The influence of the Coulomb interaction on the electronic spectrum of quantum dots

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Abstract

The spectral properties of up to *four* interacting electrons confined within a quasi–one dimensional system of finite length are determined by numerical diagonalization. The ground state energy as a function of the number of the electrons and the lengths of the system is investigated. The energetically lowest lying excitations are identified with vibrational and tunneling modes of the charge distribution. The limits of a dilute, Wigner–type arrangement of the electrons, and a dense, more homogeneous distribution are discussed.

1 Introduction

Interaction effects play a crucial role in the understanding of the electric transport in very small condensed matter systems [1]. Most prominent are the Coulomb blockade and the single–electron oscillations in quantum mechanical tunneling of electrons through very small tunnel junctions [2], and the resonance–like oscillations of the conductance of quantum dots at milli-Kelvin temperatures [3]. They are commonly discussed in terms of the tunneling resistances and capacitances [4, 5]. However, the microscopic justification of the latter is not obvious [6, 7].

One possibility to investigate whether or not a capacitance can be defined for small systems is to compare the quantum mechanical ground state energy E_0 of several, N, interacting confined electrons with the charging energy of a capacitor. In this paper we present results for E_0 obtained by numerical diagonalization of the corresponding Hamiltonian. In contrast to previous work for harmonic confinement [8, 9] which was restricted to $N \leq 2$ we consider rectangular confinement and $N \leq 4$.

In addition we discuss the spectral properties, especially in the asymptotic regions of low (Wigner electron lattice) and high density (almost homogeneous charge distribution). We identify two kinds of elementary excitations, namely vibrational and tunneling modes that are related to the Coulomb repulsion, and the exchange interaction, respectively.

We conclude from our microscopic results that for the system parameters realized in inversion layer based quantum dots the quantum mechanics of the electron–electron interaction cannot be neglected.

2 Interacting electrons in a square well potential

We consider N–electrons within a 1D square well of length L. We use the interaction potential

$$V(x,x') \propto \frac{1}{\sqrt{(x-x')^2+\lambda^2}}. \tag{1}$$

which behaves Coulombically at large distances. λ is a measure for the width of the electron wave functions in transversal direction. For most of our results $\lambda/L = 2\cdot 10^{-4} \ll 1$. Then, the energy eigenvalues of the Hamiltonian

$$H = E_{\rm H}\frac{a_{\rm B}}{L}\left(\frac{a_{\rm B}}{L}H_0 + H_{\rm I}\right) \tag{2}$$

depend only weakly on λ. $E_{\rm H} = e^2/a_{\rm B}$ is the Hartree energy, $a_{\rm B} = \varepsilon\hbar^2/me^2$ the Bohr radius, ε the relative dielectric constant and m the electron mass. The relative importance of the the kinetic energy of the electrons within the square well,

$$H_0 = \sum_{n,\sigma} \varepsilon_n c^+_{n,\sigma} c_{n,\sigma} \tag{3}$$

($\varepsilon_n \propto n^2$), and the interaction energy,

$$H_{\rm I} = \sum_{n_1 \ldots n_4, \sigma_1, \sigma_2} V_{n_4 n_3 n_2 n_1} c^+_{n_4\sigma_1} c^+_{n_3\sigma_2} c_{n_2\sigma_2} c_{n_1\sigma_1} \tag{4}$$

changes with the system length. The total electron spin S is conserved. All eigenvalues have degeneracy $2S+1$.

The interaction matrix elements $V_{n_4 n_3 n_2 n_1}$ are real, and do not depend on the spin state σ. They fulfill the symmetry relations $V_{n_4 n_3 n_2 n_1} = V_{n_4 n_2 n_3 n_1} = V_{n_1 n_3 n_2 n_4} = V_{n_3 n_4 n_1 n_2}$. Furthermore, $V_{n_4 n_3 n_2 n_1} = 0$ if $\sum_i n_i =$ odd. For $\lambda/L \ll 1$

$$V_{n_4 n_3 n_2 n_1} \approx -8\pi \int_0^\infty {\rm d}q \; (\ln(q\lambda/L) + C)\, \hat{f}_{14}(q)\hat{f}_{23}(q) \quad .$$

$\hat{f}_{ij}$ is the Fourier transform of the product $\varphi^*_{n_i}(x)\varphi_{n_j}(x)$ of the one–electron eigenfunctions of H_0, and $C = 0.577$ the Euler constant.

