

# Interacting electrons in a 2D quantum dot

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## Abstract

The exact numerical diagonalization of the Hamiltonian of a 2D circular quantum dot is performed for 2, 3, and 4 electrons. The results are compared with those of the perturbation theory. Our numerical results agree reasonably well for small values of the dimensionless coupling constant  $\lambda = \frac{a}{a_B}$  where  $a$  is the dot radius and  $a_B$  is the effective Bohr radius. Exact diagonalization results are compared with the classical predictions, and they are found to be almost coincident for large  $\lambda$  values.

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## I. INTRODUCTION

There is considerable interest in the basic science and technological applications of quantum dots [1-5]. The electron motion in quantum dots are confined to a region with dimensions comparable to the de Broglie wavelength of the particle. The result is the quantization of energy. However, since the quantization in the vertical direction is much stronger than in the planar directions, a quantum dot can well be treated as a 2D disc of finite radius.

Although quantum dots and natural atoms contain comparable number of electrons, their electronic properties can have gross differences due to the nature of the confinement potential [6]. In quantum dots confinement potential is experimentally controllable [4], and usually parabolic and much shallower than the  $\frac{1}{r}$  potential of the natural atoms. One recalls, however, that parabolic structures are not the only ones because hard wall type confinement can also be obtained by etching techniques [7-10]. Electron electron correlations in quantum dots have been worked out for parabolic and hard wall confinements in the classical limit and finite temperature in [11], and for hard wall confinement at zero temperature in [12].

In this work we perform an exact numerical analysis of a few electrons confined in a circular 2D quantum dot. We believe that such analyses of 2D structures can shed light on the nature of the electron correlations in quantum dots.

The organization of the paper is as follows. In Sec. 2 we formulate the second quantized Hamiltonian and specify its symmetries. In Sec. 3 we perform a numerical diagonalization of the Hamiltonian obtained its energy levels as a function of the dot dimension. We also present a comparative analysis of the quantum mechanical and classical energy levels.

## II. MODEL AND THE METHOD OF CALCULATION

We consider a many electron system in a two-dimensional circular quantum dot with radius  $a$ . The system is described by the Hamiltonian

$$H = \sum_{i=1}^N \left\{ -\frac{\hbar^2}{2m^*} \vec{\nabla}_i^2 + U(\vec{\mathbf{x}}_i) \right\} + \frac{e^2}{2\epsilon} \sum_{i \neq j} \frac{1}{|\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j|}, \quad (1)$$

where  $m^*$  is the electron effective mass and  $\epsilon$  is the dielectric constant of the medium. The second term in the paranthesis,  $U(\vec{\mathbf{x}})$ , is the hard-wall confinement potential which vanishes for  $|\vec{\mathbf{x}}| < a$ , and infinite for  $|\vec{\mathbf{x}}| \geq a$ . For convenience, we introduce the dimensionless Hamiltonian  $\mathcal{H}$  via the definition

$$H = \frac{\hbar^2}{m^* a_B^2 \lambda^2} \mathcal{H}, \quad (2)$$

where  $\lambda = a/a_B$  is the dimensionless coupling constant. The dimensionless Hamiltonian  $\mathcal{H}$  is given by

$$\mathcal{H} = \sum_{i=1}^N \left( -\frac{1}{2} \right) \vec{\nabla}_i^2 + \frac{\lambda}{2} \sum_{i \neq j} \frac{1}{|\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j|}. \quad (3)$$

One notes that energy is measured in units of  $\frac{\hbar^2}{m^* a_B^2 \lambda^2}$  which depends on  $\lambda$ , and length is measured in units of  $a$ , the dot radius.

