponding to the ground state of $(d-1)$ -spherium for various dimensionalities. The analytical procedure for calculating the entanglement of s -states of spherium has been checked by the numerical computation of entanglement for some of these states.

It can be seen in table 3 that, for a given dimensionality d , the amount of entanglement associated with the ground state of spherium increases with the radius R . This trend is akin with what has been recently observed in other two-electron models [5]; see also the recent review [8]. In fact, we know from previous experience with two-electron systems that, for a constant strength of the interaction between the particles, entanglement tends to increase when the confinement becomes weaker. This behavior has been observed in several systems, such as the Moshinsky model, the Hooke atom, the Crandall model, and the Helium iso-electronic series [5]. The connection between entanglement and confinement has also been detected in two-electron systems in a uniform magnetic field [4]. In these systems confinement decreases, and entanglement increases, when the intensity of the applied magnetic field becomes weaker. In spherium confinement decreases, and entanglement increases, for increasing values of the radius R . In figure 2 we plotted, for $d = 3$ (that is, when the two electrons are confined to an ordinary two-dimensional sphere), the wavefunction $\psi_{10}(\theta_1, \phi_1, \theta_2, \phi_2)$ as a function of the angular coordinates (θ_1, ϕ_1) of one of the particles, keeping constant the values of the coordinates (θ_2, ϕ_2) of the other particle (here we use the standard notation for the polar and azimuthal coordinates on a two-dimensional sphere). Since

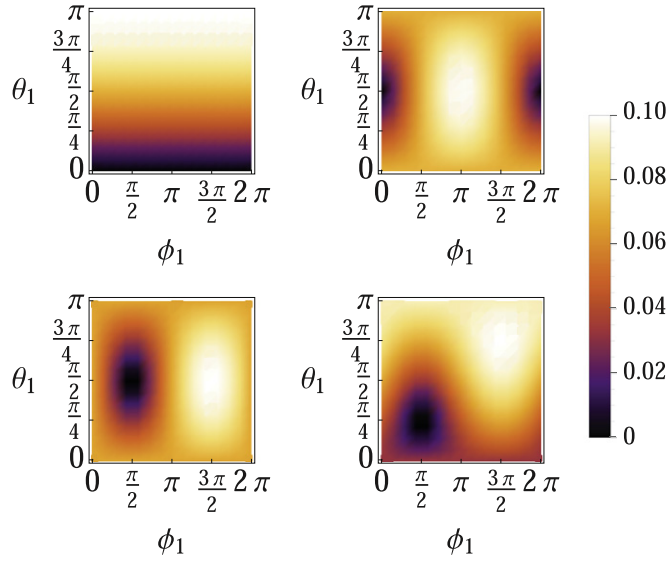


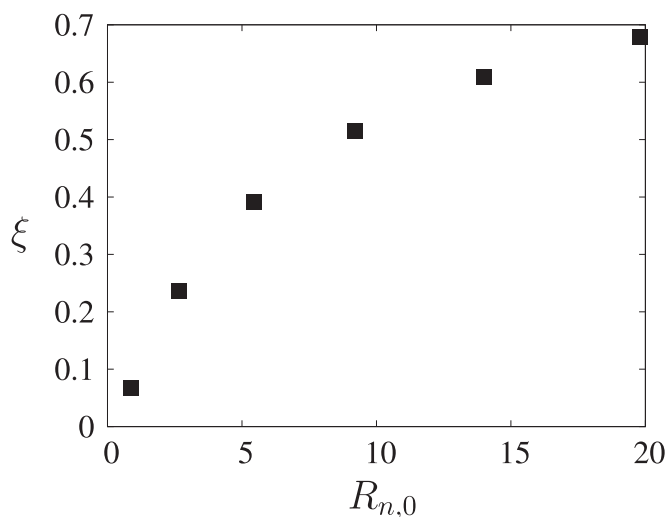
Figure 2. Wave function $\psi(\theta_1, \phi_1, \theta_2, \phi_2)$ as a function of the angular coordinates θ_1, ϕ_1 of one of the electrons for constant values θ_2 and ϕ_2 of the coordinates of the other electron. On the upper left plot we have $\theta_2 = 0$ and $\phi_2 = 0$ and on the upper right one $\theta_2 = \frac{\pi}{2}$ and $\phi_2 = 0$. The lower left plot corresponds to $\theta_2 = \frac{\pi}{2}$ and $\phi_2 = \frac{\pi}{2}$ and the lower right one to $\theta_2 = \frac{\pi}{4}$ and $\phi_2 = \frac{\pi}{2}$. The different aspect of the four figures illustrates the fact that the wavefunction ψ is entangled.

