The addition spectrum of a classical short-range interaction model for a disordered quantum dot

1998 J. Phys.: Condens. Matter 10 6515

(http://iopscience.iop.org/0953-8984/10/29/011)

J. Phys.: Condens. Matter **10** (1998) 6515–6522. Printed in the UK PII: S0953-8984(98)91574-0

The addition spectrum of a classical short-range interaction model for a disordered quantum dot

E Eisenberg and R Berkovits

The Jack and Pearl Resnick Institute of Advanced Technology, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

Received 11 February 1998, in final form 24 April 1998

Abstract. The addition spectrum of a classical short-range interaction model for a disordered quantum dot is calculated numerically. The average change in the chemical potential needed to add a particle, as well as the fluctuations in this quantity, are proportional to the interaction strength, and their ratio is one for a wide range of interaction strengths. Analytical arguments which lead to the same result are also presented. On the basis of these results the behaviour of these quantities for real Coulomb interactions at the high-density limit may be reproduced, and speculations on the behaviour at low densities are presented.

1. Introduction

Due to the great advances in microstructure fabrication and measurement techniques, the addition spectra of quantum dots have recently became experimentally accessible [1–4]. When the conductance is measured as a function of an applied gate voltage V_g, a series of conductance peaks appears. Each peak corresponds to an additional electron in the dot, and the spacings between the conductance peaks ΔV_g are proportional to the change in the chemical potential of the dot as an additional electron enters. This may be expressed by

$$e\,\Delta V_g \propto \mu_{N+1} - \mu_N = \Delta\mu_N. \tag{1}$$

The conductance peak spacing is mainly determined by the charging energy and is proportional to e^2/C, which is the well known Coulomb blockade phenomenon [5].

For small quantum dots, in which the single-electron-level spacing is already significant, careful measurements [2–4] of the conductance peak spacings show fluctuations. One would expect fluctuations of the order of the single-level spacings which do not depend on the charging energy (or the interaction between the electrons), but some of these experiments seem to indicate larger fluctuations [2, 3]. An exact-diagonalization study on a small many-particle tight-binding model with long-range Coulomb interactions indicates that such large fluctuations appear in the low-density regime, i.e., when the ratio of the Coulomb interaction between neighbouring electrons and their kinetic energy

$$r_s = e^2/v_F = 1/\sqrt{\pi n}a_B \geqslant 1$$

(where v_F is the Fermi velocity, n is the electronic density and a_B is the Bohr radius) [2, 6]. This density region includes the density of the experimental dots.

The numerical study indicates that for $r_s \geqslant 1$ the peak spacing fluctuations depend on the interaction strength and are proportional to the peak spacing [2]. At these densities, short-range correlations also appear in the electronic density, although the system is far from

0953-8984/98/296515+08$19.50

the Wigner crystallization regime [6]. It was suggested that the behaviour of the fluctuation is due to the essentially classical appearance of the short-range correlations in the system, which lead to interaction-dependent fluctuations.

This work has motivated several studies of the addition spectrum based on classical models such as the Coulomb glass [7] and the Wigner crystal island [8], in which long-range Coulomb interactions for classical models are considered. In the study of the Coulomb glass it was shown that the average conductance peak spacing, as well as the fluctuations of the peak spacing, increase with interaction strength and their ratio is of order 0.3.

The experiments described in references [1–4] were carried out at a temperature of 30 mK, and thus the configuration is expected to be the ground state. In order to rule out the possibility of extremely long thermalization times, such that the ground state was not attained during the experiment, the sweep along the gate voltage was done both up and down. Comparison of the peak positions confirms that the system did enter its ground state. We thus study the spacing of the ground states of the system for different numbers of electrons.

