

**INTERACTING ELECTRONS IN PARABOLIC QUANTUM DOTS:
ENERGY LEVELS, ADDITION ENERGIES,
AND CHARGE DISTRIBUTIONS**

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We investigate the properties of interacting electrons in a parabolic confinement. To this end we numerically diagonalize the Hamiltonian using the Hartree-Fock based diagonalization method which is related to the configuration interaction approach. We study different types of interactions, Coulomb as well as short range. In addition to the ground state energy we calculate the spatial charge distribution and compare the results to those of the classical calculation. We find that a sufficiently strong screened Coulomb interaction produces energy level bunching for classical as well as for quantum-mechanical dots. Bunching in the quantum-mechanical system occurs due to an interplay of kinetic and interaction energy, moreover, it is observed well before reaching the limit of a Wigner crystal. It also turns out that the shell structure of classical and quantum mechanical spatial charge distributions is quite similar.

1. Introduction

Nanostructured electronic systems like quantum wells, quantum wires, or quantum dots are one of the most active areas of research in today's condensed matter physics. On the one hand they are of fundamental interest, allowing the fabrication and investigation of artificial atoms, molecules and even solids with well-defined and highly adjustable properties. On the other hand, they are of immediate importance to applications, e.g. electronic devices. The problem of interacting electrons in a parabolic confinement potential is one of the paradigmatic examples in this field. It has attracted considerable attention recently, both from experiment and from theory. Experiments on parabolic quantum dots¹ have revealed peculiar properties of such systems, in particular the "bunching" of energy levels. This means that at certain gate voltages two or more electrons enter the dot simultaneously corresponding to a negative chemical potential. This is in contradiction to the picture of single-particle energy levels plus a homogeneous charging energy. To understand these properties, first a model of classical point charges in a parabolic potential was investigated.² It was found that the system displays a shell structure which is essentially independent of the type of interaction. However, the opposite is true for the addition energies: For Coulomb interaction the shell structure is nearly unimportant while a short-range interaction leads to fluctuations in the addition energies which can give rise to level bunching.

The approximation of electrons by classical point charges becomes exact in the zero-density limit, but in the experiments¹ the density is rather high, and the system is likely to be in the Fermi liquid regime. Therefore a quantum-mechanical investigation is necessary. However, the interacting many-particle problem is not exactly solvable, and numerical calculations beyond the Hartree-Fock (HF) level are complicated since the dimension of the many-particle Hilbert

space grows exponentially with the number of particles. Recently, a multilevel blocking Monte-Carlo method was used to investigate the crossover between the Fermi liquid and Wigner crystal regimes.³

In this paper we investigate the problem of interacting electrons in a parabolic confinement using the Hartree-Fock based diagonalization (HFD) method⁴ which is related to the quantum chemical configuration interaction approach. The paper is organized as follows: In section 2 we define the model Hamiltonian and describe our method, and the results are presented in section 3.

2. Model and Method

In the experiments the parabolic quantum dot is formed in the two-dimensional electron gas at a GaAs/AlGaAs interface. Thus, the confinement in lateral direction is very strong while the much weaker, approximately parabolic confinement in the layer is produced by a gate voltage. We model this situation by considering a system of electrons in two dimensions in a parabolic confinement interacting via a screened Coulomb potential (in the experiments screening is produced by the gate). The Hamiltonian reads

$$H = \sum_{\sigma} \int d^2r \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{m}{2} \omega^2 \mathbf{r}^2 \right] \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d^2r d^2r' \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \frac{e^2 e^{-K_0|\mathbf{r}-\mathbf{r}'|}}{\epsilon|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}). \quad (1)$$

The problem contains three length scales, the oscillator length scale, $l_0 = (\hbar/m\omega)^{1/2}$, the Bohr radius of the host, $a_0 = \hbar^2\epsilon/me^2$, and the screening length, K_0^{-1} . Rescaling all lengths by l_0 , and defining $\alpha = l_0/a_0$, $k_0 = K_0 l_0$ leads to

$$H = \sum_{\sigma} \int d^2r \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} \mathbf{r}^2 \right] \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d^2r d^2r' \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \frac{\alpha e^{-k_0|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}). \quad (2)$$

