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Entanglement properties of the two-electron quasi-one dimensional Gaussian quantum dot

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Abstract We analyse the entanglement characteristics of the quasi one-dimensional quantum dot containing two Coulombically interacting electrons in an inverted Gaussian potential. The linear entropy of the lowest energy states is calculated in the whole range of the effective interaction strength g for different parameters of the longitudinal potential and the lateral radius of the quantum dot. We employ the configuration interaction method with complex-coordinate rotation, since the considered states become autoionizing resonances at the interaction strenght above the critical value g_{th}. We study the dependence of the linear entropy on the parameters of the quantum dot and discuss how the stability properties of the system are characterized by the entanglement between the electrons.

Keywords Autoionization · Entanglement · Linear Entropy

1 Introduction

In recent years, the application of quantum information tools has contributed new insights into the physics of many-body systems [1; 2]. Entanglement provides interesting characteristics of highly correlated states, so that's why the entropies started to be used to analyze quantum phase transitions with much effort focused on spin systems [1; 3; 4]. Few-body systems such as semiconductor quantum dots [5] can be also investigated from quantum information perspective. It is a pleasant feature of quantum dots that their geometry, the number of constituents and the interactions between them can be experimentally controlled. This gave an impetus for studying theoretically two-body systems subjected to external potentials and discussing their characteristics in dependence on varying parameters. The autoionization problem has been discussed for two-electron quantum dots of various geometries [6; 7; 8; 9; 10; 11]. Application of quantum information tools to stability studies was discussed for spherically symmetric

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two-particle systems in Refs. [12; 13; 14; 15]. The critical behavior of entanglement near the ionization point has been observed.

Here, the two-particle quasi-one dimensional quantum dots will be analysed from quantum information perspective. Such simple systems, that can be realized in semiconductor quantum wires [16] or carbon nanotubes [17], are particularly important as possible building blocks of quantum information processors. We consider a system of two Coulombically interacting particles that are strongly confined laterally and weakly confined by the longitudinal Gaussian potential which supports both bound and continuum stationary states. The system will be modelled by a quasi-one-dimensional Hamiltonian with the parameters describing the shape of the potential and the interparticle interaction strength. The energies and widths of autoionizing resonances of the model have been discussed by us previously [11]. Here, we will study how the entropic entanglement characteristics depend on the details of the confining potential and the interaction strength, paying particular attention to the values in the vicinity of the stability limit.

2 The model

We consider a quasi-one-dimensional Hamiltonian

$$\hat{H} = \sum_{i=1}^{2} \left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} - V_0 e^{-x_i^2} \right] + V^{\delta}(|x_1 - x_2|), \tag{1}$$

where the effective interaction potential is taken in the truncated Coulomb form

$$V^{\delta}(|x_1 - x_2|) = \frac{g}{\sqrt{(x_1 - x_2)^2 + \delta}}. \tag{2}$$

The model can be regarded as describing a two-electron system in an axially symmetric anisotropic trap, where the lateral confinement is much stronger than the longitudinal one [18]. The parameter g is the strength of the effective interaction and δ is related to the lateral dimension of the confinement. The limit of $\delta \to 0$ corresponds to the strictly one-dimensional system. The longitudinal confinement in the considered system (1) is taken in the form of an attractive Gaussian potential of the depth V_0, which is commonly used to model quantum dots [19].

The two-particle Hamiltonian (1) spectrum is continuous above the threshold energy $\varepsilon_{th}^{(2)} = \varepsilon^{(1)}$, where $\varepsilon^{(1)}$ is the one-particle energy in the Gaussian well. The bound-states are associated with the solutions of the Schrö dinger equation under vanishing boundary conditions, the eigenenergies of which are real and less than $\varepsilon_{th}^{(2)}$. The autoionizing resonances correspond to the discrete solutions that satisfy outgoing boundary conditions. The resonance eigenvalues are complex numbers, $E = \varepsilon - i\frac{\Gamma}{2}$, which determine the binding energy ε and the inverse of the resonance lifetime Γ.

