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Entanglement in Hooke's Law Atoms: an Effect of the Dimensionality of the Space

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Abstract We study a singlet ground-state of the D -dimensional Hooke's law model for $D = 1, 2, 3$. We explore an effect of the dimensionality of the space D on the entanglement in the whole range of the repulsive interaction. Among other features, it is found that there exists a critical interaction strength above which for $D = 3$ the amount of entanglement contained in the singlet ground-state becomes larger than that for $D = 2$.

1 Introduction

In recent years, there has been a considerable interest in studies of entanglement properties of systems of interacting particles because of their possible application in quantum information technology [1]. In particular, quantum entanglement in systems of two interacting particles confined in a harmonic trap has attracted much attention [2–8]. In this Letter we study the singlet ground-state of the Hooke's law atom in one, two and three dimensions. The main aim of this Letter is to investigate the effect of the dimensionality of the space on the entanglement, which, to the best of our knowledge, has not been done so far.

The Hamiltonian of the D -dimensional system consisting of two electrons that repel Coulombically and are bound by the harmonic potential is of the form

$$H = \sum_{i=1}^2 \left[\frac{\mathbf{p}_i^2}{2m} + \frac{m\omega^2 \mathbf{x}_i^2}{2} \right] + \frac{\lambda}{|\mathbf{x}_2 - \mathbf{x}_1|}, \quad (1)$$

where $\mathbf{x}_1 = (x_1, \dots, x_D)$ and $\mathbf{x}_2 = (y_1, \dots, y_D)$. Stationary states of the Hamiltonian (1) have the form

$$\Psi(\zeta_1, \zeta_2) = \psi(\mathbf{x}_1, \mathbf{x}_2)\chi(\sigma_1, \sigma_2), \quad (2)$$

where ϱ is a spin function.

After the scaling $\mathbf{x} \mapsto \sqrt{\frac{\hbar}{m\omega}}\mathbf{x}$, $E \mapsto \hbar\omega E$, the Schrödinger equation takes the form

$$H\psi(\mathbf{x}_1, \mathbf{x}_2) = E\psi(\mathbf{x}_1, \mathbf{x}_2), \quad (3)$$

with

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$$H = \sum_{i=1}^2 \left[-\frac{1}{2} \Delta_{\mathbf{x}_i} + \frac{\mathbf{x}_i^2}{2} \right] + \frac{g}{|\mathbf{x}_2 - \mathbf{x}_1|}, \quad (4)$$

where $g = \lambda \sqrt{\frac{m}{\omega \hbar^3}}$ represents the ratio of Coulomb interaction strength.

Introducing the variables

$$\mathbf{Z} = \frac{\mathbf{x}_1 + \mathbf{x}_2}{\sqrt{2}}, \quad \mathbf{z} = \frac{\mathbf{x}_2 - \mathbf{x}_1}{\sqrt{2}}, \quad (5)$$

the Hamiltonian (4) separates as $H = H^{\mathbf{Z}} + H^{\mathbf{z}}$. Since the Hamiltonian $H^{\mathbf{Z}} = -\frac{1}{2} \left[\frac{\partial^2}{\partial Z_1^2} + \frac{\partial^2}{\partial Z_2^2} + \dots + \frac{\partial^2}{\partial Z_D^2} \right] + \frac{Z_1^2}{2} + \frac{Z_2^2}{2} + \dots + \frac{Z_D^2}{2}$ is exactly solvable, the problem is reduced to the eigenvalue equation

$$H^{\mathbf{z}} \varphi(\mathbf{z}) = \varepsilon^{\mathbf{z}} \varphi(\mathbf{z}), \quad (6)$$

with

$$H^{\mathbf{z}} = -\frac{1}{2} \left[\frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} + \dots + \frac{\partial^2}{\partial z_D^2} \right] + \frac{z_1^2}{2} + \frac{z_2^2}{2} + \dots + \frac{z_D^2}{2} + \frac{g}{\sqrt{2} \sqrt{z_1^2 + z_2^2 + \dots + z_D^2}}. \quad (7)$$

