We study influence of electron-electron interaction on statistics of Coulomb blockade peak spacings in disordered quantum dots. It is shown that the interaction combined with fluctuations of eigenfunctions of the Fermi sea, enhances the peak spacing fluctuations, in accordance with recent experiments. In addition, account of the spin degrees of freedom leads to a pronounced odd-even structure for weak interaction ($e^2/\epsilon \ll v_F$); in the opposite case ($e^2/\epsilon \gtrsim v_F$) this structure is washed out.

PACS numbers: 73.23.Hk, 73.61.-r, 05.45.+b

Recent experimental studies of chaotic quantum dots in the Coulomb blockade regime showed unusually large fluctuations of conductance peak spacings. The r.m.s. fluctuation of the spacing between consecutive peaks was found to exceed the mean level spacing $\Delta$ [1,2]. These fluctuations can not be explained from the point of view of the standard “charging energy” model (CEM) [3] which assumes that the spacing between the consecutive peaks is equal to $S_N = e^2/C + \delta \xi_N$. Here $C$ is the capacitance of the quantum dot, while $\delta \xi_N$ is the distance between the last filled single-particle level and the previous one. Since the charging energy $e^2/C$ is a non-fluctuating quantity in CEM, the peak spacing fluctuations are solely due to the single-particle energies. Assuming the applicability of the random matrix theory (RMT) one obtains [4] (we consider the case of broken time reversal symmetry throughout the paper)

$$r.\ m.\ s. (S_N) = \Delta (3\pi/8 - 1)^{1/2},$$

(1)

that is less than observed experimentally.

Below we study the fluctuations of peak spacings in the Coulomb blockade regime. First we investigate the Coulomb interaction in the finite system, and find corrections to CEM. Then we demonstrate that these corrections, being combined with fluctuations of eigenfunctions, lead to enhancement of spacing fluctuations. This becomes important for a sufficiently strong interaction and may account for experimentally observable effects. In addition, we study the effect of spin degree of freedom and find a pronounced odd-even structure of conductance peaks, which for strong interactions is washed out.

Recently Sivan et al [2] made an attempt to explain the large fluctuations of $S_N$ observed in experiment using numerical diagonalization of a Coulomb system with $N \sim 10$ electrons. However, they considered the range of very strong interaction $e^2/C > E_F$, where $E_F$ is the Fermi energy, while in the experiment [2] $e^2/C \sim 0.6$ meV and $E_F \sim 12$ meV. Effect of spin has been also recently studied by Prus et al [5] in terms of a disordered Hubbard model.

We consider a diffusive quantum dot ($R \gg l$, $R$ and $l$ being the size of the dot and the mean free path, respectively) with a large number of electrons. Most of them are compensated by a positive background with the density $\bar{\rho}$; in addition, there is a number $N$ of excess (uncompensated) electrons, so that the total charge of the dot is $Ne$. The Hamiltonian of the system is

$$H = \sum_{\lambda} \epsilon_\lambda a_\lambda^+ a_\lambda + \frac{1}{2} \sum_{\lambda_1, \lambda_2} a_\lambda^+ a_\lambda U_{\lambda_1, \lambda_2} a_{\lambda_1} a_{\lambda_2},$$

(2)

$$U_{\lambda_1, \lambda_2} = \int \mathbf{dr}_1 \mathbf{dr}_2 \psi_{\lambda_1}^* (\mathbf{r}_1) \psi_{\lambda_2}^* (\mathbf{r}_2) U (\mathbf{r}_1 - \mathbf{r}_2) \times \psi_{\lambda_1} (\mathbf{r}_2) \psi_{\lambda_2} (\mathbf{r}_1).$$

(3)

Here $\lambda$ labels eigenstates of non-interacting system with eigenfunctions $\psi_\lambda (\mathbf{r})$ and energies $\epsilon_\lambda$; the correlations of these states have been calculated in Ref. [6]. Furthermore, $U (\mathbf{r}) = U_0 (\mathbf{r}) \equiv e^2/\epsilon \rho$ is the Coulomb interaction, $\epsilon$ being the dielectric constant. The interaction with positive background should be added to Eq. (2).

