Measures of spatial entanglement in a two-electron model atom

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Different entropies which can characterize the inseparable quantum correlation in a two-electron entangled artificial atom proposed by Moshinsky are analyzed. The analysis is based on an exact representation for the trace of the q-order one-body reduced density matrix in terms of the interparticle coupling. The entanglement spectrum of the model system and the possible role of the entropy-maximum concept to practical applications of matrices are discussed as well. The ground-state energy, readily obtained from the Schrödinger Hamiltonian, is recalculated within a density-matrix-functional representation for its components.

I. INTRODUCTION

The symmetrization postulate states that two fermions, say electrons, have only antisymmetric states. In other words, the full state function must change sign when the electrons are interchanged. When the two electrons are moving in an external confining field, as in an atom, the spatial part of the full ground-state function is symmetric. Therefore, it must be multiplied by an antisymmetric singlet spin-state function. This construction remains true if, beyond the confinement, there is interaction between the electrons which depends on their coordinates. With no coupling between the two electrons, the spatial wave function is a simple product of single-particle eigenstates. The product eigenfunctions describe stationary states of the system, and the position probability density does not exhibit correlation between the positions of the two electrons.

In the ground state of the two-electron system the spin part is a singlet and thus is always maximally entangled. When there is an interparticle coupling, the spatial function can show positional correlation. One then expects that interaction-induced correlation, named as spatial entanglement, can have important effects in various applications. This spatial entanglement depends on the interplay of the interelectron interaction and the strength of the external confining field. Currently, the characterization of *inseparable* correlation has become one of the most active research fields and an intense interdisciplinary effort is directed at analyzing this remarkable feature of quantum mechanics.

The present paper is devoted to a specific application along this line. Namely, we deduce different entropies motivated by a model two-electron atom introduced by Moshinsky [1]. The Hamilton operator of our system is taken as follows:

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}m\omega_0^2(\mathbf{r}_1^2 + \mathbf{r}_2^2) + \frac{1}{2}m\Lambda\omega_0^2(\mathbf{r_1} - \mathbf{r_2})^2,$$

(1)

where Λ is a convenient coupling parameter; $\Lambda=0$ refers to the noninteracting case. From now on we shall use Hartree atomic units, $e^2 = \hbar = m = 1$. Values $\Lambda < 0$ describe a repulsive electron-electron interaction, whereas $\Lambda > 0$ corresponds to an attractive interaction. The ground state is always bounded

for attractive pair interaction for any $0 < \Lambda < \infty$, however, a strong repulsive interaction destabilizes (see Sec. II below) the system for $\Lambda < -1/2$.

Of course, since the entropies are not expectation values of operators of the Hilbert space of the system like most of the fundamental quantities in position and momentum space, elucidation of their physical significance is important to understand their role in characterizing and representing electronic systems. Detailed knowledge of different entropies, combined with other concepts of physics (such as the maximum-entropy principle), may contribute to the practical problem of characterization of correlation in a sufficiently precise way.

The exact solution of Moshinsky's model was used [2] to a detailed discussion on the capability of the energy-optimal Hartree-Fock (HF) method which is based on a product-state approximation for the spatial wave function. In this standard method, which may be considered as a variational attempt, the last term of the rewritten Hamiltonian,

$$\hat{H} = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}\Omega_0^2(\mathbf{r}_1^2 + \mathbf{r}_2^2) - \Lambda\omega_0^2\mathbf{r}_1 \cdot \mathbf{r}_2,$$

