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Correlation and Entanglement in Elliptically Deformed Two-Electron Quantum Dots

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Abstract We study quantum correlation in a two-dimensional system of two Coulombically interacting electrons trapped in an anisotropic harmonic potential in dependence on the interaction strength. The linear entropy and von Neumann entropy that measure the entanglement between the electrons are compared with the correlation energy and the statistical correlation coefficient. We observe that the entanglement properties are dramatically influenced by the anisotropy of the confining potential.

1 Introduction

Recently, quantum correlation measures have received noteworthy attention as a tool for better understanding the structure of strongly coupled many-body systems. Both the atoms and molecules as well as artificially fabricated few-particle systems are investigated from this point of view.

Here, we compare various methods of measuring correlations for the ground state of the two-dimensional Hamiltonian $H = \sum_{i=1}^{2}\left[\frac{\mathbf{p}_i^2}{2m^*} + \frac{m^*}{2}(\omega_x^2 x_i^2 + \omega_y^2 y_i^2)\right] + \frac{e^2}{\varepsilon^*|\mathbf{r}_2-\mathbf{r}_1|}$, where ε^* and m^* represent the effective dielectric constant and electron mass of a two-electron quantum dot (2eQD). The transformation $\mathbf{r} \mapsto \sqrt{\frac{2\hbar}{m^*\omega_x}}\mathbf{r}$, $E \mapsto \frac{\hbar\omega_x E}{2}$, brings the Hamiltonian to the dimensionless form

$$H = \sum_{i=1}^{2}\left[-\frac{1}{2}\triangle_{\mathbf{r}_i} + 2x_i^2 + 2\epsilon^2 y_i^2\right] + \frac{g}{|\mathbf{r}_2 - \mathbf{r}_1|}. \tag{1}$$

The coupling $g = \frac{e^2}{\varepsilon^*}\sqrt{\frac{2m^*}{\omega_x\hbar^3}}$ represents the ratio of the Coulomb repulsion to the confinement energy and $\epsilon = \frac{\omega_y}{\omega_x}$ measures the anisotropy of the confining potential.

2 Correlation Measures

Energetic and statistical correlation measures were created for quantum chemical applications. Recently, the development of quantum information theory led to investigation of correlations in few-particle systems using entropic entanglement measures. Below, we present the representative measures of those three kinds and compare their behavior on the example of an anisotropic 2eQD.

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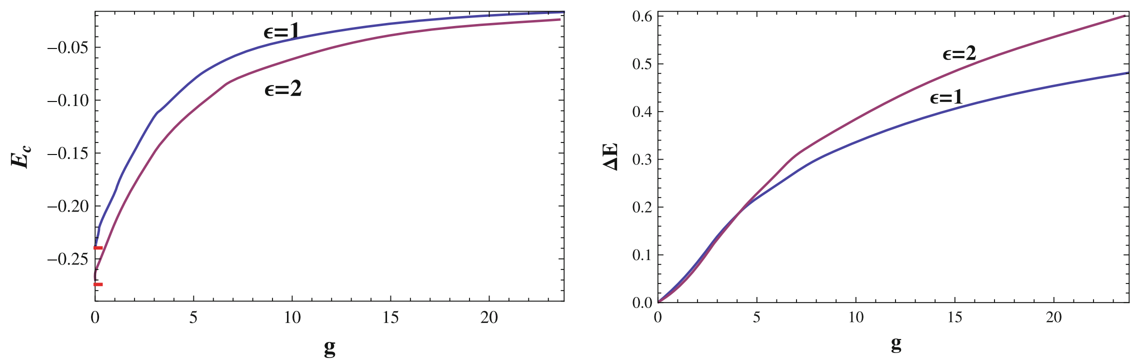

Fig. 1 Correlation energy (*left*) and relative correlation energy (*right*) as functions of the interaction strength

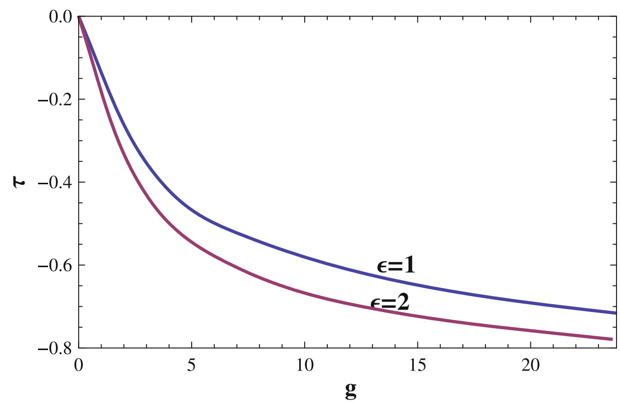

Fig. 2 Kutzelnigg coefficient as a function of the interaction strength

Correlation energy In quantum chemistry, the amount of correlations is usually measured by the correlation energy, defined as the difference between the Hartree Fock approximation and the exact energy $E_c = E_{HF} - E_{exact}$. The relative correlation energy $\Delta E = |\frac{E_{HF} - E_{exact}}{E_{exact}}|$ has been proposed [1] as a better correlation measure. In Fig. 1 we compare the behavior of E_c and ΔE in function of the interaction strength g for 2eQDs of different anisotropies. In contrast to E_c, ΔE vanishes in the case of no correlations, i.e. at $g \to 0$, which confirms its superiority.

