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The relationship between entanglement, energy and level degeneracy in two-electron systems

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Abstract

The entanglement properties of two-electron atomic systems have been the subject of considerable research activity in recent years. These studies are still somewhat fragmentary, focusing on numerical computations on particular states of systems such as helium, or on analytical studies of model systems such as the Moshinsky atom. Some general trends are beginning to emerge from these studies: the amount of entanglement tends to increase with energy and, in the case of excited states, entanglement does not necessarily tend to zero in the limit of vanishing interaction between the two constituting particles. A physical explanation of these properties, shared by the different two-electron models investigated so far, is still lacking. As a first step towards this goal, we perform here, via a perturbative approach, an analysis of entanglement in two-electron models that sheds new light on the physical origin of the aforementioned features and on their universal character.

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1. Introduction

Entanglement constitutes one of the most fundamental phenomena in quantum mechanics [1–6]. Entangled states of composite quantum systems exhibit non-classical correlations that give rise to a rich variety of physical phenomena of both fundamental and technological significance. Quantum entanglement can be considered in two different and complementary ways. On the one hand, entanglement can be viewed as a resource. The controlled manipulation of entangled states is at the basis of 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 (for a comprehensive and up to date review on this subject see [6]). 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 above-mentioned approaches, several researchers have investigated in recent years the phenomenon of entanglement in atomic physics [6–17]. This line of enquiry is contained within the more general programme of applying tools and concepts from information theory to the analysis of atomic and molecular systems [18–27]. Most of the studies on entanglement in two-electron systems focused on the properties of the concomitant ground states. However, the entanglement features exhibited by excited states of two-electron atomic systems have also been explored [13, 14]. In this regard, the most detailed results have been obtained from analytical investigations of the entanglement properties of exactly soluble models, especially the Moshinsky one [13]. The behaviour of these soluble models is consistent with some (partial) results yielded by numerical explorations of entanglement in helium based on high-quality, state-of-the-art wavefunctions. Some general trends begin to emerge from these investigations. First, and not surprisingly, entanglement is found to increase with the strength of the inter-particle interaction. Second, entanglement also tends to increase with energy. Finally, the entanglement of excited states does not necessarily vanish in the limit of zero interaction. The last two properties are, perhaps, less intuitively clear than the first one. In fact, in a recent comprehensive review article on entanglement in atomic and molecular systems by Tichy *et al* [6] it is said that '*. . . the limit of vanishing interaction strengths does not necessarily yield a non-entangled state. . . it remains open whether this discontinuity effect has to be considered an artefact of the entanglement measures that are used, or whether a physical explanation will be provided in future*'.

It is remarkable that the various two-electron models where entanglement has been studied so far share the basic qualitative features mentioned above. This suggests that these features may constitute generic properties of these kinds of two-fermion models. In this regard, we share the opinion expressed by Tichy *et al* [6]: '*Due to the non-integrability of any non-hydrogen-like atom, theoretical studies of multielectron systems have, so far, mainly focused on exactly solvable model atoms. While such models differ strongly from real multielectron atoms as concerns the interelectronic interaction and the definition of the confining potential, they allow insight in some qualitative features*.'

The aim of this work is to clarify the origin of the aforementioned properties. To this end we are going to consider a perturbative approach to this problem, regarding the term in the Hamiltonian describing the interaction between the two electrons as a small perturbation. We shall show that the eigenvalue degeneracy of the unperturbed Hamiltonian (describing independent particles) plays a crucial role in explaining the entanglement features of the 'perturbed' system.

2. Quantum entanglement in systems of two identical fermions

Correlations between two identical fermions that are only due to the antisymmetric nature of the two-particle state do not contribute to the state's entanglement [28–32, 35, 36, 34, 33]. The entanglement of the two-fermion state is given by the quantum correlations existing on top of these minimum ones. For example, a two-fermion state of Slater rank 1 (that is, a state whose wavefunction can be expressed, in terms of an appropriate single-particle orthonormal basis, as one single Slater determinant) must be regarded as non-entangled. There are deep, fundamental physical reasons for this. On the one hand, the correlations exhibited by such states are not useful as a resource to perform non-classical information transmission or information processing tasks [28]. On the other hand, the non-entangled character of these states is consistent with the possibility of associating complete sets of properties with both parts of the composite system (see [29–31] for a detailed analysis of various aspects of this approach).