In the second quantized language, the dimensionless Hamiltonian takes the form

$$\mathcal{H} = \sum_K \mathcal{E}_K a_K^\dagger a_K + \frac{\lambda}{2} \sum_{K,L,M,N} V_{K,L,M,N} a_K^\dagger a_M^\dagger a_L a_N, \quad (4)$$

where  $\mathcal{E}_K$  is the single particle energy level, and

$$V_{K,L,M,N} = \int \int d^2 \vec{x} d^2 \vec{x}' \varphi_K^*(\vec{x}) \varphi_L(\vec{x}) V(\vec{x} - \vec{x}') \varphi_M^*(\vec{x}') \varphi_N(\vec{x}') \quad (5)$$

is the matrix element of the Coulombic interaction term in (3). Here  $\varphi_A(\vec{x})$  ( $A = K, L, M, N$ ) is the single particle eigenstate of the free Hamiltonian, and  $A$  is a collective index designating the radial ( $n_A$ ), angular momentum ( $m_A$ ) and spin ( $\sigma_A$ ) quantum numbers. Solution of the eigenvalue problem for the free Hamiltonian yields

$$\varphi_A(\vec{x}) = \phi_{n_A, m_A}(\vec{x}) \chi_{\sigma_A}, \quad (6)$$

where  $\chi_\sigma$  is the spin wavefunction, and  $\phi_{n,m}(\vec{x})$  is the normalized orbital eigenfunction given by

$$\phi_{n,m}(\vec{x}) = \frac{1}{\sqrt{\pi}} \frac{1}{|J_{|m|+1}(k_{n,|m|})|} e^{im\theta} J_{|m|}(k_{n,|m|}|\vec{x}|), \quad (7)$$

with the eigenvalues  $\mathcal{E}_K = \frac{1}{2} k_{n_K, |m_K|}^2$  which is independent of both spin and the sign of  $m$ . Here  $k_{n,|m|}$  are the zeroes of the Bessel function ( $J_{|m|}(k_{n,|m|}) = 0$ ).

In determining the spectrum of the total Hamiltonian in (3), it would be convenient to find a representation for the Coulombic potential  $V(\vec{x} - \vec{x}') = \frac{1}{|\vec{x} - \vec{x}'|}$  in terms of Bessel functions, as the single particle eigenstates in (7) do depend only on the Bessel functions. Accordingly, we use the following decomposition for  $1/|\vec{x} - \vec{x}'|$

$$\frac{1}{|\vec{x} - \vec{x}'|} = \sum_{m=-\infty}^{\infty} \int_0^{\infty} dk e^{im(\theta - \theta')} J_m(k\rho) J_m(k\rho') e^{-k(z_> - z_<)}, \quad (8)$$

where we let  $z_> - z_< \rightarrow 0$  as the vertical dimension of the dot is vanishingly small.

By inserting the equations (6), (7) and (8) into equation (5), we obtain the final form of the spin independent potential matrix element  $V_{K,L,M,N}$  as follows

$$\begin{aligned} V_{m_K, m_L, m_M, m_N}^{n_K, n_L, n_M, n_N} &= 4 \frac{1}{|J_{|m_K|+1}(k_{n_K, |m_K|})|} \frac{1}{|J_{|m_L|+1}(k_{n_L, |m_L|})|} \frac{1}{|J_{|m_M|+1}(k_{n_M, |m_M|})|} \\ &\frac{1}{|J_{|m_N|+1}(k_{n_N, |m_N|})|} \int_0^{\infty} dk \int_0^1 d\rho \rho J_{|m_K|}(k_{n_K, |m_K|} \rho) J_{|m_L|}(k_{n_L, |m_L|} \rho) \\ &J_{m_K - m_L}(k\rho) \int_0^1 d\rho' \rho' J_{|m_M|}(k_{n_M, |m_M|} \rho') J_{|m_N|}(k_{n_N, |m_N|} \rho') J_{m_N - m_M}(k\rho'). \end{aligned} \quad (9)$$

Integration over the azimuthal angle  $\theta$  in (5) drops the sum over  $m$  in (8), and the difference between the orbital angular momentum quantum numbers becomes the order

of the Bessel function. In (9)  $J_{m_K-m_L}$  and  $J_{m_N-m_M}$  arise from such angular integrations, and unlike the other Bessel functions in (9), they have negative or positive order index. As  $J_{-|m_K-m_L|} = (-1)^{m_K-m_L} J_{|m_K-m_L|}$  and  $J_{-|m_N-m_M|} = (-1)^{m_N-m_M} J_{|m_N-m_M|}$ , these two Bessel functions create sign differences among different potential matrix elements.