the wavefunction is in this case real, we depict in figure 2 the wave function ψ_{10} itself, not its squared modulus. In figure 2 we have $\theta_2 = 0; \phi_2 = 0$ (upper left) and $\theta_2 = \frac{\pi}{2}; \phi_2 = 0$ (upper right); $\theta_2 = \frac{\pi}{2}; \phi_2 = \frac{\pi}{2}$ (lower left) and $\theta_2 = \frac{\pi}{4}; \phi_2 = \frac{\pi}{2}$ (lower right). Figure 2 provides an illustration of the entangled character of the associated two-electron state. If it were a non-entangled state, it would be of the form $\Phi(\theta_1, \phi_1)\Phi(\theta_2, \phi_2)\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})$. We would have a factorizable spatial wavefunction (remember that the spatial parts of the wavefunctions corresponding to the states that we are considering are symmetric) and a singlet spin wavefunction. With a factorized spatial wavefunction the four graphics depicted in figure 2 would be identical. All of them would correspond to $\Phi(\theta_1, \phi_1)$. The differences between the four graphics in figure 2 constitute a concrete pictorial illustration of the entanglement of the concomitant two-electron state.

The connection between entanglement and the radius R of the spherium system can be appreciated in figure 3. In this figure we plotted the amount of entanglement versus the radius of the confining sphere for several singlet states wavefunctions $\psi_{n,0}(r_{12})$ of the two-dimensional ($d = 3$) spherium, with the integer parameter n (characterizing the radius' values $R_{n,m}$ leading to exact analytical solutions) adopting values $n = 1, \dots, 6$. We observe that entanglement grows with the radius. The dependence of entanglement on the spherium radius is, however, nonlinear. For small values of R (corresponding to small values of the parameter n) the rate of growth of entanglement with R is greater than for larger values of R . The monotonically increasing behavior of entanglement with R illustrated in figure 3 corresponds to the particular case $d = 3$. However, the same trend is observed for other values of the spatial dimensionality d , as can be seen in table 3 for dimensions up to $d = 6$. The observed decreasing rate of growth of entanglement with the spherium's radius R does not rule out the

Table 3. Radius, energy and entanglement values of the of the $(d-1)$ -dimensional spherium with singlet ground-state wavefunctions $\Psi_{n,0}(r_{12})$, $n = 1, 2, 3$, for various dimensionalities $d = 3, 4, 5, 6$.

State	d	$R_{n,0}$	$E_{n,0}$	$\xi[\Psi_{n,0}\rangle]$
$n = 1$	3	0.866025	1	0.0677386
	4	1.58114	0.5	0.0436006
	5	2.29129	0.333333	0.0323117
	6	3.0	0.25	0.0256836
$n = 2$	3	2.64575	0.285714	0.235892
	4	4.06202	0.181818	0.160622
	5	5.47723	0.133333	0.121691
	6	6.89202	0.105263	0.0979235
$n = 3$	3	5.43118	0.127128	0.391247
	4	7.51536	0.0929523	0.293556
	5	9.61594	0.0729996	0.232591
	6	11.7241	0.0600194	0.191796

**Figure 3.** Entanglement against the radius R for the singlet state wavefunctions $\psi_{n,0}(r_{12})$, $n = 1, \dots, 6$, of $(d-1)$ -dimensional spherium with $d = 3$.

possibility that the (increasing) entanglement measure ξ tends to its maximum possible value ($\xi = 1$) in the limit $R \rightarrow \infty$. Unfortunately, the case by case (exact) evaluation of the entanglement of each exactly solvable eigenstate of spherium does not allow us to analytically determine the aforementioned limit value. However, the behavior of other two-electron systems suggests that entanglement in spherium does indeed approach its maximum value as $R \rightarrow \infty$. In the $d = 3$ case the $R \rightarrow \infty$ limit of spherium can be related to a limit case of the two-dimensional Hooke atom. In the $R \rightarrow \infty$ limit, as the radius of curvature of the confining sphere tends to zero, the Schrödinger equation describing spherium approaches that of two electrons moving in a two-dimensional Euclidean plane. This suggests that the limit value of

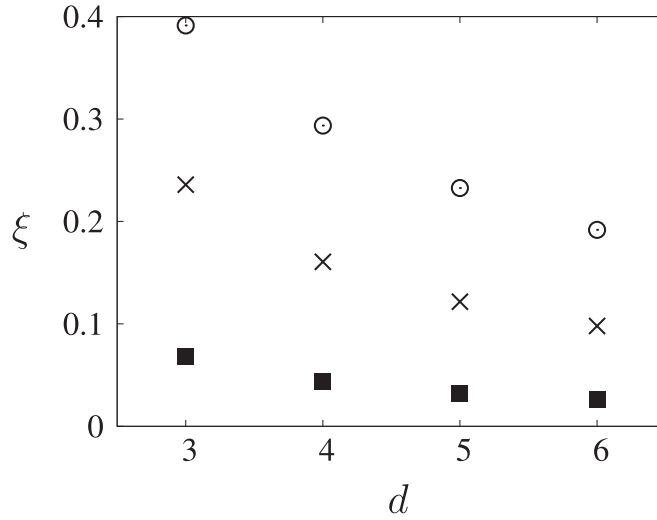


Figure 4. Entanglement against dimensionality for the singlet state wavefunctions $\psi_{n,0}(r_{12})$ with $n = 1$ (■), $n = 2$ (×), $n = 3$ (○), of $(d-1)$ -dimensional spherium with $d = 3, \dots, 6$.

entanglement in $d = 3$ spherium should coincide with the limit value of entanglement in the two-dimensional Hooke system when the confining potential becomes negligible compared with the electron–electron interaction potential. Results reported by Kościk and Hassanabadi in [18] provide numerical evidence that the entanglement of the two dimensional Hooke system tends to its maximum value in this limit.