Two useful quantitative measures for the amount of entanglement of a pure state $|\psi\rangle$ of a system of two identical fermions are expressed in terms of (see [37] and references therein) the linear entropy

$$\varepsilon_L(|\psi\rangle) = 1 - 2\,\mathrm{Tr}[\rho_r^2] \tag{1}$$

and the von Neumann entropy

$$\varepsilon_{vN}(|\psi\rangle) = -\mathrm{Tr}[\rho_r \ln \rho_r] - \ln 2 \tag{2}$$

of the single-particle reduced density matrix ρ_r. Note that according to the entanglement measures given by equations (1) and (2) a pure state that can be represented by a single Slater determinant has no entanglement (that is, it is separable).

The fermionic entanglement measures (1) and (2) are closely related to the Schmidt decomposition of pure states of systems constituted by two identical fermions [32]. For any pure state $|\psi\rangle$ of two identical fermions it is possible to find an orthonormal basis $\{|i\rangle,\ \ i = 0, 1, \ldots\}$ of the single-particle Hilbert space such that the state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_i \sqrt{\frac{\lambda_i}{2}}\ (|2i\rangle|2i+1\rangle - |2i+1\rangle|2i\rangle), \tag{3}$$

where the Schmidt coefficients λ_i verify $0 \leqslant \lambda_i \leqslant 1$ and $\sum_i \lambda_i = 1$. (In the case of systems with a single-particle Hilbert space of finite dimension N, we assume that N is even and that the sums on the index i run from $i = 0$ to $i = N/2$.) Then one has that the entanglement measures (1) and (2) can be expressed in terms of the Schmidt coefficients of the state $|\psi\rangle$ respectively as [32, 37]

$$\varepsilon_L(|\psi\rangle) = 1 - \sum_i \lambda_i^2 \tag{4}$$

and

$$\varepsilon_{vN}(|\psi\rangle) = -\sum_i \lambda_i \ln \lambda_i. \tag{5}$$

In a particular case of systems of two fermions with a single-particle Hilbert space of dimension 4, the quantity $2\varepsilon_L$ reduces to the entanglement measure (usually referred to as squared concurrence) studied in [28] (see also [35]). The entanglement measure given by equations (1) and (4) has been recently applied to the analysis of various physical systems or processes, including electron–electron scattering processes [34], the study of entanglement-related aspects of quantum brachistochrone evolutions [35] and the entanglement properties of two-electron atomic models [13]. As a final remark on entanglement in the fermionic system we mention that in this work we deal with the fermionic case of the concept of *entanglement between particles*. This is not the only possible conception of entanglement in systems of identical particles. In particular, there is an approach to the study of entanglement in systems of indistinguishable particles which focuses on the entanglement between different modes (see, for instance, [6] and references therein).

3. Perturbative approach

Let us consider a system of two identical fermions (electrons) governed by a Hamiltonian of the form $H = H_0 + \lambda H'$, where the unperturbed Hamiltonian H_0 corresponds to two independent (non-interacting) particles, $\lambda H'$ describes the interaction between the electrons and λ is a small parameter. When this system is treated perturbatively, the perturbative corrections to the eigenenergies correspond to some 'fine structure' sitting on top of the main pattern due to

the spectrum of H_0. It is plain that within this scenario the leading, zeroth-order contribution to the energy spectrum is independent of the detailed structure of the perturbation H'. As we presently see, the situation is completely different when, instead of energy, we calculate the entanglement of the system's eigenstates. When the unperturbed energy eigenvalues are degenerate the leading (zeroth-order) contribution to the eigenfunction's entanglement does depend, in general, on the details of the perturbation.

