Universal Scrambling Properties of Spectra and Wave functions in Disordered Interacting Systems

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Recent experiments on quantum dots in the Coulomb Blockade regime have shown how adding successive electrons into a dot modifies the energy spectrum and the wave functions of the electrons already present in the dot. Using a microscopic model, we study the importance of electron-electron interaction on these “scrambling” effects. We compute the Hartree-Fock single particle properties as function of the number \( p \) of added electrons. We define parametric correlation functions that characterize the scrambling properties of the Hartree-Fock wave functions and energy spectra. We find that each of these correlation functions exhibit a universal behavior in terms of the ratio \( p/p^* \) where \( p^* \) is a characteristic number that decreases with increasing either the interaction strength, the disorder strength or the system size.

1 Introduction

At very low temperature, by applying a gate voltage \( V_g \) to a Quantum Dot (QD) weakly connected to leads by tunnel contacts, one obtains a series of Coulomb blockade conductance peaks of height \( G_N \) at positions \( V_g^N \). The peak positions \( V_g^N \) are directly related to difference \( E_{N+1} - E_N \) between the ground state energies of the dot with \( N \) and \( N + 1 \) electrons (in zero bias). The heights \( G_N \) are related to the overlap of the \( |N> \) and \( |N + 1> \) ground state wave functions at the contacts. During the last few years, many experiments have shown that the statistical properties of the successive peak positions \( V_g^N \) could not be described within the framework of the random matrix theory (RMT). For the addition spectrum (e.g. statistical properties of the differences \( \Delta_2 = V_g^{N+1} - V_g^N \)), qualitative agreement with experimental results can only be obtained by taking into account fluctuations of the charging energy that originate from the spatial fluctuations of wave function amplitudes. Although such fluctuations of wave functions already exist in RMT, the resulting charging energy fluctuations are parametrically to small if one ignores the reorganization or “scrambling” (of the wave functions and of the spectrum) induced by the addition of the successive electrons. In fact, in a recent experimental study of the peak to peak heights correlation, Patel et al. have unambiguously shown that this reorganization is important and could essentially be attributed to electron-electron interaction effects. Recently, Alhassid et al. have confirmed the importance of scrambling using a phenomenological model based on Gaussian Random Matrix Process (GRMP, and have obtained good agreement with Patel et al. experiment.

In the present work based on a microscopic model of a quantum dot, we present a detailed numerical study that shows directly the importance of the electron-electron interaction on the scrambling of the single particle properties obtained within a self consistent Hartree-Fock (SCHF) method.

2 Microscopic model

We model a two dimensional disordered dot of size \( A = L_x \times L_y \) by the following Hamiltonian:

\[
H = \sum_i w_i c_i^\dagger c_i - t \sum_{<ij>} [c_i^\dagger c_j + h.c.] + \frac{U}{2} \sum_{i,j=1}^{A} M_{ij} n_i n_j, \tag{1}
\]

where \( <ij> \) denotes nearest neighbors on a square lattice of size \( A = L_x \times L_y \) and \( t = 1 \). \( c_i^\dagger \) and \( c_i \) are creation and annihilation operators for an electron (spinless) on site \( i \) and \( n_i = c_i^\dagger c_i \).
The random on-site disorder potential $w_i$ are uniformly distributed over $[-\frac{W}{2}, \frac{W}{2}]$. Because of the disorder, the electronic charge density exhibits fluctuations in space. We consider that the natural bare interaction between these charge fluctuations has a long range Coulomb form $M_{ij} = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$. We choose a torus geometry to prevent from electrostatic effects that tend to accumulate the charge on the surface. The distance $|\mathbf{r}_i - \mathbf{r}_j|$ is calculated from the shortest path relating the two sites $i$ and $j$ on the torus.

