Even-odd correlations in capacitance fluctuations of quantum dots

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We investigate effects of short range interactions on the addition spectra of quantum dots using a disordered Hubbard model. A correlation function $S(q)$ is defined on the inverse compressibility versus filling data, and computed numerically for small lattices. Two regimes of interaction strength are identified: the even/odd fluctuations regime typical of Fermi liquid ground states, and a regime of structureless $S(q)$ at strong interactions. We propose to understand the latter regime in terms of magnetically correlated localized spins.

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Coulomb interactions and disorder in electronic systems have posed a major challenge to condensed matter physics for quite some time.

Quantum dots with discrete electronic spectra offer a new avenue to this problem. A direct probe to the ground state energy is given by Coulomb blockade peaks in the conductance as the gate voltage is varied [1–4]. Theory of spectral fluctuations of non interacting electrons has made much progress during the last decade due to the advent of semiclassical approximations, random matrix theory and the non linear sigma model approach [1,5]. However since Coulomb interactions are essential for the “Coulomb blockade” effect, one may wonder as to the validity of non interacting approximations to quantum dots in general. In particular: Is the ground state qualitatively similar or different than a Fock state of the lowest single electron orbitals?

To gain insight into this question, we consider a system of interacting electrons on a finite tight binding lattice with onsite disorder. The inverse compressibility at consecutive fillings is

$$ \Delta(N) = E(N + 1) - 2E(N) + E(N - 1) $$

where $E(N)$ is the ground state energy of a dot with $N$ electrons. (We assume weakly coupled leads such that $N$ is well defined within the area of the dot.) By varying a gate potential $\varphi$, the dot’s energy is modified to $E_{N}^{\varphi} = E(N) - \varphi N$. Conductance peaks through the leads are observed at $E_{N}^{\varphi}(N) = E^\ast(N + 1)$, i.e. at potentials $\varphi_{N} = E(N + 1) - E(N)$. Thus differences between the peak potentials $\varphi_{N}$ yield direct measurements of $\Delta(N)$ which can be defined as $e^2$ times the discrete inverse capacitance of the dot.

We shall model the single electron part of the dot’s Hamiltonian by a site-disordered tight binding model

$$ \mathcal{H}_{0} = \sum_{i,s} w_{i}c_{i,s}^{\dagger}c_{i,s} - \sum_{\langle ij \rangle} t_{ij}(B)c_{i,s}^{\dagger}c_{j,s} $$

$$ = \sum_{n,s} \epsilon_{n}\alpha_{ns}^{\dagger}\alpha_{ns} $$

where $c_{i,s}^{\dagger}$ creates an electron at site $i$ with spin $s$, $\langle ij \rangle$ denote nearest neighbors on the lattice, and $w_{i}$ are random site energies taken from a uniform distribution in the domain $[-W/\sqrt{3}, W/\sqrt{3}]$. $\alpha_{ns}^{\dagger}$ creates an electron in eigenstate $\phi_{n}$ and spin $s$. An orbital coupling to a magnetic field is included by defining $t_{ij}(B) = te^{i\mathbf{A} \cdot \mathbf{x}_{ij}}$, where $\mathbf{\nabla} \times \mathbf{A} = B$.

In the absence of electron interactions, the inverse compressibility is given by

$$ \Delta_{0}(N) = \begin{cases} 0 & N = 2n + 1 \\ \epsilon_{n+1} - \epsilon_{n} & N = 2n \end{cases} $$

where $\epsilon_{n}$ are defined in (3). We find it useful to define the “Ising” variables

$$ S(N) = \frac{\Delta(N) - \Delta(N - 1)}{[\Delta(N) - \Delta(N - 1)]} $$

and a corresponding correlation function on a series of $L$ consecutive data points,

$$ S(q) \equiv \frac{1}{L^{2}} \sum_{i,j=1}^{L} S(N_{i})S(N_{j}) \exp(-i(N_{i} - N_{j})q) $$

Obviously, the non interacting spectrum has perfect “long range antiferromagnetic correlations” i.e. $S_{0}(\pi) = 1$.

Coulomb interactions are treated by separating the interactions into the long and short range parts. A crude
approximation to these two terms is given by an onsite and an infinite range parts
\[ H_{int} = e^2 \frac{N(N-1)}{2C} + U \sum_i n_{is} n_{is}. \] (7)

where \( n_{is} = c_i^\dagger c_is \), \( s = \uparrow, \downarrow \). It is clear that the first term simply adds a constant \( \frac{\pi}{2} \) to \( \Delta(N) \), and therefore does not alter \( S(q) \). Thus in our model, deviations of \( S(q) \) from \( S_0(q) \) must therefore be a consequence of the Hubbard interactions described by the second term in (6). We restrict ourselves to a square lattice of \( N \) sites with periodic boundary conditions, and to disorder strength \( W \) appropriate for the “diffusive” regime, i.e. the mean free path \( l \) for the non interacting electrons is of the order of, or smaller than, the system’s linear length \( L \). Using \( l = v_F \tau \), where the inverse lifetime is calculated in the Born approximation to be \( \tau = \frac{\pi \hbar}{2eW} \), we find \( L/l = \frac{\pi}{16} \sqrt{N} (W/t)^2 \).