A value of $\alpha = 0$ corresponds to non-interacting electrons, experimentally realistic values of α are around 1...10. A numerically exact solution of this quantum many-particle system requires the diagonalization of a matrix whose dimension increases exponentially with the number of particles in the dot. This severely limits the possible particle numbers. In order to calculate the properties of this model we therefore use the HFD method.⁴ The basic idea is to work in a truncated Hilbert space consisting of the HF ground state and the low-lying excited Slater states. For each disorder configuration three steps are performed: (i) find the HF solution of the problem, (ii) determine the B Slater states with the lowest energies, and (iii) calculate and diagonalize the Hamiltonian matrix in the subspace spanned by these states. The number B of basis states determines the quality of the approximation, reasonable values have to be found empirically. For the results reported here we have worked in a plane wave basis with up to 961 k -points. This leads to accurate results for non-interacting electrons, the relative energy error is smaller than 10^{-9} for up to 20 electrons and smaller than 10^{-6} for up to 50 electrons. The truncated many-particle Hilbert space used in the HFD method consisted of up to $B = 4000$ Slater states.

3. Results

We have first carried out calculations for classical point charges (which corresponds to neglecting the gradient term in eq. (2)). Here the ground state is determined simply by minimizing the total energy with respect to the positions of the point charges in the dot. Figure 1(a) shows

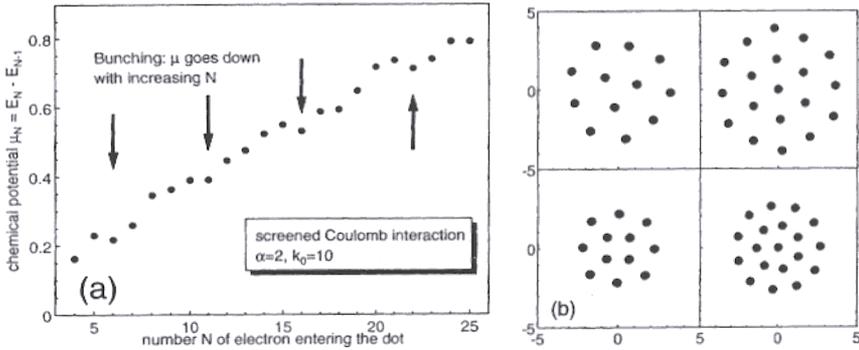


Fig. 1. (a) Addition spectrum for a system of classical point charges. (b) Real space configurations of the charges, the upper two configurations for 12 and 19 electrons are for unscreened interaction ($\alpha = 4, k_0 = 0$), the lower two are for $\alpha = 4$ and $k_0 = 1$.

the resulting addition energies $\mu_N = E_N - E_{N-1}$ and the corresponding configurations of the point charges in real space. While μ_N generally increases with N , it decreases for some N . If $\mu_N > \mu_{N+1}$ two electrons will enter the dot simultaneously if the gate voltage reaches μ_N , i.e. the system shows bunching. Figure 1(b) shows the sensitivity of the real space configurations to screening by comparing the charge configurations for screened and unscreened interactions.

It is clear that the kinetic energy term in the Hamiltonian which was neglected in the classical calculations will have a tendency to suppress the energy fluctuations connected with different real space configurations. As a first check we compare the radial charge densities of the classical and quantum-mechanical calculations in Figure 2. For the classical case the point charges are replaced by Gaussians whose width is half the minimum particle distance. The qualitative shell structures of the two systems are very similar. The kinetic energy leads to a slightly wider charge cloud in the quantum case.

