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Quantum entanglement in a soluble two-electron model atom

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Abstract. We investigate the entanglement properties of bound states in an exactly soluble two-electron model, the Moshinsky atom. We present exact entanglement calculations for the ground, first and second excited states of the system. We find that these states become more entangled when the relative interparticle interaction becomes stronger. As a general trend, we also observe that the entanglement of the eigenstates tends to increase with the states' energy. There are, however, "entanglement level-crossings" where the entanglement of a state becomes larger than the entanglement of other states with higher energy. In the limit of weak interaction, we also compute (exactly) the entanglement of higher excited states. Excited states with anti-parallel spins are found to involve a considerable amount of entanglement even for an arbitrarily weak (but non zero) interaction. This minimum amount of entanglement increases monotonically with the state's energy. Finally, the connection between entanglement and the Hartree-Fock approximation in the Moshinsky model is addressed. The quality of the ground-state Hartree-Fock approximation is shown to deteriorate, and the corresponding correlation energy to grow, as the entanglement of the (exact) ground state increases. The present work goes beyond previous related studies because we fully take into account the identical character of the two constituting particles in the entanglement calculations, and provide analytical, exact results both for the ground and the first few excited states.

PACS. 03.65.-w Quantum mechanics – 03.67.-a Quantum information – 03.67.Mn Entanglement measures, witnesses, and other characterizations

1 Introduction

The application of information-theoretic ideas to the study of atomic structure has attracted the attention of several researchers in recent years [1–9]. This line of inquiry provides an interesting and potentially fertile new channel of cross-pollination between the mature field of atomic physics and the emerging field of quantum information theory. These two areas of research also exhibit an intensive interaction, of course, due to the fact that some of the systems studied by contemporary atomic physics, such as ion traps, constitute promising candidates for the experimental implementation of quantum computer technology [10]. Furthermore, the investigation of information-theoretical aspects of atomic structure has interesting points of contact with other important areas of physics, such as the theory of critical phenomena [5].

A key ingredient in quantum information theory is the phenomenon of quantum entanglement [10,11]. There is wide consensus that it constitutes one of (if not the) most fundamental features of quantum physics. The study of quantum entanglement has been the focus of intense research efforts in recent years, leading to the discovery of novel quantum information processes such as quantum teleportation, superdense coding, and quantum computation [10,12], that may have important practical applications. Besides its revolutionary technological implications, current research in quantum entanglement is providing a deeper understanding of various basic aspects of quantum physics, such as, for instance, quantum interference [13], the foundations of quantum statistical mechanics [14], the origin of the quantum-to-classical transition [15] and the limits on the speed of quantum evolution (see [16] and references therein).

From both fundamental and practical points of view, it is imperative to investigate in a systematic way all the facets of the concept of entanglement. It must be realized that quantum entanglement is not just a fashionable research subject. Entanglement is a fundamental concept of quantum physics that plays a deep role within all

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applications of quantum mechanics involving composite systems (e.g., problems involving more than one particle).

The aim of the present contribution is to investigate some aspects of the relationship between quantum entanglement and atomic physics. In order to do this, we are going to consider the entanglement properties of the energy eigenstates of the Moshinsky atom [17,18] and its connection with the correlation energy in the framework of the Hartree-Fock approximation. The Moshinsky system has in recent years attracted the interest of researchers, as a testing ground to investigate fundamental aspects of atomic physics [6,7,18]. In particular, it has been used to explore the application of ideas from information theory to this field [6,7]. The Moshinsky atom provides a solvable system where some fundamental aspects of atomic physics (in particular, the role of entanglement) can be investigated by recourse to detailed, exact analytical computations. Furthermore, exact information about the eigenstates of the Moshinsky model can be used to develop valuable approximation techniques to treat more realistic models [18]. Some interesting results related to the entanglement properties of the Moshinsky model have been recently reported by Amovilli and March in [7], but these authors limited their considerations only to the ground state of the system. Entanglement in a system similar to the Moshinsky model has also been studied in connection with the entropy-area relationship for massless free fields [19]. However, the results reported in [19] refer only to the system's ground state.

The structure of the paper is the following. First, in Section 2 we briefly review the quantitative measures of entanglement for pure states, with special emphasis on measures appropriate for two electrons systems. Second, in Section 3, we describe the eigensolutions of the Hamiltonian of the Moshinsky atom. Then, in Section 4, the entanglement properties of the ground and various excited states of this model atom are investigated in detail. In Section 5 we analyze the entanglement of the Hartree-Fock ground state of the Moshinsky atom, and its relationship with the correlation energy and the validity of the approximation itself. Finally, some conclusions are drawn in Section 6.

2 Entanglement measure for two electron systems

It is useful to consider first a quantum system constituted by two distinguishable subsystems A and B. If $\mathcal{H}_A$ and $\mathcal{H}_B$ denote the Hilbert spaces describing, respectively, the subsystems A and B, the Hilbert space associated with the composite system has the tensor-product form $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. Pure states of this composite system can be classified into separable (factorizable) pure states and entangled pure states. Separable pure states are those that can be written as the tensor product of two states, $|\phi\rangle = |\phi\rangle_A \otimes |\phi\rangle_B$, where $|\phi\rangle_k$ $(k = A, B)$ are pure states of the k-subsystem. On the other hand we have entangled states, which are those that cannot be factorized in such a way. In the case of factorizable states, each subsystem is described by an individual pure state of its own. On the contrary, when we have an entangled state it is not possible to assign an individual pure state to each subsystem, and the subsystems are in mixed states. In general, if our bipartite system is in a (pure) state $|\psi\rangle$, its subsystems are described by the (marginal) density matrices ρ_k given by

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B(|\psi\rangle\langle\psi|), \\ \rho_B &= \mathrm{Tr}_A(|\psi\rangle\langle\psi|). \end{aligned} \tag{1}$$

The degree of mixedness of these marginal density matrices constitute quantitative measures of the amount of entanglement exhibited by the joint (pure) state $|\psi\rangle$. The larger the mixing of the subsystems, the larger the amount of entanglement of the (global) pure state. There are various ways to measure the degree of mixedness of the marginal density matrices and, consequently, the amount of entanglement associated with the global pure state of the composite system. Let us just mention the measure of entanglement based upon the von Neumann entropy of either marginal density matrices ρ_k,

$$-\mathrm{Tr}(\rho_A \ln \rho_A) = -\mathrm{Tr}(\rho_B \ln \rho_B) \tag{2}$$

and the measure defined in terms of the traces of the squared marginal density matrices (see, e.g., [20–23]) which is given by the linear entropies of these density matrices,

$$\mathcal{E}(|\psi\rangle) = 1 - \mathrm{Tr}\left(\rho_A^2\right) = 1 - \mathrm{Tr}\left(\rho_B^2\right). \tag{3}$$