From the symmetries of the problem it is seen that the  $z$  component of the total spin  $S_z = \sum_{i=1}^N s_i$  and the  $z$  component of the orbital angular momentum  $M = \sum_{i=1}^N m_i$  are conserved quantum numbers. The diagonalization of the Hamiltonian is done in the single particle basis by taking the constraints coming from the conservation of  $z$  component of total spin and orbital angular momentum. Hence, dimension of the total Hamiltonian matrix depends on  $S_z$  and  $M$ . In the next section we shall present the result of the exact diagonalization of the many body Hamiltonian matrix for 2, 3 and 4 electrons.

### III. NUMERICAL RESULTS AND DISCUSSION

In this section we present the  $\lambda$  dependence of the ground state energies for 2, 3 and 4 electrons. For each electron number we consider certain values of  $S_z$  and  $M$ . In the figures below we plot the ground state energy of the dimensionless Hamiltonian  $\mathcal{H}$  in (3) as a function of  $\lambda$ .

The dimensionless coupling constant  $\lambda$  measures the dot dimension in units of Bohr radius. In plotting the figures we shall vary  $\lambda$  from 0 to 3. For  $0 \leq \lambda < 1$  one can analyze this problem using perturbation theory as was already done in [13]. However when  $\lambda$  exceeds unity perturbation theory methods do not work, and one has to resort to some other technique, such as numerical diagonalization. Hence, ground state energies will be obtained by the exact diagonalization of the dimensionless many body Hamiltonian.

In Fig.1 depicted is the  $\lambda$  dependence of the ground state energy for 2 electrons. Here solid curve is for  $2S1$  ( $M = 0, S_z = 0$ ), dashed curve for  $2S2$  ( $M = 1, S_z = 0$ ), and short-dashed curve for  $2T1$  ( $M = 1, S_z = 1$ ).

Fig.2 displays the  $\lambda$  dependence of the ground state energy for 3 electrons. In this figure curves correspond to the ground state energies of  $3D1$  ( $|M| = 1, S_z = 1/2$ ) (solid curve),  $3D3$  ( $|M| = 0, S_z = 1/2$ ) (short-dashed curve),  $3D2$  ( $|M| = 2, S_z = 1/2$ ) (dashed curve), and  $3Q1$  ( $|M| = 0, S_z = 3/2$ ) (dotted curve).

In Fig.3 we present the case of 4 electrons. The solid curve is for  $4S1$  ( $M = 2, S_z = 0$ ), dashed curve for  $4S2$  ( $M = 0, S_z = 0$ ), short-dashed curve for  $4S3$  ( $M = 1, S_z = 0$ ), dotted curve for  $4T1$  ( $M = 0, S_z = 1$ ), and dot-dashed curve for  $4T2$  ( $M = 1, S_z = 1$ ).

As is seen in these three figures, our exact diagonalization results are comparable with those ones which are obtained from perturbation theory [13]. However, there are some differences between our numerical results and perturbative results. For instance,  $2S2$  state in Fig.1 and  $3D3$  state in Fig.2 are energetically more favoured than  $2T1$  and  $3Q1$  states, respectively. Also in Fig.3,  $4S2$  and  $4S3$  states are more stable than  $4T1$  and  $4T2$  respectively.

