

Entanglement in resonances of two-electron quantum dots

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Bound and resonance states of a two-electron quantum dot are studied using a variational expansion with real basis-set functions. The two-electron entanglement (von Neumann entropy) is calculated as a function of the quantum-dot size at both sides of the critical size, where the ground (bound) state becomes a resonance (unbound) state. The use of von Neumann entropy is proposed as a method for the determination of the energy of a resonance.

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I. INTRODUCTION

The entanglement of a quantum state may be considered as a resource, which is the point of view of quantum information [1], or may serve to further characterize the state, as the case when the concept is applied to well-known models [2]. In other few cases, concepts that are motivated by quantum information considerations shed some new light in problems otherwise unsolved or poorly understood, for example, the scaling of block entropies is related to the efficient simulability using matrix product states of many-body systems [3].

The calculation of entanglement in atoms, molecules, and quantum dots obeys to the aforementioned reasons. Among the applications oriented to quantum information there are proposals for using quantum dots as a source on demand of entangled pairs [4], for entanglement generation in a quantum-dot structure [5], or entanglement distribution in a quantum-dot processor [6].

In atomic systems the behavior of the entanglement near the ionization threshold has been obtained for both ground and first excited states of the spherical helium atom [7,8]. Carlier *et al.* [9] studied a one-dimensional two-electron atom and calculated the entanglement carried by the two-electron eigenstates. Shi and Kais [10] studied the near-threshold scaling of the Shannon entropy for the two-electron atom, and Amovilli and March [11] studied the Shannon correlation and Jaynes entropy for an exactly solvable artificial two-electron atom. Fedorov *et al.* [12] considered the entanglement shared by an electron and an ion in a photoionization and photodissociation setup. Another context in which the entanglement of quantum states in “atomic systems” is of interest arises in the implementation of quantum gates [13].

Interestingly, the works cited above only deal with L^2 bound states (the discrete spectrum) or the δ -function-normalized continuum states which occur over a continuous range of energies, bounded below by a threshold for scattering but not bounded above. However, it is well known that this is not the whole spectrum for a whole kind of systems

since there is a part of the spectrum called *singular continuous spectrum* or *resonances* [14]. These resonance states can be observed in two-electron quantum dots [15,16] and two-electron atoms [17]. The behavior of the entanglement near the ionization threshold is determined by the characteristics of the spectrum near the threshold [7,8], so it should be influenced by the presence of resonance states. However the cases analyzed so far have not been studied in the region where the resonance states should be expected. The present work deals with the behavior of the entanglement near the ionization threshold in systems with resonance states. To this end we studied the von Neumann entropy of two closely related models, a two-electron quantum dot, as considered by Bylicki *et al.* [15], and a simplified version of this model which allows us to obtain more numerical accuracy. As we shall see our results are general and could be relevant for realistic problems; this is the reason why we should pay particular attention to one special model of quantum dot.

The properties of the von Neumann entropy as an entanglement measure are discussed by Ghirardi and Marinatto [18]. This entropy has been used to study a number of problems: heliumlike atom [7,8], generation of entanglement via scattering [19], the dynamical entanglement of small molecules [20], and entanglement in Hooke’s atoms [21]. Anyway it is noteworthy that the quantification of entanglement for identical particles admits other possibilities, see, for example, the Slater formation measure [22] which is analogous to the concurrence introduced by Wootters [23] in the context of arbitrary states of two qubits.

The model of quantum dot that we consider is one of spherical symmetry. The electrons are confined in a spherical square-well potential, and the interactions of the materials that compound the quantum dot with the electrons are taken into account by considering that the electrons have an effective mass, and the Coulombic repulsion between the electrons is affected by a dielectric constant. Of course there are other ways to include the interactions of the electrons with the materials of the quantum dot, see, for example, the work by Liu *et al.* [24], but this model is used when one is interested in other issues such as the decoherence of states prepared on the quantum dot.

This paper is organized as follows: in Sec. II we present the models and give a brief account of the numerical results that shows the presence of resonance states in them. In Sec. III we discuss the general aspects of the von Neumann entropy. In Sec. IV we present the numerical results about the

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von Neumann entropy and energy of a resonance. Finally, in Sec. V we discuss our results and present our conclusions.