In this paper we check the behaviour of a classical model which incorporates the features of short-range correlations and disorder. We will show that in this model the peak spacing fluctuations increase with interaction strength and are proportional to the average peak spacing, as is the case for the quantum model in reference [2] and the Coulomb glass model of reference [7]. This is rather surprising, since naively one would expect the fluctuations for short-range interactions to depend on the disorder and not on the interaction strength.

On the other hand, the proportionality ratio is of the order of one, which is much larger than the ratio in the full quantum treatment, or the Coulomb glass case. The reason for this behaviour lies in the different roles played by short- and long-range interactions in determining the average and fluctuations in the ground-state energies of the systems. The average value of the peak spacing is mainly determined by the long-range part of the interactions, while the short-range correlations determine the dependence of the fluctuations on the interaction strength. If we add an infinite-range component to the interaction, the average peak spacing will increase, with no influence on the fluctuations. Thus, by such a combination any desired ratio between the peak spacing fluctuations and the average peak spacing can be achieved. When the magnitudes of both components of the interaction are compared on physical grounds, the proportionality ratio coincides with the one obtained from RPA (random-phase approximation) results.

2. The model and results

The model that we study is one of classical spinless electrons on a disordered 2D square lattice, which only interact with nearest neighbours. In fact, this is similar to the Coulomb glass Hamiltonian with the long-range interactions replaced by nearest-neighbour interactions. The Hamiltonian is given by

$$H = \sum_i (h_i - \mu) n_i + U \sum_{\langle ij \rangle} n_i n_j \tag{2}$$

where $n_i = 0, 1$. The disordered on-site potential h_i is randomly chosen from a uniform distribution $U[-1, 1]$, and μ is the chemical potential proportional to the external gate voltage V_g applied to the dot. As μ gets higher, the ground state of the dot becomes more and more populated. As can be seen from equation (1), the conductance peak spacings are proportional to the change in μ needed to add an additional particle to the dot, and hence we study the statistics of the change in μ needed to add another particle to the ground-state

configuration of the dot, i.e., $\Delta\mu_N = \mu_{N+1} - \mu_N$. We study the relative fluctuations of the spacings

$$\sqrt{\langle \delta^2\, \Delta\mu \rangle}/\langle \Delta\mu \rangle$$

where

$$\langle \delta^2\, \Delta\mu \rangle = \langle \Delta\mu^2 \rangle - \langle \Delta\mu \rangle^2$$

and $\langle \cdots \rangle$ denotes averages with respect to disorder realizations.

Numerical calculations of the ground state of this system become simpler on using the mapping of the problem to a related network problem, as suggested in [9]. A network is defined such that its minimum-cut capacity is equal to the ground-state energy of the Hamiltonian (2) [10]. To determine the capacity of the minimum cut, the '*max-flow min-cut*' theorem is used [11]. This theorem states that the minimum cut is equal to the maximal flow in the network. The maximal flow, in turn, can be calculated by employing the Ford–Fulkerson algorithm [11, 12]. Using this mapping, the ground state can be exactly determined in a polynomial time, $O(n^2)$, where n is the lattice size.