It might be interesting to compare the exact diagonalization results with those of the classical considerations. Modelling the quantum dot by an isolated conducting disc with the capacitance  $C = (2\epsilon a)/\pi$  one gets the classical interaction energy  $E_{int}^{class.} = \frac{1}{\lambda}$ , in units of  $\frac{\hbar^2}{m^* a_B^2} \frac{\pi N^2}{4}$ , where  $N$  is the number of electrons. In Fig.4 we present the  $\lambda$  dependence of the quantum mechanical interaction energies for  $2S1$  (solid curve),  $3D1$  (dashed curve) and  $4S2$

(short dashed curve) in units of  $\frac{\hbar^2}{m^* a_B^2} \frac{\pi N^2}{4}$ . The dotted curve in this figure corresponds to the classical interaction energy. In fact, we see that exact diagonalization results always remain below the classical result [13], and approach to it for large  $\lambda$  values. One further observes that for small  $\lambda$  values, quantum mechanical and classical results behave differently, as opposed to the case of large  $\lambda$ . This can be attributed to the effect of electron-electron correlations, which implies that the ground state energy cannot be written as the sum of the contributions of kinetic energy and interaction potential [12].

Figure 5 shows the dependence of the dimensionless ground state energy per particle,  $\mathcal{E}_0/N$ , on the particle number  $N$  for different  $\lambda$  values. For small  $\lambda$  values,  $\mathcal{E}_0/N$  deviates from a linear behaviour due to the dominance of the free Hamiltonian. On the other hand, when the interaction potential becomes dominant with increasing  $\lambda$  value,  $\mathcal{E}_0/N$  changes almost linearly with  $N$ , as is observed in the figure.

In conclusion, we have worked out the exact diagonalization of the total Hamiltonian for 2, 3 and 4 electrons in a 2D circular quantum dot as a function of the dot dimension. Our results approximately agree with those of the perturbation theory for small radii, but disagreement sets in for larger radii. We have also compared exact diagonalization results with the classical predictions, and found that they almost coincide for large  $\lambda$  values.

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#### IV. FIGURE CAPTIONS

- Figure 1: The ground state energy levels for 2 electrons  
Figure 2: The ground state energy levels for 3 electrons  
Figure 3: The ground state energy levels for 4 electrons  
Figure 4: Comparison of the classical interaction energy with the lowest three quantum mechanical interaction energies  
Figure 5: Dimensionless ground state energies per particle  $\mathcal{E}_0/N$  versus the particle number  $N$  for  $\lambda = 5(\diamond)$ ,  $\lambda = 10(+)$ ,  $\lambda = 50(\square)$ ,  $\lambda = 100(\times)$