Here we consider the cases $D = 1, 2, 3$ and restrict our investigation to the study of the singlet ground-state $\Psi(\zeta_1, \zeta_2) = e^{-\frac{Z^2}{2}} \varphi(\mathbf{z}) \chi_S(\sigma_1, \sigma_2)$, where $\chi_S = \frac{1}{\sqrt{2}}(\alpha(1)\beta(2) - \alpha(2)\beta(1))$ is the spin singlet function. We will solve (6) by the Rayleigh-Ritz (RR) method. In the $D = 2$ and $D = 3$ cases, to solve the radial Schrödinger equation we use in the RR calculations the basis of two and three dimensional radial harmonic oscillator eigenfunctions with frequency $\omega = 1$, respectively. The RR method enables to obtain very accurate results. As an example, in the $D = 3$ case, for the smallest positive value of g at which an exact ground-state wavefunction is known i.e., $g = \sqrt{2}$; $\varepsilon^{\mathbf{z}} = 2.5$ [9], a good approximation to the energy is already obtained using 10 basis functions i.e., $\varepsilon_{RR}^{\mathbf{z}} = 2.50098$.

In the case of $D = 1$, because the Coulombic interaction $1/|z_1|$ diverges when $z_1 \rightarrow 0$, the symmetric spatial ground-state wavefunction $\psi^+(x_1, y_1)$ is given by $\psi^+(x_1, y_1) = |\psi^-(x_1, y_1)|$, where ψ^- is the lowest energy antisymmetric spatial wavefunction i.e., $\psi^-(x_1, y_1) = e^{-\frac{z_1^2}{2}} \varphi_1(z_1)$ (see, for example, a discussion in [10]). Since $\varphi_1(z_1)$ is odd under inversion $z_1 \rightarrow -z_1$, to obtain it we use the RR method with a set of odd eigenfunctions of the one-dimensional harmonic oscillator.

2 The Participation Ratio

The one-particle reduced density matrix (RDM) is defined as

$$\rho_{red}(\zeta, \zeta') = \text{tr}_{\zeta_2} [|\Psi\rangle\langle\Psi|]. \quad (8)$$

The RDM corresponding to (2) factors into spatial and spin components

$$\rho_{red}(\zeta, \zeta') = \rho(\mathbf{x}, \mathbf{x}') \rho^{(spin)}(\sigma, \sigma'), \quad (9)$$

where $\rho(\mathbf{x}, \mathbf{x}') = \int \psi^*(\mathbf{x}, \mathbf{x}_2) \psi(\mathbf{x}', \mathbf{x}_2) d\mathbf{x}_2$. To measure the amount of entanglement in the pure state $|\Psi\rangle$, we use the participation ratio defined as [11]

$$\mathbf{R} = \frac{1}{\text{tr}[\rho_{red}^2]}. \quad (10)$$

It approximately measures the ‘average’ number of Slater orbitals involved in the Slater expansion of Ψ . For the singlet states we have $\text{tr}[\rho_{red}^2] = \text{tr}[(\rho^{(spin)})^2] \text{tr}[\rho^2] = \frac{1}{2} \text{tr}[\rho^2]$, and the participation ratio can be expressed as $\mathbf{R} = 2 / \sum_l \lambda_l^2$, where $\{\lambda_l\}$ are the eigenvalues (occupancies) of the spatial RDM i.e., $\int \rho(\mathbf{x}, \mathbf{x}') v_l(\mathbf{x}') d\mathbf{x}' = \lambda_l v_l(\mathbf{x})$.

The Schmidt decomposition of the real and symmetric spatial wavefunction may be written down as

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \sum_{l=0}^{\infty} k_l v_l(\mathbf{x}_1) v_l(\mathbf{x}_2), \quad (11)$$

where the coefficients k_l and the orbitals v_l satisfy the integral equation $\int \psi(\mathbf{x}_1, \mathbf{x}_2) v_l(\mathbf{x}_1) d\mathbf{x}_1 = k_l v_l(\mathbf{x}_2)$. The former are related to λ_l through $\lambda_l = k_l^2$.

The nature of degeneracy appearing in the spectrum of the RDM of the singlet ground-state in the $D = 2$ and the $D = 3$ cases has been recently explained in [4] and [5], respectively. In the former case, the results for \mathbf{R} have already been obtained in [4]. In the latter one, to calculate \mathbf{R} , we apply the method of Ref. [5].

3 Results

The main numerical results of this paper are presented in Fig. 1, where the values of \mathbf{R} are displayed as a function of g for $D = 1, 2, 3$. As we mentioned earlier, in the case of $D = 1$, the spatial wavefunction of the singlet ground-state is given by $\psi^+(x_1, y_1) = |\psi^-(x_1, y_1)|$ as long as $g \neq 0$. This is the reason why for $D = 1$ the participation ratio \mathbf{R} has a discontinuity at the point $g = 0$. For $g = 0$, the value of \mathbf{R} of the singlet ground-state Ψ equals, of course, exactly 2, regardless of D . Obviously, only in that case Ψ may be represented by a Slater determinant and the state can be regarded as non-entangled.