(2)

does not contribute to the ground-state energy due to parity considerations in angle integration. The shifted frequency is $\Omega_0 = \omega_0\sqrt{1+\Lambda}$, and the ground-state energy is $E_{\mathrm{gr}}^{\mathrm{HF}} = 2(D/2)\Omega_0$ in dimension D. This expression gives a $\Lambda=-1$ limit value for the coupling. The $[E_{\mathrm{gr}}^{\mathrm{HF}}(\Lambda) - E_{\mathrm{gr}}^{\mathrm{HF}}(\Lambda=0)]$ interaction-energy scales as $(D/2)\Lambda\omega_0$ for $\Lambda \to 0$. At $\Lambda \to -1$ (from above) in the repulsive case the HF product wave function,

$$\psi^{\mathrm{HF}}(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{\Omega_0}{\pi}\right)^{D/2} e^{-(1/2)\Omega_0 r_1^2} e^{-(1/2)\Omega_0 r_2^2},$$

(3)

becomes more and more extended ($\Omega_0 \to 0$), showing an effect of interparticle repulsion. The antisymmetry of the complete two-particle wave function is ensured by multiplying the spin free part ψ^{HF} by the singlet two-particle spin function. The form of the Hamilton operator and the above Hartree-Fock expressions show that it is the $\Lambda\omega_0^2\mathbf{r}_1 \cdot \mathbf{r}_2$ term which results in an inseparable correlation in Moshinsky's two-electron model.

Recent studies, based on the exact solution [1–3], have been dedicated to the pair function at electron coincidence

[4], the one-particle density matrix [5], and the so-called Fisher information [6]. Amovilli and March [7] studied Shannon entropies based on one-particle and two-particle density functions analytically and the Jaynes entropy by using an expansion based on nonorthogonal basis functions to model the natural orbitals of the one-particle density matrix *approximately*. This fact gives a particularly strong motivation to the present work on entropies. In this work we give an *exact* representation for the trace of the *q*-order one-body reduced density matrix in terms of the interparticle coupling.

The paper is organized as follows. In Sec. II A, we outline the exact solution for the spatial wave function based on Eq. (1). Section II B is devoted to the details of deducing various entropies and the entanglement spectrum. Comparisons of the entropies are given there with relevant discussions. The paper ends with a short summary in Sec. III.

II. THEORY AND RESULTS

In order to provide a self-contained presentation and to summarize notation, we start by outlining the exact solution for the spatial wave function in Sec. II A. Then an analysis of entropies is given in Sec. II B.

A. Wave function and one-particle density matrix

Following the earlier works [1,2], we introduce the variables $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/\sqrt{2}$ and $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)/\sqrt{2}$ and write the Hamiltonian (in a.u.) as

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial \mathbf{R}^2} + \frac{\partial^2}{\partial \mathbf{r}^2}\right) + \frac{1}{2}\omega_+^2 \mathbf{R}^2 + \frac{1}{2}\omega_-^2 \mathbf{r}^2, \quad (4)$$

where $\omega_+^2 = \Omega_0^2 - \Lambda\omega_0^2 = \omega_0^2$ and $\omega_-^2 = \Omega_0^2 + \Lambda\omega_0^2 = \omega_0^2(1+2\Lambda)$. Thus one has two uncoupled harmonic oscillators in Eq. (4), and the ground-state space wave function is a product of two Gaussian functions of the variables $\mathbf{R}$ and $\mathbf{r}$. By an inverse transformation, one arrives at the normalized eigenfunction of Eq. (1), given by

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{\omega_-\omega_+}{\pi^2}\right)^{D/4} e^{-(1/2)\Omega_1(r_1^2 + r_2^2)} e^{(1/2)\Omega_2 \mathbf{r}_1 \cdot \mathbf{r}_2}, \quad (5)$$

in which $\Omega_1 = (\omega_- + \omega_+)/2$ and $\Omega_2 = (\omega_- - \omega_+)$ are abbreviations. Again, antisymmetry is ensured by multiplying Eq. (5) by the antisymmetric spin function,

$$\chi(\sigma_1, \sigma_2) = -\chi(\sigma_2, \sigma_1) = 2^{-1/2}[\alpha(\sigma_1)\beta(\sigma_2) - \beta(\sigma_1)\alpha(\sigma_2)]. \quad (6)$$