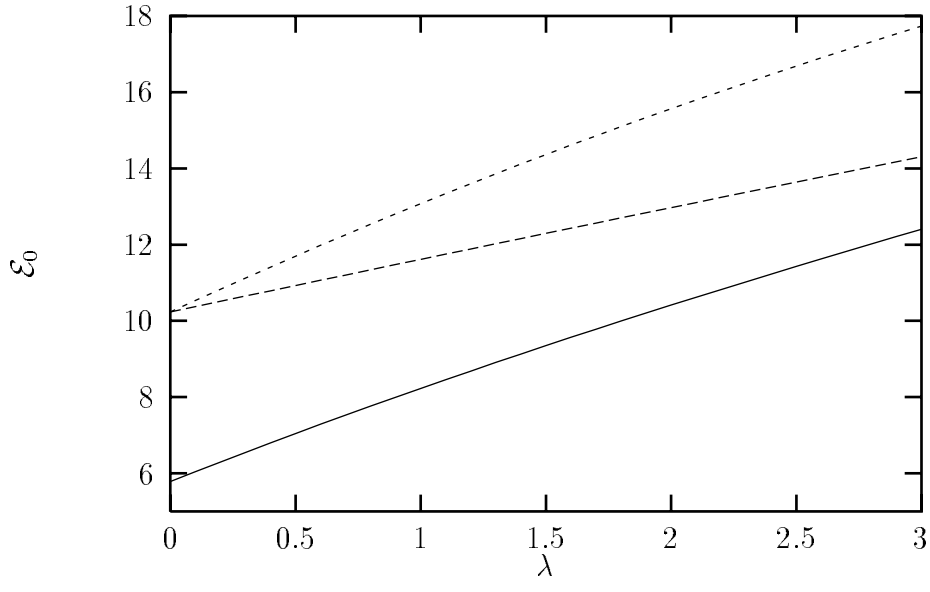


Fig.1



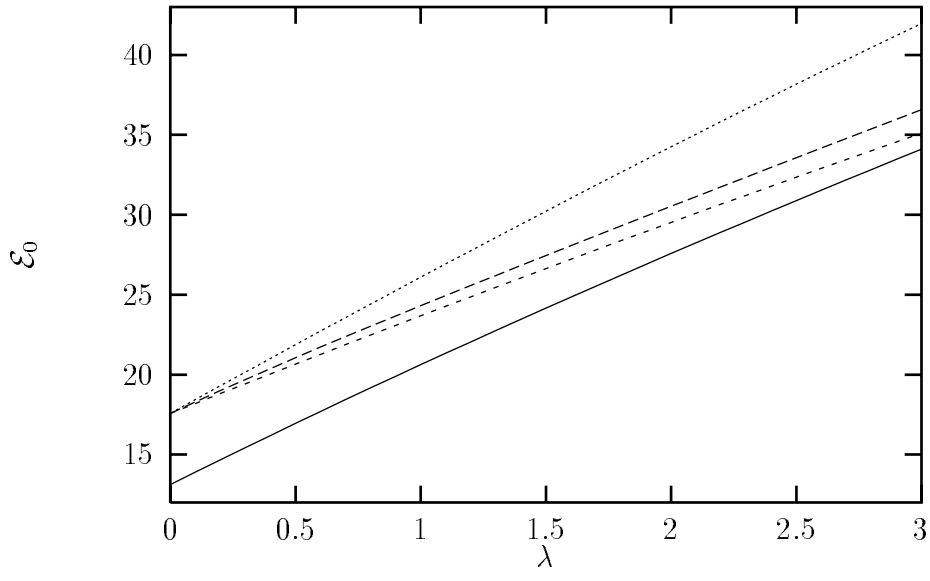
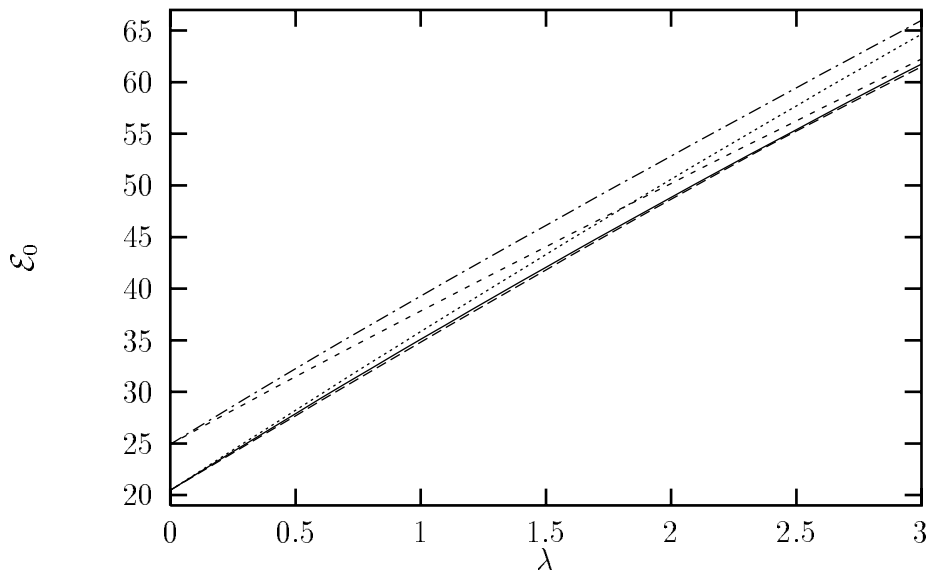