**Random-phase approximation in restricted geometry.** As is well known, it is not sufficient to consider the Coulomb interaction in the first order of perturbation theory due to its long-range nature. A common way to improve it is the random phase approximation (RPA). Whereas it is trivial to solve the RPA equation in infinite system, restricted geometry makes the situation more complicated (cf. [6]). In the 3D case the RPA equation for the effective potential $U$ is

$$U (\mathbf{r}, \mathbf{r}') = U_0 (\mathbf{r} - \mathbf{r}') - \int \mathbf{dr}_1 \mathbf{dr}_2 U_0 (\mathbf{r} - \mathbf{r}_1) \times K (\mathbf{r}_1, \mathbf{r}_2) U (\mathbf{r}_2, \mathbf{r}'),$$

(4)

where the polarization operator $K$ has the form

$$K (\mathbf{r}, \mathbf{r}') \approx \nu \left( \delta (\mathbf{r} - \mathbf{r}') - V^{-1} \right) = \nu \sum_{\alpha \neq 0} \phi_\alpha (\mathbf{r}) \phi_\alpha (\mathbf{r}').$$

Here $\nu$ is the density of states, $\phi_\alpha (\mathbf{r})$ is the eigenfunction of the Laplace operator with eigenvalue $-E_\alpha$;
\[ \phi_0 = V^{-1/2} \] is the so-called zero-mode. In addition, the function \( K \) contains also a random part. The latter gives rise to the fluctuations of the charging energy and is for a moment ignored. The bare Coulomb potential \( U_0 \) can be expanded as follows:

\[
U_0(r - r') = \sum_{\alpha \neq 0} \frac{4\pi e^2}{\epsilon} E_\alpha^{-1} \phi_\alpha(r) \phi_\alpha(r') + V^{-1/2} \sum_{\alpha \neq 0} u_{\alpha 0} [\phi_\alpha(r) + \phi_\alpha(r')] + V^{-1} u_{00}, \tag{5}\]

where we have denoted

\[
u = e^2 \int dr \phi_\alpha(r) \Phi(r), \quad u_{00} = \frac{e^2}{\epsilon V} \int dr \Phi(r),
\]

\[
\Phi(r) = \int dr' |r - r'|^{-1}. \tag{6}\]

Then the solution to the equation (6) reads as

\[
U(r, r') = \sum_{\alpha \neq 0} \frac{4\pi e^2 / \epsilon}{(E_\alpha + \kappa^2)^{-1}} \phi_\alpha(r) \phi_\alpha(r') + V^{-1/2} \sum_{\alpha \neq 0} u_{\alpha 0} (E_\alpha + \kappa^2)^{-1} [\phi_\alpha(r) + \phi_\alpha(r')] + V^{-1} (u_{00} - \nu \sum_{\alpha \neq 0} (1 + \kappa^2 / E_\alpha)^{-1} u_{\alpha 0}), \tag{7}\]

with \( \kappa = \sqrt{4\pi e^2 / \epsilon} \) being the inverse screening length. One can show (3) that in the limit \( \kappa R \gg 1 \) (\( R \) is characteristic size of the system), which we assume from now on, RPA result (3) can be also obtained from the Thomas-Fermi approximation (TFA), that assumes proportionality between effective potential and excess charge density.

Up to a constant, the first term in Eq. (7) is the usual 3D screened Coulomb interaction,

\[
U_\kappa(r_1, r_2) = \frac{e^2}{\epsilon r} \exp(-\kappa r),
\]

where \( r = |r_1 - r_2| \). Two other terms appear due to the restricted geometry. The last one is a constant, \( e^2 / C \), and \( C \) is usual electrostatic capacitance of the system; for the sphere with radius \( R \) we recover \( C = \epsilon R \). Relative correction to \( C \) due to the finite value of screening parameter \( \kappa \) is found to be of the order \( (\kappa R)^{-1} \). Finally, the second term (to be denoted as \( \tilde{U}(r) + \tilde{U}(r') \)) is a single-particle (rather than a two-particle) contribution. It vanishes in the electrostatic limit \( \kappa \to \infty \), and for the sphere takes the explicit form (up to a constant)

\[
\tilde{U}(r) = -\frac{e^2}{\epsilon \kappa R^2} \exp(-\kappa R - r)), \tag{8}\]

i.e. it is localized in a narrow layer of thickness \( \kappa^{-1} \) near the boundary. Thus, the Coulomb interaction in the restricted geometry is given by

\[
U(r, r') = U_\kappa(r_1, r_2) + \tilde{U}(r) + \tilde{U}(r') + e^2 / C; \tag{9}\]

\[
\int dr U_\kappa(r, r') = \int dr \tilde{U}(r) = 0.
\]
$E(N + 1) - E(N)$; the distance between two adjacent peaks is the difference $S_N = \mu_{N+1} - \mu_N$.