In figure 4 the ground state’s entanglement is plotted against the spatial dimensionality d . We have computed the entanglement measure based on the linear entropy of the single particle reduced density matrix for spatial dimensionalities in the range $3 \leq d \leq 6$, and for $n = 1, 2, 3$. We see that the range of possible values of entanglement, as well as the largest adopted value (for the above range of n -values) decreases with d .

It can be appreciated from figure 4 that, for given constant values of the integer parameter n determining the special radius $R_{n,m}$ for which spherium admits closed analytical solutions, the amount of entanglement exhibited by the ground state of spherium decreases monotonically with the spatial dimensionality. We conjecture that entanglement behaves in this way for all values of the parameter n . In the particular case of $n = 1$, since we have an analytical expression for $R_{1,0}$, we can obtain a closed analytical expression for the entanglement of the states $\psi_{1,0}$ for all values of the spatial dimension d . The corresponding behavior of entanglement as a function of d is shown in figure 5, where it can be seen that entanglement decreases with d . This trend might be related to a well-known, but counterintuitive, feature of multi-dimensional spheres: the surface area of a $(d - 1)$ -hypersphere of radius 1 (that is, the total hyper-solid angle $\int_{\text{sphere}} d\Omega$) tends to zero as $d \rightarrow \infty$ (for an interesting discussion on the physical implications of the geometry of hyperspheres see, for instance, [46] and references therein). The above can be construed as implying that, as far as the hyperspherical angular degrees of freedom are concerned, the particles constituting the spherium system can be regarded as becoming more confined as d increases. These geometrical considerations suggest a tentative explanation of the behavior of entanglement with spatial dimensionality d in spherium: entanglement decreases with d , because an increasing spatial dimensionality

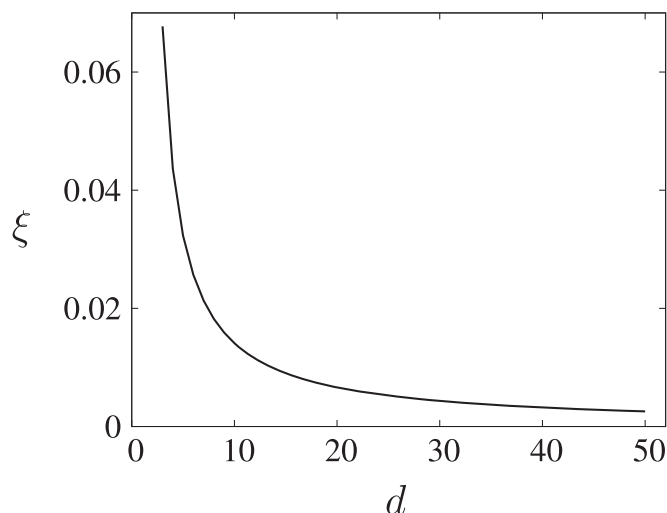


Figure 5. Entanglement against dimensionality for the singlet state wavefunction $\psi_{1,0}(r_{12})$.

tends to make the system more confined. Then, according to this explanation, the entanglement-dimensionality relation in spherium would be another instance of the entanglement-confinement relation observed in several two-electron systems [5]. These considerations have some plausibility in connection with the behavior of entanglement with dimensionality for large values of d . However, a simple, direct connection between entanglement and the area of the unit hyper-sphere seems unlikely, since for $n = 1$ entanglement decreases monotonically with the spatial dimension for all d -values, while the surface area of a unit hyper-sphere does not behave monotonically with d : for moderately small values of d it first increases with d , reaching a maximum for $d \approx 7$, and then decreases monotonically for all d . The decreasing behavior of entanglement with spatial dimension in spherium might be related to the properties of other quantum mechanical models where the limit of high dimensionality leads to classical behavior [47].

The effect of space dimensionality on entanglement has also been studied in the Hooke atom by Kościk and Hassanabadi [18]. These authors studied the behavior of entanglement in the Hooke system for one, two, and three spatial dimensions. The dependence of entanglement on spatial dimension is not as clear in the Hooke atom as it is in spherium. Indeed, the dependence of entanglement with dimension in the Hooke system depends on the strength of the electron–electron interaction (as compared with the strength of the confining potential). This more complicated behavior is probably due to the fact that in the Hooke atom the entanglement features of the system’s eigenstates depend on both the radial and angular behaviors of the concomitant wavefunctions. In spherium, in contrast, the effective configuration space solely involves the angular variables.