The numerical diagonalization requires a restriction of the number of considered one particle states $c^+_{n\sigma} \mid 0\rangle$ to $1 \le n \le M$. Their anti–symmetrized products form a complete N–particle basis, which includes also the spin degree of freedom. It can easily been generated for arbitrary N using a binary code representation. Although the size of the Hamiltonian matrix, given by the binomial coefficient $R = (2M)!/N!(2M-N)!$, is rapidly increasing with N there are only relatively few non–vanishing elements. It is very economic to determine only the latter. Applying two creation operators to a certain $(N-2)$–particle state, generates an N–particle state with proper sign, which corresponds to a certain row of the Hamiltonian matrix. Creating from the same $(N-2)$–particle state a (different or the same) N–particle state identifies a certain column. Independent summation over all possible two–particle excitations and subsequent summation over all $(N-2)$–particle states generates eventually all non–vanishing elements of the Hamiltonian matrix. In our calculations $R \le 10^4$ even when using Lanczos procedures.

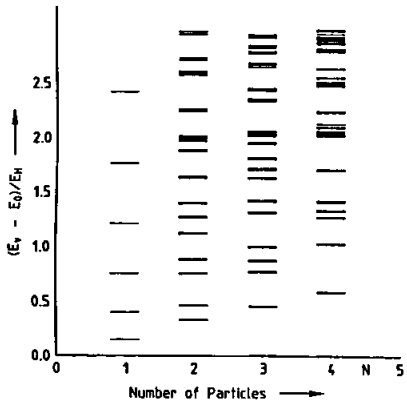

Figure 1: Energy spectra for different electron numbers for a system of length $9.45a_B$ in atomic energy units E_H. The ground state energies E_0 are substracted. The low lying eigenvalues form multiplets with very small internal level separations which are not resolved in the figure. The corresponding states differ in the total spin quantum number.

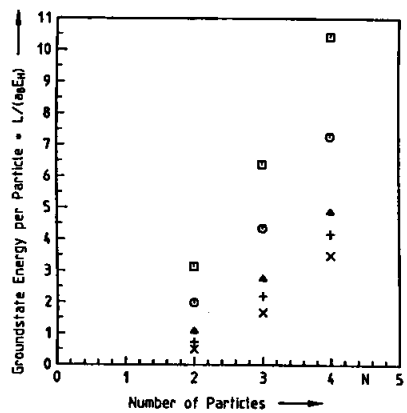

Figure 2: Ground state energies per particle E_0/N multiplied by L/a_B versus the particle number N in atomic units for $L = 6.61a_B$ (□) $L = 16.1a_B$ (o) $L = 94.5a_B$ (△) $L = 944.8a_B$ (+). (×) denote the energy of N electrons at fixed, equally spaced positions, $L/(N-1)$. They are the limiting values of E_0 as $L \to \infty$.

3 The Eigenvalue Spectrum

Typical examples of N–electron spectra are shown in Figure 1. Not only the average total number of levels per energy interval is considerably increasing with N, but also their density within certain energy regions. The lowest eigenvalues form *multiplets* that are energetically extremely narrow when $L \gg Na_B$. The total number of states within each multiplet, including degeneracies, is 2^N.

Figure 2 shows the dependence of E_0/N on N for different L. The data are multiplied by L in order to eliminate the trivial L–dependence. $E_0(N)$ is *not* proportional to $N(N-1)$, as expected for the classical charging model. For the smaller systems the contribution of the kinetic energy leads to considerable deviations. On the other hand, for very large L, one can approximate $E_0(N)$ by the Coulomb energy of N electrons at equal distances $r_s = L/(N-1)$ (Wigner lattice).