Perturbation theory: We diagonalize \( H_0 \) on a square lattice of size \( N \), with periodic boundary conditions for a given realization \( \{ w_i \} \). The single electron eigenenergies \( \{ \epsilon_n \} \) and wavefunctions \( \psi_n(i) \) are assumed to be known. The first order correction to Eq. (4) are given by second differences of the first order energies
\[ E_1(N) = U \sum_{n_{\uparrow} \leq n_{\uparrow}; n_{\downarrow} \leq n_{\downarrow}} |\psi_{n_{\uparrow}}|^2 |\psi_{n_{\downarrow}}|^2. \] (8)

Here we appeal to the random matrix properties of \( H_0 \) in the diffusive regime, in order to estimate the magnitude and fluctuations of \( E_1 \) analytically. We assume a Random Vector Model (RVM) where all eigenvectors \( \psi_n \) are random complex unit vectors of dimension \( N \) whose ensemble averaged correlations are
\[ \langle \psi_n(x_i) \psi_m(x_j) \rangle_{RVM} \propto \delta_{ij} \delta_{nm}. \] (9)

Using the orthonormalization constraints for \( \psi_n \) we obtain after some algebra \( \psi_n \) that the RVM estimate for the average first order correction to \( \Delta \) is
\[ \Delta_1^{RVM}(N) = \begin{cases} \frac{3U}{N^2 + 2} & N \text{ odd} \\ \frac{2U}{N^2 + 2} & N \text{ even} \end{cases} \] (10)

We have compared the RVM estimates to numerical results for disorder averaged \( \Delta_1^{num}(N) \) for odd and even \( N \) respectively. Calculations have been done for lattice sizes \( N = 56, 110, 210, 420 \), with the disorder varied in the range \( l/L \in [0.1, 2.5] \). We find that
\[ \Delta_1^{num}(N) = \begin{cases} [2.3, 3.5] \times \frac{L}{N} & N \text{ odd} \\ [-1.3, -2.7] \times \frac{L}{N} & N \text{ even} \end{cases} \] (11)

Comparison of (10) to (11) shows the RVM estimates to be in the right ball park as those gotten by numerically determining \( \psi_n \) of the disordered tight binding model. The main lesson learned by this calculation is that first order Hubbard corrections reduce on average the fluctuations in \( \Delta(N) \) since they are positive for odd \( N \) and negative (on average) for even \( N \).

Variational Theory for Sign Flips. The weak coupling regime is defined where the non interacting ground state \( |\Psi_0 \rangle \) is variationally stable against particle hole excitations. When interaction strength exceeds a certain threshold, it is variationally advantageous to create spin polarized electron-hole pairs e.g. \( c_{n \uparrow}^\dagger c_{n \downarrow}^\dagger |\Psi_0 \rangle \) which reduce the Hubbard interaction energy at the expense of enhanced single particle (kinetic) energy \( \epsilon_{n \uparrow} - \epsilon_{n \downarrow} \). In this variational theory, for an even number of electrons the threshold for forming a triplet is given by the inequality
\[ 0 > \Delta \epsilon - (E_1^\uparrow(2n) - E_1^\downarrow(2n)) = \Delta \epsilon + U \mathcal{F} \]
\[ \mathcal{F} = \sum_i \left( |\psi_{n+1}(x_i)|^2 - |\psi_n(x_i)|^2 \right) \left( \sum_{n' \neq n} |\psi_{n'}(x_i)|^2 \right) + |\psi_n(x_i)|^4 \] (12)

where \( \Delta \epsilon = \epsilon_{n+1} - \epsilon_n \) and \( E_1^\uparrow, E_1^\downarrow \) are the interaction corrections to the singlet and triplet energies respectively. Eq. (12) can alternatively be written as an inequality for \( \Delta(N) \) which includes up to first order corrections in \( U \):
\[ 0 > \Delta(2n) - \Delta(2n-1) - U \sum_i \left( |\psi_{n+1}(x_i)|^2 - |\psi_n(x_i)|^2 \right) \left( \psi_n(x_i) \right)^2 \] (13)

For extended random wave functions, the last term in (13) is readily seen to be of order \( N^{-3/2} \) and thus negligible in comparison to \( \Delta(2n) - \Delta(2n-1) \). Eqs. (12, 13) establish the connection between formation of triplets and sign flips of \( S(N) \) (defined in (6)). The sign flips degrade the “antiferromagnetic” correlations of \( S(q) \) as \( U \) is increased. We shall proceed to estimate the leading dependence of \( S(\pi;U) \) by a statistical calculation based on the properties of the non interacting spectrum of \( H_0 \) with and without an orbital magnetic field.

We assume that the level spacing statistics of \( H_0 \) in the diffusive regime of \( L/l \approx 1 \) is that of a random matrix in the Gaussian Orthogonal Ensemble (GOE). In the presence of a magnetic field \( B \) whose flux through the dot is of order of one flux quantum divided by \( N^{1/3} \), the level spacing statistics of \( H_0 \) turns into the Gaussian Unitary Ensemble (GUE). These assumptions were checked numerically and verified quite well for the Hamiltonian with and without external flux, on lattices up to \( N = 420 \) sites.