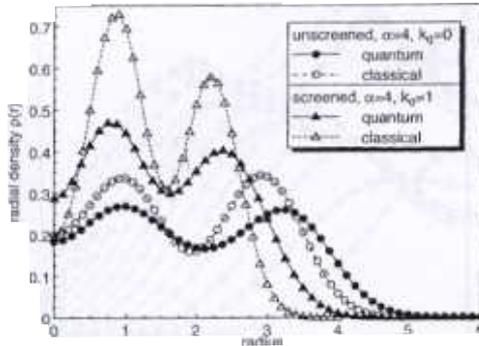


Fig. 2. Comparison of the classical and quantum-mechanical results for the radial charge densities for a quantum dot with 12 electrons, full spin-polarized case, $S = 6$.

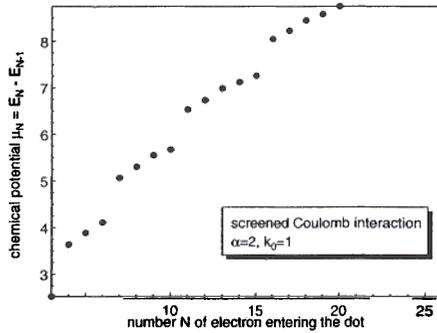


Fig. 3. Addition energies for the quantum-mechanical case, $\alpha = 2$, $k_0 = 1$, spin-polarized case, $S=N/2$.

In Figures 3 and 4 we present the addition energies and the radial charge distribution for quantum-mechanical electrons in the fully spin polarized case $S = N/2$, respectively. The parameters $\alpha = 2$ and $k_0 = 1$ are chosen to roughly correspond to the experiments¹ while the number of electrons we simulate in the dot is almost one order of magnitude smaller.

Figure 4 shows, that the charge distribution in the dot sometimes completely reorganizes when an electron is added. However, the fluctuations in the ground state energies caused by these reorganizations are not strong enough to lead to bunching as can be seen from Figure 3. The addition energies are rather dominated by the single-particle levels which possess the degeneracies due to rotational symmetry. However, if the interaction becomes larger, bunching can be observed already for the small electron numbers accessible in our simulation, as can be seen from Figure 5.

For a direct comparison of our results with the experiment our calculations have to be

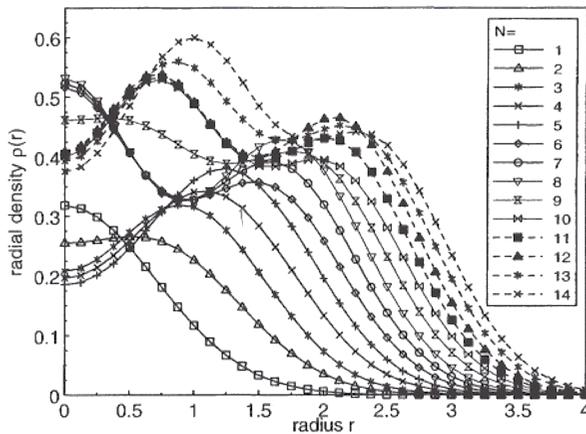


Fig. 4. Radial charge distribution for the quantum-mechanical case, $\alpha = 2$, $k_0 = 1$, spin-polarized case, $S=N/2$.

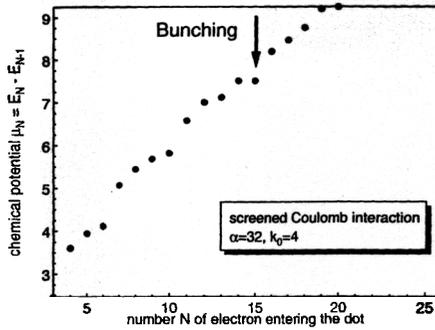


Fig. 5. Addition energies for a quantum-mechanical dot with strong interactions, full spin-polarized case

extended to larger electron numbers. Furthermore, the spin degrees of freedom which have been suppressed in our calculations so far, probably play an important role. In particular, the spin structure will also change with increasing particle number. This leads to larger fluctuations in the ground state energy and enhances the possibility of bunching. Investigations along these lines are underway.

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