3 The method

To determine both the bound and resonant states, we apply the configuration interaction (CI) expansion

$$\Psi_{s,t}(x_1, x_2) = \sum_{i,j} a_{ij} \psi_{ij}^{\pm}(x_1, x_2) \tag{3}$$

where

$$\psi_{ij}^{\pm}(x_1,x_2) = c_{ij}\left(\phi_i(x_1)\phi_j(x_2) \pm \phi_j(x_1)\phi_i(x_2)\right),\ c_{ij} = \begin{cases} \frac{1}{\sqrt{2}} & i \neq j \\ \frac{1}{2} & i = j \end{cases}, \tag{4}$$

where (+) and (−) correspond to the singlet (s) and triplet (t) states, respectively. The single particle orbitals are taken as the harmonic oscillator eigenfunctions

$$\phi_i(x) = \left(\frac{1}{\sqrt{\pi}2^i i!}\right)^{1/2} H_i(x)e^{-\frac{x^2}{2}}. \tag{5}$$

The CI method is generalised to resonant states by using the complex scaling transformation $U(\theta) : x \mapsto xe^{I\theta}$. The spectrum of the complex-rotated Hamiltonian $\hat{H}_\theta = U(\theta)\hat{H}U^{-1}(\theta)$ is described by the Balslev-Combes theorem [20], which states that the real bound-state eigenvalues, the complex resonance eigenvalues and the thresholds are the same as those of the original Hamiltonian, but the eigenvalues of the continuous spectrum are rotated about the thresholds by an angle 2θ into the lower energy half-plane, exposing complex resonance eigenvalues. Although this theorem is proven only for dilatation analytic potentials [20; 21] (i.e. the functions that can be analytically continued into the complex plane for any value of x), the complex scaled CI method is successfully applied for potentials that do not have this property [22; 23; 24; 25]. It has been argued [26] that such an approach can be viewed as finite matrix approximation to the mathematically precise exterior complex scaling [27]. In Ref. [11], we applied thus complex scaling to the model system (1), where the soft Coulombic potential (2) is non dilatation analytic. The eigenstates of the system were determined through diagonalization of the truncated Hamiltonian matrix $[H]^{\eta}_{M\times M}$, the elements of which are obtained as

$$H^{\eta}_{nmij} = \left(\psi_{nm}(x_1\eta, x_2\eta)|\hat{H}|\psi_{ij}(x_1\eta, x_2\eta)\right). \tag{6}$$

Note that the c-scalar product $(f|g) = \int_{-\infty}^{\infty} f(x)g(x)dx$ is to be used to calculate the Hamiltonian matrix elements [21]. The matrix elements are analytical functions of η and therefore we can analytically continue them to the complex plane by substituting $\eta = \alpha e^{-i\theta}$ as first proposed by Moiseyev and Corcoran [23]. The optimal value of the parameter η is fixed through the stabilization procedure [7] by requiring the eigenvalue of the considered state E^{η}_k to be stationary in the complex space

$$\left.\frac{dE^{\eta}_k}{d\eta}\right|_{\eta=\eta_{opt}} = 0. \tag{7}$$

4 The linear entropy

The correlations in many-body quantum systems can be naturally described by particle entanglement [1; 2]. Bipartite entanglement in pure states is generally quantified by measures such as the linear entropy or the von Neumann entropy. Both entropies are considered suitable to analyze properties of the systems in the neighborhoods of quantum critical points. We have checked that the dependence of the linear and von Neumann entropy on the parameters of the system (1) is very similar; therefore, in the following we discuss only the linear entropy.

The entanglement entropies are defined from the spectrum of the one-particle reduced density matrix [28]. In the case of two-particle bound-states with the real wave-function $\Psi(x_1, x_2)$ the one-particle reduced density matrix reads

$$\rho(x_1, x_1^{'}) = \int \Psi(x_1, x_2)\Psi(x_1^{'}, x_2)dx_2. \tag{8}$$

The linear entropy is defined as

$$L = 1 - \mathrm{Tr}[\rho^2]. \tag{9}$$

In the resonant case the left and right wave-function $\Psi^{\theta}_{L,R}(x_1, x_2)$, determined by the complex scaling method, satisfy the following equations

$$H^{\theta}\Psi^{\theta}_{R}(x_1, x_2) = E^{\theta}\Psi^{\theta}_{R}(x_1, x_2) \quad , \quad (H^{\theta})^{T}\Psi^{\theta}_{L}(x_1, x_2) = E^{\theta}\Psi^{\theta}_{L}(x_1, x_2), \tag{10}$$

and the one-particle reduced density matrix is defined by

$$\rho^{\theta}(x_1, x_1^{'}) = \int \Psi^{\theta}_{L}(x_1, x_2)\Psi^{\theta}_{R}(x_1^{'}, x_2)dx_2. \tag{11}$$