It is clear that, according to these two measures (2) and (3), factorizable pure states have zero entanglement. In the present work we are going to use the measure (3), which exhibits various computational advantages from both analytical and numerical points of view. The quantity (3) constitutes a very useful entanglement measure for pure states that has been applied by several researchers to the study of various problems related to quantum entanglement [20–23], particularly in connection with the entanglement features of systems of two identical fermions [22,23]. It is useful to write the entanglement measure (3) in terms of the Schmidt decomposition of the joint state. For any state $|\psi\rangle$ it is always possible to find orthonormal basis $\{|\phi_i^{(A)}\rangle\}$ and $\{|\phi_i^{(B)}\rangle\}$ for subsystems A and B, respectively, such that

$$|\psi\rangle = \sum_i \sqrt{\lambda_i} |\phi_i^{(A)}\rangle \otimes |\phi_i^{(B)}\rangle, \tag{4}$$

where $0 \geq \lambda_i \geq 1$ and $\sum_i \lambda_i = 1$. In terms of the Schmidt decomposition the entanglement measure (3) can be cast as

$$\mathcal{E}(|\psi\rangle) = 1 - \sum_i \lambda_i^2. \tag{5}$$

When dealing with systems consisting of two *identical particles* it is physically problematic (at least from the conceptual, fundamental point of view) to speak about the marginal states describing each of the alluded particles

(even if the corresponding reduced density matrix may be very useful for many practical purposes). Consequently, definitions of the amount of entanglement of fermionic systems based on expressions like (2) or (3) should be handle with care. However, the Schmidt decomposition does admit a natural generalization to systems of two identical particles (see [22] for a detailed discussion) leading to a physically meaningful definition of entanglement for pure states of this kind of systems. In the case of *two identical fermions* it is always possible to find an orthonormal basis $\{|i\rangle,\ i = 0, 1, \ldots\}$ of the single-particle Hilbert space, such that the two-particle pure state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_i \sqrt{\frac{\lambda_i}{2}}\Big(|2i\rangle|2i+1\rangle - |2i+1\rangle|2i\rangle\Big), \qquad (6)$$

with $0 \geq \lambda_i \geq 1$ and $\sum_i \lambda_i = 1$ (if the single-particle Hilbert space has a finite dimension N, we assume that N is even and that the sums on the index i go from $i = 0$ to $i = \frac{N}{2} - 1$). In terms of this fermionic Schmidt decomposition the amount of entanglement exhibited by the pure state $|\psi\rangle$ is [22]

$$\mathcal{E}(|\psi\rangle) = 1 - \sum_i \lambda_i^2 = 1 - 2\mathrm{Tr}\,(\rho_1^2), \qquad (7)$$

where $\rho_1 = \mathrm{Tr}_2\,(|\psi\rangle\langle\psi|)$ is the reduced single-particle density matrix obtained by tracing the global, two-particle density matrix $\rho = |\psi\rangle\langle\psi|$ over one of the two particles. The measure (7) has been recently applied to the study of electron-electron scattering processes [23].

One of the main features of the entanglement measure (7) for systems of two identical fermions is that correlations between the two particles that are due solely to the antisymmetric character of the fermionic states do not contribute to the state's amount of entanglement. The amount of entanglement associated with a two-fermions state corresponds, basically, to the quantum correlations exhibited by the state on top of the minimum correlations needed to comply with the antisymmetric constraint on the fermionic wave function [22–26]. For instance, for a two-fermions state of Slater rank equal to one (that is, a state whose wave function can be represented as a single Slater determinant) one of the λ's appearing in the fermionic Schmidt decomposition is equal to 1 and the rest are equal to zero. It is plain from (7) that such a state has zero entanglement. Indeed, even though the concept of entanglement in systems of indistinguishable particles is more controversial than it is in the case of distinguishable subsystems, there is by now general consensus among researchers working on entanglement theory and on the foundations of quantum mechanics that two-fermion states of Slater rank one must be regarded as non-entangled [22–29]. There are profound physical reasons for this. On the one hand, the correlations exhibited by such states can't be used as a resource to implement non-classical information transmission or information processing tasks [24]. On the other hand, the non-entangled character of states represented by one Slater determinant is consistent with the possibility of associating complete sets of properties to both parts of the composite system (see [25,26] for a detailed discussion of this approach).

Let us now consider the application of the above measure to a pure state of a two electrons system. In the present work we are going to focus mainly on states described by wave functions of the form

$$\phi(x_1, x_2)\,\chi(\sigma_1, \sigma_2), \qquad (8)$$

where the global wave function can be factorized as the product of a coordinate wave function $\phi(x_1, x_2)$ and a spin wave function $\chi(\sigma_1, \sigma_2)$, x_1 and x_2 being the coordinates of the two electrons. In general, the eigenstates of the Moshinsky aton have the factorized form (8). In the special case of vanishing interaction, however, the degeneracy of the eigenenergies of the Moshinsky model allow for constructing non-factorized eigenstates that have the form of Slater determinants and, consequently, have no entanglement.

The density matrix corresponding to a factorized wave function of the form (8) has the form

$$\rho = \rho^{(\mathrm{coord.})} \otimes \rho^{(spin)}, \qquad (9)$$

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

$$\langle x_1', x_2'|\rho^{(\mathrm{coord.})}|x_1, x_2\rangle = \phi(x_1', x_2')\phi^*(x_1, x_2). \qquad (10)$$

The entanglement measure (7) evaluated on a state with the wave function (8) (and density matrix (9)) is given by

$$\mathcal{E} = 1 - 2\,\mathrm{Tr}\left[\tilde{\rho}^2\right]\,\mathrm{Tr}\left[\tilde{\rho}_s^2\right], \qquad (11)$$

where $\tilde{\rho}$ are $\tilde{\rho}_s$ are, respectively, the single particle reduced coordinate and spin density matrices. To evaluate (11) we have now to consider separately the cases of a spin wave function describing parallel spins or antiparallel spins. If we have parallel spins (that is, if the coordinate wave function is antisymmetric and the spin wave function is either χ_{++} or χ_{--}) the entanglement measure (7) corresponding to a two-electrons state of the form (8) (which is given by (11)) reduces to

$$\xi(|\psi\rangle) = 1 - 2\int |\langle x_1'|\tilde{\rho}|x_1\rangle|^2\, dx_1' dx_1. \qquad (12)$$

