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Correlation Effects in the Moshinsky Model

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Abstract We investigate quantum correlations in the ground state of the Moshinsky model formed by N harmonically interacting particles confined in a harmonic potential. The model is solvable which allows an exact determination of entanglement between the subset of p particles and the remaining $N-p$ particles. We study linear entropies and von Neumann entropies of the bipartitions and compare their behavior with that of the relative correlation energy and of the statistical Kutzelnigg coefficient.

1 Introduction

In recent years there has been a growing interest in systems of interacting particles trapped in potential wells because of their possible use in quantum information processing. Artificially fabricated objects, such as atomic clusters or quantum dots, theoretically described as harmonically confined systems with adjustable control parameters, are promising candidates for quantum computers. This gives the motivation to study their quantum information properties. In this work we perform such a study for the Moshinsky model where the interparticle interaction is harmonic. Being solvable, the model is useful for an approximate description of realistic systems and as benchmark for many-body approximation methods [1]. Its entanglement properties have been studied in the case of $N = 2$ [2] and $N = 3$ [3]. Here we consider the ground state (GS) entanglement in the N-particle Moshinsky system.

After rescaling ($x \mapsto \sqrt{\frac{\hbar}{m\Omega}}x,\ E \mapsto \hbar\Omega E$), the one-dimensional system of particles confined by $V(x) = \frac{m\Omega^2 x^2}{2}$ and interacting via $\lambda(x_i - x_j)^2$ is described by the Schrödinger equation $H\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = E\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ with the Hamiltonian

$$H = \sum_{i=1}^{N} -\frac{1}{2}\frac{d^2}{dx_i^2} + \frac{1}{2}x_i^2 + \sum_{i<j} g(x_i - x_j)^2, \tag{1}$$

where the parameter $g = \frac{\lambda}{m\Omega^2}$ represents the ratio of the interaction to the confinement strength. In Jacobi coordinates: $Y = \frac{x_1+x_2+\ldots+x_N}{\sqrt{N}}$, $y_i = \sqrt{\frac{i-1}{i}}\left(x_i - \frac{1}{i-1}\sum_{k=1}^{i-1} x_k\right)$, $i = 2,\ldots,N$, the Hamiltonian separates into $H = H_Y + H_y = -\frac{1}{2}\frac{d^2}{dY^2} + \frac{1}{2}Y^2 + \sum_{i=2}^{N}\left(-\frac{1}{2}\frac{d^2}{dy_i^2} + \frac{1}{2}\omega^2 y_i^2\right)$, where $\omega = \sqrt{1+2Ng}$. The exact

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expression for the GS wave function is obtained in the form $\Psi(Y, y_2, \ldots, y_N) = (\frac{\omega}{\pi})^{\frac{N-1}{4}} e^{-\frac{wr^2}{2}} (\frac{1}{\pi})^{\frac{1}{4}} e^{-\frac{Y^2}{2}}$, where $r^2 = \sum_{i=2}^{N} y_i^2 = \sum_{i=1}^{N} x_i^2 - Y^2$, with the GS energy $E = \frac{1}{2}(N-1)\omega + \frac{1}{2}$.

2 Correlation Measures

Correlations in the system may be quantified by entropic, energetic or statistical measures.

2.1 Entropic Correlation Measures

From a quantum information viewpoint the entanglement in an N-particle state $\Psi(x_1, \ldots, x_N)$ is described by the correlations of p of the N particles with the remainig $N - p$ ones. The p-particle reduced density matrix (p-RDM)

$$\rho^{(p)}(\mathbf{r}_1,\ldots,\mathbf{r}_p,\mathbf{r'}_1,\ldots,\mathbf{r'}_p) = \int \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_p,\mathbf{r}_{p+1},\ldots,\mathbf{r}_N)\Psi(\mathbf{r'}_1,\ldots,\mathbf{r'}_p,\mathbf{r}_{p+1},\ldots,\mathbf{r}_N)d^3r_{p+1}\ldots d^3r_N \quad (2)$$

can be represented in the Schmidt form

$$\rho^{(p)}(\mathbf{r}_1,\ldots,\mathbf{r}_p,\mathbf{r'}_1,\ldots,\mathbf{r'}_p) = \sum \lambda_k^{(p)} u_k(\mathbf{r}_1,\ldots,\mathbf{r}_p) u_k(\mathbf{r'}_1,\ldots,\mathbf{r'}_p). \quad (3)$$