The quite simple expression, $E_{gr}(\Lambda) = (D/2)(\omega_+ + \omega_-) = (D/2)\omega_0(1 + \sqrt{1+2\Lambda})$, gives the ground-state energy. Wigner's correlation energy, $E_c(\Lambda) = [E_{gr}(\Lambda) - E_{gr}^{HF}(\Lambda)]$, behaves as $-(D/8)\Lambda^2\omega_0$, while $[E_{gr}(\Lambda) - E_{gr}(\Lambda=0)]$ as $(D/2)\Lambda\omega_0$ at small $(\Lambda \to 0)$ interparticle coupling. The above exact expressions show that the physical limit is, in fact, $\Lambda = -1/2$ in the repulsive case [3]. The destabilization occurs at smaller absolute value of the coupling than in the HF approximation showing a remarkable effect of an inseparable correlation.

The one-particle density matrix is based on the standard definition

$$\gamma(\mathbf{r}_1, \mathbf{r}_2) = \int \psi(\mathbf{r}_1, \mathbf{r}_3)\psi^*(\mathbf{r}_2, \mathbf{r}_3)d\mathbf{r}_3 \quad (7)$$

and has the following illustrative form in our case:

$$\gamma(\mathbf{r}_1, \mathbf{r}_2) = A e^{-a(r_1^2 + r_2^2)} e^{b\mathbf{r}_1 \cdot \mathbf{r}_2}. \quad (8)$$

Here $a = (8\Omega_1^2 - \Omega_2^2)/16\Omega_1$, $b = \Omega_2^2/8\Omega_1$, and $A = [(2a - b)/\pi]^{D/2}$ using von Neumann's normalization Tr $\gamma = 1$. The spin part of the density matrix is $\Sigma_{\sigma_3}\chi(\sigma_1, \sigma_3)\chi^*(\sigma_2, \sigma_3) = \mathcal{I}_s/2$, where $\mathcal{I}_s$ is the identity matrix in the spin space with Tr $\mathcal{I}_s/2 = 1$.

The diagonal, $\mathbf{r}_1 = \mathbf{r}_2 \equiv \mathbf{x}$, of the one-particle density-matrix results in the density distribution,

$$\rho(\mathbf{x}) = \left(\frac{2a - b}{\pi}\right)^{D/2} e^{-(2a-b)x^2}, \quad (9)$$

where $(2a - b) = 2\omega_+\omega_-/(\omega_+ + \omega_-) = 2\omega_0\sqrt{1+2\Lambda}/(1 + \sqrt{1+2\Lambda})$. This density distribution, the $n_2(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi^2(\mathbf{r}_1, \mathbf{r}_2)$ two-particle density [3,4], and the ground-state energy, similarly to the exact eigenfunction, show a clear difference between the attractive $(\Lambda > 0)$ and repulsive $(\Lambda < 0)$ cases. The different *entropies* are, however, *not able* to distinguish between these physical cases of interparticle coupling as we will show below.

B. Quantum entropies of the ground state

Following recent studies [8,9] on spatial entanglements of two electrons, first we calculate the linear entropy L from the following equation,

$$L = 1 - \Pi(\gamma), \quad (10)$$

using the reduced density matrix to the purity $\Pi(\gamma) = \text{Tr } \gamma^2$. The square is given by

$$\gamma^2(\mathbf{r}_1, \mathbf{r}_2) = \int \gamma(\mathbf{r}_1, \mathbf{r}_3)\gamma(\mathbf{r}_3, \mathbf{r}_2)d\mathbf{r}_3, \quad (11)$$

and one has a quite simple form,

$$\Pi(\gamma) = \int \gamma^2(\mathbf{r}, \mathbf{r})d\mathbf{r}, \quad (12)$$

to the implementation of a measure on the interaction-driven spatial entanglement. Using Eq. (8) and performing the integrations in the above equations, we obtain

$$L = 1 - \lambda^D, \quad (13)$$

where $\lambda = 2\sqrt{\omega_+\omega_-}/(\omega_+ + \omega_-)$, i.e., the ratio of the geometric and arithmetic means of frequencies introduced at Eq. (4); $\lambda(\Lambda) \in [0, 1]$. In the noninteracting $(\Lambda = 0)$ case $\lambda = 1$. For small values of Λ we get $\Pi(\Lambda) = 1 - (D/8)\Lambda^2$, which results in a quadratic dependence of L on coupling, as in the case of the dimensionless correlation energy $E_c(\Lambda)/\omega_0$.

