Statistical Properties of The First Excited State of an Interacting Many Particle Disordered System

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The distribution $P_1$ of the first many-body excitation energy of a weakly and moderately interacting electron gas in a finite conductor (in the diffusive regime) is calculated. As the interaction is increased, $P_1$ crosses over from Wigner-Dyson to Poisson. We characterize this transition through the inverse participation ratio in Hilbert space, and examine its manifestation in a projected 2-dimensional space.

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One of the most important physical quantities used to characterize finite conductors is energy level statistics. Not only does it provide an efficient mathematical framework to study such systems, but it is also correlated with other physical observables (conductance, spectral correlations, absorption spectrum, orbital magnetization, heat capacity when the number of electrons is fixed, etc.). This, in principle, allows for the “measurement of level statistics”. In weakly disordered conductors (“diffusive disorder”, as well as in chaotic cavities), it is known that the energy gap between the ground-state and the first-excited state is very small. Hereafter $\langle \ldots \rangle$ denotes an average taken over disorder realizations. One can further investigate the many-body spectra of such systems. Let us first take the interaction strength to vanish. In this case the distribution of the normalized energy gap between the ground-state $|0\rangle$ and the first-excited $|1\rangle$, $s \equiv (E_1 - E_0)/(E_1 - E_0)$, follows the WD distribution (a single particle-hole pair at the Fermi energy is involved). Hereafter $\langle \ldots \rangle$ denotes an average taken over disorder realizations. Once we consider the gap between the $m^{th}$ and the $m + 1^{st}$ many-body states with $m >> 1$, we expect the statistics to follow the Poisson distribution. This is due to the fact that, typically, the $m^{th}$ and the $m + 1^{st}$ many-body states correspond to mutually very different particle and hole configurations. Since they are not connected with each other through a single-particle operator, level repulsion is greatly reduced. Once we turn on electron-electron interaction, we expect the gap between the $m^{th}$ and the $m + 1^{st}$ many-body states ($m >> 1$) of such a system to satisfy the WD distribution. Indeed, the motivation behind the introduction of random matrix theories was to account for high-lying spectra of interacting systems. Table 1 summarizes the existing knowledge regarding the statistics of the excitation spectrum of a non-integrable electron gas. For the sake of definiteness we shall consider hereafter spinless electrons moving under the influence of weak disorder which renders the motion of a single electron

| first excitation | non-interacting | interacting |
|------------------|----------------|-------------|
| higher excitations | Wigner-Dyson | Poisson | Wigner-Dyson |

TABLE I: The many-body spacing statistics of diffusively systems: the item marked by ? is found to cross-over (with increasing interaction strength) from WD to Poisson.

diffusive.

The item in Table 1 which is marked by a question mark represents the distribution of the first excitation energy of a (weakly or moderately weakly) interacting electron gas, $P_1(s)$. This quantity is indeed the main object of our investigation. Earlier studies of $P_1$ have addressed different parameter regimes, or were at times inconclusive.

The main results of our analysis are:

1. We find numerically that as the electron-electron interaction strength is increased, the statistics of the first excitation energy crosses over from WD to Poisson (cf. Fig. 1). We characterize this transition quantitatively (cf. Fig. 2 and Eq. 4).

2. We relate the WD-to-Poisson transition to the statistics of the diagonal and off-diagonal elements of an effective $2 \times 2$ matrix, depicting the mixing of the many-body-sates $|0\rangle$ and $|1\rangle$ (Fig. 3 and Eqs. 6,7,8).

3. We show how the WD-to-Poisson crossover is manifest in the distribution of the participation ratio, i.e., the structure of the many-body wave function in Hilbert space.

4. Finally, and very importantly, we show that as the interaction is increased the first excited state, which originally (at zero interaction) corresponds to a single particle-hole excitation, involves an increasing
number of particle-holes. But this is up to a certain value of the interaction \( r_s \approx 1 \). Upon further increase of the interaction strength this trend reverses. This picture is obtained by computing (numerically) the inverse participation ratio of the ground and first-excited states (in Hilbert space) as function of the interaction (cf. Fig. 3).