On the other hand, if we have anti-parallel spins (that is, if the coordinate wave function is symmetric and the spin wave function is $\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})$ or, alternatively, if the coordinate wave function is antisymmetric and the spin wave function is $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+})$) the amount of entanglement is given by

$$\xi(|\psi\rangle) = 1 - \int |\langle x_1'|\tilde{\rho}|x_1\rangle|^2\, dx_1' dx_1. \qquad (13)$$

In equations (12) and (13) we have

$$\langle x_1'|\tilde{\rho}|x_1\rangle = \int_{-\infty}^{\infty} \phi(x_1', x_2)\phi^*(x_1, x_2)\, dx_2. \qquad (14)$$

Notice that a two-electrons state with a wave function of the form

$$\frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_2(x_2)-\phi_2(x_1)\phi_1(x_2)\right]\chi_{kk},\quad k=\pm, \tag{15}$$

with $\phi_1(x)$ and $\phi_2(x)$ orthogonal single-particle (coordinate) wave functions, has zero entanglement. This example illustrates an important point already mentioned. The wave function (15) is a Slater determinant. The associated correlations between the two electrons, due entirely to the anti-symmetry requirement on the fermionic state, do not contribute to the entanglement of the state.

3 The Moshinsky atom

The Moshinsky atom [17,18] is a system formed by two harmonically interacting particles confined in a common, external isotropic harmonic potential. In the present work we shall consider only the one dimensional case. The generalization of the present results to higher dimensions is straightforward.

The total Hamiltonian of the system is

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x_1^2}-\frac{1}{2}\frac{\partial^2}{\partial x_2^2}+\frac{1}{2}\omega^2x_1^2+\frac{1}{2}\omega^2x_2^2+\frac{1}{2}\lambda^2(x_1-x_2)^2 \tag{16}$$

where x_1 and x_2 are the coordinates of the two particles, ω is the natural frequency of the external harmonic field, and λ is the natural frequency of the interaction harmonic field. We have used atomic units ($m=1$, $\hbar=1$) throughout the paper, unless indicated otherwise.

Introducing the centre of mass and relative coordinates,

$$R=\frac{1}{\sqrt{2}}(x_1+x_2)\qquad r=\frac{1}{\sqrt{2}}(x_1-x_2), \tag{17}$$

the Hamiltonian factorizes in the following form

$$H=\left(-\frac{1}{2}\frac{\partial^2}{\partial R^2}+\frac{1}{2}\omega^2R^2\right)+\left(-\frac{1}{2}\frac{\partial^2}{\partial r^2}+\frac{1}{2}\Lambda^2r^2\right) \tag{18}$$

where $\Lambda^2=2\lambda^2+\omega^2$. The general eigenfunctions of the system are

$$\Psi(x_1,x_2)=\Psi(R,r)=\hat{\Psi}_{n_R}(R)\tilde{\Psi}_{n_r}(r) \tag{19}$$

with

$$\hat{\Psi}_{n_R}(R)=\left(\frac{\omega^{1/2}}{2^{n_R}n_R!\pi^{1/2}}\right)^{1/2}e^{-\frac{1}{2}\omega R^2}H_{n_R}(\sqrt{\omega}R) \tag{20}$$

and

$$\tilde{\Psi}_{n_r}(r)=\left(\frac{\Lambda^{1/2}}{2^{n_r}n_r!\pi^{1/2}}\right)^{1/2}e^{-\frac{1}{2}\Lambda r^2}H_{n_r}(\sqrt{\Lambda}r), \tag{21}$$

where $H_n(x)$ denote the Hermite polynomials. The eigenenergy of this state is

$$E=E_R+E_r=\omega\left(n_R+\frac{1}{2}\right)+\Lambda\left(n_r+\frac{1}{2}\right). \tag{22}$$

We will denote by $|n_R,n_r\rangle_{Rr}$ the eigenfunctions of the Hamiltonian (18), which are characterized by the two quantum numbers n_R and n_r (to fully define the two-electron system's eigenstates we have to specify also the spin wave function $\xi(\sigma_1,\sigma_2)$). All the (coordinate) wave functions $|n_R,n_r\rangle_{Rr}$ have definite parity, which is determined by the quantum number n_r: even values of n_r correspond to symmetric coordinate eigenfunctions and odd values of n_r to antisymmetric ones. A final remark concerning our notation is in order. A cursory glance at the ket $|n_R,n_r\rangle_{Rr}$ may suggest that it represents a separable state. However, in general, it represents an entangled state of the two electron system (remember that the quantum numbers n_R and n_r refer, respectively, to the centre of mass and relative coordinates of the two particles).

4 Entanglement in the Moshinsky atom

From our previous discussion of quantum entanglement in a two-particle system, it follows that the integrals,

$$\tilde{\rho}(x_1',x_1)=\int_{-\infty}^{\infty}\Psi^*(x_1,x_2)\Psi(x_1',x_2)dx_2, \tag{23}$$

and

$$\mathrm{Tr}[\tilde{\rho}^2]=\int_{-\infty}^{+\infty}|\langle x'|\tilde{\rho}|x\rangle|^2\,dx\,dx', \tag{24}$$

have to be computed in order to evaluate the entanglement associated with a wave function $\Psi(x_1,x_2)$. Both integrals can be calculated exactly for a general eigenfunction (19) of the Moshinsky system. However, since the resulting expressions becomes rather awkward for highly excited states, we are going to compute these quantities only for the ground and first two excited states. Next we are going to provide the final closed expressions for $\mathrm{Tr}[\tilde{\rho}^2]$ (arising from the evaluation of the aforementioned integrals) and discuss the corresponding amounts of entanglement exhibited by each eigenstate. In what follows $\mathrm{Tr}[\tilde{\rho}^2]_{n_R\,n_r}$ denotes value of $\mathrm{Tr}[\tilde{\rho}^2]$ when evaluated on the wave function $|n_R,n_r\rangle_{Rr}$.

4.1 Ground state $|00\rangle_{Rr}$

In this case we have

$$\mathrm{Tr}[\tilde{\rho}^2]_{00}=\frac{2\sqrt{\Lambda\omega}}{\Lambda+\omega}=\frac{\sqrt{2}\sqrt[4]{2\tau^2+1}}{\sqrt{\tau^2+\sqrt{2\tau^2+1}+1}} \tag{25}$$

where

$$\tau=\frac{\lambda}{\omega}. \tag{26}$$

The dimensionless parameter τ constitutes a measure of the relative strength of the interaction between the two particles in the Moshinsky system. When the system is

decoupled we have $\tau = 0$. The larger the value of τ, the larger is the (relative) contribution of the interaction term in the Moshinsky atom. We see from (25) that the entanglement $\mathcal{E}_{00} = 1 - \mathrm{Tr}[\tilde{\rho}^2]_{00}$ of the ground state depends upon the parameters of the Moshinsky atom only through the dimensionless quantity τ.