Notice at this point that a similar quadratic deviation from unity in the corresponding Π at small coupling appears in the one-dimensional problem [9] of interaction-induced orbital entanglement of two electrons incident on a quantum dot in a spin-singlet state. In our problem and in the HF approxima-

tion, $\Pi^{HF}(\Lambda)=1$ (as in the noninteracting, $\Lambda=0$, case) independently of the sign of the (allowed) coupling parameter. The exact purity behaves as $\Pi(\Lambda)\to 0$ for $\Lambda\to\infty$ in the attractive case and for $\Lambda\to-1/2$ (from above) in the repulsive case. Therefore, the effect of an inseparable correlation is robust in these measures. A destabilization, due to a finite interparticle repulsion in a given confinement field, results in a similar effect in L as an infinite interparticle attraction in the same external field.

A logical extension of the above concept is to investigate Rényi's entropy [10] of order q,

$$S_q = \frac{1}{1-q}\ln \mathrm{Tr}\,\Gamma^q \quad \text{for } 0 < q < \infty, \quad q\neq 1, \quad (14)$$

where, in the most general case, Γ is the one-particle density matrix containing spin variables as well. Considering the remark after Eq. (8) easily follows $\Gamma^q=\gamma^q\mathcal{I}_s/2^q$ with $\mathrm{Tr}\,\Gamma^q = 2^{1-q}\,\mathrm{Tr}\,\gamma^q$ resulting in the simple expression

$$S_q = \ln 2 + \frac{1}{1-q}\ln \mathrm{Tr}\,\gamma^q. \quad (15)$$

The lower bound of S_q is $\ln 2$ instead of the usual relation $S_q\geq 0$. As we have already emphasized in [11], the presence of the term $\ln 2$ is a strict consequence of indistinguishability of electrons, leading to a lack of information, which manifests in a minimum amount of the entropy. We have shown that this is a special case of a more general result obtained from the Pauli principle for density operators, related to the N-representability problem of Γ. As the constant $\ln 2$ is a natural consequence of the Pauli principle, we will simply omit this term in the following discussions. Thus the remaining problem is to calculate the qth power of the density matrix γ. Below we will show that it is possible to derive a closed analytic form of γ^q for arbitrary positive powers q.

For any *integer* $n>1$ the powers of γ can be defined by recursion

$$\gamma^{n+1}(\mathbf{r}_1,\mathbf{r}_3) = \int \gamma(\mathbf{r}_1,\mathbf{r}_2)\,\gamma^n(\mathbf{r}_2,\mathbf{r}_3)d\mathbf{r}_2. \quad (16)$$

Using explicit form (8) one can verify the general expression

$$\gamma^n(\mathbf{r}_1,\mathbf{r}_2) = A_n e^{-a_n(r_1^2+r_2^2)}e^{b_n\mathbf{r}_1\cdot\mathbf{r}_2}, \quad (17)$$

where the constants are obtained ($a_1=a$ and $b_1=b$) by the recursive formulas,

$$a_{n+1} = a - \frac{b^2}{4(a+a_n)} = a_n - \frac{b_n^2}{4(a+a_n)}, \quad (18)$$

$$b_{n+1} = \frac{bb_n}{2(a+a_n)}, \quad (19)$$

$$A_{n+1} = \pi^{D/2}AA_n(a+a_n)^{-D/2}. \quad (20)$$

The second equality of Eq. (18) is based on the fact that $(2a_n-b_n)(2a_n+b_n)=(2a-b)(2a+b)$, which in turn follows from

