Quantum opening of the Coulomb gap in two dimensions

Giuliano Benenti\textsuperscript{(a)}, Xavier Waintal\textsuperscript{(a)}, Jean-Louis Pichard\textsuperscript{(a)}, and Dima L. Shepelyansky\textsuperscript{(b)}
\textsuperscript{(a)}CEA, Service de Physique de l’Etat Condensé, Centre d’Etudes de Saclay, F-91191 Gif-sur-Yvette, France
\textsuperscript{(b)}Laboratoire de Physique Quantique, UMR C5626 du CNRS, Université Paul Sabatier, 31062 Toulouse, France
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For a constant density of spinless fermions in strongly disordered two dimensional clusters, the energy level spacing between the ground state and the first excitation is studied for increasing system sizes. The average indicates a smooth opening of the gap when the Coulomb energy to Fermi energy ratio \(r_s\) increases from 0 to 3, while the distribution exhibits a sharp Poisson-Wigner-like transition at \(r_s \approx 1\). The results are related to the transition from Mott to Efros-Shklovskii hopping conductivity recently observed at a similar ratio \(r_s\).

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In disordered insulators, a crossover \(\square\) in the temperature dependence of the resistivity \(\rho(T)\) is induced by Coulomb interactions from the Mott variable range hopping law \(\rho(T) = \rho_M \exp(T_0/T)^{1/3}\) to the Efros-Shklovskii behavior \(\rho(T) = \rho_{ES} \exp(T_{ES}/T)^{1/2}\). The long range nature of the interactions leads to a dip in the single particle density of states, and the assumption that single electron hopping dominates the transport leads this change in the resistivity. However, a single electron hop may reorganize the location of the other particles, inducing complex many particle excitations. This makes the Coulomb gap problem difficult and gives us the motivation to study the first quantum excitation above the ground state. For \(d = 2\), the strength of Coulomb interactions is very often given in units of the Fermi energy by the dimensionless ratio \(r_s\). For strong disorder, the first excitation energy is expected to become larger when \(r_s\) increases, and to decay as \(1/L\) (instead of \(1/L^2\) for free electrons) when the system size \(L\) increases. But one cannot estimate the threshold \(r_s^C\) where the Coulomb gap opens without taking into account all complex of many body quantum processes. Considering spinless fermions in 2d strongly disordered clusters, we confirm from numerical calculations that the gap opens at a value \(r_s^C \approx 1.2\), and we point out that this is indeed for a similar value \(r_s \approx 1.7\) that a change in the hopping conductivity from Mott hopping to Coulomb gap behavior has been reported \(\square\) for an electron gas created at a GaAs/AlGaAs heterostructure. For a statistical ensemble of clusters, we have calculated the many body states at the mean field level given by the Hartree-Fock approximation and we have added the effects of the residual interaction. Keeping constant the carrier density \(n_c\), and increasing the size \(L\), the average gap between the ground state and the first excitation behaves as \(1/L^\alpha\), with \(\alpha\) decreasing from 2 to 1 when \(r_s\) increases from 0 to 3. Another remarkable effect of the interaction is to yield a sharp transition for the gap distribution: it tends to Poisson or to Wigner-like distributions for small or large \(r_s\) respectively at the thermodynamic limit. A critical threshold \(r_s^C \approx 1.2\) is characterized by a scale invariant gap distribution, reminiscent of the one particle problem \(\square\) at a mobility edge. However, it is only the distribution of the first spacing which exhibits such a transition, the distributions of the next spacings remain Poissonian and are essentially unchanged when \(r_s\) varies. Eventually, we discuss the implications for the hopping conductivity and we confirm that the transition for the gap takes place at a smaller \(r_s\) than \(r_s^C \approx 4 - 5\) where a change in the topology of the persistent currents carried by the ground state has been observed \(\square\).

We consider a disordered square lattice with \(N = L^2\) sites occupied by \(N\) spinless fermions. The Hamiltonian reads

\begin{equation}
H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_i v_i n_i + U \sum_{i \neq j} \frac{n_i n_j}{r_{ij}}
\end{equation}

where \(c_i^\dagger (c_i)\) creates (destroys) an electron in the site \(i\), the hopping term \(t\) between nearest neighbours characterizes the kinetic energy, \(v_i\) the site potentials taken at random inside the interval \([-W/2, +W/2]\), \(n_i = c_i^\dagger c_i\) is the occupation number at site \(i\) and \(U\) measures the strength of the Coulomb repulsion. The boundary conditions are periodic and \(r_{ij}\) is the inter-particle distance for a 2d torus. If \(a_B^2 = \hbar^2/(m^* e^2)\), \(m^*, e, a\) and \(n_s = N/(aL^2)\) denote respectively the effective Bohr radius, the effective mass, the dielectric constant, the lattice spacing and the carrier density, the factor \(r_s\) is given by:

\begin{equation}
r_s = \frac{1}{\sqrt{\pi n_s a_B^2}} = \frac{U}{2 \hbar^2 \sqrt{\pi n_c}}
\end{equation}

since in our units \(\hbar^2/(2m^* a^2) \rightarrow t, e^2/(ea) \rightarrow U\) and \(n_c = N/L^2\).