Let us consider an m-fold degenerate energy level of H_0, with an associated set of m orthonormal eigenstates $|\psi_j\rangle$, $j = 1, \ldots, m$. Since H_0 describes two non-interacting particles, the m eigenstates $|\psi_j\rangle$ can always be chosen to be Slater determinants written in terms of a family of orthonormal single-particle states $|\phi_j^{(1,2)}\rangle$, so that $|\psi_j\rangle = (1/\sqrt{2})(|\phi_j^{(1)}\rangle|\phi_j^{(2)}\rangle - |\phi_j^{(2)}\rangle|\phi_j^{(1)}\rangle)$. All the members of the subspace $\mathcal{H}_s$ spanned by the states $|\psi_j\rangle$ are eigenstates of H_0 corresponding to the same eigenenergy. That is, energywise they are all equivalent. However, the different members of this subspace have, in general, different amounts of entanglement. Typically, the interaction H' will lift the degeneracy of the degenerate energy level. If we solve the eigenvalue problem corresponding to the (perturbed) Hamiltonian H and take the limit $\lambda \to 0$, the perturbation H' will 'choose' one particular basis $\{|\psi'_k\rangle_{\lambda\to 0}\}$ among the infinite possible basis of $\mathcal{H}_s$. The states constituting this special basis will in general be entangled. These states are of the form $|\psi'_k\rangle_{\lambda\to 0} = \sum_{j=1}^{m} c_{kj}|\psi_j\rangle$ and are determined (according to standard perturbation theory [38]) by the eigenvectors of the $m \times m$ matrix $\tilde{H}$ with elements given by $\tilde{H}_{ij} = \langle\psi_i|H'|\psi_j\rangle$. It is then clear that in the limit $\lambda \to 0$, the eigenstates of H will in general be entangled.

Let $\tilde{m}$ be the number of different single-particle states within the family $\{|\phi_j^{(1,2)}\rangle,\ 1, \ldots, m\}$. It is a quite typical behaviour that $\tilde{m}$ tends to increase with the degree of degeneracy m of the energy levels of H_0 which, in turn, tends to increase with energy (that is, it tends to increase as one considers higher excited states). This explains (at least in part) why the range of entanglement values available to the eigenstates $\{|\psi'_k\rangle_{\lambda\to 0}\}$ tends to increase with energy. Indeed, the maximum amount of entanglement (as measured by (2)) that can be achieved by a linear combination of Slater determinants constructed from the single-particle states $\{|\phi_j^{(1,2)}\rangle\}$ is

$$\varepsilon = \ln \Omega, \tag{6}$$

where Ω is the integer part of $\tilde{m}/2$. Expression (6) provides an upper bound for the entanglement of the states $\{|\psi'_k\rangle_{\lambda\to 0}\}$.

In this work, we are going to focus on the entanglement properties exhibited by the eigenstates $\{|\psi'_k\rangle_{\lambda\to 0}\}$ and on the entanglement upper bound (6). In this regard, our perturbative approach is unusual, since we are focusing on 'zeroth-order properties'. However, it must be stressed that the amounts of entanglement of the states $\{|\psi'_k\rangle_{\lambda\to 0}\}$ are in general finite quantities that do not vanish when $\lambda \to 0$ and, consequently, constitute dominant aspects of the entanglement-related features characterizing the system.

4. Two interacting spin-1/2 fermions in an external confining potential

We apply now the previous considerations to a system consisting of two interacting spin-1/2 fermions in an external confining potential $U(x)$. The interaction between the particles is described by the potential function $V(x_1 - x_2)$, with V being an even function. The Hamiltonian of this system is then

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + U(x_1) + U(x_2) + \lambda V(x_1 - x_2), \tag{7}$$

where x_1 and x_2 are the coordinates of the two particles. We use atomic units ($m = 1$, $\hbar = 1$). A relevant instance of this system corresponds to the case of harmonic confinement $U(x) = \frac{1}{2}\omega^2 x^2$, where ω is the natural frequency of the external harmonic field. This case includes the Moshinsky atom [7, 13, 39], where the interaction between the particles is also harmonic, $\lambda V(x_1 - x_2) = \frac{1}{2}\lambda\omega^2(x_1 - x_2)^2$, with $\lambda\omega^2 \geqslant 0$ being the square of the natural frequency of the interaction harmonic field. The Moshinsky atom is an exactly solvable system whose entanglement properties have been studied in detail. The examples considered here indicate that some important entanglement-related features of the Moshinsky model are also encountered in more general systems.