$$2a_n + b_n = \frac{P_n(a,b)}{Q_n(a,b)}(2a+b), \quad (21)$$

$$2a_n - b_n = \frac{Q_n(a,b)}{P_n(a,b)}(2a-b). \quad (22)$$

Recurrence relations (18) and (19) imply

$$\begin{pmatrix} P_{n+1} \\ Q_{n+1} \end{pmatrix} = \begin{pmatrix} 2a+b & 2a-b \\ 2a+b & 2a+b \end{pmatrix}\begin{pmatrix} P_n \\ Q_n \end{pmatrix} = (2a+b)^n\begin{pmatrix} 1 & \lambda^2 \\ 1 & 1 \end{pmatrix}^n\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (23)$$

in which $\lambda=\sqrt{(2a-b)/(2a+b)}=2\sqrt{\omega_+\omega_-}/(\omega_++\omega_-)=2(1+2\Lambda)^{1/4}/(1+\sqrt{1+2\Lambda})$. Note at this point that the $\lambda(\Lambda)$ function has its maximum at $\Lambda=0$. It becomes zero in the limiting cases, i.e., $\Lambda=-1/2$ for repulsion and $\Lambda\to\infty$ for attraction.

The vector $\begin{pmatrix} P_n \\ Q_n \end{pmatrix}$ can be expressed in closed form using the eigenvector decomposition of the initial constraint $\begin{pmatrix} P_1 \\ Q_1 \end{pmatrix}=\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. Using Eqs. (21) and (22) one gets the exponents of γ^n,

$$a_n = \frac{2a+b}{4}\lambda\left[\frac{(1+\lambda)^n + (1-\lambda)^n}{(1+\lambda)^n - (1-\lambda)^n} + \frac{(1+\lambda)^n - (1-\lambda)^n}{(1+\lambda)^n + (1-\lambda)^n}\right], \quad (24)$$

$$b_n = \frac{2a+b}{2}\lambda\left[\frac{(1+\lambda)^n + (1-\lambda)^n}{(1+\lambda)^n - (1-\lambda)^n} - \frac{(1+\lambda)^n - (1-\lambda)^n}{(1+\lambda)^n + (1-\lambda)^n}\right], \quad (25)$$

and $(2a+b)=[(\omega_++\omega_-)/2]=(\omega_0/2)(1+\sqrt{1+2\Lambda})$ in terms of the physical variables. The normalization coefficient in Eq. (17) satisfies according to Eq. (20),

$$A_{n+1} = \pi^{nD/2}A^{n+1}z_n^{-D/2}, \quad (26)$$

where

$$z_n = \prod_{i=1}^{n}(a+a_i). \quad (27)$$

As Eq. (18) implies

$$a + a_n = 2a - \frac{b^2}{4(a+a_{n-1})} \quad (28)$$

we have

$$z_n = 2az_{n-1} + \frac{b^2}{4}z_{n-2} \quad (29)$$

and using standard techniques z_n can be expressed as a linear combination of the two particular solutions in the form $z_n = \theta^n$. We arrive finally at

$$A_n = \left[\frac{2a-b}{\pi\lambda}\frac{(2\lambda)^{2n}}{(1+\lambda)^{2n} - (1-\lambda)^{2n}}\right]^{D/2}. \quad (30)$$

It is clear that all formulas (24), (25), and (30) can straightforwardly be extended for arbitrary positive *noninteger* values $n\to q$ as well. Moreover, the extension satisfies

$$a_{p+q} = a_p - \frac{b_p^2}{4(a_p + a_q)} = a_q - \frac{b_q^2}{4(a_p + a_q)}, \qquad (31)$$

$$b_{p+q} = \frac{b_p b_q}{2(a_p + a_q)}, \qquad (32)$$

$$A_{p+q} = \pi^{D/2} A_p A_q (a_p + a_q)^{-D/2}, \qquad (33)$$

corresponding to the functional equation of the product property $\Gamma^{p+q} = \Gamma^p \Gamma^q$ for arbitrary $p > 0$ and $q > 0$.