II. MODELS

A. Two-electron quantum dot

The electrons in the quantum dot are confined by the potential

$$V(r) = \begin{cases} -V_0, & r < R \\ 0, & r \geq R, \end{cases} \quad (1)$$

where V_0 is the depth of the square well and R is its radius. So, the Hamiltonian of the system, in a.u., is

$$H = -\frac{1}{2m^*} \nabla_{\mathbf{r}_1}^2 - \frac{1}{2m^*} \nabla_{\mathbf{r}_2}^2 + V(r_1) + V(r_2) + \frac{1}{\epsilon |\mathbf{r}_2 - \mathbf{r}_1|}, \quad (2)$$

where m^* is the effective mass, ϵ is the dielectric constant, and \mathbf{r}_i is the position operator of electron $i=1,2$. The model given by Eqs. (1) and (2) describes a quantum dot built of a narrow-gap semiconductor nanocrystal of radius R , surrounded by a wide-gap semiconductor (or a dielectric medium) with the conduction-band offset equal to V_0 . For more details about the precise physical conditions simulated by the model considered here see Refs. [15,25,26]. In order to compare with the results of Bylicki *et al.* [15], we used the same parameters considered in this reference, namely, $m^*=0.1m_e$, $\epsilon=5$, and $V_0=0.0198$ a.u. ~ 0.54 eV.

The discrete spectrum and the resonance states of the model given by Eqs. (1) and (2) can be obtained approximately using L^2 variational functions [15,27]. So, if $|\psi_j(1,2)\rangle$ are the exact eigenfunctions of the Hamiltonian, we look for variational approximations

$$|\psi_j(1,2)\rangle \approx |\psi_j^{(v)}(1,2)\rangle = \sum_{i=1}^M c_i^{(j)} |\Phi_i\rangle, \quad (3)$$

$$c_i^{(j)} = (\mathbf{c}^{(j)})_i; \quad j = 1, \dots, K,$$

where the $|\Phi_i\rangle$ must be chosen adequately and M is the basis-set size.

Since we are interested in the behavior of the system near the ground-state ionization threshold, we choose as a basis set the s -wave singlets given by

$$|\Phi_i\rangle \equiv |n_1, n_2; l\rangle = (\phi_{n_1}(r_1) \phi_{n_2}(r_2))_s \mathcal{Y}_{0,0}^l(\Omega_1, \Omega_2) \chi_s, \quad (4)$$

where $n_2 \leq n_1$, $l \leq n_2$, χ_s is the singlet spinor, and the $\mathcal{Y}_{0,0}^l(\Omega_1, \Omega_2)$ are given by

$$\mathcal{Y}_{0,0}^l(\Omega_1, \Omega_2) = \frac{(-1)^l}{\sqrt{2l+1}} \sum_{m=-l}^l (-1)^m Y_{lm}(\Omega_1) Y_{l-m}(\Omega_2), \quad (5)$$

i.e., they are eigenfunctions of the total angular momentum with zero eigenvalue and the Y_{lm} are the spherical harmonics. The radial term $(\phi_{n_1}(r_1) \phi_{n_2}(r_2))_s$ has the appropriate symmetry for a singlet state,

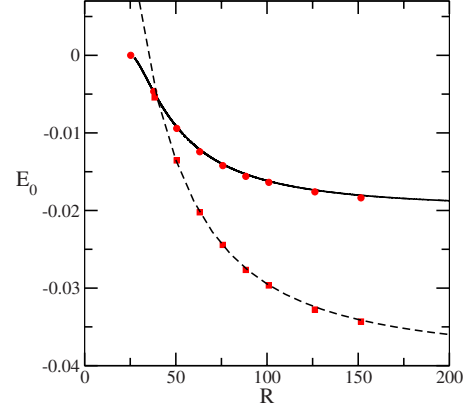


FIG. 1. (Color online) The ground-state energy for the one- and two-electron quantum dots vs R for $m^*=0.1$, $\epsilon=5$, and $V_0=0.0198$ a.u.. The solid line is the exact ground-state energy for one electron. The dashed line is the ground-state energy for the two-electron problem obtained with the variational approximation with $N=14$. The square and circle dots correspond to the values found in Refs. [15,25]. R_c and E_{th} for the two-electron system are given by the point where both curves intersect.