The natural orbital occupation numbers λ^{θ}_i are complex numbers that are determined by the Schmidt decomposition

$$\rho^{\theta}(x_1, x_1^{'}) = \sum_{i=0} \lambda^{\theta}_i u^{\theta}_i(x_1)u^{\theta}_i(x_1^{'}), \tag{12}$$

where $\sum_{i=0} \lambda^{\theta}_i = 1$. The linear entropy can be calculated as

$$L^{\theta} = 1 - \mathrm{Tr}[(\rho^{\theta})^2] = 1 - \sum_i (\lambda^{\theta}_i)^2 \tag{13}$$

For $\theta = 0$, $\Psi^{\theta=0}_{L} = \Psi^{\theta=0}_{R}$, and the one-particle reduced density matrix is real and the corresponding natural orbital occupancies are real numbers. In this case we recover the well known definition of linear entropy (9), which is real-valued.

Using the wave function of the system (1) determined by the CI method, we solved the integral equation

$$\int \rho^{\theta}(x_1, x_1^{'})u^{\theta}_i(x_1^{'})dx_1^{'} = \lambda^{\theta}_i u^{\theta}_i(x_1) \tag{14}$$

through discretization technique. The so determined occupation numbers λ_i were used to calculate the entanglement entropies. It should be noted that the reduced density matrices (11) are defined for square integrable wave functions $\Psi^{\theta}_{L,R}(x_1, x_2)$. To obtain the corresponding operator for resonance wave functions, it is necessary to use inverse coordinate transformation $U^{-1}(\theta) : x \mapsto xe^{-I\theta}$. However, the transformation does not change the occupation numbers λ^{θ}_i in the equation (12). Thus, the linear entropy can be directly obtained from (13) and is complex-valued. As suggested in [15], the real part of complex entanglement entropy (13) can by identified as the entropy of resonant states and the imaginary part gives the uncertainty of measuring it.

5 Results

The energy spectrum of the two-particle Hamiltonian (1) has been discussed in Ref. [11]. The calculations were performed with the number of basis functions $M = 342$ in the singlet case and M=324 in the triplet case, which proved sufficient to obtain convergent results. In Sect.5.1, we show the plots illustrating how the energies of the lowest states depends on the depth of the longitudinal potential V_0, and the interaction strength g. In Sect. 5.2 we discuss the entanglement properties of the system in dependence on the parameters of the system.

5.1 Energy

The energies ε and resonance widths Γ of the lowest singlet and triplet state of the system (1) are presented in Fig. 1 at fixed lateral confinement with the related parameter $\delta = 0.01$ as functions of the interaction strength g at different depths V_0 of the trapping potential.

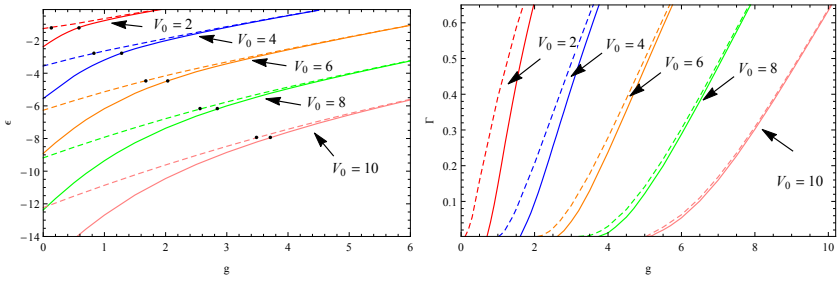

Fig. 1 The energies (left) and widths (right) of the singlet (solid curve) and triplet (dashed curve) states as functions of the interaction strength g for different depths V_0 of the trap. The black points represent the thresholds g_{th} which separate the bound states from resonances.

We observe that the dependence on the interaction strength is monotonous and smooth. The only sign of critical behaviour is the appearance of the imaginary part above critical value g_{th}. The depth of the trap has an important effect on the critical value of the interaction strength g_{th} at which the bound state is transformed into a resonance, namely the larger is the value of V_0, the larger is g_{th}.