Statistical correlation coefficient As an example of a statistical correlation measure in a two-body state $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ we calculate the scalar Kutzelnigg coefficient $\tau = \frac{\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle - \langle \mathbf{r} \rangle^2}{\langle \mathbf{r}^2 \rangle - \langle \mathbf{r} \rangle^2}$, where $\langle \mathbf{r}^n \rangle = \int \mathbf{r}^n |\Psi(\mathbf{r}, \mathbf{r'})|^2 d\mathbf{r'} d\mathbf{r}$ and $\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle = \int \mathbf{r}_1 \cdot \mathbf{r}_2 |\Psi(\mathbf{r}_1, \mathbf{r}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2$. The results in Fig. 2 show that anisotropy increases statistical correlations.

Correlation entropies Quantum information tools for measuring quantum correlations are derived from the reduced density matrix $\hat{\rho}(1, 1') = Tr_2[|\Psi(1, 2)\rangle\langle\Psi(1', 2)|]$, where the trace is taken over spin and space coordinates of particle 2. The von Neumann entropy for the singlet state may be represented as $S = -Tr[\hat{\rho} Log_2 \hat{\rho}] = 1 - \sum_{l=0} \lambda_l Log_2 \lambda_l$, where the natural orbital occupancies λ_l are the eigenvalues of the spatial reduced density matrix $\rho(\mathbf{r}, \mathbf{r}') = \int \psi^*(\mathbf{r}, \mathbf{r}_2) \psi(\mathbf{r}', \mathbf{r}_2) d\mathbf{r}_2$ which fulfill $\int \rho(\mathbf{r}, \mathbf{r}') v_l(\mathbf{r}') d\mathbf{r}' = \lambda_l v_l(\mathbf{r})$. The linear entropy $\mathbf{L} = 1 - Tr\hat{\rho}^2$ is easier to calculate since diagonalization of the reduced density matrix is not needed. The entropies presented in Fig. 3 show a very similar dependence on g. The differences are most pronounced at $g \to \infty$, where L approaches a finite value for any value of ϵ, whereas $S \to \infty$, when $\epsilon = 1$.

3 Discussion

Quantum correlations increase with increasing interaction strength. This is clearly evidenced in our plots of energetic (Fig. 1), statistical (Fig. 2) and entropic correlation measures (Fig. 3) for the 2eQD. However, the detailed behavior of the measures is quite different. The Collins' conjecture [2] that the correlation energy is

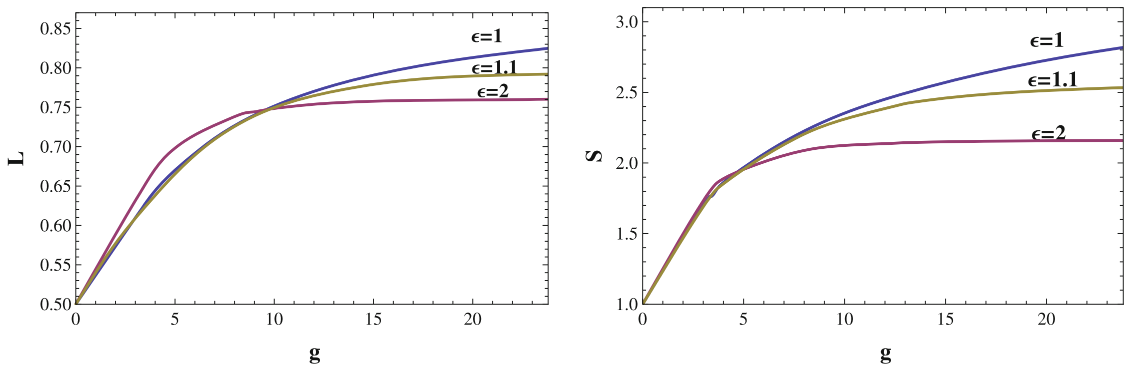

Fig. 3 Linear entropy (*left*) and von Neumann entropy (*right*) as functions of the interaction strength

proportional to the von Neumann entropy appears to fail since E_c does not vanish for no correlations, i.e. at $g \to 0$. This agrees with the observation for the Hooke'e atom [1], which resulted in the modification of the conjecture that the relative correlation energy should be compared with entropic correlations. In the isotropic case ($\epsilon = 1$) the modified conjecture works better, as the dependence of ΔE on g is very similar as that of S and L. However, the comparison of the isotropic case with that of $\epsilon = 2$, which corresponds to strong anisotropy [3], shows that the influence of anisotropy on the correlation measures is very different. We observe that the energetic and statistical correlations get stronger, whereas the entropic measures show weakening of the correlations with anisotropy.

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