The model. We consider the following tight-binding Hamiltonian, describing spinless interacting electrons moving in the presence of a random potential:

\[
\hat{H} = \sum_{k,j} \epsilon_{k,j} n_{k,j} - V \sum_{k,j} \left[ a_{k,j+1}^\dagger a_{k,j} + a_{k,j+1,j}^\dagger a_{k,j} + h.c. \right] + U \sum_{k,j} n_{k,j} n_{k\pm 1,j\pm 1}. \tag{1}
\]

Here \( \{k,j\} \) denotes a lattice site, the number operator is \( n_{k,j} \) and \( \epsilon_{k,j} \) is the site energy, selected randomly and uniformly over the interval \([-W/2, W/2]\]. We study two-dimensional arrays with periodic boundary conditions. Only nearest-neighbor interactions \( U \) are considered.

We present numerical results pertaining to \( N = 4 \times 8 \) electrons residing on \( 4 \times 4 \) lattices with \( M = 16 \) sites \((\nu \equiv N/M)\). Data for larger systems appeared to be compatible with our results. The disorder strength \( W = 8V \) was chosen so that the single-particle localization length is larger than the system size, with spectral correlations following the Gaussian orthogonal ensemble (GOE) on small energy scales (i.e., for energy differences \( \Delta \epsilon < \hbar/t_{\text{flight}} \); \( t_{\text{flight}} \) is the time-of-flight of the electron throughout the system). The motion of the electron is diffusive or marginally diffusive, \( l_{\text{el}} \leq L \), with \( L \) being the quantum dot’s linear size and \( l_{\text{el}} \) – the elastic mean-free-path.) Varying the electron density in the experiment amounts to varying the dimensionless parameter \( r_s \).

We have carried out exact diagonalization of the many-particle Hamiltonian using the Lanczos method, and obtained the eigenvalues \( \epsilon_n \) and eigenvectors \( |\alpha\rangle, \alpha = 0, 1 \).

To establish a useful frame of reference for discussing the results of our analysis, it is convenient to study the self-consistent Hartree-Fock (SCHF) Hamiltonian corresponding to this system. This Hamiltonian reads

\[
\hat{H}_{\text{SCHF}} = \sum_{k,j} \epsilon_{k,j} n_{k,j} - V \sum_{k,j} \left[ a_{k,j+1}^\dagger a_{k,j} + a_{k,j+1,j}^\dagger a_{k,j} + h.c. \right] + \sum_{k,j} n_{k,j} U (n_{k\pm 1,j\pm 1})_0 - \sum_{k,j} a_{k,j}^\dagger a_{k,j} + U (n_{k\pm 1,j\pm 1})_0. \tag{2}
\]

Here \( \langle \ldots \rangle_0 \) denotes a quantum average taken over the ground state, the latter being calculated self-consistently. The SCHF single-electron eigenvectors \( \{\psi_n\} \) and eigenvalues \( \{\epsilon_n\} \) are obtained through a self-consistent diagonalization of the Hartree-Fock Hamiltonian.

The exact many-body states may be expressed in terms of Fock determinants:

\[
|\alpha\rangle = \sum_{i_1,i_2,...,i_N} C_{i_1,i_2,...,i_N}^{(\alpha)} c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_N}^\dagger |\text{vac}\rangle, \tag{3}
\]

where the sum is over all possible permutations of \( N \) states out of \( M \) with \( M \geq i_N > i_{N-1} > \ldots > i_2 > i_1 \geq 1 \), \( c_{i_n}^\dagger \) is the creation operator of the \( n^\text{th} \) single-particle HF state and \( |\text{vac}\rangle \) is the vacuum state. For the non-interacting case, as well as for the case for which the SCHF provides an exact solution, the ground state (the first excited state) corresponds to \( C_{1,2,...,N-1,N+1} = 1 \) \((C_{1,2,...,N-1,N+1} = 1) \) while all other coefficients are equal to zero. This is compatible with a Koopmans-like picture. In this case the participation ratio (see below) is equal to 1.

An important quantity which is particularly suitable to describe scenarios intermediate between the WD \((\eta = 0)\) and the Poisson \((\eta = 1)\) limits is

\[
\eta = \frac{\int_0^{0.4729} P_1(s)ds - \int_0^{0.4729} P_{\text{wd}}(s)ds}{\int_0^{0.4729} P_1(s)ds - \int_0^{0.4729} P_{\text{wd}}(s)ds}. \tag{4}
\]

**WD to Poisson crossover.** The distribution of \( s \) as function of the interaction strength for 1000 different realizations of disorder is plotted in Fig. 1. It is seen that \( P_1(s) \) crosses over from a Poisson-like to a WD-like distribution as the interaction strength is increased, with the canonical signatures of such a transition in finite systems. The functional \( \eta \) is depicted in Fig. 2. Each curve represents averaging over 10000 different disorder realizations. In all cases \( \eta \) increases (the distribution becomes more “Poisson-like”) as the interaction strength \( U \) is increased. This increase in \( \eta \) becomes more pronounced the higher the filling factor, and tends to saturate at higher interaction strengths. At filling factors \( \nu > 1/4 \) (and \( \nu \neq 1/2 \) our data suggest that \( \eta \) collapses onto a single scaling function up to \( \nu \)-specific values where saturation takes place.