5.2 Entanglement entropy

The linear entropy L^θ obtained from the complex scaled formula (13) becomes complex-valued if the interaction strength $g > g_{th}$. In Fig.2 and Fig.3 the results for the real part of entropy for the lowest singlet and triplet states are presented as functions of the interaction strength g. We observe that the entropy increases with increasing interaction strength. In the vicinity of the threshold values of the interaction strength g_{th}, which are marked by black dots, the character of the increase of linear entropies

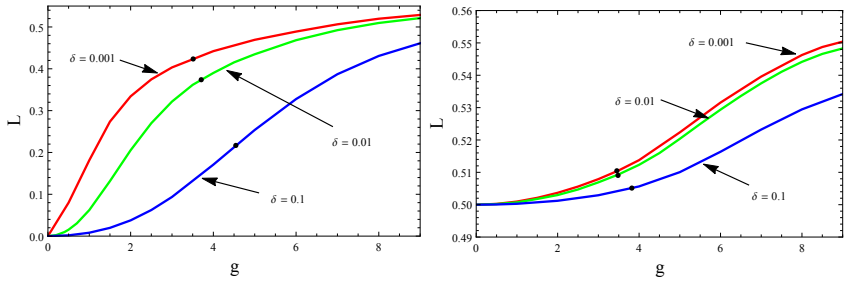

Fig. 2 The real parts of the linear entropy for the lowest singlet (left) and triplet (right) states of the Hamiltonian (1) with $V_0 = 10$ for three different values of δ. The black points represent the thresholds g_{th} which separate the bound states from resonances.

changes. About $g = g_{th}$, the entropy curves have inflection points, it is they change from being concave to convex functions.

In Fig. 2 the real parts of linear entropy are presented as functions of the interaction strength g at three different lateral confinement range δ for a trap of fixed depth $V_0 = 10$. As expected the difference between entropy obtained with different δ parameter tend to vanish in the limit of $g \to \infty$ for both singlet and triplet state. At strong interactions, it is interesting to observe that the real parts of complex linear entropies in the resonant singlet states exceed the value of entropy of the ionized state which is equal $L^{ion} = \frac{1}{2}$, as the state is described by the symmetrized product of one-electron QD and a free electron wave functions.

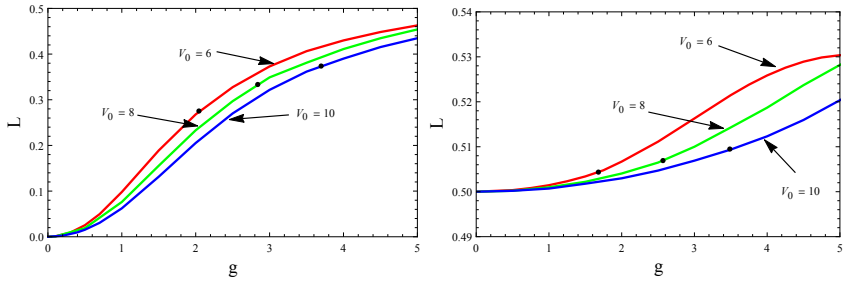

Fig. 3 The real parts of the linear entropy for the lowest singlet (left) and triplet (right) states of the Hamiltonian (1) with $\delta = 0.01$ for three different values of V_0. The black points represent the thresholds g_{th} which separate the bound states from resonances.

Fig. 3, shows the real parts of linear entropy of the singlet and triplet states as functions of the interaction strenght g at three different depths V_0 of the trapping potential. We observe that the real part of complex linear entropy of both the singlet and triplet states depends on the depth of the longitudinal trap V_0 in a similar way.

6 Conclusion

Using the reduced density matrix obtained by the complex scaling method (11) we calculated the linear entropy of bound and resonant states of the Gaussian QD with the quasi-one dimensional Hamiltonian (1). In both cases the entropy curves are monotonously increasing functions of g and do not show discontinuities in the vicinity of g_{th}. However, as opposed to the very smooth behavior of energy curves, the character of the increase of linear entropies changes around g_{th}, namely the functions change from being concave to convex. The linear entropy of the quasi-one dimensional two-electron quantum dot depends strongly on the shape of the confining potential and the interaction strength g. The effect of the interaction on entanglement between electrons is more pronounced in the singlet case. Also the lateral dimension of the QD, described by the δ parameter, influences the entanglement entropy more strongly in the singlet states. The stronger influence of the interaction on the entropy can be attributed to the fact that at $g = 0$ the lowest singlet state is occupied by electrons in the lowest one-particle states.**Whereas, the decrease with increasing depth of the longitudinal trap V_0 appears similar for the singlet and triplet entropies.**