The occupancies $\lambda_k^{(p)}$ of the natural p-orbitals characterise the bipartite entanglement in the system. Its amount can be quantified by the von Neumann entropy $S^{(p)} = -Tr[\rho^{(p)} \log_2 \rho^{(p)}] = -\sum_{n=0}^{\infty} \lambda_n^{(p)} \log_2 \lambda_n^{(p)}$, or the linear entropy $L^{(p)} = 1 - Tr[\rho^{(p)}]^2 = 1 - \sum_{n=0}^{\infty} [\lambda_n^{(p)}]^2$. In the Moshinsky model, the p-RDM can be obtained analytically [4] and defining $t = \frac{1}{N}\sqrt{N^2 - 2Np + 2p^2 + \frac{2p(gN+1)(N-p)}{\omega}}$, its eigenvalues are given by

$$\lambda_n^{(p)} = \frac{2(t-1)^n}{(t+1)^{n+1}}, \quad (4)$$

leading to exact expressions for the von Neumann entropy

$$S^{(p)} = \frac{1}{2} log_2[(t+1)^{t+1}(t-1)^{1-t}] - 1, \quad (5)$$

and the linear entropy

$$L^{(p)} = 1 - \frac{1}{t}. \quad (6)$$

2.2 Energetic Correlation Measure

The correlation in the GS is measured with respect to the mean field (MF) approximation to its energy $E_{MF} = \langle \Psi_{MF}|H|\Psi_{MF}\rangle$. The MF wave function is a product $\Psi_{MF}(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N} \psi_{MF}(x_i)$, where Ψ_{MF} fulfills $-\frac{1}{2}\frac{d^2\psi_{MF}(x)}{dx^2} + \frac{1}{2}x^2\psi_{MF}(x) + g(N-1)\psi_{MF}(x)\int_{-\infty}^{\infty} \psi_{MF}^2(x_1)(x-x_1)^2 dx_1 = \epsilon\psi_{MF}(x)$. The energetic correlation measure is defined [5] as the relative error of the MF energy $\Delta E = \frac{E_{MF} - E_{exact}}{E_{exact}}$. In the Moshinsky model, $\psi_{MF}(x) = \frac{\sqrt[8]{2g(N-1)+1} e^{-\frac{1}{2}x^2\sqrt{2g(N-1)+1}}}{\sqrt[4]{\pi}}$, GS energy $E_{MF} = \frac{1}{2}N\sqrt{2g(N-1)+1}$ and the relative correlation energy takes a form

$$\Delta E = \frac{N\sqrt{\omega^2 - 2g}}{(N-1)\omega + 1} - 1. \quad (7)$$

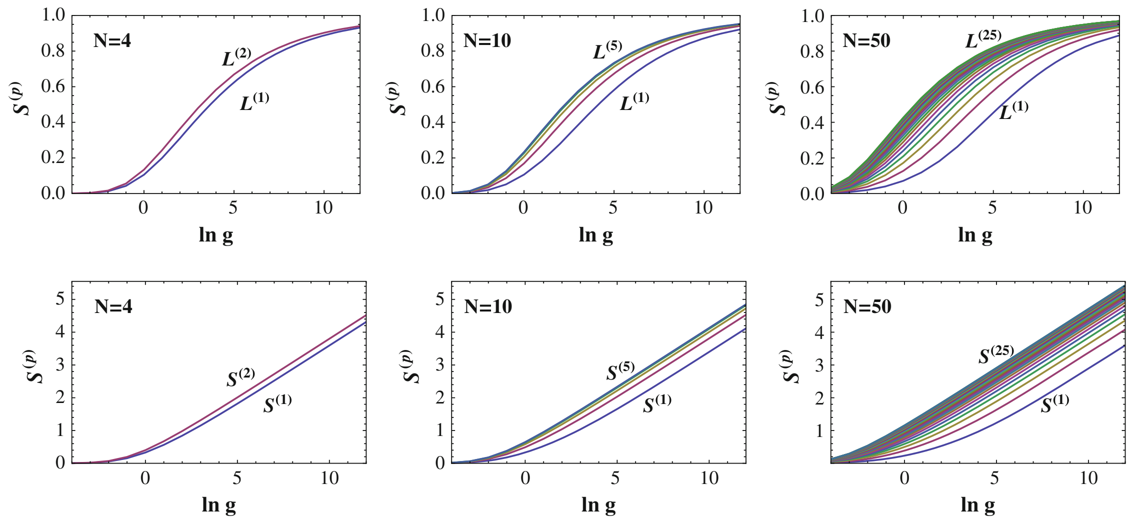

Fig. 1 The bipartite entanglement between a subset of p particles and the remaining ones for $N = 4, 10, 50$ as functions of $\ln g$. *Top* linear entropies, *bottom* von Neumann entropies

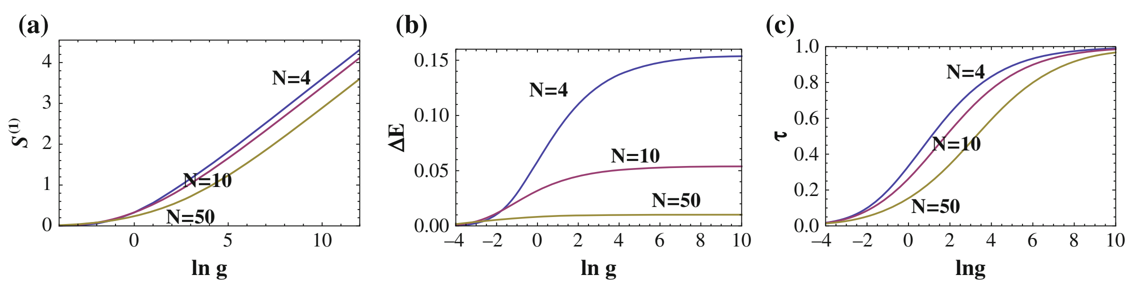

Fig. 2 (**a**) von Neumann entropy $S^{(1)}$, (**b**) relative correlation energy ΔE and (**c**) the Kutzelnigg coefficient τ as functions of $\ln g$ for $N = 4, 10, 50$