In figure 6 we depict the amount of entanglement against the energy of the singlet state for $d = 3, 4, 5$ and 6 . We observe that entanglement of $(d-1)$ -dimensional spherium tends to increase with energy. A similar behavior has been observed in other models, such as the Crandall and the Hooke ones [5], as well as for the singlet states of the Helium atom employing high-quality, state-of-the-art wavefunctions [12] (although for more general states of Helium the energy-entanglement connection seems to be much more complicated [28, 29]).

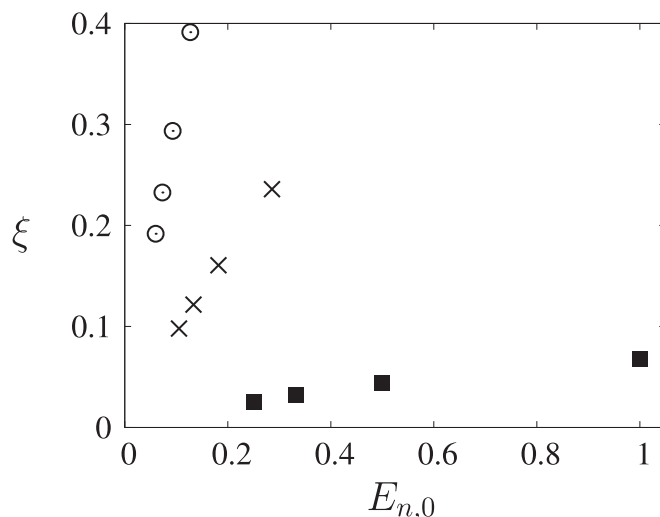


Figure 6. Entanglement against energy for the singlet state wavefunctions $\psi_{n,0}(r_{12})$ with $n = 1$ (■), $n = 2$ (×), $n = 3$ (○) of the $(d-1)$ -dimensional spherium with $d = -6$.

Finally, let us comment on the excited states of the spherium. There are no excited states for the singlet wavefunction with $n = 1$ and $n = 2$. This is due to the fact that the equation allowing for the calculation of the energy for each n has only one root which correspond to $m = 0$. For $n \geq 3$ the excited states begin to appear because the equation mentioned above has a degree equal or greater than 2. So e.g., for $n = 3$ there are two possible values for $m = 0, 1$, and therefore one exact analytical excited state can be obtained (corresponding to $m = 1$).

5. Conclusions

We have explored the entanglement related features of $(d-1)$ -spherium. This quantum system consists of two electrons interacting via a Coulomb potential and confined to the surface of a d -dimensional ball (that is, a $(d-1)$ -hypersphere) of radius R . This system is quasi-exactly solvable: its Schrödinger eigenvalue equation can be solved in a closed analytical fashion for particular values of the radius R and particular eigenstates. In the present contribution we computed in an exact analytical way the amount of entanglement (as measured by the linear entropy of the single-particle reduced density matrix) of the ground state of spherium, for several values of the radius R (corresponding to different values of the parameter n) and of the space dimension d . To the best of our knowledge this is the first two-electron system with Coulomb interaction for which exact entanglement calculations have been done. We investigated the dependence of entanglement on the radius R of the spherium system and on the spatial dimensionality d . The relation between entanglement and energy was also considered.

We have found that the amount of entanglement of the ground state of spherium increases with the radius R of the hypersphere where the particles are confined. This behavior is consistent with a general property exhibited by other two-electron systems: entanglement tends to increase when, for a given value of the interaction strength, the confinement due to the external common fields acting on both particles decreases. For instance, in the helium isoelectronic series the entanglement of the ground state increases when one considers

decreasing values of the nuclear charge Z [5, 12]. Likewise, in the three-dimensional Moshinsky model with a uniform magnetic field the entanglement of the ground state increases for decreasing values of the applied magnetic field [4].

The results reported in the present work indicate that in spherium the amount of entanglement exhibited by the ground state decreases with the spatial dimensionality d , a behavior that can also be related to the entanglement-confinement connection. In addition, we have observed that entanglement of spherium tends to increase with energy. This relation between entanglement and energy is similar to what is observed in other two-electron models, such as the Moshinsky system, the Hooke atom, and the Crandall model [5].

We hope that the techniques developed in the present work may stimulate new analytical approaches to the study of entanglement in systems with Coulomb interactions. Any further developments in this direction will be very welcome.