We now apply the formalism of perturbation theory to a system described by the Hamiltonian (7) with harmonic confinement and a generic interaction V between the particles. The unperturbed Hamiltonian is then

$$H_0 = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}\omega^2 x_1^2 + \frac{1}{2}\omega^2 x_2^2, \tag{8}$$

and the perturbation

$$\lambda H' = \lambda V(x_1 - x_2). \tag{9}$$

When $\lambda = 0$, the model consists of two independent harmonic oscillators with the same natural frequency. Let $|n\rangle$ ($n = 0, 1, 2, \ldots$) be the eigenstates of each of these oscillators. Then, the kets $|n, \pm\rangle$ constitute a single-particle orthonormal basis (the signs $\pm$ correspond, in standard notation, to the spin state of the spin-1/2 particle). The eigenstates of H_0 are characterized by two quantum numbers n_1 and n_2 corresponding to the alluded pair of independent oscillators. The corresponding eigenenergies depend only on the value of the sum $n_1 + n_2$ and are m-fold degenerate with $m = 2(n_1 + n_2) + 1$ ($m = 2(n_1 + n_2) + 2$) if $n_1 + n_2$ is even (odd). Assuming that $n_1 + n_2$ is odd, with $n_1 = n_2 - 1$, and taking spin into consideration, we can choose the following set of m antisymmetric eigenstates (all with the same energy):

$$\begin{aligned}
|\psi_1\rangle &= \frac{1}{\sqrt{2}}(|n_1, +\rangle|n_2, +\rangle - |n_2, +\rangle|n_1, +\rangle)\\
|\psi_2\rangle &= \frac{1}{\sqrt{2}}(|n_1, +\rangle|n_2, -\rangle - |n_2, -\rangle|n_1, +\rangle)\\
|\psi_3\rangle &= \frac{1}{\sqrt{2}}(|n_1, -\rangle|n_2, +\rangle - |n_2, +\rangle|n_1, -\rangle)\\
|\psi_4\rangle &= \frac{1}{\sqrt{2}}(|n_1, -\rangle|n_2, -\rangle - |n_2, -\rangle|n_1, -\rangle)\\
&\vdots\\
|\psi_{m-3}\rangle &= \frac{1}{\sqrt{2}}(|0, +\rangle|n_2 + n_1, +\rangle - |n_2 + n_1, +\rangle|0, +\rangle)\\
|\psi_{m-2}\rangle &= \frac{1}{\sqrt{2}}(|0, +\rangle|n_2 + n_1, -\rangle - |n_2 + n_1, -\rangle|0, +\rangle)\\
|\psi_{m-1}\rangle &= \frac{1}{\sqrt{2}}(|0, -\rangle|n_2 + n_1, +\rangle - |n_2 + n_1, +\rangle|0, -\rangle)\\
|\psi_m\rangle &= \frac{1}{\sqrt{2}}(|0, -\rangle|n_2 + n_1, -\rangle - |n_2 + n_1, -\rangle|0, -\rangle),
\end{aligned} \tag{10}$$

which are represented by single Slater determinants and consequently have zero entanglement. A similar set of separable eigenstates of H_0 can be chosen when $n_1 + n_2$ is even.