Fig.2



**Fig.3**

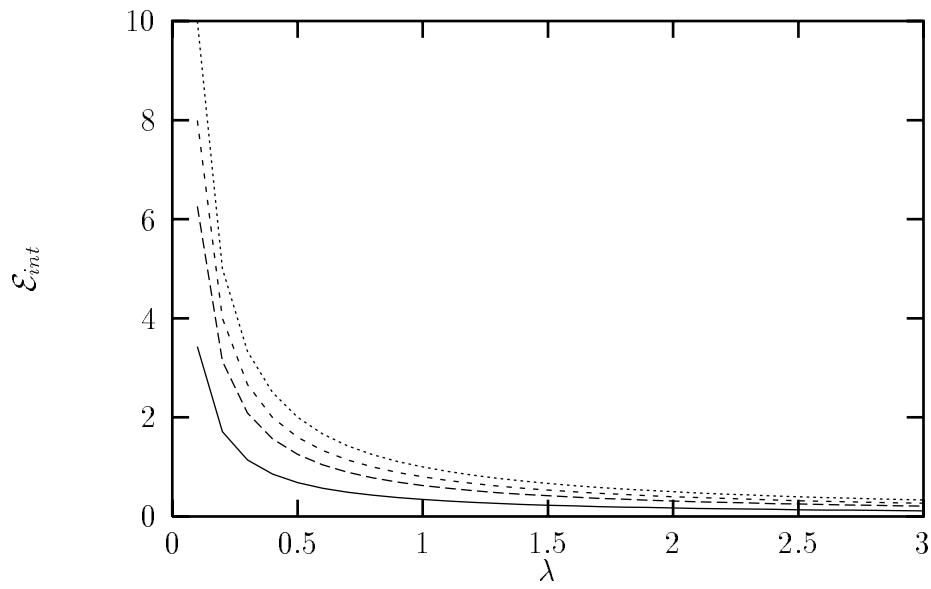


Fig.4

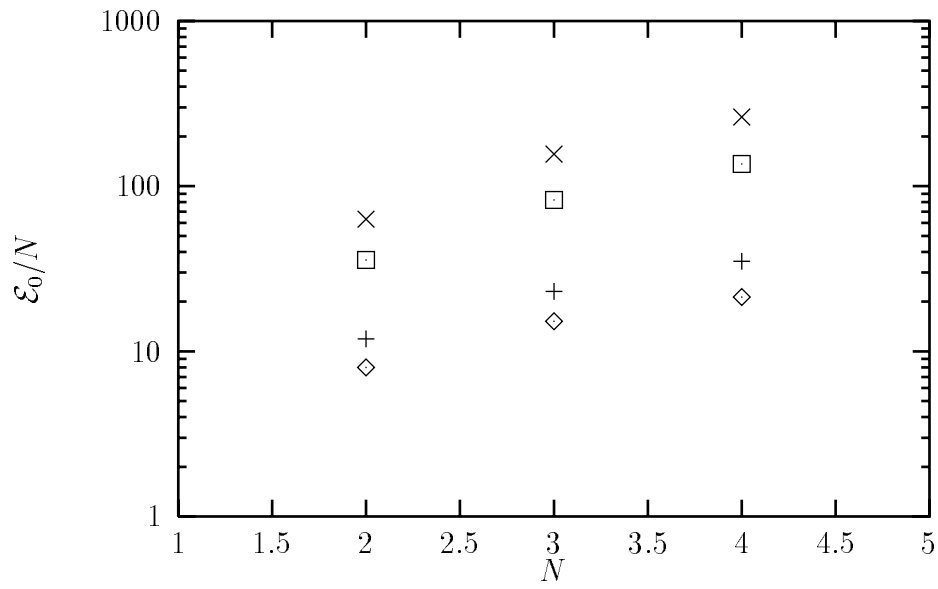


Fig.5