Based on this fact and due to the above details, we can write

$$\gamma^q(\mathbf{r_1}, \mathbf{r_2}) = (\text{Tr } \gamma^q) \left(\frac{2a_q - b_q}{\pi} \right)^{D/2} e^{-a_q(r_1^2 + r_2^2)} e^{b_q \mathbf{r_1} \cdot \mathbf{r_2}}, \quad (34)$$

where the trace of γ^q, i.e., the input to different entropies, is given by

$$\text{Tr } \gamma^q = \left[\frac{(2\lambda)^q}{(1+\lambda)^q - (1-\lambda)^q} \right]^D \qquad (35)$$

in terms of the previously introduced informative $\lambda(\Lambda) = 2(1+2\Lambda)^{1/4}/(1+\sqrt{1+2\Lambda})$. Due to the special character of the $\lambda(\Lambda)$ function, to any $-1/2 < \Lambda < 0$ repulsive coupling there exists a corresponding attractive one $\Lambda' > 0$ for which $\lambda(\Lambda) = \lambda(\Lambda')$. Therefore, all entropic quantities depending on trace (35) have the dual property $S_q(\Lambda) = S_q(\Lambda')$. As a simple and nice illustration one can consider $S_2(\lambda) = D \ln(1/\lambda)$.

For small enough interparticle coupling ($\Lambda \to 0$) we have the $\lambda = 1 - \Lambda^2/8$ expansion; thus the asymptotic forms of entropies are $S_q(\Lambda) = D[q/(q-1)](\Lambda^2/16)$ for $q > 1$ and $S_q(\Lambda) = D[1/(1-q)](\Lambda^2/16)^q$ for $q < 1$. Therefore, for small coupling we have a Λ^2 scaling, as in Wigner's correlation energy, in all higher-order ($q > 1$) entropies. Notice that a similar quadratic scaling can be obtained from the so-called correlation Shannon entropies defined by Amovilli and March [7]. On the other hand, only $S_{1/2}$ scales linearly (similarly to the interaction energy) with the coupling as $S_{1/2}(\Lambda) = (D/2)|\Lambda|$ in the perturbative limit. A combination of these details with the additional constraint based on the maximum-entropy principle suggests the $(1/2) < q < 1$ range to practical applications of density matrices γ^q.

Motivated partly by this possibility of practical nature, we investigate the $(2a_q - b_q)/\omega_0$ quantity which is a measure of the spatial extension of $\gamma^q(\mathbf{r}, \mathbf{r})/\text{Tr } \gamma^q$. We interpret this ratio, a kind of density distribution, as a physical quantity. It is a monotonically growing function of the coupling $\Lambda \in [-0.5, \infty)$ for $q > 1/2$. At $q = 1/2$ one gets $(2a_{1/2} - b_{1/2}) = \omega_0$ for all $\Lambda \geq 0$, where $\text{Tr } \gamma^{1/2} = (1+2\Lambda)^{D/8}$ and $S_{1/2} = (D/4)\ln(1+2\Lambda)$. When $-(1/2) < \Lambda < 0$, one gets $(2a_{1/2} - b_{1/2}) = \omega_0 \sqrt{1+2\Lambda}$ and $S_{1/2} = -(D/4)\ln(1+2\Lambda)$. For $q < 1/2$ there is a maximum in $(2a_q - b_q)/\omega_0$ at $\Lambda = 0$. This behavior for $q < 1/2$ is similar to one in $\lambda(\Lambda)$. Thus, the ratio $\gamma^q(\mathbf{r}, \mathbf{r})/\text{Tr } \gamma^q$ is uniquely determined by the interaction strength Λ only for $q \geq 1/2$, otherwise the repulsive and attractive cases are not distinguishable.