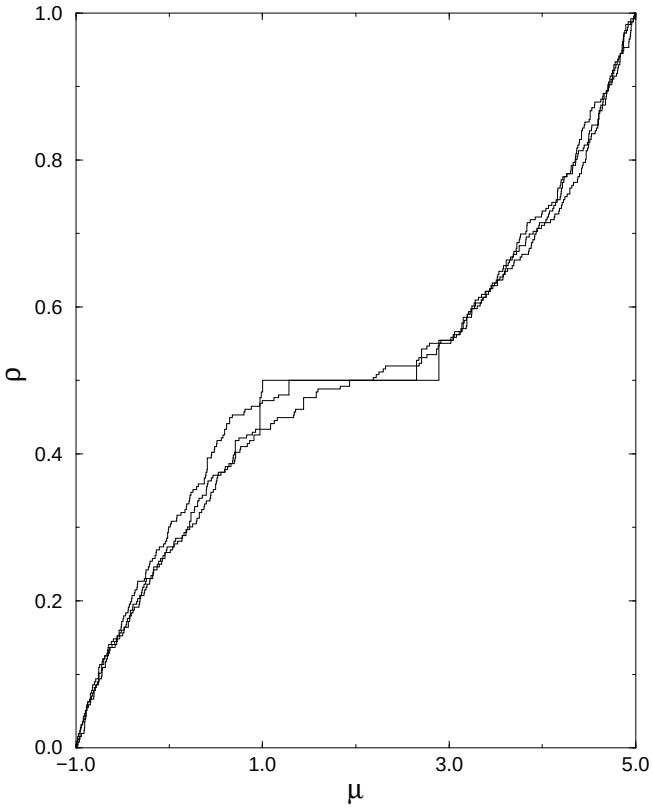

Figure 1. The ground-state density ρ versus the chemical potential μ for three disorder realizations of a 16×16 lattice. $U = 1.0$.

The numerical calculation was done as follows. For each realization of the disordered system, we started with a very low value of the chemical potential μ such that the ground-state density was zero, and then searched for the value of μ for which the density changes.

The process thus continues until all of the lattice is filled. Thus we generate for each realization a density versus μ plot. Such a plot is presented in figure 1. Usually, a change in the density involves the addition of one new particle, but in many cases, especially close to half-filling, two or even more particles were added simultaneously. This happens whenever there is an electron or a domain which is located in a potential well in a non-optimal way, such that it prevents new particles from coming in. It takes then a big change in μ to make it possible to add a new electron, but when this happens, the whole domain moves and there is room for more electrons.

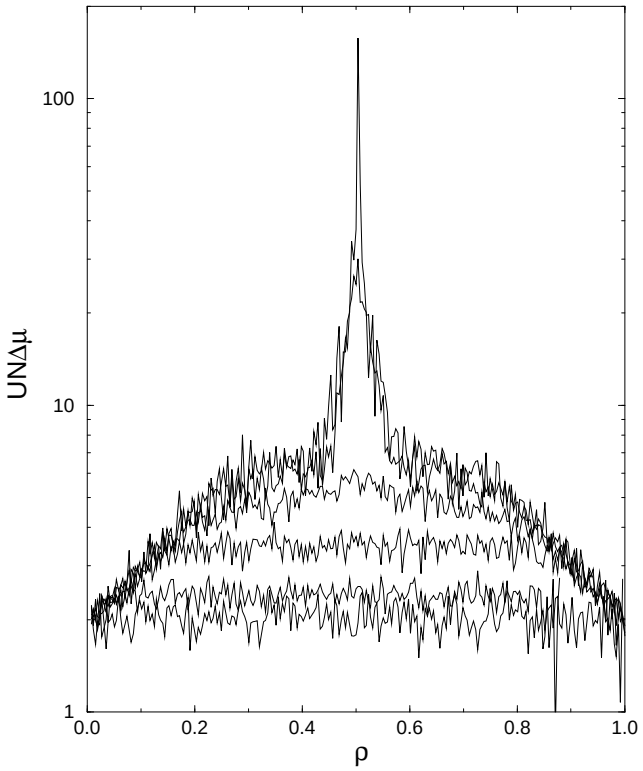

Figure 2. The average gap $\Delta\mu$ as a function of the ground-state density ρ. The various lines correspond to different values of U/H, where U takes the values (from bottom to top) 10^{-2}, 0.1, 0.3, 0.5, 0.8, 1.0.