In this study, a large disorder to hopping ratio \(W/t = 15\) is imposed for having Anderson localization and Poissonian spectral statistics for the one particle levels at \(r_s = 0\) when \(L \geq 8\). We study \(N = 4, 9\) and 16 particles inside clusters of size \(L = 8, 12\) and 16 respectively. This corresponds to a constant low carrier density \(n_c = 1/16\).
A numerical study via exact diagonalization techniques for sparse matrices is possible only for small systems \[3\], and does not allow us to vary \( L \) for a constant density. We are obliged to look for an approximate solution of the problem, using the Hartree-Fock (HF) orbitals, and to control the validity of the approximations. One starts from the HF Hamiltonian where the two-body part is reduced to an effective single particle Hamiltonian \[6–8\]

\[
U(\sum_{i \neq j} \frac{1}{r_{ij}} |n_i\rangle \langle n_j| - \sum_{i \neq j} \frac{1}{r_{ij}} c_i^\dagger c_j c_j^\dagger c_i),
\]

(3)

where \( \langle \ldots \rangle \) stands for the expectation value with respect to the HF ground state, which has to be determined self-consistently. For large values of the interaction and large system sizes the single-particle problem \(3\) is still non-trivial, since the self-consistent iteration can be trapped in metastable states. This limits our study to small \( r_s \) and forbids us to study by this method charge crystallization discussed in \[4\] at a larger \( r_s^{\text{W}} \approx 12 \).

The mean field HF results can be improved using a method \[9,10\] known as the configuration interaction method (CIM) in quantum chemistry \[11\]. Once a complete orthonormal basis of HF orbitals has been calculated \((H_{HF}|\psi_\alpha\rangle = \epsilon_\alpha |\psi_\alpha\rangle\) with \( \alpha = 1, 2, \ldots, L^2 \), it is possible to build up a Slater determinants’ basis for the many-body problem which can be truncated to the \( N_H \) first Slater determinants, ordered by increasing energies. The two-body Hamiltonian can be written as

\[
H_{\text{int}} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} Q_{\alpha\beta}^{\gamma\delta} d_\alpha^\dagger d_\beta^\dagger d_\delta d_\gamma,
\]

(4)

with

\[
Q_{\alpha\beta}^{\gamma\delta} = U \sum_{i \neq j} \frac{\psi_\alpha(i)\psi_\beta(j)\psi_\gamma(i)\psi_\delta(j)}{r_{ij}}
\]

(5)

and \( d_\alpha^\dagger = \sum_j \psi_\alpha(j)c_j^\dagger |0\rangle \). One gets the residual interaction subtracting Eq. \[3\] from Eq. \[4\]. This keeps the two-body nature of the Coulomb interaction, and if \( N \gg 2 \) it is still possible to take advantage of the sparsity of the matrix and to diagonalize it via the Lanczos algorithm.

We have first compared HF and CIM results. Labelling the levels by increasing energy and studying an ensemble of \( 10^4 \) samples, we have studied the first spacing \( \Delta_0 = E_1 - E_0 \). The role of the residual interaction can be seen in Fig. \[3\]. When \( r_s > 1 \), the residual interaction reduces the mean gap, and slightly changes the distribution. The CIM results agree with the results given from exact diagonalization with an accuracy of the order 2% when one takes into account the \( N_H = 10^3 \) first Slater determinants when \( r_s = 5 \) and \( L = 8 \). This means that a basis spanning only 0.2% of the total Hilbert space is sufficient for studying the first excitations. For larger \( L \), exact diagonalization is no longer possible, but one can look if the results vary when \( N_H \) increases. In the worst case considered \((L = 16, r_s = 2.8)\) the accuracy in the first four spacings can be estimated of the order 5% when \( N_H = 2 \times 10^3 \).

Therefore the CIM method allows to study low energy level statistics for \( r_s < 3 \). However, its accuracy is not sufficient to determine a small change of the ground state energy when the boundary conditions are twisted (i.e. the persistent currents).

**FIG. 1.** CIM result (full circle) compared to HF approximation (empty circle) for \( N = 9 \) and \( L = 12 \). Mean gap < \( \Delta_0 \) > and gap distribution at \( r_s = 4.5 \) (insert).