We use Hartree-Fock (HF) approximation and account for $e-e$ interaction by introducing the effective single-particle Hamiltonian $\hat{H}_N$ which depends explicitly on the number of excess electrons $N$. Its spectrum is schematically shown on Fig. 1. First empty state is separated from the last filled one by a gap of order $e^2/C$. The key point for the further discussion is that the Hamiltonian $\hat{H}_N$ is essentially random for each $N$. Namely, we assume that the statistical properties of its single-particle excited states (with the exception of the gap mentioned above) are the same as that of single electron states in a random potential. In particular, in the leading approximation they obey RMT, an assumption which is in agreement with the experiment [10].

![Energy states of the HF Hamiltonian with $N$ (left) and $N + 1$ (right) excess electrons.](image)

The distance between two adjacent peaks can be decomposed in a following way (Fig. 1):

$$S_N = \mu_{N+1}^{(N+2)} - \mu_N^{(N+2)} + (\mu_N^{(N+2)} - \mu_N^{(N+1)}) \equiv E_1 + E_2.$$ 

Here $\mu_j^{(j)}$ is the energy of single-particle eigenstate $j$ of the (HF) Hamiltonian $\hat{H}_N$.

Both quantities $E_1$ and $E_2$ are random. The statistical properties of the latter one are trivial, since it is just a distance between two adjacent single-particle levels of the same random Hamiltonian $\hat{H}_N$. Hence, they obey RMT; in particular, the average $\langle E_2 \rangle = \Delta$, while the fluctuations are given by Eq. (10).

On the other hand, the quantity $E_1$ is the shift of the $N + 2$-th single-particle level due to addition of a new electron in the $N + 1$-th state. It can be expressed as

$$E_1 = \int dr_1 dr_2 \mathcal{U}(r_1, r_2) \left[ |\psi_{N+1}(r_1)\psi_{N+2}(r_2)|^2 - |\psi_{N+1}^*(r_1)\psi_{N+1}(r_2)|^2 \right].$$ (13)

Here $\psi_{N+1}$ and $\psi_{N+2}$ are eigenfunctions of two first excited single-particle states of the Hamiltonian $\hat{H}_N$ (with corresponding energies $\mu_N^{(N+1)}$ and $\mu_N^{(N+2)}$, respectively; see Fig. 1). The quantities $E_1$ and $E_2$ are statistically independent; therefore fluctuations of $S_N$ are given by the sum of fluctuations of $E_1$ and $E_2$. In other words, since $E_1$ is related to the change in the Hamiltonian (from $\hat{H}_N$ to $\hat{H}_{N+1}$), it leads to fluctuations, additional to those given by RMT.

Statistical properties of this quantity can be investigated with the use of the expressions for correlations of eigenfunctions [8]:

$$V^2(|\psi_k(r_1)\psi_l(r_2)|^2) - 1 = k_d(r)\delta_{kl} + \Pi(r_1, r_1)$$

$$+ \Pi(r_1, r_2)\delta_{kl} + (1/2)\Pi^2(r_1, r_2).$$ (14)

The short-range function $k_d(r)$ is defined as

$$k_d(r) = (\pi v)^{-2} \frac{\text{Im} G^R(r)}{\rho} =$$

$$\approx \exp(-r/l) \left\{ \frac{J_0^2(p_F r)}{(p_F r)^{-2} \sin^2 p_F r}, \begin{array}{ll} 2D & 3D \end{array} \right.,$$ (15)

and $\Pi(r_1, r_2)$ is the diffusion propagator. For $r \gg l$ and for the case of spherical (3D) and circular (2D) particle

$$\Pi(r_1, r_2) \approx \left\{ \begin{array}{ll} (\pi g)^{-1} \ln r/r, & 2D \\frac{2D}{3D} & \end{array} \right.,$$ (15)

with $g = 2\pi E_c/\Delta$ being the dimensionless conductance; $E_c = D/R^2$ and $D$ are the Thouless energy and the diffusion coefficient, respectively. For a moment we assume electrons to be spinless, then the wave functions $\psi_{N+1}$ and $\psi_{N+2}$ are different.