$$(\phi_{n_1}(r_1) \phi_{n_2}(r_2))_s = \frac{\phi_{n_1}(r_1) \phi_{n_2}(r_2) + \phi_{n_1}(r_2) \phi_{n_2}(r_1)}{[2(1 + \langle n_1 | n_2 \rangle^2)]^{1/2}}, \quad (6)$$

where

$$\langle n_1 | n_2 \rangle = \int_0^\infty r^2 \phi_{n_1}(r) \phi_{n_2}(r) dr, \quad (7)$$

with the ϕ 's being chosen to satisfy $\langle n_1 | n_1 \rangle = 1$. The numerical results are obtained by taking the Slater-type forms for the orbitals

$$\phi_n(r) = \left[\frac{\alpha^{2n+3}}{(2n+2)!} \right]^{1/2} r^n e^{-\alpha r/2}. \quad (8)$$

It is clear that in terms of the functions defined in Eq. (4) the variational eigenfunctions take the form

$$|\psi_i^{(v)}(1,2)\rangle = \sum_{n_1 n_2 l} c_{n_1 n_2 l}^{(i)} |n_1, n_2; l\rangle, \quad (9)$$

where $N \geq n_1 \geq n_2 \geq l \geq 0$. Then the basis-set size is given by

$$M = \sum_{n_1=0}^N \sum_{n_2=0}^{n_1} \sum_{l=0}^{n_2} 1 = \frac{1}{6} (N+1)(N+2)(N+3), \quad (10)$$

so we refer to the basis-set size using both N and M . The matrix elements of the kinetic energy, the Coulombic repulsion between the electrons, and other mathematical details involving the functions $|n_1, n_2; l\rangle$ are given in Refs. [28,29].

Figure 1 shows the ground-state energies of the one- and two-electron quantum dots against the dot radius. The crossing point of both curves defines the critical radius R_c and the threshold energy E_{th} for the two-electron dot. Values obtained in Refs. [15,25] are added for comparison.

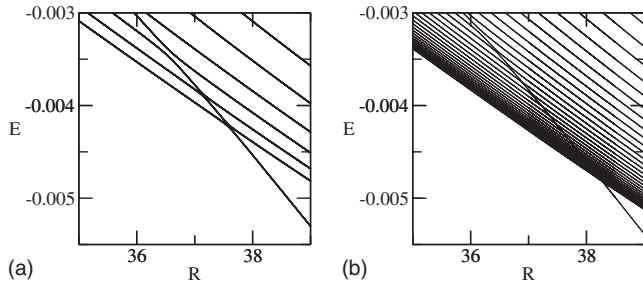


FIG. 2. The energy levels for the (a) full Coulombic repulsion potential with $N=14$ and (b) the spherical Coulomb potential with $N=50$. For $R > R_c$, the lowest eigenvalue corresponds to the ground-state energy; for $R < R_c$ the behavior of the eigenvalues at energies close to E_r is evident.

B. Simplified version of a quantum dot

It is possible to simplify the model given by Eq. (2) by taking

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_l \sum_{r'_l}^{r'_l < r'_l} P_l(\cos(\theta_{12})) \rightarrow \frac{1}{r_>}, \quad (11)$$

where $r_< = \min(r_1, r_2)$ and $r_> = \max(r_1, r_2)$. The approximation given by Eq. (11) is known as the ‘‘spherical’’ Coulomb potential since there are no angular variables in the potential. Then, an adequate basis set for s waves depends only on (r_1, r_2) , allowing to reach larger values of N in the basis functions defined in Eqs. (6) and (8). In this case, the basis-set size is given by

$$M(N) = \sum_{n_1=0}^N \sum_{n_2=0}^{n_1} 1 = \frac{1}{2}(N+1)(N+2). \quad (12)$$

For this approximation, we used up to $N=50$ instead of the value $N=14$ for the full Coulombian potential.

As shown in Fig. 2, bound states and resonances are similar for both models (see Sec. II C). Moreover, the spherical model has the same near-threshold behavior as the model with full Coulombic repulsion between the electrons. The details about the numerical solution of the simplified model can be found in Ref. [30].

C. Resonance states

Resonance states have isolated complex eigenvalues, $E_{\text{res}} = E_r - i\Gamma/2$, $\Gamma > 0$, whose eigenfunctions are not square integrable. These states are considered as quasibound states of energy E_r and inverse life time Γ . For the Hamiltonian Eq. (2), the resonance energies belong to the interval $(\varepsilon, 0)$, where ε , the threshold energy, is the ground-state energy of the one-electron quantum dot.