We consider now a harmonically confined two-fermion system with an interaction potential given by a repulsive Dirac delta function

$$\lambda V = \tfrac{1}{2}\lambda\delta(x_1 - x_2). \tag{11}$$

For the first excited energy level of H_0 ($n_1 + n_2 = 1$) which is fourfold degenerate, we then have

$$\tilde{H} = \frac{1}{4}\sqrt{\frac{\omega}{2\pi}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{12}$$

and the corresponding eigenvectors can be written as

$$\begin{aligned} |\psi_1'\rangle &= \frac{1}{\sqrt{2}}(-|\psi_2\rangle + |\psi_3\rangle) \\ |\psi_2'\rangle &= |\psi_4\rangle \\ |\psi_3'\rangle &= |\psi_1\rangle \\ |\psi_4'\rangle &= \frac{1}{\sqrt{2}}(|\psi_2\rangle + |\psi_3\rangle). \end{aligned} \tag{13}$$

In the limit of vanishing interaction, $\lambda \to 0$, the eigenstates corresponding to the first two excited energy levels of the full Hamiltonian tend to the states (13), which have the following amounts of entanglement:

$$\varepsilon_L(|\psi_2'\rangle) = \varepsilon_L(|\psi_3'\rangle) = 0 \tag{14}$$

$$\varepsilon_{vN}(|\psi_2'\rangle) = \varepsilon_{vN}(|\psi_3'\rangle) = 0 \tag{15}$$

$$\varepsilon_L(|\psi_1'\rangle) = \varepsilon_L(|\psi_4'\rangle) = \tfrac{1}{2} \tag{16}$$

$$\varepsilon_{vN}(|\psi_1'\rangle) = \varepsilon_{vN}(|\psi_4'\rangle) = \ln 2. \tag{17}$$

It can be verified after some algebra that the eigenvectors (and the associated amounts of entanglement) obtained in this case coincide with those corresponding (in the $\lambda \to 0$ limit of the two first excited energy levels) to a harmonic interaction. That is, they are the same as those associated with the Moshinsky model. We thus see that the harmonic and the Dirac delta interactions lead, for particles confined by an external harmonic well, to the same entanglement behaviour of the first excited states in the limit of weak interaction.

We now consider the case of generic external (one-dimensional) potential $U(x)$ and interaction $V(x_1 - x_2)$ (with V an even function) so that $H_0 = \sum_{i=1}^{2}\left(\frac{\partial^2}{\partial x_i^2} + U(x_i)\right)$ and $\lambda H' = \lambda V(x_1 - x_2)$, which leads to

$$\tilde{H} = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \tag{18}$$

with

$$\begin{aligned} a &= \tfrac{1}{2}(\langle 0|\langle 1|H'|0\rangle|1\rangle - \langle 0|\langle 1|H'|1\rangle|0\rangle - \langle 1|\langle 0|H'|0\rangle|1\rangle + \langle 1|\langle 0|H'|1\rangle|0\rangle) \\ b &= \tfrac{1}{2}(\langle 0|\langle 1|H'|0\rangle|1\rangle + \langle 1|\langle 0|H'|1\rangle|0\rangle) \\ c &= -\tfrac{1}{2}(\langle 0|\langle 1|H'|1\rangle|0\rangle + \langle 1|\langle 0|H'|0\rangle|1\rangle) \end{aligned} \tag{19}$$

where $|0\rangle$ and $|1\rangle$ are the ground and first excited eigenstates corresponding to the external confining potential $U(x)$. The eigenvectors of $\tilde{H}$ are

$$\begin{aligned} |\psi_1'\rangle &= \frac{1}{\sqrt{2}}(-|\psi_2\rangle + |\psi_3\rangle) \\ |\psi_2'\rangle &= |\psi_4\rangle \\ |\psi_3'\rangle &= |\psi_1\rangle \\ |\psi_4'\rangle &= \frac{1}{\sqrt{2}}(|\psi_2\rangle + |\psi_3\rangle). \end{aligned} \tag{20}$$

The values of entanglement exhibited by these states are $\varepsilon_L = \varepsilon_{vN} = 0$ associated with $|\psi_2'\rangle$ and $|\psi_3'\rangle$ and $\varepsilon_L = \frac{1}{2}$, $\varepsilon_{vN} = \ln 2$ associated with $|\psi_1'\rangle$ and $|\psi_4'\rangle$. This result generalizes the previous one, as we have solved the problem for generic interactions and external confining potentials. Here it is possible to obtain general results for an arbitrary confining potential $U(x)$ for the case where one has (in the limit of vanishing interaction) one particle in the ground state and one particle in the first excited state of $U(x)$ because the degeneracy of the concomitant energy level (of the two-partile system) can be determined directly without knowing the detailed energy spectrum associated with $U(x)$. On the other hand, the properties exhibited by states of higher excitation in the limit of vanishing interaction do depend (via the degeneracy appearing in this limit case) on the detailed eigenenergies of the confining potential $U(x)$. Consequently, the analysis of the limit of vanishing interaction can be performed only in a case-by-case way. In the following section, we are going to consider higher excited states in the case of a generic interaction potential $V(x_1 - x_2)$ and a harmonic confining potential.