We see from Fig. 1 that the amount of correlation depends strongly not only on g but also on D . We may extract four regimes of the interaction strength with different behaviors of \mathbf{R} with respect to D . In the first (I) regime $0 < g \lesssim 8$, generally a decrease in D causes an increase in \mathbf{R} . In the second (II) regime $8 \lesssim g \lesssim 11$, the entanglement in the system with $D = 1$ becomes smaller than that in the system with $D = 2$, but still remains larger than that in the one with $D = 3$. As g exceeds the value $g \approx 11$ (the beginning of the III regime), the system with $D = 1$ starts to exhibit the smallest entanglement compared with the entanglements in the remaining cases. Interestingly, when it comes to the cases $D = 2$ and $D = 3$, the situation changes essentially in the fourth (IV) regime $g \gtrsim 20$, namely the entanglement in the former case becomes smaller than that in the latter one. We find that both in the $D = 2$ and the $D = 3$ case, \mathbf{R} increases monotonically with the increase in the interaction strength g and tends to ∞ as $g \rightarrow \infty$. On the other hand, for $D = 1$, \mathbf{R} saturates at a constant value in the regime of strong interaction (in fact, already above $g \approx 8$). We find the value of \mathbf{R} to be about 4 as $g \rightarrow \infty$, which suggests that the corresponding total two-electron wavefunction $\Psi^{g \rightarrow \infty}(\zeta_1, \zeta_2)$ can be well approximated by a combination of two Slater determinants. We have found numerically that $k_0^{g \rightarrow \infty} \approx 0.7$, $k_1^{g \rightarrow \infty} \approx -0.7$ which gives $\lambda_0^{g \rightarrow \infty} = \lambda_1^{g \rightarrow \infty} \approx 0.49$. Hence, because of the conservation of probability $\sum_l \lambda_l = 1$, it immediately follows that in (11) only two terms are important as $g \rightarrow \infty$ and, as a result, the spatial wavefunction approaches the form

$$\psi^{g \rightarrow \infty}(x_1, y_1) \approx 0.7[v_0(x_1)v_0(y_1) - v_1(x_1)v_1(y_1)]. \quad (12)$$

Combining (12) and the spin singlet function, we get that indeed $\Psi^{g \rightarrow \infty}(\zeta_1, \zeta_2)$ constitutes a sum of two Slater determinants. We want to stress at this point that, in the case of $D = 1$, all eigenvalues of the spatial RDM

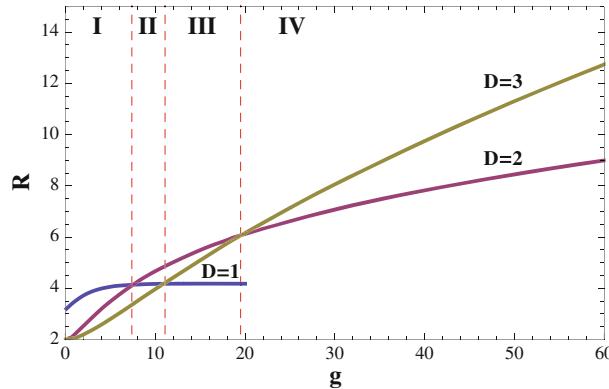


Fig. 1 The participation ratio \mathbf{R} calculated as a function of g for $D = 1, 2, 3$

become doubly degenerate at $g \rightarrow \infty$ limit. This can easily be proved in the framework of the harmonic approximation, in a similar way as it has been done in [8] in the case of $D = 2$ with the anisotropic harmonic trap. Also, it should be stressed that the approximation given by Eq. (12) has already been obtained in [8] where calculations are performed in the presence of strong anisotropy of the harmonic trap.

4 Summary

In conclusion, we carried out the calculation for the participation ratio of the singlet ground-state of the D -dimensional Hooke's law atom for $D = 1, 2, 3$, thereby investigating the effect of D on the entanglement. In particular, we have found that above $g = \lambda \sqrt{\frac{m}{\omega \hbar^3}} \approx 20$ the entanglement contained in the singlet ground-state of the system with $D = 3$ becomes larger than that in the system with $D = 2$.

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