It can be shown [8], that the average $\langle E_1 \rangle = e^2/C$, with negligible corrections of the order $\Delta(\rho F)^{1-d}$. Thus, the average spacing between the Coulomb blockade peaks is $\langle S_N \rangle = e^2/C + \Delta$, in agreement with CEM.

Now we turn to fluctuations of the quantity $E_1$. In accordance with decomposition [8], there are three contributions. First, the charging energy $e^2/C$ is a fluctuating quantity due to fluctuations in the polarization operator $K(r, r')$. A direct calculation [8] shows r.m.s. $(e^2/C) \sim \alpha_2^2 \Delta \ln g/g.$ Here the parameters $\alpha_3 = 4\pi e^2/\hbar c^2$ and $\alpha_2 = 2\pi e^2/\hbar c$ are equal to unity for the case of weak interaction ($k \ll p_F$ – see below).

Next, we evaluate the fluctuations due to the screened interaction $\tilde{U}_k$. Expanding the average of eight wave functions in the cumulants [11] and using Eq. (11) we find that these fluctuations are of order r.m.s. $|E_1(\tilde{U}_k) - \langle E \rangle| \sim \alpha_d g^{-1/2} \Delta$. Finally, the fluctuations due to the potential $\tilde{U}$ can be directly evaluated with the use of Eq. (14), yielding

$$\text{r.m.s. } E_1(\tilde{U}) = \left\{ \begin{array}{ll} 2 \int dr_1 dr_2 \tilde{U}(r_1, r_2) |\psi_{N+1}(r_1)|^2 \psi_{N+1}^2(r_2)|^2 \right\}^{1/2} \sim \begin{array}{ll} \alpha_2 g^{-1/2} \Delta, & 2D \\ \alpha_3 g^{-1/2} \Delta, & 3D \end{array},$$ (16)
which constitutes the main contribution to the fluctuations of the quantity $E_1$. This result reflects the fact that fluctuations of the density of the last added electron lead to fluctuations of its energy in the non-uniform potential $U(r)$.

In the above treatment the screened Coulomb potential has been calculated within RPA, and thus we have assumed $\kappa \ll p_F$, that implies $\alpha_d = 1$. If the interaction is strong (but still the ground state of the dot is Fermi-liquid-like), the range of the screened potential is determined by the Fermi wavelength. The quantity $\alpha_d$ is then of order of $\alpha_d \sim e^2/\epsilon v_F > 1$. The limitation on $\alpha_d$ given by the Wigner crystallization is $\alpha < \alpha_c$, where $\alpha_c \simeq 100$ in 2D (see e.g. [12]). Therefore, even for $\alpha$ well below the Wigner crystallization threshold, the fluctuations (16) can exceed $\Delta$, if the dimensionless conductance $g$ is not too large.

Although the above results are derived for diffusive systems ($R \gg l$), we believe also that they are valid for chaotic ballistic systems ($R < l$) as well. For the latter case the parameter $g$ can be roughly estimated as the ratio of inverse time of flight $t_F$ to the level spacing, $g \sim (t_F \Delta)^{-1} \sim v_F/(R \Delta)$, up to a geometry-dependent coefficient.

**Spin effects.** We denote as $\uparrow$ and $\downarrow$ two states with the same energy but different values of spin; their eigenfunctions are identical. If the state $\uparrow$ is occupied by an electron, the energy of the state $\downarrow$ is shifted, the shift being

$$E_1 = \int dr_1 dr_2 U_c(r_1, r_2)|\psi_\lambda(r_1)|^2|\psi_\lambda(r_2)|^2. \quad (17)$$