5. Entanglement upper bound for excited states in the limit of weak interaction

We consider now two spin-1/2 particles (in one dimension) confined by an external harmonic potential and having a generic interaction $\lambda V(x_1 - x_2)$. We shall calculate general upper bounds for the entanglement of the eigenstates of this system in the limit $\lambda \to 0$. These bounds, expressed in terms of the quantum numbers n_1 and n_2 characterizing the eigenfunctions of H_0, are

$$\varepsilon_L(|n_1 n_2\rangle) \leqslant \frac{n_1 + n_2}{n_1 + n_2 + 1} \tag{21}$$

$$\varepsilon_{vN}(|n_1 n_2\rangle) \leqslant \ln(n_1 + n_2 + 1). \tag{22}$$

Equation (22) constitutes a particular instance, corresponding to a harmonic confining potential, of the general upper bound (6). In figure 1, we plot the entanglement bounds against $n_1 + n_2$. These curves represent the maximum possible entanglement compatible with those quantum numbers (the bounds do not depend on the interaction and are, in this sense, universal).

In the particular case $n_1 + n_2 = 2$, besides the above upper bound, we can calculate the exact amount of entanglement (in the limit $\lambda \to 0$) for an arbitrary interaction potential $V(x_1 - x_2)$. This case corresponds to a fivefold degenerate energy level of H_0 shared by a set of eigenvectors of the form (10), with $m = 5$. The generic matrix $\tilde{H}$ is of the form

$$\tilde{H} = \begin{pmatrix} a & 0 & 0 & 0 & 0 \\ 0 & b & c & 0 & d \\ 0 & c & b & 0 & -d \\ 0 & 0 & 0 & a & 0 \\ 0 & d & -d & 0 & e \end{pmatrix}, \tag{23}$$

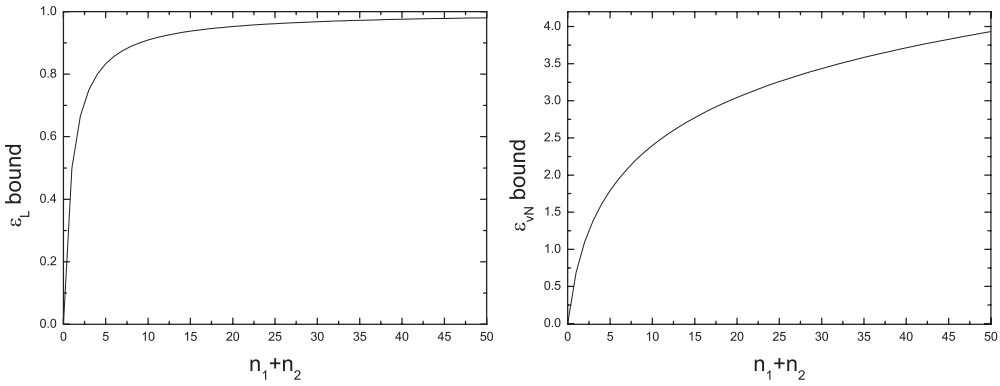

Figure 1. Entanglement bound as a function of the sum of the quantum numbers $n_1 + n_2$. All depicted quantities are dimensionless.