Decoupling the system, that is, making $\tau \to 0$ (which corresponds, for instance, to $\lambda \to 0$ or equivalently $\Lambda \to \omega$) makes

$$\lim_{\tau\to 0} \mathrm{Tr}[\tilde{\rho}^2]_{00} = 1 \tag{27}$$

showing that in the decoupled system the ground state is not entangled ($\mathcal{E}_{00} = 0$). On the other hand, with maximum coupling ($\tau \to \infty$) we find that

$$\lim_{\tau\to \infty} \mathrm{Tr}[\tilde{\rho}^2]_{00} = 0. \tag{28}$$

Consequently, in this limit we have $\mathcal{E}_{00} = 1 - \mathrm{Tr}[\tilde{\rho}^2]_{00} = 1$. That is, the entanglement measure adopts its maximum possible value.

4.2 First excited states $|10\rangle_{Rr}$ and $|01\rangle_{Rr}$

In this case we have

$$\begin{aligned}\mathrm{Tr}[\tilde{\rho}^2]_{10} &= \frac{\sqrt{\Lambda\omega}\left(3\Lambda^2 + 2\omega\Lambda + 3\omega^2\right)}{2(\Lambda+\omega)^3} \\ &= \frac{\sqrt[4]{2\tau^2+1}\left(3\tau^2 + \sqrt{2\tau^2+1} + 3\right)}{\left(\sqrt{2\tau^2+1}+1\right)^3}\end{aligned} \tag{29}$$

and, consequently,

$$\lim_{\tau\to 0} \mathrm{Tr}[\tilde{\rho}^2]_{10} = \frac{1}{2}. \tag{30}$$

showing that, even if we decouple the system, the state $|10\rangle_{Rr}$ still exhibits a finite, non-vanishing amount of entanglement. However, when $\tau = 0$ we have $\omega = \Lambda$ and the energy eigenvalue corresponding to the eigenstate $|10\rangle_{Rr}$ becomes four-fold degenerate. It then becomes possible to choose a new set of four eigenstates (with the same eigenenergy) exhibiting zero entanglement. If we consider the Moshinsky atom in the original coordinate system $x_{1,2}$, we see that when $\lambda = 0$, the Moshinsky system consists of two independent one-dimensional harmonic oscillators with the same natural frequency. Let us denote by $|n\rangle$ $(n = 0, 1, 2, \ldots)$ the eigenstates of each of these oscillators. The kets $|n, \pm\rangle$ $(n = 0, 1, 2, \ldots)$, using standard self-explanatory notation, constitute a single-particle orthonormal basis. For $\tau = 0$ we can choose the four eigenstates (all with the same energy as $|10\rangle_{Rr}$)

$$\begin{aligned}&\frac{1}{\sqrt{2}}(|0,+\rangle|1,+\rangle - |1,+\rangle|0,+\rangle),\\ &\frac{1}{\sqrt{2}}(|0,+\rangle|1,-\rangle - |1,-\rangle|0,+\rangle),\\ &\frac{1}{\sqrt{2}}(|0,-\rangle|1,+\rangle - |1,+\rangle|0,-\rangle),\\ &\frac{1}{\sqrt{2}}(|0,-\rangle|1,-\rangle - |1,-\rangle|0,-\rangle),\end{aligned} \tag{31}$$

which are represented by a Slater determinant and thus have zero entanglement. It must be stressed that the case $\tau = 0$ allows for this particular set of eigenstates because of the degeneracy exhibited by the energy levels of the Moshinsky model when there is no interaction between the particles. On the contrary, eigenstates of zero entanglement do not exist for arbitrary values of τ.

In the limit of maximum coupling we have

$$\lim_{\tau\to \infty} \mathrm{Tr}[\tilde{\rho}^2]_{10} = 0, \tag{32}$$

which means maximum entanglement $\mathcal{E}_{10} = 1$, as expected.

For the first excited state $|01\rangle_{Rr}$ the quantity $\mathrm{Tr}[\tilde{\rho}^2]_{01}$ is also given by expression (29). Therefore, the measures of entanglement of the states $|10\rangle_{Rr}$ and $|01\rangle_{Rr}$ are exactly the same (and also the conclusions).

4.3 Second excited state $|11\rangle_{Rr}$

In this case we have

$$\begin{aligned}\mathrm{Tr}[\tilde{\rho}^2]_{11} &= \frac{\sqrt{\Lambda\omega}\left(9\Lambda^4 - 4\omega\Lambda^3 + 118\omega^2\Lambda^2 - 4\omega^3\Lambda + 9\omega^4\right)}{8(\Lambda+\omega)^5} \\ &= \frac{\sqrt[4]{2\tau^2+1}\left(9\tau^4+68\tau^2 - 2\left(\tau^2+1\right)\sqrt{2\tau^2+1} + 34\right)}{2\left(\sqrt{2\tau^2+1}+1\right)^5}\end{aligned} \tag{33}$$

then

$$\lim_{\tau\to 0} \mathrm{Tr}[\tilde{\rho}^2]_{11} = \frac{1}{2}. \tag{34}$$

We see that, also in this case, the eigenstate $|11\rangle_{Rr}$ remains entangled even in the decoupled limit $\tau \to 0$. Again, when $\tau = 0$ and the two particles are non-interacting, the degeneracy of the concomitant energy level allows for choosing a new set of eigenstates exhibiting zero entanglement.

In the limit of maximum coupling we have

$$\lim_{\tau\to \infty} \mathrm{Tr}[\tilde{\rho}^2]_{11} = 0, \tag{35}$$

corresponding to maximum entanglement $\mathcal{E}_{11} = 1$.