In Figure 3 E_0/N is shown as a function of r_s. Pronounced deviations from the Coulombic $1/L$ behavior occur below $r_s \lesssim r_1 \approx 50a_B$. These deviations cannot be attributed to a simple additive influence of the kinetic part of the Hamiltonian.

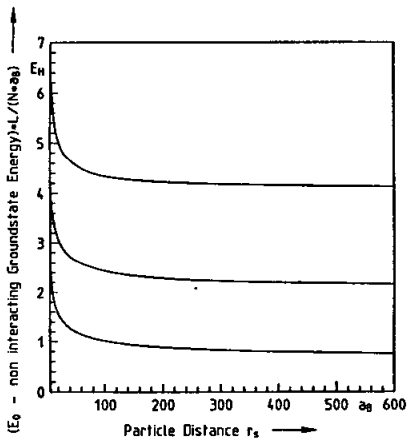

Figure 3: Ground state energy per particle E_0/N multiplied by L/a_B versus the mean particle distance $r_s = L/(N-1)$. Ground state energies of the corresponding non-interacting systems were subtracted. Data for $N = 2$, $N = 3$ and $N = 4$ are shown (from bottom to top). Deviations from Coulombic behavior occur for $r_s \lesssim 50 a_B$.

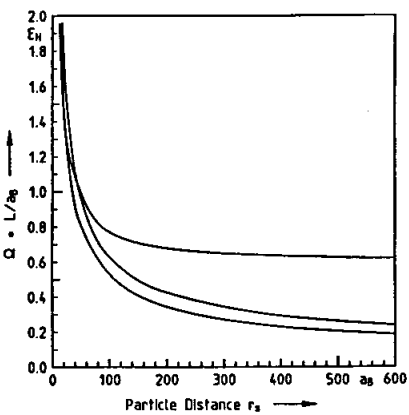

Figure 4: Energy difference between the two lowest multiplets, Ω, multiplied by L/a_B versus the mean particle distance r_s. Data for $N = 2$, $N = 3$ and $N = 4$ are shown (from bottom to top). Ω decreases stronger than $\sim r_s^{-1}$ for $N = 2$ and 3.

For $L \gg N a_B$ certain aspects of the spectra can be understood using the Wigner crystal picture. In this limit, the electron density shows N approximately equidistant peaks within L. One type of excitation is phonon like due to the Coulomb forces between these charge density maxima.

For charge clouds at equal distance r_s the typical phonon frequencies should behave $\sim r_s^{-\nu}$ with $\nu = 3/2$ or $= 1$ if δ-function like or Gaussian charge distributions with a variance inversely proportional to the phonon frequency, respectively, are assumed. The energy of the lowest excitation of vibrational type is given by the distance Ω between the lowest two multiplets in our spectra. Figure 4 shows $\Omega L/a_B$ as function of r_s for different N. The behavior at large r_s is consistent with $\nu \gtrsim 1$, indicating that the charge density distributions are more localized than Gaussians. For $r_s \lesssim r_2 \approx 100 a_B$ the strong deviations from the asymptotic behavior signalize the breakdown of the Wigner crystal.

Each of the multiplets consists of a series of energy levels that are $(2S+1)$-fold degenerate since the corresponding states are simultaneously eigenstates of $\hat{S}^2$. They transform according to the irreducible representation A_2 of the permutation group P_N

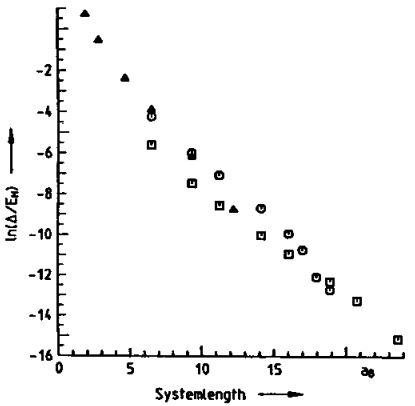

Figure 5: Logarithm of the energy difference Δ between the ground state and the first excited state within the lowest multiplet versus the system length for $N = 2$, $M = 11$ ($\Box$), $N = 3$, $M = 13$ (o), and $N = 4$, $M = 10$ (Δ). From the slope of the data we estimate $L_\Delta \approx 1.5 a_B$.