As we have already mentioned, the resonance states can be analyzed using the spectrum obtained with a basis of L^2 functions. The levels above the threshold have several avoided crossings that ‘‘surround’’ the real part of the energy of the resonance state. The presence of a resonance can be made evident looking at the eigenvalues obtained numerically. Figure 2 shows the typical spectrum obtained from the

variational method, in this case, for a quantum dot with $V_0 = 0.54$ eV and for both models.

III. VON NEUMANN ENTROPY

If $\hat{\rho}^{\text{red}}$ is the reduced density operator for one electron, then the von Neumann entropy is given by

$$S = -\text{Tr}(\hat{\rho}^{\text{red}} \log_2 \hat{\rho}^{\text{red}}), \quad (13)$$

where the reduced density operator is

$$\hat{\rho}^{\text{red}}(\mathbf{r}_1, \mathbf{r}'_1) = \text{Tr}_2 |\Psi\rangle\langle\Psi|. \quad (14)$$

In Eq. (14) the trace is taken over one electron, and $|\Psi\rangle$ is the total two-electron wave function. As the two-electron wave function is not available we instead use the variational approximation Eq. (9). As has been noted in previous works (see [7], and references therein), when the total wave function factorizes in spatial and spinorial components, it is possible to single out both contributions. Then the analysis of the behavior of the von Neumann entropy is reduced to analyze the behavior of the spatial part S since the spinorial contribution is constant. In this case, if $\varphi(\mathbf{r}_1, \mathbf{r}_2)$ is the two-electron wave function and the $\rho(\mathbf{r}_1, \mathbf{r}'_1)$ is given by

$$\rho(\mathbf{r}_1, \mathbf{r}'_1) = \int \varphi^*(\mathbf{r}_1, \mathbf{r}_2) \varphi(\mathbf{r}'_1, \mathbf{r}_2) d\mathbf{r}_2, \quad (15)$$

then the von Neumann entropy S can be calculated as

$$S = -\sum_i \lambda_i \log_2 \lambda_i, \quad (16)$$

where the λ_i are given by

$$\int \rho(\mathbf{r}_1, \mathbf{r}'_1) \phi_i(\mathbf{r}'_1) d\mathbf{r}'_1 = \lambda_i \phi_i(\mathbf{r}_1). \quad (17)$$

In the heliumlike atom, the behavior of the von Neumann entropy as a function of the nuclear charge Z for s -wave states is quite simple to describe. The ground-state entropy is discontinuous at the threshold; conversely an excited-state entropy is continuous at the threshold. These behaviors are described by the critical exponents associated to each entropy μ , which is zero for the ground state and nonzero for the excited states [7,8]. The behavior of the entropy near the critical charge Z_c is given by

$$S(Z) - S_{\text{th}} \sim (Z - Z_c)^\mu. \quad (18)$$

When the two-electron atom loses an electron the state of the system can be described as one electron bounded to the nuclear charge and one unbounded electron *at infinity*. As a consequence the spatial wave function can be written as a symmetrized product of one-electron wave functions so $S = S_c = 1$. But what happens when the system has resonance states? A resonance state keeps its two electrons ‘‘bounded’’ before the ionization for a finite time given by the inverse of the imaginary part of the energy. Of course the life time of a bounded state is infinite. So, if the von Neumann entropy for an ionized system is equal to one, what is its value for a resonance state with a finite life time? Before addressing this

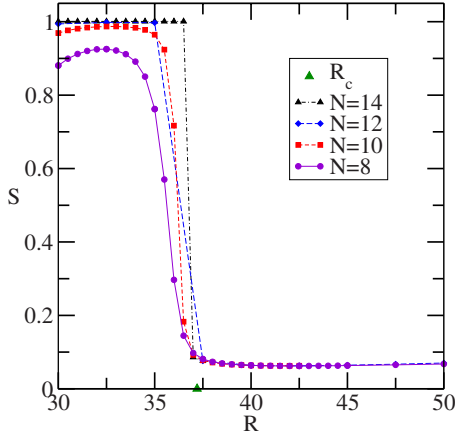


FIG. 3. (Color online) The von Neumann entropy for the ground state vs the radius R for the Coulombian model for different basis-set sizes N . All the curves give similar values for $R > R_c$. For $R < R_c$ the critical value $S_c=1$ can be observed for the largest basis-set sizes available, $N=12$ and 14 .

question, it is interesting to take a closer look at the ground-state entropy.