4.4 Second excited states $|20\rangle_{Rr}$ and $|02\rangle_{Rr}$

Now we find

$$\begin{aligned}&\mathrm{Tr}[\tilde{\rho}^2]_{20} = \\ &\frac{\sqrt{\Lambda}\sqrt{\omega}\left(41\Lambda^4 + 60\omega\Lambda^3 + 182\omega^2\Lambda^2 + 60\omega^3\Lambda + 41\omega^4\right)}{32(\Lambda+\omega)^5} \\ &= \frac{\sqrt[4]{2\tau^2+1}\left(41\tau^4+132\tau^2+30\left(\tau^2+1\right)\sqrt{2\tau^2+1}+66\right)}{8\left(\sqrt{2\tau^2+1}+1\right)^5}.\end{aligned} \tag{36}$$

In the decoupled limit we have

$$\lim_{\tau\to 0} \mathrm{Tr}[\tilde{\rho}^2]_{20} = \frac{3}{8}, \tag{37}$$

and, consequently, a non-zero amount of entanglement $\mathcal{E}_{20} = \frac{5}{8}$. As happens with the eigenstates discussed previously, when $\tau = 0$ the entangled eigenstate $|20\rangle_{Rr}$ corresponds to a degenerate energy level and due to this degeneracy it is possible to find another set of eigenstates exhibiting no entanglement. In the limit of strong coupling we have

$$\lim_{\tau\to\infty} \mathrm{Tr}[\tilde{\rho}^2]_{20} = 0, \tag{38}$$

corresponding to maximum entanglement.

In the case of the second excited state $|02\rangle_{Rr}$ the expression for $\mathrm{Tr}[\tilde{\rho}^2]_{02}$ is again given by (36). Consequently, the behavior of the entanglement measure $\mathcal{E}$ as a function of the parameter τ is the same for states $|02\rangle_{Rr}$ and $|20\rangle_{Rr}$. In both cases we have maximum entanglement in the limit $\tau \to \infty$. In the decoupled limit, the state $|02\rangle_{Rr}$ still has non-vanishing entanglement. When $\tau = 0$ this eigenstate corresponds to the same degenerate eigenvalue as $|20\rangle_{Rr}$ and, as we already said, there is another set of eigenstates (for the same energy eigenvalue) endowed with no entanglement.

An interesting feature of the above analytical expressions for $\mathrm{Tr}[\tilde{\rho}^2]_{n_R\, n_r}$ (and, consequently, of the expressions for the amount of entanglement $\mathcal{E}$ exhibited by the eigenstates of the Moshinsky atom) is that these expressions are symmetrical in the frequencies ω and Λ. In order to shed some light on this symmetry let us consider the Moshinsky Hamiltonian H' corresponding to permuted values of the frequencies ω and Λ. That is, the frequencies ω' and Λ' associated with H' are related to the frequencies ω and Λ of H by

$$\begin{aligned} \omega' &= \Lambda \\ \Lambda' &= \omega. \end{aligned} \tag{39}$$

The relations (39) are equivalent to the following relations between the parameters ω' and λ' characterizing the Hamiltonian H' and the parameters ω and λ corresponding to H,

$$\begin{aligned} \omega'^2 &= 2\lambda^2 + \omega^2 \\ \lambda'^2 &= -\lambda^2. \end{aligned} \tag{40}$$

It can be verified that the Moshinsky Hamiltonian H' with parameters given by (40) can be written in terms of ω and λ as,

$$H' = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}\omega^2 x_1^2 + \frac{1}{2}\omega^2 x_2^2 + \frac{1}{2}\lambda^2 (x_1 + x_2)^2. \tag{41}$$

Now, if $\Psi(x_1, x_2)$ is an eigenfunction of the Moshinsky Hamiltonian H (given by Eq. (16)) it is clear that

$$\Psi'(x_1, x_2) = \Psi(x_1, -x_2), \tag{42}$$

is an eigenfunction of H'. The quantum numbers n'_R and n'_r corresponding to $\Psi'(x_1, x_2)$ are related to those of $\Psi(x_1, x_2)$ by

$$n'_R = n_r; \quad n'_r = n_R. \tag{43}$$

It is also plain from (42) that the quantity $\mathrm{Tr}[\tilde{\rho}^2]$ has the same value when evaluated upon $\Psi(x_1, x_2)$ or $\Psi'(x_1, x_2)$. Consequently, remembering that the Moshinsky Hamiltonian H' is obtained from H by permuting the frequencies ω and Λ, it follows that

$$\mathrm{Tr}[\tilde{\rho}^2]^{(\omega,\Lambda)}_{n_R\, n_r} = \mathrm{Tr}[\tilde{\rho}^2]^{(\Lambda,\omega)}_{n_r\, n_R}. \tag{44}$$

An immediate consequence of the last equation is that, for those eigenstates of the Moshinsky atom with equal quantum numbers, $n_R = n_r$, *the expression for* $\mathrm{Tr}[\tilde{\rho}^2]_{n_r\, n_r}$ *is symmetrical in* ω *and* Λ. We have already verified this property in the particular cases of $\mathrm{Tr}[\tilde{\rho}^2]_{00}$ and $\mathrm{Tr}[\tilde{\rho}^2]_{11}$. The explicit expressions obtained for $\mathrm{Tr}[\tilde{\rho}^2]_{01}$ and $\mathrm{Tr}[\tilde{\rho}^2]_{02}$ are also symmetrical in ω and Λ. We conjecture that this symmetry holds in general for all values of the quantum numbers n_R and n_r, but a general proof of this property has eluded us. Notice that the symmetry that we are conjecturing is different from the one given by (44) because it requires the invariance of $\mathrm{Tr}[\tilde{\rho}^2]_{n_R\, n_r}$ under the permutation of ω and Λ without permuting at the same time the quantum numbers n_R and n_r.

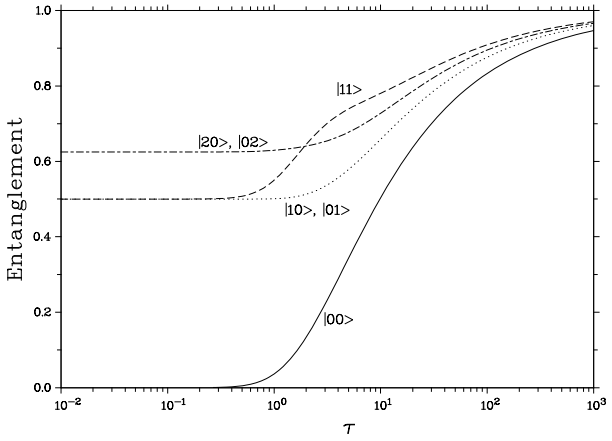

Fig. 1. Entanglement of the ground, first, and second excited states (with anti-parallel spins) of the Moshinsky atom as a function of the parameter τ. All depicted quantities are dimensionless.