Now, we outline the result for the von Neumann entropy S_1 which can be derived by a limiting ($q \to 1$) procedure. In order to perform this L'Hospital procedure for a (0/0)-type

expression, we use the $\lambda = (1-\xi)/(1+\xi)$ variable change to Eq. (35). Thus we get

$$\text{Tr } \gamma^q = \left[(1-\xi)^q \frac{1}{1-\xi^q} \right]^D. \qquad (36)$$

Applying also the $(a^x)' = a^x \ln(a)$ standard rule of derivation, we easily obtain the

$$S_1 = -D \ln(1-\xi) - D \frac{\xi}{1-\xi} \ln(\xi), \qquad (37)$$

expression in terms of ξ. For small coupling one has $\xi(\Lambda \to 0) = \Lambda^2/16$. With this we get a $S_1 \propto \Lambda^2 \ln(1/\Lambda^2)$ characteristic dependence at small values of the interelectron coupling. Thus, in contrast to numerical results [8] for Hook's atom, in the case of Moshinsky's atom the linear and von Neumann entropies do not scale onto each other.

It may have a general interest to note at this point that S_1 is equivalent to the entropy of a *single* harmonic oscillator specified by frequency $\bar{\omega} = \sqrt{\omega_+ \omega_-} = \omega_0 \sqrt{1+2\Lambda}$ and temperature (T) defined from $\lambda = \tanh(\bar{\omega}/2k_B T)$. Furthermore, it can be written [12], alternatively, as $(S_1/D) = -\sum_{n=0}^{\infty} p_n \ln p_n$ in terms of the eigenvalues p_n of the one-dimensional density matrix; $\sum_{n=0}^{\infty} p_n = 1$. The p_n are natural occupation numbers to the spectral [13] representation of the one-particle density matrix. Since the one-dimensional ($D=1$) trace is equal to $\sum_{n=0}^{\infty} (p_n)^q$, we get the simple $p_n = (1-\xi)\xi^n$ representation; $\xi(\Lambda) \in [0,1]$.

The deviations of the natural occupation numbers from 1 or 0 describe, beyond the HF approximation, the phenomenon of correlation on the one-particle level. For example, in the weak entanglement ($\Lambda \to 0$) limit $p_0(\Lambda) - p_1(\Lambda) = 1 - \Lambda^2/8$. This difference clearly shows the role of correlation, and thus it can be interpreted [14] as a quasiparticle weight similarly to the renormalization of the electron-gas momentum distribution. Furthermore, a correlation tail [14] can be defined from $(\sum_{n=1}^{\infty} p_n) = \xi$. This measure becomes $\Lambda^2/16$ in the investigated limit.

Other interesting interpretation can be based on the recently introduced [15] concept of *entanglement spectrum*. Namely, using the so-called "excited state" eigenvalues ζ_n, the von Neumann entropy is given, alternatively, as $(S_1/D) = \sum_{n=0}^{\infty} \zeta_n \exp(-\zeta_n)$. From $p_n = \exp(-\zeta_n)$ and $p_n = (1-\xi)\xi^n$ we get the following simple expression,

$$\zeta_n = -\ln(1-\xi) - n \ln \xi, \qquad (38)$$

for the spectrum of excited state eigenvalues. At weak entanglement ($\Lambda \to 0$) one gets an "energy gap," $\zeta_1(\Lambda) - \zeta_0(\Lambda) = \ln(16/\Lambda^2)$, which becomes infinite in the limit of a simple product state with vanishing entropy. We stress the point that the entanglement spectrum is a property of the ground-state wave function itself, so it allows direct comparison between approximate states and exact ones.