with

$$
\begin{aligned}
a &= \tfrac{1}{2}(\langle 0|\langle 2|H'|0\rangle|2\rangle - \langle 0|\langle 2|H'|2\rangle|0\rangle - \langle 2|\langle 0|H'|0\rangle|2\rangle + \langle 2|\langle 0|H'|2\rangle|0\rangle)\\
b &= \tfrac{1}{2}(\langle 0|\langle 2|H'|0\rangle|2\rangle + \langle 2|\langle 0|H'|2\rangle|0\rangle)\\
c &= -\tfrac{1}{2}(\langle 0|\langle 2|H'|2\rangle|0\rangle + \langle 2|\langle 0|H'|0\rangle|2\rangle)\\
d &= \tfrac{1}{2}(\langle 0|\langle 2|H'|1\rangle|1\rangle + \langle 2|\langle 0|H'|1\rangle|1\rangle)\\
e &= \langle 1|\langle 1|H'|1\rangle|1\rangle.
\end{aligned}
\tag{24}
$$

The corresponding normalized eigenvectors can be expressed as follows:

$$
\begin{aligned}
|\psi_1'\rangle &= |\psi_1\rangle\\
|\psi_2'\rangle &= |\psi_4\rangle\\
|\psi_3'\rangle &= \frac{1}{\sqrt{2}}(|\psi_2\rangle + |\psi_3\rangle)\\
|\psi_4'\rangle &= \frac{1}{\sqrt{2r_1^2+1}}(-r_1|\psi_2\rangle + r_1|\psi_3\rangle + |\psi_5\rangle)\\
|\psi_5'\rangle &= \frac{1}{\sqrt{2r_2^2+1}}(-r_2|\psi_2\rangle + r_2|\psi_3\rangle + |\psi_5\rangle),
\end{aligned}
\tag{25}
$$

where r_1 and r_2 are the functions of the matrix elements b, c, d and e given by the expressions

$$
r_1 = \frac{C_1 + cR}{C_2 + dR}, \qquad r_2 = \frac{C_1 - cR}{C_2 - dR},
\tag{26}
$$

with

$$
C_1 = -bc + c^2 + 2d^2 + ce, \qquad C_2 = d(b + 3c - e)
\tag{27}
$$

and

$$
R = \sqrt{b^2 + c^2 + 8d^2 + 2ce + e^2 - 2b(c + e)}.
\tag{28}
$$

Now we calculate the amounts of entanglement of the states $|\psi_4'\rangle$ and $|\psi_5'\rangle$ that depend (in the same way) on r_1 and r_2, respectively. The values adopted by these two constants depend on the

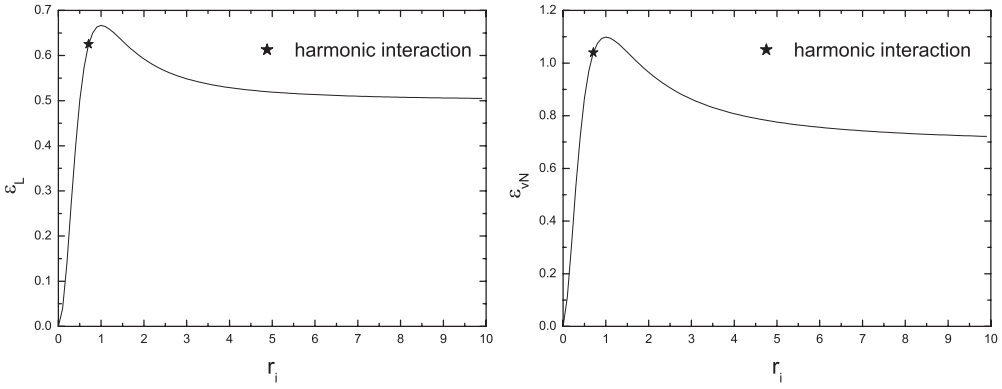

Figure 2. ε_L (left panel) and ε_{vN} (right panel) as the functions of r_i for the case $n_1 + n_2 = 2$ and an arbitrary interaction $V(x_1 - x_2)$. The stars in both plots correspond to the entanglement amount for the Moshinsky atom (harmonic interaction). All depicted quantities are dimensionless.

form of the interaction $V(x_1 - x_2)$. The general expressions for the amount of entanglement of the states $|\psi_4'\rangle$ and $|\psi_5'\rangle$ are

$$\varepsilon_L(r_i) = 1 - \frac{2r_i^4 + 1}{(2r_i^2 + 1)^2} \qquad i = 1, 2, \tag{29}$$

$$\varepsilon_{vN}(r_i) = \ln(2r_i^2 + 1) - \frac{4r_i^2}{2r_i^2 + 1} \ln r_i \qquad i = 1, 2. \tag{30}$$

We plot these expressions in figure 2. Note that the particular value $r_i = \frac{1}{\sqrt{2}}$ corresponds to the harmonic interaction in the Moshinsky model.