The behavior of the amount of entanglement $\mathcal{E}$ as a function of τ for various eigenstates of the Moshinsky atom is shown in Figures 1 and 2 as a function of the relative interaction strength τ of its two constituent particles. In Figure 1 the entanglement $\mathcal{E}$ is plotted against τ for eigenstates with anti-parallel spins (eigenstates with symmetric coordinate wave functions and eigenstates with antisymmetric coordinate wave functions, are both represented in this figure). In Figure 2 we compare (for eigenstates with anti-symmetric coordinate wave functions) the entanglement exhibited by states with parallel (dashed line) and anti-parallel (continuous line) spins.

We encounter two general trends: (i) the entanglement increases monotonically with τ and, consequently, with the strength of the interaction between the particles and (ii) the amount of entanglement also tends to increase when we consider higher excited states (that is, it increases with the energy). There are, however, exceptions to this last rule. For large enough values of the interaction parameter τ the state $|11\rangle_{Rr}$ (with anti-parallel

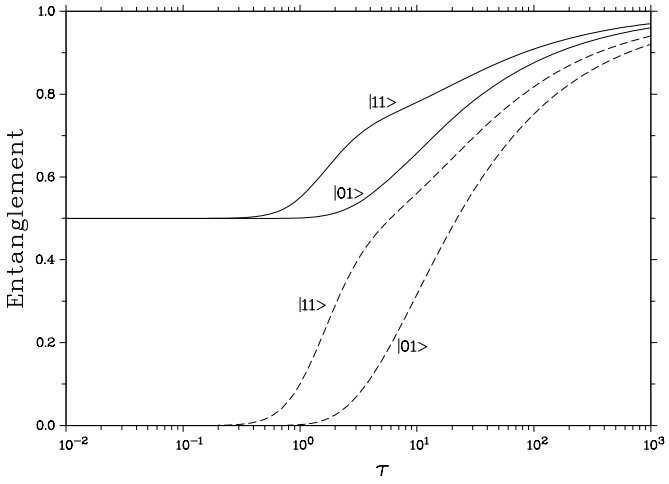

Fig. 2. Entanglement of the first and second excited states of the Moshinsky model with antisymmetric coordinate wave function. Solid lines correspond to eigenstates with anti-parallel spins and dashed lines to eigenstates with parallel spins. All depicted quantities are dimensionless.

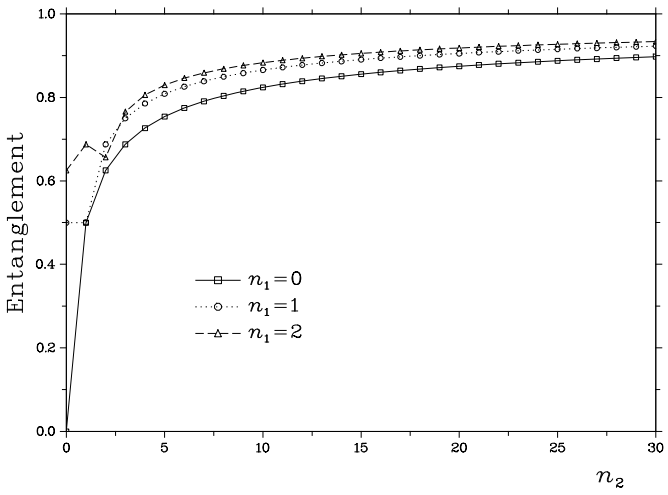

Fig. 3. Entanglement in the limit of weak interaction, as a function of the quantum number n_2, exhibited by the eigenstates $|0,n_2\rangle$, $|1,n_2\rangle$, and $|2,n_2\rangle$ (with anti-parallel spins). All depicted quantities are dimensionless.

spins) has higher entanglement than the state $|02\rangle_{Rr}$ (also with anti-parallel spins). In point of fact, as the parameter τ increases, these two states exhibit an interesting "entanglement level-crossing".

It can be appreciated in Figure 2 that, for eigenstates sharing the same anti-symmetric coordinate wave functions, the eigenstates with parallel spins have less entanglement than the eigenstates with anti-parallel spins. In fact, this is a general property of the eigenstates with anti-symmetric coordinate wave functions, not restricted to the states considered in Figure 2. This property follows directly from equation (11). The eigenstates with parallel spins have $\mathrm{Tr}\left[\tilde{\rho}_s^2\right] = 1$, while the eigenstates with anti-parallel spins have $\mathrm{Tr}\left[\tilde{\rho}_s^2\right] = 1/2$ and, as a consequence of (11), are endowed with a larger amount of entanglement.

It is also interesting that, as already mentioned, the entanglement of excited eigenstates with anti-parallel spins does not go to zero in the limit $\tau \to 0$. This means that *an arbitrarily weak (but non-zero) interaction already leads to excited eigenstates exhibiting a considerable amount of entanglement*. On the other hand, as already explained, in the decoupled system corresponding to $\tau = 0$ these states correspond to degenerate eigenenergies and the degeneracy enables one to find an alternative set of non-entangled eigenstates with the same energies. However, when $\tau > 0$ the degeneracy is lifted by the interaction and the aforementioned eigenstates are now necessarily entangled. It is worth stressing that the finite amount of entanglement corresponding to the limit $\tau \to 0$ is not due to the correlations arising exclusively from the antisymmetric nature of the (global) fermionic states. As already mentioned, these correlations do not contribute to the entanglement of the state. The amount of entanglement exhibited by the excited states (with anti-parallel spins) in the limit of weak interaction increases monotonically with the energy of the states. This behavior can be clearly observed in Figure 3, where the entanglement corresponding to the limit $\tau \to 0$ is plotted as a function of the quantum number n_2 for states of the form $|0,n_2\rangle$, $|1,n_2\rangle$, and $|2,n_2\rangle$, all with anti-parallel spins. It is remarkable that the entanglement exhibited by these states (which is clearly a non-classical feature) increases with n_2 in spite of the fact that various important properties of states with large quantum numbers yield to a semiclassical description.