The Wigner distributions of \( \Delta \epsilon \) are
\[ P_2^{\text{GOE}}(\Delta \epsilon) = \frac{\Delta \epsilon \pi}{2 \Delta^2} e^{-\frac{\pi (\Delta \epsilon)^2}{4 \Delta^2}} \]
\[ P_2^{\text{GUE}}(\Delta \epsilon) = \frac{32 (\Delta \epsilon)^2}{\pi^2 \Delta^3} e^{-\frac{4 (\Delta \epsilon)^2}{\pi^2 \Delta^2}} \]  

(14)

where \( \Delta \) is the mean level spacing.

The probability distribution of the interaction term in \[ P(\Delta \epsilon) \]

is denoted by

\[ P_1(U,F) = \frac{1}{U} P_1(F), \]

(15)

where \( P_1 \) is a dimensionless function of its dimensionless argument. The probability of satisfying Eq. (12) is given by the double integral

\[ P^{\text{flip}}(U) = \int_0^\infty dF P_1(F) \int_0^{U,F} d(\Delta \epsilon) P_2(\Delta \epsilon) \]

(16)

which at weak coupling \( U \ll \Delta \) we can evaluate using the low energy expansion of \( P_2 \) and obtain

\[ P^{\text{flip}}_{\text{GOE}} \approx U^2 \frac{\pi}{2 \Delta^2} \int_0^\infty dx P_1(x) \int_0^{x} dx \epsilon = U^2 \frac{\pi}{4 \Delta^2} \langle F^2 \rangle \]
\[ P^{\text{flip}}_{\text{GUE}} \approx U^3 \frac{32}{\pi^2 \Delta^3} \int_0^\infty dx P_1(x) \int_0^{x} dx \epsilon = U^2 \frac{32}{3 \pi^2 \Delta^3} \langle F^3 \rangle \]  

(17)

At weak coupling the reduction in the perfect even-odd correlations are proportional to \( P^{\text{flip}} \), and therefore we find that

\[ 1 - S(\pi) \propto P^{\text{flip}}(U) \propto \left\{ \begin{array}{ll}
U^2 & \text{GOE} \\
U^3 & \text{GUE}
\end{array} \right. \]  

(18)

Numerical Diagonalizations. The variational theory and the random matrix estimates were checked by numerically diagonalizing the full interacting Hamiltonian on a lattice size \( 3 \times 3 \) with periodic boundary conditions with a magnetic flux \( \phi \) threading the lattice at its center. We varied the number of electrons for each specific realization from \( N = 5 \) to \( N = 13 \), each time diagonalizing the corresponding \( \left( \frac{N}{2A} \right)^2 \) matrix (i.e., maximum matrices of size \( 48620 \times 48620 \) for \( N = 9 \)) for various values of \( U \).

Then \( S(\pi) \) was calculated and averaged over 500 different realizations.

Two different values of \( \phi \) were considered: \( \phi = 0 \) and \( \phi = \pi/2 \) which should correspond to the GOE and GUE statistics. Because of the small size of the samples the maximum flux of \( \phi = \pi/2 \) is not strong enough to completely remove time reversal symmetry, and the level spacing is a combination of the GOE and GUE level spacing. The results of \( S(\pi) \) for both cases are presented in Fig. 1. It can be seen that the general behavior predicted in Eqs. (13) is observed. A reasonable fit for the numerical results in the regime \( U \leq 1 \) is obtained by \( S(\pi) = 1 - 0.3 U^2 \) for \( \phi = 0 \) and \( S(\pi) = 1 - 0.2 U^3 \). This supports the validity of the GOE (GUE) statistics for the case \( \phi = 0 \) (\( \phi = \pi/2 \)).

Experimental \( S(q) \). In Fig. (2) we have plotted three sets of data for \( \Delta(N) \) and \( S(q) \). The top two sets were measured on two GaAs samples at different fillings. The bottom data, measured on InO, was taken from Ref. [9]. It is interesting to note that \( S(q) \) shows strong even-odd correlations only for the middle data set, while it has no remnant of these correlations for the top and bottom sets. Although we do not attempt to provide a quantitative understanding of the data in this paper, we dare to speculate that the flatness of \( S(q) \) correlations is definitively associated with strongly correlated samples where ground states significantly differ from Fermi-liquid Fock states. The fluctuations in \( \Delta(N) \) due to the direct Coulomb interaction and its interplay with disorder are discussed in Ref. [1].

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FIG. 1. Averaged $S(q)$, Eq. (6), for the disordered Hubbard model on a $3 \times 3$ torus. Inset: $S(\pi)$ for the $\phi = 0$ and $\phi = \pi/2$ cases, fitted to estimates of RVM variational theory.

FIG. 2. Experimental second energy differences from quantum dots of GaAs, Ref. [9] (top and middle), and InO, Ref. [10], (bottom), with corresponding correlations $S(q)$. Correlations indicate that the top and bottom data are in the strongly interacting regime.