Acknowledgments

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Appendix A. ($d-1$)-Spherium Hamiltonian

Here we are going to briefly review some basic aspects of the Hamiltonian describing the two-electron system spherium. For more details on spherium and the solutions of the concomitant Schrödinger equation see [1, 2] and references therein. Spherium consists of two electrons confined to a $(d-1)$ -sphere (that is, the surface of a d -dimensional ball) and interacting via a Coulomb potential. The corresponding Schrödinger eigenvalue equation reads

$$-\left(\frac{\hbar^2}{2m}\right)\frac{1}{R^2}\left[\Delta_{S^{d-1}}^{(1)} + \Delta_{S^{d-1}}^{(2)}\right]\Psi + \frac{e^2}{r_{12}}\Psi = E\Psi, \quad (\text{A1})$$

where R is the radius of the $(d-1)$ -sphere, r_{12} is the distance between the two electrons (evaluated in the d -dimensional euclidean space in which the $(d-1)$ -sphere is embedded), Ψ is the two-electron eigenfunction, E is the corresponding eigenenergy, and $\Delta_{S^{d-1}}^{(1,2)}$ are the angular Laplacian operators acting on the angular coordinates of each electron. Note that the wavefunction Ψ is a function of the hyper-spherical angular coordinates of both electrons, $\{\theta_1^{(k)}, \dots, \theta_{d-2}^{(k)}, \phi^{(k)}\}$, with $0 \leq \theta_j^{(k)} \leq \pi$ for $j = 1, \dots, d-2$, and $0 \leq \phi^{(k)} \leq 2\pi$. The upper index $k = 1, 2$ refers to the two electrons. The spherical Laplacian operator (Laplace–Beltrami operator on the $(d-1)$ -sphere) acts on a function f defined on the $(d-1)$ -sphere according to the following recurrence relation

$$\Delta_{S^{d-1}} f(\theta_1, \zeta) = (\sin \theta_1)^{2-d} \frac{\partial}{\partial \theta_1} \left[(\sin \theta_1)^{d-2} \frac{\partial f}{\partial \theta_1} \right] + (\sin \theta_1)^{-2} \Delta_{\zeta} f, \quad (\text{A2})$$

where $\zeta = \{\theta_2, \dots, \theta_{d-2}, \phi\}$ denotes the set of all the angular coordinates on the $(d-1)$ -sphere except θ_1 , and Δ_{ζ} is the spherical Laplacian corresponding to a $(d-2)$ -sphere with hyper-spherical coordinates $\zeta = \{\theta_2, \dots, \theta_{d-2}, \phi\}$. That is, the operator Δ_{ζ} only involves derivatives with respect to the coordinates appearing in the set ζ . For instance, for $d = 3$ the spherical Laplacian adopts the well known form

$$\Delta_{S^2} f(\theta, \phi) = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}. \quad (\text{A3})$$

It is convenient to recast the Schrödinger equation (A1) in a dimensionless form, using atomic units. In order to do that we divide equation (A1) by the constant $m e^4 / \hbar^2$ (which has dimensions of energy) obtaining

$$-\frac{1}{2\tilde{R}^2} \left[\Delta_{S^{d-1}}^{(1)} + \Delta_{S^{d-1}}^{(2)} \right] \Psi + \frac{1}{\tilde{r}_{12}} \Psi = \tilde{E} \Psi, \quad (\text{A4})$$

where

$$\tilde{R} = \frac{m e^2}{\hbar^2} R, \quad (\text{A5})$$

$$\tilde{r}_{12} = \frac{m e^2}{\hbar^2} r_{12}, \quad (\text{A6})$$

$$\tilde{E} = \frac{\hbar^2}{m e^4} E. \quad (\text{A7})$$

Note that in its dimensionless form (A4) the Schrödinger equation for spherium only has one parameter, the dimensionless radius \tilde{R} given by (A5). This parameter is a dimensionless quantity involving the parameter e^2 , measuring the strength of the interaction between the electrons, and the radius R of the confining sphere. When studying entanglement in spherium we investigate, among other things, its dependence on the dimensionless parameter \tilde{R} , which can be regarded as proportional to the quotient between the quantities e^2 (interaction strength) and $1/R$ (amount of confinement). In the rest of the present article, since we are going to deal exclusively with the dimensionless form (A4) of the spherium's Schrödinger equation, we are going to drop the upper 'tilde' from R , r_{12} and E (as in equation (10)).