(Pauli principle). However, when exchanging spatial coordinates only, they transform according to *any* irreducible representation of P_N since H does not contain spin operators.

In general, the states are not simple products of spatial and spin parts, as is shown for $N = 3$ in [10]. The quantum number of the total spin increases with increasing energy within each multiplet, in agreement with the theorem of Lieb and Mattis [11] for 1D interacting electrons.

For a better understanding of the level structure within one multiplet we consider the configuration space of dimensionality L^N. The modulus of the N-particle probability amplitude has maxima there at $N!$ different points corresponding to the number permutations of N particles. The eigenfunctions can be approximately identified with linear combinations of states $|j>$, with $1 \leq j \leq N!$, each of them corresponding to one of the $N!$ maxima. The coefficients for the linear combination are determined by the respective irreducible representation of P_N. The differences between the energy expectation values are proportional to the finite overlap integrals between the states $|j>$. Assuming an asymptotic exponential decay of the $|j>$ wave functions suggests $\Delta \propto \exp(-L/L_\Delta)$, where Δ is the energy difference between the ground state and the first excited state within the lowest multiplet. L_Δ is a characteristic length scale beyond which the non-interacting spectrum is changed into the multiplet structure characteristic for the influence of the Coulomb interaction. The tunneling energies Δ depend on λ, due to the finiteness of the height of the potential barrier between different maxima of the N-electron probability amplitude given approximately by $V(x,x) \propto \lambda^{-1}$ (eq. (1)).

In Figure 5 the L-dependence of $\ln(\Delta/E_H)$ is plotted for different N. From the slope of the linear part of the data we obtain $L_\Delta \approx 1.5 a_B$.

4 Conclusion

We have calculated numerically the energy spectra of up to $N = 4$ electrons confined within a quasi-one dimensional potential well of finite length. We demonstrated that the $E_0(N)$ deviates from the classically expected N^2-behavior due to the quantum mechanical influences of the kinetic energy, and the formation of a Wigner-lattice like structure for small and large L, respectively. For low electron numbers it is only a limited range

of variables where a capacitance–type of behavior can be obtained.

We discussed the dependence of the energies for the lowest (vibrational and tunneling mode) excitations. Deviations from the Wigner–type arrangement due to the influence of the kinetic energy part is found for quite large system sizes r_2. The ground state energy cannot be obtained by adding kinetic and potential energy eigenvalues separately. It turns out that exponentially decaying states $|j>$ describe our data well down to system lengths $L \approx L_\Delta \approx 1.5 a_B$ (Figure 5), although the single particle charge density can be expected to be more or less homogeneous for $L \lesssim N \cdot 100 a_B$ (Figure 4).

Given the geometry and the electron numbers in the AlGaAs/GaAs–based quantum dots showing the resonance–like conductance oscillations [3] (area of the dot $\approx 2 \cdot 10^5 \mathrm{nm}^2$, number of electrons $\approx 10^2$ effective mass $\approx 0.07m$, dielectric constant ≈ 10) one can estimate a mean distance of $r_s \approx 2a_B$ such that $L_\Delta \approx r_s \ll r_1, r_2$. Although in general, especially at lower electron density [12], quantum mechanical effects cannot be discarded for the understanding of the conductance oscillations, we conclude from the results of our investigations (Fig. 2) that for this relatively high density the physical situation can be approximately described by a semi–classical picture taking into account only the Coulombic part of the electron-electron interaction.

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