IV. ENTROPY AND ENERGY OF A RESONANCE

In this section we analyze the behavior of the entropy of a resonance and we suggest a method for calculation of the real part of the resonance energy E_r . Figure 3 shows the behavior of the von Neumann entropy for the ground state vs the radius of the quantum dot for different sizes of the variational basis set. The steep change near the critical radius is due to the ionization of the system and suggests a discontinuity of the entropy at the critical radius. We performed a finite-size scaling analysis on the data and found a null critical exponent, which is the same critical behavior of the two-electron atom described in Ref. [7], corresponding to the existence of an L^2 wave function at the threshold, as expected for a two-identical fermion system [31].

For values of R smaller than R_c , the system has no bound states, and the Ritz-variational method gives a L^2 approximation of scattering and resonances energies, as shown in Fig. 2. Then, in order to calculate the entropy of the resonance, we calculated the entropies for all negative eigenvalues of the variational solution. We numbered the eigenvalues in increasing order, irrespective of whether they were bound states or not. Figure 4 shows the von Neumann entropy vs R for the ground state and the negative-eigenvalue states for both systems.

As shown in Fig. 3 the ground-state entropy S_0 is very small below the threshold and jumps to its critical value, $S_c=1$, at the threshold. The entropies for the first, second, and third states (S_1, S_2, S_3, \dots) behave differently. At threshold their value is 1, and for smaller values of R they present a single minimum. After the minimum is reached the entropy of any of these states goes to $S=1$ when R decreases. As can be seen from Fig. 4, when the value of the entropy of the ground state, S_0 , jumps to its value after the ionization, the entropy for the first state, S_1 , drops almost to the value of S_0

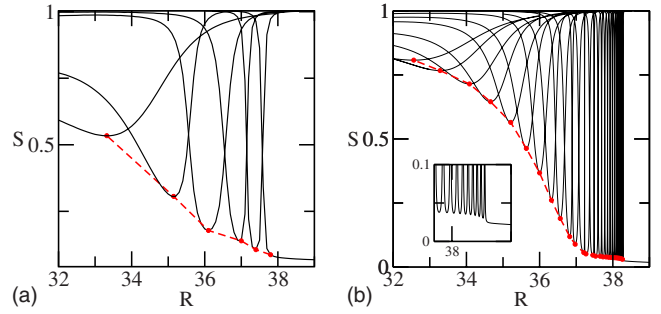


FIG. 4. (Color online) The von Neumann entropy vs R for successive eigenvalues. The curves correspond to the entropy for the first, second, and third states (S_1, S_2, S_3, \dots), the minima are ordered from right to left, the first minimum correspond to S_1 , the second to S_2 , and so on. (a) The full Coulombian potential with $N=14$, and (b) the spherical Coulomb potential with $N=50$. The inset in (b) shows a magnification from the first ten entropies.

prior to the jump. For larger values of R there are similar interchanges between S_1 and S_2 , and so on. These results lead us to conclude that the von Neumann entropy follows the resonance of the quantum dot. In Fig. 4 we sketched qualitatively the envelope following the minima of the curves S_1, S_2, \dots . This envelope is quite stable against N and provides a method to obtain the real part of the energy of the resonance state; if R_i^m is the radius where $S_i(R)$ gets its minimum then the real part of the energy is $E_r = E_i(R_i^m) = E_i^m$, where E_i is the i th energy level of the L^2 spectrum. Following this recipe we obtain the values shown in Fig. 5 as (red) dots.