2.3 Statistical Correlation Coefficient

Quantum correlations of a many-body system can be also measured by the Kutzelnigg coefficient [6] $\tau = \frac{\langle x_1 x_2\rangle - \langle x\rangle^2}{\langle x^2\rangle - \langle x\rangle^2}$, where the averages are defined as $\langle f(x)\rangle = \int f(x)|\psi(x, x_2, x_3, \ldots, x_N)|^2 dx dx_2 \ldots dx_N$, and $\langle x_1 x_2\rangle = \int x_1 x_2 |\psi(x_1, x_2, x_3, \ldots, x_N)|^2 dx_1 dx_2 \ldots dx_N$. In the Moshinski model, it takes a form

$$\tau = \frac{\omega - 1}{\omega + N - 1}. \tag{8}$$

3 Results

The linear entropies $L^{(p)}$ and von Neumann entropies $S^{(p)}$ are presented in Fig. 1 for all possible bipartitions $p = 1, \ldots, [N/2]$ of the Moshinsky systems with various numbers of particles N. Both entropies increase with the number of extracted particles p. The entropies $L^{(p)}$ are bounded, whereas $S^{(p)}$ are not, but at all p they show a similar, monotonically increasing behaviour, reflecting the fact that the number of noticeably occupied $p-$orbitals increases with g.

The Fig. 2 compares the one-particle entanglement $S^{(1)}$ with the relative correlation energy ΔE and the Kutzelnigg coefficient τ as functions of g. All the measures show a monotonic increase with g. A similar comparison but in function of N is made in Fig. 3 for three different values of g. We observe the decrease to zero for large N, which is monotonic only for the relative correlation energy and for the Kutzelnigg coefficient. Interestingly enough, the entropic measure $S^{(1)}$ displays a maximum at N_{max}, suggesting that entanglement is maximal when the number of particles of the Moshinsky system $N = N_{max}$.

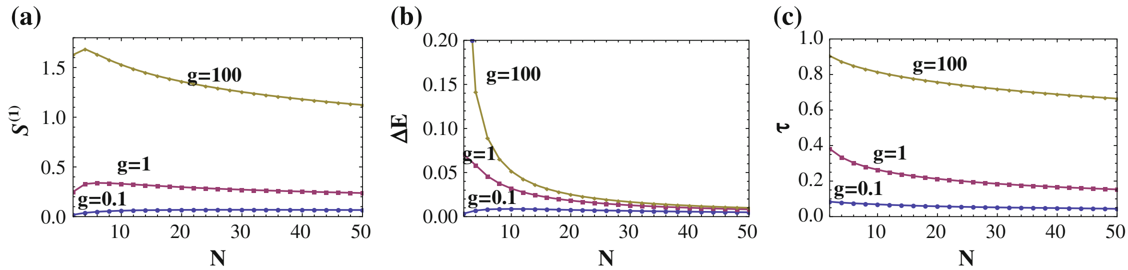

Fig. 3 (**a**) von Neumann entropy $S^{(1)}$, (**b**) relative correlation energy ΔE and (**c**) the Kutzelnigg coefficient τ as functions of N for $g = 0.1, 1, 100$

4 Conclusion

In the Moshinsky model, the bipartite entropies $L^{(p)}$ and $S^{(p)}$ monotonically increase with g for all p. The entropies show a maximum at some number of particles $N = N_{max}$, which does not happen for the correlation energy or the Kutzelnigg coefficient.

References

1. Moshinsky, H.M.: How good is the Hartree-Fock approximation. Am. J. Phys. 36, 52-53 (1968); Erratum: M. Moshinsky, Am. J. Phys. 36, 763 (1968)
2. Yañez, R., Plastino, A., Dehesa, J.: Quantum entanglement in a soluble two-electron model atom. Eur. Phys. J. D **56**, 141–150 (2010)
3. Bouvrie, P.A., et al.: Quantum entanglement in exactly soluble atomic models: the Moshinsky model with three electrons and with two electrons in a uniform magnetic field. Eur. Phys. J. D **66**, 15 (2012)
4. Pruski, S., Maćkowiak, J., Missuno, O.: Reduced density matrices of a system of n coupled oscillators. 3. The eigenstructure of the p-particle matrix for the ground state. Rep. Math. Phys. **3**, 241–246 (1972)
5. Ziesche, P., et al.: The He isoelectronic series and the Hooke's law model: Correlation measures and modifications of the Collins' conjecture. J. Chem. Phys. **110**, 6135–6142 (1999)
6. Kutzelnigg, W., del Re, G., Bertier, G.: Correlation coefficients for electronic wave functions. Phys. Rev. **172**, 49–59 (1968)