Using Eq. (14), we find

$$\langle E_1 \rangle = \left\{ \begin{array} {l}
 c_2 \Delta (\kappa/p_F)^{d-1} \ln(p_F/\kappa), \quad e^2/\epsilon \ll v_F \\
 \alpha_d \Delta, \quad e^2/\epsilon \gtrsim v_F
\end{array} \right., \quad (18)$$

with the coefficients $c_1 = 1/2$ and $c_2 = 1/\pi$. In the weak interaction regime ($e^2/\epsilon \ll v_F$) we obtain $\langle E_1 \rangle \ll \Delta$. This means that the set of peaks is split into pairs; the reduced spacing $S_N - e^2/C$ between two peaks of the same pair (states $\uparrow$ and $\downarrow$) is equal to $\langle E_1 \rangle$, while that between two different pairs is of order $\Delta$. Furthermore, since the eigenfunctions of states $\uparrow$ and $\downarrow$ are identical, the corresponding peak heights are correlated, and the resulting picture is a set of pairs with small reduced spacings and correlated heights - a pronounced odd-even structure. Fluctuations of $E_1$ are given by Eq. (16) multiplied by a factor of 2, and do not destroy the pair structure. For strong interaction ($e^2/\epsilon \gtrsim v_F$) the splitting (18) exceeds $\Delta$, and reordering of energy levels takes place. However, the spacing fluctuations are still enhanced in comparison with the spinless value, since a new type of ensemble is created, with the spectrum formed by a superposition of a RMT-type set of levels and the same set shifted by $E_1$,

$$\nu(E) = \sum_\lambda \left[ \delta(E - E_\lambda) + \delta(E + E_1 - E_\lambda) \right].$$

In particular, the two-point correlation function is given by ($\Delta$ is now the mean level spacing for a system with removed spin degeneracy, $s = \pi \omega/2\Delta$, $\tilde{s} = \pi E_1/2\Delta$)

$$R(\omega) \equiv \langle \nu(E)\nu(E + \omega) \rangle/\langle \nu(E) \rangle \langle \nu(E + \omega) \rangle = \frac{1}{2} R_{RMT}(s) + \frac{1}{4} R_{RMT}(s - \tilde{s}) + \frac{1}{4} R_{RMT}(s + \tilde{s}), \quad (19)$$

where $R_{RMT}(s) = 1 - s^{-2} \sin^2 s$ is the RMT two-point correlation function. The level repulsion in the ensemble (13) is clearly reduced. Thus, fluctuations of peak spacings are enhanced by spin effects, in addition to their enhancement due to fluctuations in $E_1$ discussed above, Eq. (16). On the other hand, even-odd correlations of heights of adjacent peaks in the strong interaction regime are washed out.

In conclusion, we have studied Coulomb interaction effects on the statistics of conductance peaks spacings in the Coulomb blockade regime. The Coulomb interaction leads, in combination with fluctuations of eigenfunctions, to enhancement of peak spacing fluctuations in comparison with the RMT value. Taking into account the spin degrees of freedom, we find in addition in the case of weak interaction ($e^2/\epsilon \ll v_F$) a pronounced odd-even structure. The peaks come in pairs, with correlated heights and small reduced spacings $S - e^2/C \ll \Delta$ within each pair. In the opposite case $e^2/\epsilon \gtrsim v_F$, which is relevant to the experiment (12), this structure is destroyed.

We are grateful to L.I. Glazman and C.M. Marcus for useful discussions. This work was supported by the Alexander von Humboldt Foundation (Y.M.B.), SFB 195 der Deutschen Forschungsgemeinschaft (Y.M.B., A.D.M.), and the German-Israeli Foundation (A.D.M.).

*Present address: Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland.

[1] J. A. Folk et al, Phys. Rev. Lett. 76, 1699 (1996); C. M. Marcus et al, Superlattices and Microstructures, ICSMM, Liege (1996) (to be published); C. M. Marcus (private communication).

[2] U. Sivan et al, Phys. Rev. Lett. 77, 1123 (1996).

[3] See e.g. M. A. Kastner, Rev. Mod. Phys. 64, 437 (1992).

[4] M. L. Mehta, *Random Matrices*, Academic Press (N.Y.) (1991).

[5] O. Prus et al, Phys. Rev. B 54, R14280 (1996).

[6] Ya. M. Blanter and A. D. Mirlin, Phys. Rev. B 53, 12601 (1996); Phys. Rev. E 55, May (1997).

[7] M. Büttiker, J. Phys. Cond. Mat. 5, 9361 (1993).

[8] R. Berkovits and B. L. Altshuler, Phys. Rev. B 46, 12526 (1992).

[9] Ya. M. Blanter, A. D. Mirlin, and B. A. Muzykantski, unpublished.

[10] U. Sivan et al, Europhys. Lett. 25, 605 (1994).

[11] Ya. M. Blanter, Phys. Rev. B 54, 12807 (1996).

[12] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. 54, 437 (1982).