**Comparison with a SCHF scheme.** It is known that in zero-dimensional systems the low-lying many-body states are made of combinations of a finite number of Slater determinants (each made up of single-particle SCHF states). This motivates the use of such a basis to describe the exact \(|0\rangle\) and \(|1\rangle\) states. We invoke the participation ratio in the Hilbert space spanned by all possible Slater determinants:

\[
\hat{P} = \sum_{i_1,i_2,...,i_N} |C_{i_1,i_2,...,i_N}^{(\alpha)}|^4. \tag{5}
\]

Koopmans’ variant of the HF approximation asserts that the effective single-particle states remain unmodified under a change of the occupancy of these states. As long as the HF-Koopmans-like picture holds, \( \hat{P} = 1 \).
whereas if this picture breaks down completely we approach $\tilde{P} \sim (N!)^{-2}$, signaling delocalization in Hilbert space.

Our results are depicted in Fig. 3. There we plot the disorder-averaged inverse participation ratio as function of the interaction for the ground-state and the first excited state, with $N = 4$ and $N = 7$. It can be seen that $1/\langle \tilde{P} \rangle \propto U^2$ for weak interactions for both states.

We note that there is some nontrivial physics taking place: the cusp of the curve $1/\langle \tilde{P} \rangle$ vs. $U$ for the first excited state, as it departs from the $U = 0.5$ for the $N = 4$ case. This cusp becomes more pronounced as $N$ becomes larger; the $N = 7$ case is a manifestation of the system becoming more localized (in Hilbert space) with interaction strength exceeding $U = 2$.

Studying the distribution of $\tilde{P}$ (cf. Fig 4) reveals that as the interaction strength is increased, the original sharp peak at 1 is initially smeared, but the function then evolves into a doubly peaked distribution.

In this context it is also useful to consider the quantity $K \equiv \langle |c_{N+1}^\dagger c_N|^2 \rangle$. We note that in the Koopmans limit $K = 1$, implying that both the ground and the first-excited states are given respectively by a single Slater determinant (they differ from each other by a particle-hole excitation). In that limit, as discussed above, the inverse participation ratio $1/\langle \tilde{P} \rangle = 1$. As we turn on the interaction $1/\langle \tilde{P} \rangle$ increases concomitantly with the decrease in $K$. The behavior of the average $K$ is depicted in Fig 4.

A two-level model. To further characterize the phenomena discussed here, we resort to the philosophy behind the Wigner surmise, and try to study the manifestation of the crossover in a truncated $2 \times 2$ Hilbert space. The latter is spanned by $|0\rangle$ and $|1\rangle$ (in a certain realization).

If the Koopmans-like scenario holds $K = 1$ while $\langle |c_{N+1}^\dagger c_N|^2 \rangle = 0$. Under such a scenario the Wigner distribution should hold: consider an arbitrary perturbation $\tilde{F} = \sum_{ij} \alpha_{ij} c_i^\dagger c_j$, $\langle \hat{F} | 0 \rangle = \sum_{i<N+1} \alpha_{ii}$ $\langle \hat{F} | 1 \rangle = \sum_{i<N} \alpha_{ii} + \alpha_{N+1,N+1}$ $\langle \hat{F} | 0 \rangle = \alpha_{N,N+1}$, (6)

 corresponds (up to a constant matrix $\hat{I} \times \sum_{i<N} \alpha_{ii}$ subtracted, where $\hat{I}$ is the unit matrix) the $2 \times 2$ matrix:

$$\hat{F}_{HF-Koopmans} = \begin{pmatrix} \alpha_{N+1,N+1} & \alpha_{N,N+1} \\ \alpha_{N+1,N} & \alpha_{N,N} \end{pmatrix}.$$ (7)

The distribution of the HF states over disorder realizations obeys RMT. Likewise, the distribution of $\{\alpha_{ij}\}$ will follow RMT (Gaussian), and will lead to the energy spacing $E_1 - E_0$ obeying the WD distribution.