We then repeat the calculation for many realizations and look at the statistics for $\Delta\mu$ needed to add the jth particle, as a function of the interaction strength U. The average $\langle\Delta\mu\rangle$ as a function of density is presented in figure 2 for various values of U. Most of the calculations were done for 250 realizations of 16×16 lattices. It can be seen that as U increases, the spacings near half-filling become larger. The reason for this behaviour is as follows. For an exactly half-filled ground state in a finite system, it is clear that for large U the electrons will be ordered on one of the two sub-lattices such that no interaction term will contribute to the energy. To put in the next electron, one needs a change in μ of the order of $4U$ (plus some disorder contribution). Thus we get a spacing which scales O(1) while all other gaps are O($1/N$). As one comes close to half-filling, the system organizes itself into the ordered phase of the half-filling ground state. As explained before, this means

moving large domains from lower-potential positions to places in which they fit the global order. Thus larger and larger spacings occur. Like in to the situation for the random-field Ising model [13], one expects that as the system size goes to infinity, the picture of an ordered ground state at half-filling breaks down. The ground state of an infinite 2D system is built up from ordered domains of linear dimension $L_c \sim \exp(U^2)$. This cut-off length controls the divergence in the $N \to \infty$ limit.

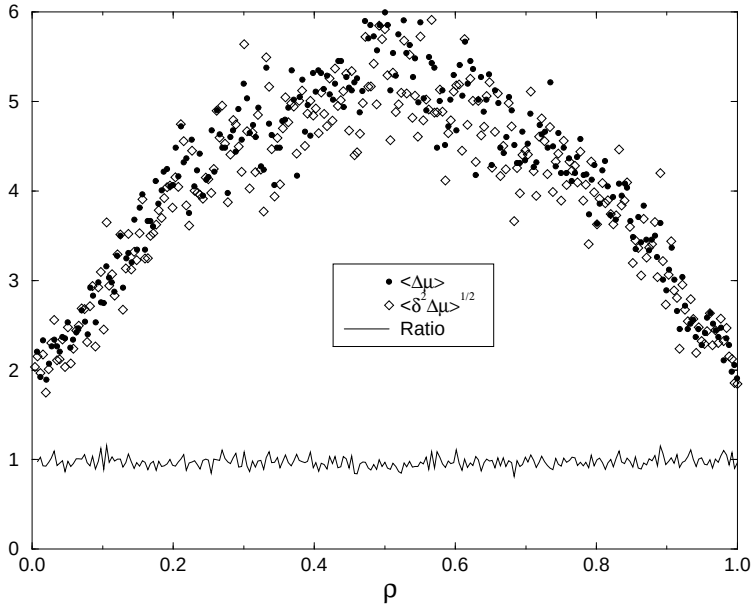

Figure 3. The average gap $\Delta\mu$ (circles) and the square root of the fluctuations $\sqrt{\langle\delta^2\,\Delta\mu\rangle}$ (diamonds) as a function of the ground-state density ρ for $U = 0.5$. The solid line shows the relative fluctuations.

We now look at the relative fluctuation. Figure 3 presents the fluctuations $\langle\delta^2\,\Delta\mu\rangle$ for $U = 0.5$, together with the average $\langle\Delta\mu\rangle$. It is clearly seen that the behaviour of the fluctuations as a function of the density is exactly the same as that of the average gap. This behaviour persists for all other values of U. We therefore obtain the result that the relative fluctuation in our model is constant with respect to changes of both the density and U.

The average $\Delta\mu$ can be crudely estimated as follows. It is clear that the first particle enters the dot when $\mu = -h_{min} \sim -1$, and the addition of the last particle costs $4U + h_{max} \sim U + 1$, i.e., the range of μ needed to fill all of the lattice is

$$-1 < \mu < 4U + 1.$$

Thus, neglecting density correlations, the average gap should be $(4U + 2)/N$. This is indeed what we get for small values of U, where interaction plays no role. We see that the average gap depends on U, and this is even more important when one takes into account the density dependency of the gap as explained before, since near half-filling the gap diverges as a function of U. This dependency on U is expected. However, we see that fluctuations in the gaps as a result of disorder in the configuration depend on U in the same manner. This is less obvious, since one might expect only the disorder to affect these fluctuations. This behaviour is in agreement with the quantum model in reference [2] and the Coulomb glass model of reference [7].