There is another way to see that the envelope of the entropy minima follows the resonance energy. Figure 6 shows the values of the energy E_i^m for different basis-set sizes. The number of negative eigenvalues changes when the basis-set size is increased, for example, in the case of the spherical Coulomb model, at $R=R_c$, this number grows from 11 for $N=14$ up to 38 for $N=50$. Despite the fact that the number of eigenvalues changes with N , and then the position of the minima, the values obtained for E_r give approximately the same curve $E_r(R)$. This behavior is observed in both model, even with the few negative eigenvalues present in the full Coulombian repulsion system for $N \leq 14$. In other words, the calculation of the von Neumann entropy using L^2 basis-set

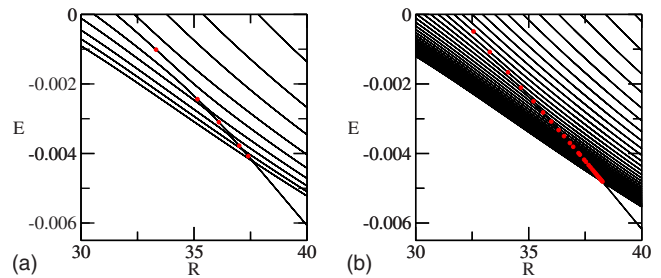


FIG. 5. (Color online) The energy levels for the (a) full Coulombian repulsion potential with $N=14$ and (b) the spherical Coulomb potential with $N=50$. The red points are the resonance energies E_r calculated using the minimum-entropy method described in Sec. IV.

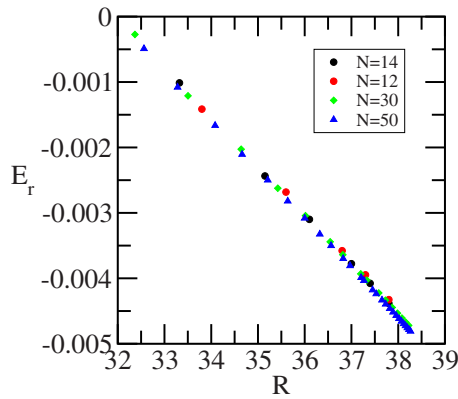


FIG. 6. (Color online) E_r vs R for different basis-set sizes and models. $N=12$ and 14 correspond to the model with full Coulombian repulsion, and $N=30$ and 50 to the spherical Coulomb approximation.

real functions provides a method to get the energy of a resonance without resorting to the use of a stabilization method.

V. CONCLUSIONS

We have performed a detailed study of bound and resonance states of a two-electron spherical quantum dot using a variational expansion with real basis-set functions. We found that the von Neumann entropy detects the resonance states of two-electron quantum dots. This information is encoded in the entropy of the eigenfunctions with negative eigenvalue in the Ritz-variational expansion when these are calculated using an L^2 basis set above the ionization threshold. We calculated an envelope for the minima of the functions S_0, S_1, \dots which follows the resonance state. Our guess is that this envelope is the von Neumann entropy of the resonance, i.e., the von Neumann entropy of the L^2 eigenstate that can be obtained performing *complex scale transformation* [14] of the Hamiltonian. Work is in progress to show this assumption in a model that accepts complex scale transformations.

Another important result of this work was the development of a method for the calculation of a resonance energy E_r with real eigenfunctions without using stabilization meth-

ods which need a free parameter. This method uses the minima of the entropies to obtain the real part of the eigenenergy of the resonance.

We performed our calculations in two related models. The two-electron quantum dot with Coulomb interaction and the two-electron quantum dot with spherical Coulomb interaction. The values of E_r obtained with the approximate model are in good agreement with the exact Coulomb system, so for this kind of quantum dot, the spherical approximation for the repulsive interaction seems to be appropriate to calculate the energy and the von Neumann entropy.

Finally, we found that the amount of entanglement in the ground state is very small and all the s -wave excited states seems to have almost the same entanglement in the region where the quantum dot effectively bound the two electrons. Moreover the entanglement is rather insensitive to the size of the quantum dot at least up to $R=50$ a.u. when $V_0 = 0.54$ eV. As pointed out, among others, by He and Zunger [32] the degree of entanglement is one of the most important quantities for successful quantum gates operations, so the knowledge of the entanglement for different structures gives an indication of its utility to implement quantum information tasks. Despite the fact that He and Zunger considered hetero-quantum-dot and homo-quantum-dot molecules, the amount of entanglement for the ground state of their systems is quite similar to the amount that we calculated for the single two-electron quantum dot. Also it is remarkable that there are, in both models, excited states whose entanglement is equal to 1. Changing the interdot distance provides a way to optimize, to some extent, the amount of entanglement of the ground state.

The use of quantum dots with tailored resonance states has been proposed to enhance the efficiency of photodetectors [16]. This possibility makes it necessary to know how the entanglement of the resonance states behaves and how it must be calculated, and our work points in this direction.

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