3 Hartree Fock picture of scrambling

We treat interaction effects in the self-consistent Hartree-Fock approximation. We thus assume that the ground state $|\Psi_0^N\rangle$ of a dot with $N$ particles is a Slater determinant of $N$ effective single particle states $\psi^{N}_\alpha(\mathbf{r}_i)$ with associated quasi-energy $\epsilon^{N}_\alpha$. These states $\psi^{N}_\alpha(\mathbf{r}_i)$ are in fact the self-consistent eigenstates of an effective one–particle Hamiltonian $h^N = \sum_i w_i^{\text{eff}} c_i^{\dagger} c_i - \sum_{<ij>} [t^{\text{eff}}_{ij} c_i^{\dagger} c_j + h.c.]$. The effective onsite potential $w_i^{\text{eff}} = w_i + U \sum_j M_{ij} < \Psi_0^N | n_j | \Psi_0^N >$ is the sum of the disorder potential and the Hartree contribution. Similarly the effective hopping $t^{\text{eff}}_{ij} = t \delta_{<ij>} + U M_{ij} < \Psi_0^N | c_i^{\dagger} c_j | \Psi_0^N >$ includes the Fock exchange term. Self consistency is obtained with an iterative procedure.

The self consistent states $\psi^N_\alpha(\mathbf{r}_i)$ are linear combinations of the non interacting $\psi^0_\alpha(\mathbf{r}_i)$. However the $\psi^N_\alpha(\mathbf{r}_i)$ depend explicitly on interaction strength and particle number $N$ and not only on disorder strength and system size as the $\psi^0_\alpha(\mathbf{r}_i)$. Therefore, by adding one by one $p$ electrons into a dot with initially $N$ particles, the effective one body Hamiltonian $h^N$ is changed into another Hamiltonian $h^{N+p}$ with the corresponding $\psi^N_{\alpha+p}(\mathbf{r}_i)$ and $c^{N+p}_\alpha$. In the Hartree-Fock approximation, one can always write $h^{N+p} = h^N + V^{N,N+p}$, such that the scrambling effects of the $p$ additional electrons is described by an effective one body term $V^{N,N+p}$, that is neither diagonal in the position basis nor in the $\psi^N_\alpha$ basis of the dot with $N$ particles. In fact this possibility of writing $h^{N+p} = h^N + V^{N,N+p}$ allows us to make a parallel with the phenomenological model of Alhassid and Malhotra. In their work, the $N+p$ interacting particles system is described by an effective one body Hamiltonian $h^{N+p} = h_0 \cos(p \delta x) + h_1 \sin(p \delta x)$ in which $h_0, h_1$ are two random Gaussian matrices and $\delta x$ is the parameter that control the scrambling strength. Their effective scrambling potential $V^{N,N+p}$ is thus given by $V^{N,N+p} \simeq h_0 \cos(p \delta x) - 1) + h_1 \sin(p \delta x)$.

4 Numerical results

4.1 Scrambling properties of SCHF single particle wave functions

In order to characterize the scrambling of the SCHF single particle wave functions, we have computed the following parametric correlation function:

$$C_\psi(p) = \left| \int d\mathbf{r} \psi^{N+p}_{\alpha}(\mathbf{r})\psi^{N+p*}_{\alpha}(\mathbf{r}) \right|^2$$

in which means averaging on disorder configurations and on the $N$ lowest single particle energy levels $\alpha$. The scrambling of wavefunctions is characterized by a decrease of $C_\psi(p)$ with increasing $p$. A similar quantity has already been studied in the context of GRMP. We have studied in detail the dependences of $C_\psi(p)$ on the disorder strength $W$ (or conductance $g$), the interaction strength $U$ and the system size $A$. The ranges of parameters considered are $W = 4 \rightarrow 10$; $U = 0.5 \rightarrow 3$, $A = 6 \times 6 \rightarrow 11 \times 10$ sites. The initial values of $N$ are chosen so that the band is quarter filled $\nu = N/A \simeq 1/4$. For each set of parameters we have averaged over 500 distinct disorder configurations. The results obtained for $C_\psi(p)$ are summarized on Figure 1a. This figure shows a quite interesting result, that the correlation function $C_\psi(p)$ can be recast...
into a one parameter scaling form \( C_\psi(p) = f_\psi(p/p_\psi) \) where \( p_\psi \) depends on the three parameters \( W, U, A \). In the range of parameters studied we further obtain the following approximate fitting form:

\[
\frac{C_\psi(p)}{p} \simeq \frac{1}{1 + \left(\frac{p}{p_\psi}\right)^{3/4}}^{1/2} \quad \frac{1}{p_\psi} = c U^2 A^2 W^3 [1 + d_A U^2].
\]