In the following we give a simple argument to show that this behaviour should be attributed to the short-range character of the interaction, and this is the reason for not finding it in the infinite-range Coulomb blockade model. In real systems, however, the interaction is long ranged but not infinite ranged, and thus we get an intermediate result, which has the characteristics of both the short-range behaviour of the fluctuations in $\Delta\mu$ and the infinite-range behaviour of the average $\Delta\mu$, as will be explained.

We make two assumptions.

(a) The effect of the deposition of the jth electron on the deposition of the $(j+1)$th electron may be neglected. This is plausible when the system is much larger than the interaction range, and generally, the jth and the $(j+1)$th particles will be positioned far enough apart that there is no interaction between them. We neglect here the possibility of a global change in the system caused by the addition of a new particle. We have checked and seen that this happens only in the vicinity of half-filling. Otherwise, almost always the correlation between the j-particle ground state and the $(j+1)$-particle ground state is maximal.

(b) The probability density of $\Delta\mu$ $P(0) \neq 0$, i.e., there is a finite probability for $\Delta\mu = 0$. This is in fact related to the first assumption. If there is no connection between the deposition of the two particles, there is nothing to prevent them entering together.

Under these two assumptions, we can state the following. We look at a given configuration, and denote by $\bar{h}_i$ the effective local field at each site (interaction + disorder). The next two particles will enter in at the two sites with the smallest effective local field. We denote the probability distribution of the effective local field by $p(x)$. It is easy to see that

$$G(\Delta) = n(n-1)\int \mathrm{d}x_0 \; p(x > x_0 + \Delta)^{n-2} P(x_0) P(x_0 + \Delta) \tag{3}$$

is the probability density for having the smallest effective potential x_0, and the next one $x_0 + \Delta$ (such that $\Delta\mu = \Delta$), integrated over all possible x_0, i.e., the probability density for having $\Delta\mu = \Delta$. This can also be written as

$$G(\Delta) = -n\,\frac{\partial}{\partial \Delta}\int \mathrm{d}x_0 \; p(x > x_0 + \Delta)^{n-1} P(x_0). \tag{4}$$

Since the spacings (apart from in the vicinity of half-filling) scale $\mathrm{O}(1/N)$, we may assume x_0, $x_0 + \Delta \ll 1$, and write

$$\begin{aligned} G(\Delta) &\sim -nP(0)\,\frac{\partial}{\partial \Delta}\int \mathrm{d}x_0 \; \exp(-(n-1)P(0)(x_0 + \Delta)) \\ &\sim (n-1)P(0)\exp(-(n-1)P(0)\Delta) \end{aligned} \tag{5}$$

where in the last equation we replaced n by $n-1$ to maintain normalization. We thus see that the probability distribution of $\Delta\mu$ is exponential and it is therefore clear that the ratio of the fluctuations should be 1.

3. Discussion

Thus, we find that the relative fluctuations for a nearest-neighbour classical model do not depend on the interaction parameter U for a considerable region of interaction strength and densities. Since the averages $\Delta\mu$ certainly do depend on U, this means that the interaction enhances the disorder-induced fluctuations. This effect is actually what is seen in reference [2] where a full quantum mechanical many-particle Hamiltonian with long-range Coulomb

interactions was treated. We therefore claim that the origin of this effect is not the quantum mechanical behaviour, but the local correlations induced by short-range interactions.

However, the ratio between the fluctuations of $\Delta\mu$ and its average value, i.e., the magnitude of the relative fluctuations, does depend on the long-range nature of the interaction. This can be seen from adding an infinite-range interaction to equation (2):

$$H = \sum_i (h_i - \mu)n_i + U\sum_{\langle ij\rangle} n_i n_j + (e^2/2C)\sum_{ij} n_i n_j. \tag{6}$$

While the fluctuations in $\Delta\mu$ will not be influenced by the additional infinite-range term, the average value of $\langle\Delta\mu\rangle \sim e^2/C$. Thus, using the value for the fluctuations obtained in the previous section, the ratio

$$\sqrt{\langle\delta^2\,\Delta\mu\rangle}/\langle\Delta\mu\rangle \sim 4UC/e^2N$$

which, since it depends on two parameters U and C, can correspond to any ratio.