6. Conclusions

By recourse to a perturbative approach, we studied the entanglement-related properties of a system consisting of two interacting spin-1/2 fermions 'electrons' confined by an external potential. Our present results clarify some aspects of the basic entanglement features exhibited by particular two-electron models studied previously, and shed some light upon the fact that these systems share important qualitative entanglement properties that are also observed in more general cases. Our analysis highlights the important role played by the degeneracy of the energy levels of the 'unperturbed' (interaction-free) Hamiltonian H_0. The non-vanishing entanglement exhibited by the interacting particles in the limit of vanishing interaction is due to the particular eigenbasis of H_0 'chosen' by the interaction. This amount of entanglement tends to increase with the alluded degeneracy which, in turn, tends to increase with energy. *This sheds light on the physical reasons behind the fact (observed in all cases studied so far) that the amount of entanglement exhibited by the eigenstates of two-electron systems tends to increase with energy*. These basic trends do not depend on the particular entanglement measure employed, as has been shown in this work, where entanglement measures based upon the linear and the von Neumann entropies were considered. In connection with this point, it is worthwhile to mention a relevant question raised in a recent review article on entanglement in atoms and molecules [6]: does the existence, for some excited states, of a finite amount of entanglement in the limit of vanishing interaction depend upon the particular entanglement measure employed? As already mentioned, the answer to this question is that the alluded

feature constitutes an intrinsic property of the systems under consideration, which does not depend on the entanglement measure used.

As particular illustrations of the above considerations we have

- computed for general confining and interaction potentials, in the limit $\lambda \to 0$, the entanglement measures based upon the linear entropy and the von Neumann entropy of the excited states associated with the fourfold degenerate unperturbed first excited state.
- obtained for a harmonic confining potential and a generic interaction potential $V(x_1 - x_2)$, the entanglement of the eigenstates corresponding in the above limit to the second excited unperturbed energy level (given by $n_1 + n_2 = 2$).
- determined, for a harmonic confining potential and an arbitrary interaction, upper bounds on the amounts of entanglement exhibited by the system's eigenstates in the limit of vanishing interaction. These upper bounds are expressed in terms of the quantum numbers n_1 and n_2.

The results advanced here corresponding to the entanglement in the limit of vanishing interaction are *exact*, and our procedure can in principle be applied to any excited state of systems of the kind considered in this work. In this sense, the perturbative method used here is not (in itself) the fundamental protagonist of our present considerations. The perturbative approach was used only as a tool to determine (exactly) the entanglement features of the system's eigenstates in the limit of vanishing interaction, in order to get some insight into the qualitative entanglement features of two-electrons models. It is worth stressing that the entanglement exhibited by these systems in the limit $\lambda \to 0$ constitutes a basic, dominant aspect of their entanglement-related characteristics. It is to be expected, on general physical grounds, that the entanglement–degeneracy relationship uncovered here constitutes a typical feature of atomic models. This provides a first step towards explaining the fact that the general entanglement features exhibited by soluble models such as the Moshinsky one are also observed in other two-electron systems.

The ideas discussed here may also be useful for the analysis of entanglement-related aspects of other scenarios involving interacting fermions, such as those appearing in molecular or solid state physics. Just to mention one example, a situation similar to the one observed in the atomic models considered here also occurs when studying the behaviour of electronic entanglement in the dissociation process of diatomic molecules [27]. One observes that, for instance, in the limit of large values of the reaction coordinate (corresponding to vanishing interaction between the electrons in the system) describing the dissociation of H_2, the electronic entanglement does not tend to zero [27].

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