Going now beyond the Koopmans limit, and employing the basis of the exact ground and first-excited states, the
FIG. 3: The inverse averaged participation ratio $1/\langle \tilde{P} \rangle$ and $1/K \equiv 1/(1|e_{N+1}^{1}c_{N}|0)$, as a function of the interaction strength $U$ for the ground state and the first excited state for the $N=4$ case. The curves correspond to the best fit to $1 + aU^2$, with $a = 0.015$ for the ground state and $a = 0.22$ for the first excited one. Inset: The same as the above for $N=7$ and a wider range of interaction of interaction strength. Here $a = 0.034$ for the ground state and $a = 0.22$ for the first excited one.

FIG. 4: The distribution function of the participation ratio, $P$, for the first excited state.

FIG. 5: The fluctuations in the matrix element, $F_{\alpha,\beta} = \langle \alpha|\hat{F}|\beta \rangle$, defined as $(\delta^2 F_{\alpha,\beta}) = (F_{\alpha,\beta}^2) - (F_{\alpha,\beta})^2$, for the diagonal ($\alpha=\beta$) and non-diagonal ($\alpha \neq \beta$) elements as function of the interaction strength $U$. For $N = 4,7$ $r_s \approx 0.56U, 0.42U$ respectively.

2-level matrix is

\begin{equation}
\hat{F} = \left( \begin{array}{cc}
\langle 1|\hat{F}|1 \rangle & \langle 1|\hat{F}|0 \rangle \\
\langle 1|\hat{F}|0 \rangle & \langle 0|\hat{F}|0 \rangle
\end{array} \right) .
\end{equation}

The WD $\rightarrow$ Poisson crossover is now manifest through $\hat{F}$. We first subtract a constant, proportional to the unit matrix, to render the resulting matrix $\delta \hat{F}$ statistically traceless. We are left to compare the fluctuations of the diagonal matrix elements, $(\delta^2 F_{\alpha,\beta}) = (F_{\alpha,\beta}^2) - (F_{\alpha,\beta})^2$ with $\alpha = \beta$, with those of the off-diagonal entries, $(\delta^2 F_{\alpha,\beta})$ with $\alpha \neq \beta$. (We note that the ensemble average of the off-diagonal entries vanishes). This is shown in Fig. 5 for two values of electron number, $N$. It is clearly seen, especially for the larger $N$, that as the interaction strength is increased (beyond $U \approx 2$ which is equivalent to $r_s = U/V \sqrt{4\pi\nu}$), the diagonal entries win over the off-diagonal, marking the suppression of level-repulsion and the cross-over to Poisson statistics. This cross-over appears to be quite sharp for our larger system.

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[1] See e.g. G. Katomeris, F. Selva and J.-L. Pichard, cond-mat/0206404; G. Benenti, X. Waintal, J.-L. Pichard and D. L. Shepelyansky, Eur. Phys. J. B 17, 515 (2000).

[2] This choice of a short range interaction is a reasonable way to model a restricted-geometry two-dimensional electron gas (quantum dot) with metallic gates in the vicinity which give rise to screening of the bare Coulomb interaction. The effects we discuss here are found for long-range Coulomb interactions too. In that case, though, one needs to consider higher values of the interaction for the effects to be appreciable.

[3] In principle we need to vary the bare potential with \( U \) to keep the “dressed” parameter \( l_{el} \) unchanged. But over the range \( U \) is varied here we have observed that \( l_{el} \) remains unchanged, the evidence for this being that the conductance is hardly modified.

[4] This is in agreement with: P. N. Walker, Y. Gefen and G. Montambaux Phys. Rev. B, 60, (1999); P. N. Walker, Y. Gefen and G. Montambaux Phys. Rev. Lett. 82, (1999); A. Cohen, K. Richter, and R. Berkovits, Phys. Rev. B, 60, 2536 (1999).

[5] Note also that the upper limit in the integrals in Eq. is 0.4729 the value of the lower intersection point of the WD and the Poisson distributions. Here we focus on the low energy limit of the distribution function which is robust and universal.

[6] B. L. Altshuler, Y. Gefen, A. Kamenev and L. S. Levitov, Phys. Rev. Lett. 78, 2803 (1997).

[7] The cusp appears to be weakly geometry dependent. It is most pronounced for square samples above quarter filling.

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