A natural extension of the classical model results into the quantum regime can be performed in the following way. U is the strength of the nearest-neighbour interaction, i.e. $U \sim e^2/a$, where a is the lattice constant. Since $C \sim L$ and $N = (L/a)^d$ (where d is the dimensionality), one obtains

$$\frac{\sqrt{\langle\delta^2\,\Delta\mu\rangle}}{\langle\Delta\mu\rangle} \sim \left(\frac{a}{L}\right)^{d-1}. \tag{7}$$

Assuming that the range of the nearest-neighbour interactions is of the order of the screening length κ^{-1}, the result is

$$\frac{\sqrt{\langle\delta^2\,\Delta\mu\rangle}}{\langle\Delta\mu\rangle} \sim \left(\frac{1}{\kappa L}\right)^{d-1} \tag{8}$$

which is exactly the RPA result for these fluctuations [6]. Since the classical behaviour of the fluctuations seems to hold for any value of U, the qualitative behaviour should not change beyond the RPA limit (i.e., $r_s > 1$, or κ^{-1} is smaller than the mean distance between particles) except for the fact that the screening length should be replaced by $\lambda \sim 1/n^{1/d}$, the mean distance between particles [7]. Thus, according to these considerations,

$$\frac{\sqrt{\langle\delta^2\,\Delta\mu\rangle}}{\langle\Delta\mu\rangle} \sim \left(\frac{\lambda}{L}\right)^{d-1} \tag{9}$$

beyond the RPA limit. On the other hand, it is possible that beyond the RPA regime there is some collective behaviour that will lead to a departure from the above behaviour. A detailed study of the size dependence of the fluctuation ratio is still needed for the full quantum model in order to clarify this point.

References

[1] For recent reviews, see
Kastner M A 1992 *Rev. Mod. Phys.* **64** 849
Meirav U and Foxman E B 1995 *Semicond. Sci. Technol.* **10** 255

[2] Sivan U, Berkovits R, Aloni Y, Prus O, Auerbach A and Ben-Yoseph G 1996 *Phys. Rev. Lett.* **77** 1123

[3] Simmel F, Heinzel T and Wharam D A 1997 *Europhys. Lett.* **38** 123

[4] Patel S R, Cronenwett S M, Stewart D R, Huibers A G, Marcus C M, Duruoz C I, Harris J S, Campman K and Gossard G 1998 *Phys. Rev. Lett.* **80** 4522

[5] Averin D V and Likhraev K K 1991 *Mesoscopic Phenomena in Solids* ed B L Altshuler, P A Lee and R A Webb (Amsterdam: North-Holland)

[6] Berkovits R and Altshuler B L 1997 *Phys. Rev.* B **55** 5297

[7] Koulakov A A, Pikus F G and Shklovkii B I 1997 *Phys. Rev.* B **54** 9223
[8] Koulakov A A and Shklovkii B I 1998 *Phys. Rev.* B **57** 2352
[9] Hartmann A K and Usadel K D 1995 *Physica* A **214** 141
[10] Pickard J P and Ratcliff H D 1975 *Networks* **5** 357
[11] Ford L R and Fulkerson D R 1956 *Can. J. Math.* **8** 399
[12] Tarjan R E 1983 *Data Structures and Network Algorithms* (Philadelphia, PA: Society for Industrial and Applied Mathematics)
[13] For a recent review, see
Belanger D P and Young A P 1991 *J. Magn. Magn. Mater.* **100** 272