where \( c \approx 8.10^{-8} \) and \( d_A = 0.03; 0.05; 0.1; 0.15; 0.2 \) for \( A = 6 \times 6; 6 \times 7; 7 \times 8; 8 \times 9; 9 \times 10 \) respectively. For a given \( p \), \( C_\psi(p) \) decreases when either \( W, U \) or \( A \) is increased. Thus the larger the system size, the stronger is the scrambling effect of a single additional electron. Let us compare the scaling (3) with the scaling obtained by Alhasid and Malhotra in the context of the GRMP model. The behavior found in this model for the correlation function is \( C_\psi^{GRMP}(p) \simeq \frac{1}{1 + (\frac{x}{\sqrt{M}})^{3/4}} \) with \( 1/p_\psi \simeq \delta x / \sqrt{M} \) for gaussian orthogonal matrices of size \( M \times M \). The difference between the functional form \( C_\psi(p) \) and \( C_\psi^{GRMP}(p_{GRMP}) \) seems to prevent any simple mapping between them. Nevertheless, if we consider only the tail of the two forms, we can identify the microscopic value \( p \) with \( p_{GRMP}^{16/3} \). We then obtain the following relation between the microscopic parameters and the parameters of the GRMP model: \( (\delta x / \sqrt{M})^{16/3} \approx c U^2 A^2 W^3 (1 + d_A U^2) \).

![Figure 1](image_url)

Figure 1: (a) \( C_\psi(p) \) as a function of the scaling variable \( p/p_\psi \). (b) \( C_\psi(p) \) as a function of the scaling variable \( p/p_c \). For a given disorder \( W \) and system area \( A \), we plot all the data points corresponding to the entire range \( p = \{1, 2, ..., 10\} \) and interaction range \( U = \{0.5, 1, ..., 3\} \).

4.2 Scrambling properties of SCHF single particle energy spectra

In order to characterize the scrambling of the SCHF single particle energy spectrum we have computed the following parametric correlation function:

\[
C_\epsilon(p) = \frac{s^{N+p}_\alpha s^{N-1}_\alpha}{s^{N}_\alpha s^{N-1}_\alpha}.
\]

where \( s^{N}_\alpha = e^{N}_{\alpha+1} - e^{N}_\alpha \) is the spacing between two consecutive levels (\( s^{N}_\alpha \) is normalized to the mean level spacing at this energy). Since the one particle density of state has a deep around the (average) Fermi level, we have used all \( \alpha \) corresponding to energy levels (empty or occupied) neither in the deep nor at the band edges. As it is illustrated on Figure 1b, we have found
that \( C_\psi(p) \) can also be recast into a one parameter scaling form \( C_\psi(p) = f_\psi(p/p_\psi) \) where \( p_\psi \) depends on the parameters \( W, U, A \). Quantitatively we obtain the following approximate fitting form:

\[
C_\psi(p) \simeq \frac{1}{1 + \left( \frac{p}{p_\psi} \right)^{2/3}},
\]

\[
1/p_\psi \simeq cU^3 A^2 W^{2.75},
\]

where \( c \simeq 5.10^{-8} \). The quantitative behavior of \( p_\psi \), in terms of \( W, A, U \), is different from that of \( p_\psi \). This contrasts with GRMP-like models in which necessarily \( p_\psi = p_\psi \). For the microscopic model, we believe that the difference found between \( p_\psi \) and \( p_\psi \) reflects the distinct statistical behavior of the diagonal and the off-diagonal elements of \( V_{N,N}^{N+N} \) in the \( \psi_N^\alpha \) basis (within a perturbative approach, the SCHF single particle energy level position depends on both the diagonal and off-diagonal terms. In contrast the reorganization of SCHF wave functions depends only on the off-diagonal elements).

5 Conclusion

Based on a microscopic model of a disordered quantum dot, we have presented detailed numerical results that show the importance of electron-electron interaction on the scrambling of the single particle properties obtained within a self consistent Hartree-Fock method. As main result of this study, we have found one-parameter scaling properties for the two quantities \( C_\psi(p), C_\psi(p) \) which describe respectively the reorganization of the one particle wave functions and of the energy spectrum when \( p \) particles are added to the system. The quantitative analysis of this one parameter scaling properties cannot be described by effective GRMP models considered until now. This suggests that new specific random matrix models are necessary to describe microscopic disordered models of Coulomb interacting particles within the Hartree-Fock approximation.

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