In the case of s -states, the solutions of spherium's Schrödinger equation are functions of the inter-particle distance r_{12} . That is, one has $\Psi = \Psi(r_{12})$, with

$$r_{12} = R \sqrt{2(1 - \cos \alpha)}, \quad (\text{A8})$$

where $\cos \alpha$ can be expressed in terms of the hyper-spherical coordinates of the two electrons

$$\begin{aligned} \cos \alpha &= \cos \theta_1^{(1)} \cos \theta_1^{(2)} \\ &+ \sin \theta_1^{(1)} \sin \theta_1^{(2)} \cos \theta_2^{(1)} \cos \theta_2^{(2)} \\ &+ \sin \theta_1^{(1)} \sin \theta_1^{(2)} \sin \theta_2^{(1)} \sin \theta_2^{(2)} \\ &\dots \\ &+ \sin \theta_1^{(1)} \sin \theta_1^{(2)} \dots \sin \theta_{d-2}^{(1)} \sin \theta_{d-2}^{(2)} \cos \phi^{(1)} \cos \phi^{(2)}. \\ &+ \sin \theta_1^{(1)} \sin \theta_1^{(2)} \dots \sin \theta_{d-2}^{(1)} \sin \theta_{d-2}^{(2)} \sin \phi^{(1)} \sin \phi^{(2)}. \end{aligned} \quad (\text{A9})$$

For s -states the Schrödinger equation (A1) can be re-expressed in terms of the derivatives of the wavefunction with respect to the variable $u = r_{12}$ [1, 2],

$$\left[\frac{u^2}{4R^2} - 1 \right] \frac{d^2 \Psi}{du^2} + \left[\frac{u(2d-3)}{4R^2} - \frac{d}{u} \right] \frac{d\Psi}{du} + \frac{\Psi}{u} = E\Psi. \quad (\text{A10})$$

Appendix B. Expansion coefficients of spherium s-eigenstates $\Psi_{n,0}(r_{12})$ with $n = 1, 2, 3$

The analytical expression for the expansion coefficients $s_k \equiv s_{k,0}(d)$ of the spherium s-eigenstates $\Psi_{n,0}(r_{12})$ with $n = 1, 2, 3$, have the following form:

$$\begin{aligned}
 s_0 &= 1 \\
 s_1 &= \frac{1}{d-2} \equiv \gamma \\
 s_2 &= \frac{1-2d}{-8d^3 + 34d^2 - 46d + 20} \\
 s_3 &= \frac{1}{48\,600} \left(-\frac{5520}{(d-2)^2} - \frac{5400}{d-1} + \frac{1600}{1-2d} + \frac{2393}{d-2} \right. \\
 &\quad \left. - \frac{4050}{d^2} + \frac{24975}{d} - \frac{42336}{2d+1} \right. \\
 &\quad \left. + \frac{900(d(14d-23) + 6) \sqrt{\frac{d(d(64(d-2)d+169)-78)+9}{d^2(d(3-2d)+2)^2}}}{(d-2)(d-1)d(2d-1)} \right). \tag{B1}
 \end{aligned}$$

They have been obtained from the recurrence relation (13).

Appendix C. Evaluation of the multidimensional integrals involved in the entanglement of spherium

Here we first give some further details of the calculation of the relevant integrals involved in the determination of the normalization constant N_1 of the ground state wavefunction $\Psi_{1,0}(r_{12})$ given by equation (15). Later on, we provide with further information of the derivation of the integral functions involved in the determination of the entanglement measure of such a state. Finally, we give indications for the similar calculation of the normalization constant N_n and the entanglement measure of the general wavefunctions $\Psi_{n,0}(r_{12})$, $n \geq 2$, of the d -dimensional spherium.

Derivation of the normalization constant N_1 given by equation (31). This issue reduces to prove that the two-center integrals J_i , $i = 0 - 2$, defined by expressions (22) have the values given by equations (28)–(30), respectively. The value (28) of the integral J_0 is straightforward since it is the product of the volumes of the hyperspheres for each electron. To obtain the values (29) and (30) of J_1 and J_2 , respectively, we use the Cohl expansion (24) for r_{12}^d in terms of the Gegenbauer polynomials, $C_m^\alpha(x)$, and then we apply the orthogonality property of these polynomials which reads [45] as

$$\int_{-1}^1 (1-t^2)^{\alpha-\frac{1}{2}} C_n^\alpha(x) C_m^\alpha(x) dx = \frac{\pi 2^{1-2\lambda} \Gamma(n+2\lambda)}{n!(n+\lambda)[\Gamma(\lambda)]^2} \delta_{m,n}, \tag{C1}$$

where $\text{Re}(\lambda) > -1/2$ with $\lambda \neq 0$ and that $C_0^\alpha(x) = 1$. Then, we obtain for the integral J_1 the following expression:

$$\begin{aligned}
 J_1 &= \sum_{n=0}^{\infty} (2n + d - 2) R\left(-\frac{1}{2}\right)_n 2^{d-2} \pi^{-1/2} \\
 &\quad \times \frac{\Gamma\left(\frac{d}{2} - 1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d + n - \frac{1}{2}\right)} \int C_n^{\frac{d}{2}-1}(\cos \theta_{12}) d\Omega_1 d\Omega_2 \\
 &= \int d\Omega_1 \sum_{n=0}^{\infty} (2n + d - 2) R\left(-\frac{1}{2}\right)_n 2^{d-2} \\
 &\quad \times \pi^{-1/2} \frac{\Gamma\left(\frac{d}{2} - 1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d + n - \frac{1}{2}\right)} \int C_n^{\frac{d}{2}-1}(\cos \theta_{12}) d\Omega_{12} \\
 &= \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \sum_{n=0}^{\infty} (2n + d - 2) R\left(-\frac{1}{2}\right)_n 2^{d-2} \pi^{-1/2} \frac{\Gamma\left(\frac{d}{2} - 1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d + n - \frac{1}{2}\right)} \\
 &\quad \times \int C_n^{\frac{d}{2}-1}(\cos \theta_{12}) C_0^{\frac{d}{2}-1}(\cos \theta_{12}) [\sin \theta_{j=1}^{(12)}]^{d-2} d\Omega_{j=1}^{(12)} \\
 &\quad \times \prod_{j=2}^{d-2} \int_0^\pi [\sin \theta_j^{(12)}]^{d-j-1} d\theta_j^{(12)} \int_0^{2\pi} d\phi^{(12)}
 \end{aligned}$$

Now we do change of integration variables

$$t = \cos \theta_{j=1}^{(12)}, \tag{C2}$$

$$\begin{aligned}
 dt &= -\sin \theta_{j=1}^{(12)} d\theta_{j=1}^{(12)} \\
 &= -(1 - t^2)^{1/2} d\theta_{j=1}^{(12)},
 \end{aligned} \tag{C3}$$

obtaining the following expression

$$\begin{aligned}
 J_1 &= \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \sum_{n=0}^{\infty} (2n + d - 2) R\left(-\frac{1}{2}\right)_n 2^{d-2} \pi^{-1/2} \frac{\Gamma\left(\frac{d}{2} - 1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d + n - \frac{1}{2}\right)} \\
 &\quad \times \int C_n^{\frac{d}{2}-1}(t) C_0^{\frac{d}{2}-1}(t) (1 - t^2)^{\left(\frac{d}{2}-1\right)-\frac{1}{2}} dt \\
 &\quad \times (2\pi) \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma\left(\frac{d-j}{2}\right)}{\Gamma\left(\frac{d-j+1}{2}\right)} \\
 &= \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \sum_{n=0}^{\infty} (2n + d - 2) R\left(-\frac{1}{2}\right)_n 2^{d-2} \pi^{-1/2} \frac{\Gamma\left(\frac{d}{2} - 1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d + n - \frac{1}{2}\right)} (2\pi) \delta_{n,0} \\
 &\quad \times \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma\left(\frac{d-j}{2}\right)}{\Gamma\left(\frac{d-j+1}{2}\right)} \frac{\pi 2^{3-d} \Gamma(n + d - 2)}{n! \left(n + \frac{d}{2} - 1\right) \Gamma\left(\frac{d}{2} - 1\right)^2} \\
 &= \frac{2^{d+1} \pi^{\frac{d}{2}+1} \Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(d - \frac{1}{2}\right)} R \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma\left(\frac{d-j}{2}\right)}{\Gamma\left(\frac{d-j+1}{2}\right)}
 \end{aligned}$$

$$= \frac{2^{d+1}\pi^{d-\frac{1}{2}}}{\Gamma\left(d-\frac{1}{2}\right)}R \tag{C4}$$

for the integral J_1 which is equal to the wanted value (29). Operating in a similar way we obtain

$$\begin{aligned} J_2 &= \int d\Omega_1 \int r_{12}^2 d\Omega_{12} \\ &= \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \int \left(2R^2 C_0^{\frac{d}{2}-1}(\cos \theta_{12}) - \frac{2R^2}{d-2} C_1^{\frac{d}{2}-1}(\cos \theta_{12}) \right) d\Omega_{12} \\ &= \frac{8\pi^{\frac{d+3}{2}}\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)^2} R^2 \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma\left(\frac{d-j}{2}\right)}{\Gamma\left(\frac{d-j+1}{2}\right)} \\ &= \frac{8\pi^d}{\Gamma\left(\frac{d}{2}\right)^2} R^2 \end{aligned} \tag{C5}$$

which is equal to the wanted value (30). Finally, by performing the sum in (21) with J_0 , J_1 and J_2 , we arrive at final expression (31) for the normalization, N_1 . It is worth to say that it is possible to compute the normalizaton of an arbitrary s -state of the d -dimensional spherium by means of the integral J_0 and the general one-center integral

$$\int r_{12}^q d\Omega_1 d\Omega_2 = \frac{2^{d+q}\pi^{d-\frac{1}{2}}\Gamma\left(\frac{d+q-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)\Gamma\left(d+\frac{q}{2}-1\right)}R^q \tag{C6}$$

with $q \geq 1$.