At the end of this section we turn our attention to a possible further application of the results obtained above. As an active research field of considerable practical importance, we mention the density-matrix-functional theory, where the basic goal is to express the total energy of an interacting system in terms of *one-particle* density matrices. Such a theory does

not rely on the concept of a fictitious noninteracting system used in current density-functional theory. Here we recalculate the ground-state energy of our two-electron model atom using the above-obtained $\gamma(\mathbf{r}_1, \mathbf{r}_2)$ matrix, its diagonal $\rho(\mathbf{r})$, and the *two-particle* density $n_2(\mathbf{r}_1, \mathbf{r}_2)$, which is the diagonal of the second-order density matrix [3,4]. Considering the normalizations of these inputs, we can write

$$E_{\mathrm{gr}} = 2 \int t(r)d\mathbf{r} + 2\frac{1}{2}\omega_0^2 \int r^2 \rho(r)d\mathbf{r}$$
$$+ \frac{1}{2}\Lambda\omega_0^2 \int \int (\mathbf{r} - \mathbf{r}')^2 n_2(\mathbf{r}, \mathbf{r}')d\mathbf{r}d\mathbf{r}', \qquad (39)$$

where the exact kinetic energy density [5], $t(r)$, is given by the following informative expression: $t(r) = \frac{1}{2}[\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}'} \gamma(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}'=\mathbf{r}} = [|\nabla\rho|^2/(8\rho)] + b(D/2)\rho$. This last form shows the important role of an inseparable correlation via the b-proportional (second order in Λ at small coupling) term. Performing the integrations in the above equation we obtain

$$E_{\mathrm{gr}}(\Lambda) = \frac{D}{4}\omega_0(1 + \sqrt{1 + 2\Lambda}) + \frac{D}{4}\omega_0\frac{(1 + \sqrt{1 + 2\Lambda})}{\sqrt{1 + 2\Lambda}}$$
$$+ \frac{D}{2}\omega_0\frac{\Lambda}{\sqrt{1 + 2\Lambda}} \qquad (40)$$

in the same order of terms as in Eq. (39). In the HF approximation, i.e., using the wave function of Eq. (3) with Ω_0 as *variational* parameter and $n_2^{\mathrm{HF}}(\mathbf{r}, \mathbf{r}')$, one gets the

$$E_{\mathrm{gr}}^{\mathrm{HF}}(\Omega_0) = \frac{D}{2}\Omega_0 + \frac{D}{2}\frac{\omega_0^2}{\Omega_0} + \frac{D}{2}\Lambda\frac{\omega_0^2}{\Omega_0}, \qquad (41)$$

decomposition which results, of course, in $\Omega_0 = \omega_0\sqrt{1 + \Lambda}$ after variation.

The decomposition of the total energy in Eq. (40) gives a rigorous background to test various approximations [16–19]

for the interaction term, the last term in Eq. (39). Namely, the exact results obtained in the present work for the density $\rho(\mathbf{r})$ and a density matrix $\gamma^q(\mathbf{r}_1, \mathbf{r}_2)$ allow a detailed research via ansatz kernels to be used in Eq. (39) instead of the exact two-particle density. Interestingly, for the present two-electron system, a simple inspection (based on the above energies) shows that a form of $[2\rho(\mathbf{r}_1)\rho(\mathbf{r}_2) - \rho(\Lambda = 0, \mathbf{r}_1)\rho(\Lambda = 0, \mathbf{r}_2)]$ reproduces the last term of Eq. (40) exactly. Further details on the capability of different approximations will be published [20] elsewhere.

III. SUMMARY

Motivated by the exact solution for the space-wave function of a two-electron entangled model atom, different entropies which can characterize inseparable quantum correlation are derived. Our main result here is the exact expression for $\gamma^q(\Lambda)$, where $0 < q < \infty$, in terms of the interparticle coupling $-0.5 < \Lambda < \infty$. The entropies are analyzed and compared with appropriate previous results on the role of correlation in other two-electron systems.

The practical applicability range of the detailed mathematical results for entropies, based on the q-order one-particle density matrix, is investigated by using the maximum-entropy principle as an additional constraint. A proposal is made to density-matrix-functional theory, which rests on one-particle density matrices, by calculating exactly the electron-electron interaction term of the ground-state energy of Moshinsky's two-electron model atom.

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