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References

1. Amico, L., Fazio, R., Osterloh, A., Vedral, V.: Entanglement in many-body systems. Rev. Mod. Phys. **80**, 517 (2008)
2. Tichy, M., Mintert, F., Buchleitner, A.: Essential entanglement for atomic and molecular physics. J. Phys. B: At. Mol. Opt. Phys. **44**, 192001 (2011)
3. Osterloh, A., Amico, L., Falci, G., Fazio, R.: Scaling of entanglement close to a quantum phase transition. Nature **416**, 608-610 (2002)
4. Ma, J., Wang, X., Sun, C.P., Nori, F.: Quantum spin squeezing. Phys. Rep. **509**, 89 (2011)
5. Jacak, L., Hawrylak, P., Wójs, A.: Quantum Dots. Springer, Berlin (1997)
6. Bylicki, M., Jaskólski, W., Stachów, A., Diaz, J.: Resonance states of two-electron quantum dots. Phys. Rev. B **72**, 075434 (2005)
7. Sajeev, Y., Moiseyev, N.: Theory of autoionization and photoionization in two-electron spherical quantum dots. Phys. Rev. B **78**, 075316 (2008)
8. Genkin, M., Lindroth, E.: Effects of screened Coulomb impurities on autoionizing two-electron resonances in spherical quantum dots. Phys. Rev. B **81**, 125315 (2010)
9. Chakraborty, S., Ho, Y.K.: Autoionization resonance states of two-electron atomic systems with finite spherical confinement. Phys. Rev. A **84**, 032515 (2011)
10. Selsto, S.: Scattering in a quantum dot: the role of resonances. J. Phys.: Condens. Matter **25**, 315802 (2013)
11. Kuroś, A., Okopińska, A.: Two-electron resonances in quasi-one dimensional quantum dots with Gaussian confinement. Int. J. Theor. Phys. (2015). DOI 10.1007/s10773-015-2533-2
12. Osenda, O., Serra, P.: Scaling of the von Neumann entropy in a two-electron system near the ionization threshold. Phys. Rev. A **75**, 042331 (2007)
13. Osenda, O., Serra, P.: Excited state entanglement on a two-electron system near the ionization threshold. J. Phys. B: At. Mol. Opt. Phys. **41**, 065502 (2008)
14. Ferrón, A., Osenda, O., Serra, P.: Entanglement in resonances of two-electron quantum dots. Phys. Rev. A **79**, 032509 (2009)
15. Pont, F.M., Osenda, O., Toloza, J.H., Serra, P.: Entropy, fidelity, and double orthogonality for resonance states in two-electron quantum dots. Phys. Rev. A **81**, 042518 (2010)
16. Bleszynski-Jayich, A. C., Frberg, L. E., Bjrk M. T., Trodahl, H. J., Samuelson, L., and Westervelt, R. M.: Imaging a one-electron InAs quantum dot in an InAs/InP nanowire. Phys. Rev. B **77**, 245327 (2008)

17. Buitelaar, M. R., Bachtold, A., Nussbaumer, T., Iqbal, M., Schnenberger, C.: Multiwall Carbon Nanotubes as Quantum Dots. Phys. Rev. Lett.**88** 156801 (2002)
18. Häusler, W., Kramer, B.: Interacting electrons in a one-dimensional quantum dot. Phys. Rev. B **47**, 16353-16357 (1993)
19. Adamowski, J., Sobkowicz, M., Szafran, B., Bednarek, S.: Electron pair in a Gaussian confining potential. Phys. Rev. B **62**, 4234-4237 (2000)
20. Balslev, E., Combes, J.M.: Spectral properties of many-body Schrödinger operators with dilatation-analytic interactions. Comm. Math. Phys. **22**, 280 (1971)
21. Moiseyev, N.: Non-Hermitian Quantum Mechanics. Cambridge University Press, (2011)
22. Yaris, R., Bendler, J., Lovett, R. A., Bender, C. M., Fedders, P. A.: Resonance calculation for arbitrary potentials. Phys. Rev. A **18**, 1816 (1978)
23. Moiseyev, N., Corcoran, C.: Autoionizing states of H_2 and H_2^- using complex-scaling method. Phys. Rev. A **20**, 814 (1979)
24. Moiseyev, N.: Resonance states by the generalised complex variational method. Mol. Phys. **47**, 585 (1982)
25. Honigmann, M., Buenker, R., Liebermann, H-P.: Complex multireference configuration interaction calculations employing a coupled diabatic representation for the $2Pi(g)$ resonance states of $N2(-)$. J. Chem. Phys. **125**, 234304 (2006)
26. Morgan, J.D., Simon, B.: The calculation of molecular resonances by complex scaling. J. Phys. B: At. Mol. Phys. **14**, L167 (1981)
27. Simon, B.: Phys.: The definition of molecular resonance curves by the method of exterior complex scaling, Phys.Lett.A**71**, 211 (1979)
28. Nielsen M. A., Chuang I. L.: Quantum Computation and Quantum Information. Cambridge University Press, (2000).