As a final remark on the entanglement properties of the eigenstates of the Moshinsky atom it must be noticed that, due to degeneracy, the energy eigenbasis of the Moshinsky atom that we have considered is not unique. We have discussed energy eigenstates of the form (8), where the spin wave function is equal to $\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{+-})$ when the coordinate wave functions is symmetric, and it is equal to either χ_{++}, χ_{--}, or $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{+-})$ when the coordinate wave function is anti-symmetric. Now, the eigenstates with a symmetric coordinate wave function are in general non-degenerate and consequently unique. On the contrary, the eigenstates with anti-symmetric coordinate wave functions are three-fold degenerate, since the three eigenstates corresponding to the three above mentioned spin wave functions (and having the same coordinate wave function) share the same eigenenergy. Consequently, any (normalized) linear combination of these three eigenstates is still a legitimate eigenstate of the Moshinsky atom sharing the alluded eigenenergy. Any of these possible eigenstates still has the factorized form (8), even if the spin wave function is not χ_{++}, χ_{--}, or $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{+-})$. The entanglement $\mathcal{E}$ associated with any of these eigenstates having the same anti-symmetric coordinate wave function (and the same eigenenergy) is within the range

$$1 - 2\mathrm{Tr}[\tilde{\rho}^2]_{n_R n_r} \leq \mathcal{E} \leq 1 - \mathrm{Tr}[\tilde{\rho}^2]_{n_R n_r}, \qquad (45)$$

where the upper bound corresponds to anti-parallel spins ($\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{+-})$) and the lower bound corresponds to

parallel spins (χ_{++} or χ_{--}). It is worth stressing that, excepting the cases of $|01\rangle_{Rr}$ and $|11\rangle_{Rr}$ with parallel spins, *all these eigenstates share the property that their entanglement tends to a finite, non-zero value when* τ *goes to zero*. However, as already mentioned, in the case of strictly zero interaction (that is when $\tau = 0$) an extra degeneracy appears, and it is then possible to construct eigenstates of zero entanglement, which are no longer of the factorized form (8). One more comment is here in order. Having the factorized form is not a sufficient, nor a necessary condition for being entangled. A state of two spin-1/2 particles having the factorized form (8) may be separable or entangled. The same happens with non-factorized states.

It would be interesting to investigate which of the entanglement properties exhibited by the excited states of the Moshinsky model are shared by the excited states of other, more realistic two-electron models. A promising way to pursue this line of research would be to investigate the entanglement properties of the (semi-analytic) approximate wave functions for the eigenstates of many-electron systems obtained by recourse to the generalized Sturmian technique developed by Avery and Avery [30].

5 Hartree-Fock approximation, correlation energy, and entanglement

The Hartree-Fock approximation has played a distinguished role in atomic and nuclear physics, and in quantum many-body physics in general. The validity of this approximation is closely related to the entanglement exhibited by the (exact) eigenstates of a given quantum many body-system. Indeed, in contemporary quantum mechanical parlance, the Hartree-Fock approximation can be described, basically, as a "zero entanglement approximation". The aim of the present section is to explore quantitatively, in the context of the exactly soluble Moshinsky model, the connection between entanglement and the Hartree-Fock approximation, emphasizing that the amount of entanglement of an exact eigenstate is the main property determining how good the corresponding Hartree-Fock approximation is.

Let us now consider the relationship between the Hartree-Fock approximation and the entanglement of the energy eigenstates of the Moshinsky atom. The Hartree-Fock ansatz is

$$\Phi(x_1, x_2) = \phi(x_1)\phi(x_2) \tag{46}$$

where $\phi(x_1)$ verifies

$$-\frac{1}{2}\frac{d^2\phi(x_1)}{dx_1^2} + \frac{1}{2}\omega^2 x_1^2\phi(x_1) + \frac{\lambda^2}{2}\left(\int_{-\infty}^{+\infty}\phi^2(x_2)(x_1-x_2)^2dx_2\right)\phi(x_1) = \epsilon\phi(x_1). \tag{47}$$

By parity considerations, this equation reduces to:

$$-\frac{1}{2}\frac{d^2\phi(x_1)}{dx_1^2} + \frac{1}{2}(\omega^2+\lambda^2)x_1^2\phi(x_1) + \frac{\lambda^2}{2}\left(\int_{-\infty}^{+\infty}\phi^2(x_2)x_2^2dx_2\right)\phi(x_1) = \epsilon\phi(x_1). \tag{48}$$

The ground state solution of the above equation is

$$\phi(x_1) = \left(\frac{\sqrt{\omega^2+\lambda^2}}{\pi}\right)^{1/4} e^{-\frac{1}{2}\sqrt{\omega^2+\lambda^2}x_1^2} \tag{49}$$

with

$$\epsilon = \frac{2\omega^2+3\lambda^2}{4\sqrt{\omega^2+\lambda^2}}. \tag{50}$$

So the Hartree-Fock solution for the ground state is [17]

$$\Phi(x_1, x_2) = \left(\frac{\sqrt{\omega^2+\lambda^2}}{\pi}\right)^{1/2} e^{-\frac{1}{2}\sqrt{\omega^2+\lambda^2}(x_1^2+x_2^2)} \tag{51}$$

with Hartree-Fock energy:

$$E_{HF} = \sqrt{\omega^2+\lambda^2}. \tag{52}$$

The correlation energy is defined as the difference between the exact and the Hartree-Fock energies of a given eigenstate, so that for the ground state one has

$$E_c = E - E_{HF} = \frac{\omega+\Lambda}{2} - \sqrt{\omega^2+\lambda^2} = \frac{\omega+\sqrt{2\lambda^2+\omega^2}-2\sqrt{\omega^2+\lambda^2}}{2}. \tag{53}$$

In terms of $\tau = \frac{\lambda}{\omega}$ this expression can be written as

$$E_c = \frac{1}{2}\omega\left(1+\sqrt{2\tau^2+1}-2\sqrt{\tau^2+1}\right). \tag{54}$$

Another important quantity indicating the quality of the Hartree-Fock approximation is given by the overlap between the exact wave function and the Hartree-Fock wave function,

$$O = \langle\Psi|\Phi\rangle = \frac{2\sqrt{2}\sqrt[4]{\omega}\sqrt[4]{\lambda^2+\omega^2}\sqrt[8]{2\lambda^2+\omega^2}}{\sqrt{\omega+\sqrt{2\lambda^2+\omega^2}}\sqrt{\omega+2\sqrt{\lambda^2+\omega^2}+\sqrt{2\lambda^2+\omega^2}}}. \tag{55}$$

In the Moshinsky system, the overlap O can be expressed in terms of τ,

$$O = \frac{2\sqrt{2}\sqrt[4]{\tau^2+1}\sqrt[8]{2\tau^2+1}}{\sqrt{\sqrt{2\tau^2+1}+1}\sqrt{2\sqrt{\tau^2+1}+\sqrt{2\tau^2+1}+1}}. \tag{56}$$