Derivation of the values (39)–(43) for the multicenter integrals I_i , $i = 0 - 4$ defined by equations (34)–(38), which are involved in the entanglement of the s -states of the d -dimensional spherium. These values are characterized by the parameter n , which determines the radius R_n of the sphere on which the particles are confined. For this issue we have first determined the following general expressions

$$\begin{aligned} &\int r_{12}^{q_1} r_{12'}^{q_2} r_{12''}^{q_3} r_{12'''}^{q_4} d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2' \\ &= \pi^{2d-2} 2^{4d+q_1+q_2+q_3+q_4-7} \\ &\quad \times \frac{\Gamma\left(\frac{d+q_1-1}{2}\right)\Gamma\left(\frac{d+q_2-1}{2}\right)}{\Gamma(d-1)\Gamma\left(d+\frac{q_1}{2}-1\right)\Gamma\left(d+\frac{q_2}{2}\right)\Gamma\left(d+\frac{q_2}{2}-1\right)\Gamma\left(d+\frac{q_2}{2}\right)} \\ &\quad \times \frac{\Gamma\left(\frac{1}{2}(d+q_3-1)\right)\Gamma\left(\frac{1}{2}(d+q_4-1)\right)}{\Gamma\left(d+\frac{q_3}{2}-1\right)\Gamma\left(d+\frac{q_3}{2}\right)\Gamma\left(d+\frac{q_4}{2}-1\right)\Gamma\left(d+\frac{q_4}{2}\right)} R^{q_1+q_2+q_3+q_4} \\ &\quad \times \left[8\Gamma(d-1)\Gamma\left(d+\frac{q_1}{2}\right)\Gamma\left(d+\frac{q_2}{2}\right)\Gamma\left(d+\frac{q_3}{2}\right)\Gamma\left(d+\frac{q_4}{2}\right) \right] \\ &\quad \times {}_5F_4\left(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, d-2; d+\frac{q_1}{2}-1, d+\frac{q_2}{2}-1, \right. \end{aligned}$$

$$\begin{aligned}
 & d + \frac{q_3}{2} - 1, d + \frac{q_4}{2} - 1; 1) \\
 & + \Gamma(d-1)\Gamma\left(d + \frac{q_1}{2} - 1\right)\Gamma\left(d + \frac{q_2}{2} - 1\right)\Gamma\left(d + \frac{q_3}{2} - 1\right)\Gamma\left(d + \frac{q_4}{2} - 1\right) \\
 & \times {}_5F_4\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, d-1; d + \frac{q_1}{2}, d + \frac{q_2}{2}, d + \frac{q_3}{2}, d + \frac{q_4}{2}; 1\right) \Big] \quad (C7)
 \end{aligned}$$

for four-center integrals

$$\begin{aligned}
 & \int r_{ij}^{q_1} r_{ik}^{q_2} r_{pk}^{q_3} d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2' = 2^{3d-3+q_1+q_2+q_3} \pi^{\frac{3}{2}(d-1)} R^{q_1+q_2+q_3} \\
 & \times \frac{\Gamma\left(\frac{d+q_1-1}{2}\right)\Gamma\left(\frac{d+q_2-1}{2}\right)\Gamma\left(\frac{d+q_3-1}{2}\right)}{\Gamma\left(d-1 + \frac{q_1}{2}\right)\Gamma\left(d-1 + \frac{q_2}{2}\right)\Gamma\left(d-1 + \frac{q_3}{2}\right)} \frac{2\pi^{d/2}}{\Gamma(d/2)}. \quad (C8)
 \end{aligned}$$

for three-center integrals

$$\begin{aligned}
 & \int r_{ij}^{q_1} r_{pk}^{q_2} d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2' \\
 & = 2^{2d-2+q_1+q_2} \pi^{d-1} R^{q_1+q_2} \frac{\Gamma\left(\frac{d+q_1-1}{2}\right)\Gamma\left(\frac{d+q_2-1}{2}\right)}{\Gamma\left(d-1 + \frac{q_1}{2}\right)\Gamma\left(d-1 + \frac{q_2}{2}\right)} \left(\frac{2\pi^{d/2}}{\Gamma(d/2)}\right)^2. \quad (C9)
 \end{aligned}$$

for two-center integrals, and

$$\int r_{ij}^{q_1} d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2' = \frac{2^{d-1+q_1} \pi^{\frac{d-1}{2}} R^{q_1} \Gamma\left(\frac{d+q_1-1}{2}\right)}{\Gamma\left(d-1 + \frac{q_1}{2}\right)} \left(\frac{2\pi^{d/2}}{\Gamma(d/2)}\right)^3. \quad (C10)$$

For one-center integrals, where the parameters $q_i \geq 1$ for $i = 1, \dots, 4$.

Apart from the value (39) of the integral I_0 , which is straightforward, these general multicenter integral expressions allow us to calculate not only the values (39)–(43) of the integrals I_i , $i = 1-4$ needed for the entanglement of the ground-state wavefunctions $\Psi_{1,0}(r_{12})$, but also the corresponding integrals involved in the entanglement of the ground-state wavefunctions $\Psi_{n,0}(r_{12})$ with $n \geq 2$, of the d -dimensional spherium in an analytical way.

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