It can be verified that the limits of the overlap (for $\tau \to 0$ and $\tau \to \infty$) are

$$\lim_{\tau\to 0} O = 1, \tag{57}$$

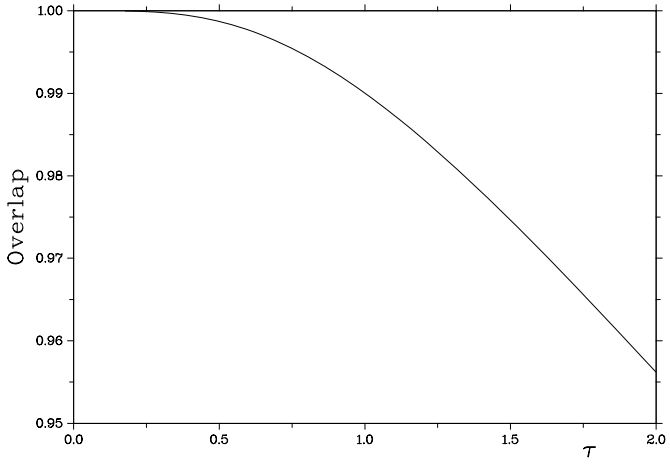

Fig. 4. Overlap between the exact ground state wave function and the corresponding Hartree-Fock approximation, plotted as a function of the parameter τ. All depicted quantities are dimensionless.

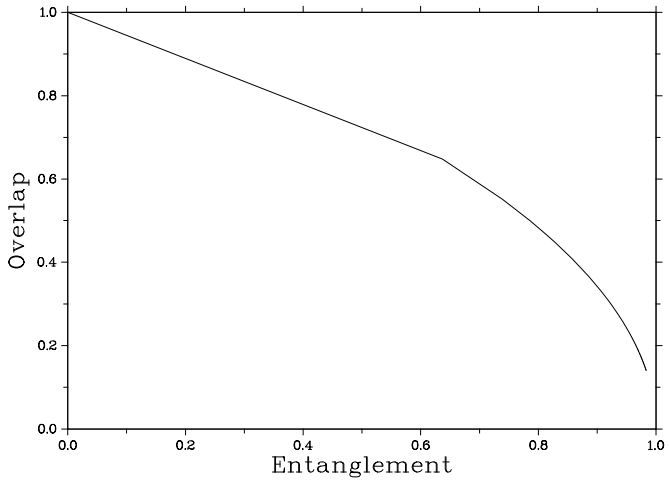

Fig. 5. Overlap between the exact ground state wave function and the corresponding Hartree-Fock approximation, plotted as a function of the ground state's entanglement $\mathcal{E}$. All depicted quantities are dimensionless.

and

$$\lim_{\tau \to \infty} O = 0. \tag{58}$$

The above limiting values are physically sensible. For the decoupled system the Hartree-Fock approximation yields an exact eigenfunction. On the other hand, as the interaction term in the Hamiltonian becomes dominant the quality of the Hartree-Fock approximation deteriorates and the overlap tends to zero. This behavior can be seen in Figure 4, where the overlap is plotted against τ.

Finally, it is instructive to consider the relationship between the overlap, the correlation energy, and the entanglement of the Moshinsky atom ground state. In Figures 5 and 6 the overlap and the correlation energy, respectively, are depicted as a function of $\mathcal{E}$, we take $\omega = 1$ without any loss of generality. As physically expected, the overlap decreases while the correlation energy increases

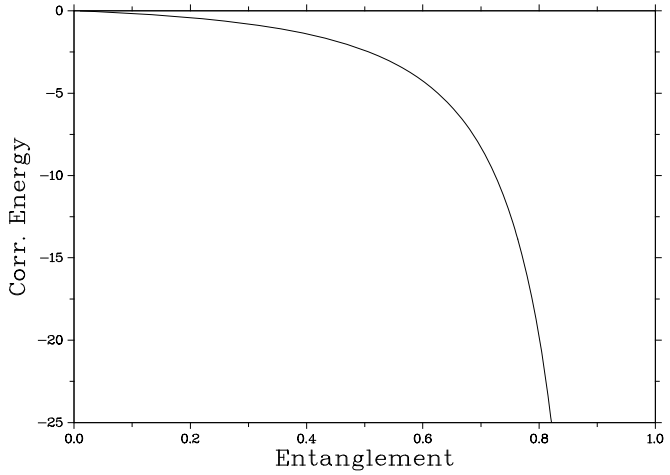

Fig. 6. Correlation energy of the ground state (in atomic units) plotted as a function of the ground state's entanglement $\mathcal{E}$ (this quantity is dimensionless).

with the the amount of entanglement exhibited by the ground state. The results presented by us in this section concerning the relationship between entanglement and the Hartree-Fock approximation in the Moshinsky model are fully consistent with the results reported by Amovilli and March (AM) in [7]. The difference between our study and the one performed by AM is that we have done exact entanglement calculations using an entanglement measure based upon the linear entropy, while AM did approximate calculations using an entanglement measure based on the von Neumann entropy.

6 Conclusions

In the present effort we have considered the entanglement properties of various energy eigenstates of the Moshinsky atom. The amount of entanglement contained in these eigenstates depends solely upon a dimensionless parameter τ that measures the (relative) weight of the interaction term in the Hamiltonian. We computed *exactly* the entanglement of the aforementioned bound states, obtaining closed analytical expressions for the entanglement as a function of τ. As a general trend we found that, as τ increases (that is, as the interaction becomes more important) the amount of entanglement exhibited by the atomic states increases as well. Moreover, entanglement tends to increase when more highly excited states are considered. There are, however, "entanglement level-crossings" where the entanglement of a state becomes larger than the entanglement of another state of higher energy.

Excited states with anti-parallel spins exhibit a considerable amount of entanglement even in the case of an arbitrarily weak (but non-zero) interaction. This amount of entanglement increases monotonically with the energy of the concomitant eigenstates. It is worth stressing that this "minimum" entanglement appearing in the limit of weak interactions is not due to the minimum correlations required to comply with the antisymmetric character of

the fermionic wave functions: these correlations do not contribute to the entanglement associated with the two-electrons states.

The connection between the entanglement of the atomic states and the celebrated Hartree-Fock approximation was also addressed. The quality of this approximation can be estimated by recourse to the overlap O between the exact wave functions and the Hartree-Fock ones. Another physically relevant quantity is the correlation energy, defined as the difference between the exact eigenenergies of the system and the energies provided by the Hartree-Fock scheme. For the Moshinsky atom both quantities depend on the system's parameter only through τ. This allows us to determine functional relationships between the entanglement of the atomic states, on the one hand, and the overlap and correlation energy, on the other one. We found that the overlap decreases when the entanglement increases, while the correlation energy increases with entanglement.

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