**FIG. 2.** Size dependence of the average gap (first spacing < \( \Delta_0 \) >) \( L^{-\alpha(r_s)} \). From bottom to top: \( r_s = 0, 0.6, 0.9, 1.1, 1.4, 1.7, 2.3, 2.8 \). Insert: \( \alpha(r_s) \) (circle, characterizing < \( \Delta_0 \) > and square, average over \( i = 1 - 3 \), characterizing < \( \Delta_i \) >).
We have calculated the first energy levels for different sizes $L$. The first average spacing $<\Delta_0>$ calculated for an ensemble of $10^4$ samples is given in Fig. 2. It exhibits a power law decay as $L$ increases, with an exponent $\alpha$ given in the insert. One finds for the first spacing that $\alpha$ linearly decreases from $d = 2$ to 1 when $r_s$ increases from 0 to 3. This proves a gradual opening of the mean Coulomb gap. The next mean spacings depend more weakly on $r_s$, as shown in Fig. 2.

For $r_s = 0$, the distribution of the first spacing $s = \Delta_0/ <\Delta_0>$ becomes more and more close to the Poisson distribution $P_P(s) = \exp(-s)$ when $L$ increases, as it should be for an Anderson insulator. For a larger $r_s$, the distribution seems to become close to the Wigner surmise $P_W(s) = (\pi s/2)\exp(-\pi s^2/4)$ characteristic of level repulsion in random matrix theory, as shown for $r_s = 2.8$ and $L = 16$ for instance. To study how this $P(s)$ goes from Poisson to a Wigner-like distribution when $r_s$ increases, we have calculated a parameter $\eta$ which decreases from 1 to 0 when $P(s)$ goes from Poisson to Wigner:

$$\eta = \frac{\text{var}(P(s)) - \text{var}(P_W(s))}{\text{var}(P_P(s)) - \text{var}(P_W(s))},$$

where $\text{var}(P(s))$ denotes the variance of $P(s)$, $\text{var}(P_P(s)) = 1$ and $\text{var}(P_W(s)) = 0.273$. In Fig. 3, one can see that three curves $\eta(r_s)$ characterizing the first spacing for $L = 8, 12, 16$ intersect at a critical value $r_s^C \approx 1.2$. For $r_s < r_s^C$ the distribution tends to Poisson in the thermodynamic limit, while for $r_s > r_s^C$ it tends to a Wigner-like behavior. At the threshold $r_s^C$, there is a size-independent intermediate distribution shown in the insert of Fig. 3, exhibiting level repulsion at small $s$ followed by a $\exp(-as)$ decay at large $s$ with $a \approx 1.52$. This Poisson-Wigner transition characterizes only the first spacing, the distributions of the next spacings being quite different. The insert of Fig. 3 does not show an intersection for the parameter $\eta$ calculated with the second spacing.

The second excitation is less localized than the first one when $r_s = 0$, since the one particle localization length weakly increases with energy. This is only for $L = 16$ that the distribution of the second spacing becomes close to Poisson without interaction, and a weak level repulsion occurs as $r_s$ increases. The observed transition, and the difference between the first spacing and the following ones is mainly an effect of the HF mean field. For the first spacing, the curves $\eta$ calculated with the HF data are qualitatively the same. At the mean field level the first excitation is a particle-hole excitation starting from the ground state and requires an energy of the order $U/L$, with fluctuations around this mean value. The second excitation is again a particle-hole excitation starting from the ground state. The energy spacing between the first and the second excited state is given by the difference of two uncorrelated particle-hole excitations and a Poissonian distribution follows naturally. For $r_s > r_s^C$, the Gaussian-like HF distributions for $\Delta_0$ become more Wigner-like when the residual interaction is included. We point out that in metallic quantum dots also, the first excitation is statistically different from the others, as shown by numerical studies within the HF approximation. The existence of a critical $r_s$ value for the opening of the Coulomb gap can be understood similarly to [4]. The single particle density of states around the Fermi

FIG. 3. Gap distribution $P(s)$ for $r_s = 0$ (empty circle) and $r_s = 2.8$ (full circle) when $L = 16$, compared to $P_P(s)$ and $P_W(s)$. Insert: size invariant $P(s)$ at $r_s^C \approx 1.2$ ; $L = 8$ (circle), 12 (square) and 16 (diamond).

FIG. 4. Parameter $\eta(r_s)$ corresponding to the first spacing $\Delta_0$ at $L = 8$ (circle), 12 (square) and 16 (diamond). Insert: $\eta(r_s)$ for the second spacing $\Delta_1$. 
energy $E_F$ is given by $\rho(E) \approx |E - E_F|/U^2$ and the gap size $\Delta_g = |E_g - E_F|$ can be estimated from the condition $\rho(E_g) \approx 7$, with $7 \approx 1/W$ mean density of states for $W \gg t$, obtaining $\Delta_g \approx U^2/W$. According to Fermi golden rule, the inverse lifetime of a Slater determinant built from electrons localized at given sites is $\Gamma_i \approx t^2(1/W)(N/L^2)$, with $N/(WL^2)$ density of states directly coupled by the hopping term of the Hamiltonian $\hat{H}$. Therefore at zero temperature quantum fluctuations melt the Coulomb gap for $\Gamma_i \approx \Delta_g$, giving $r_s \approx r_s^C \approx 1$. We conclude that a crossover from Efros-Shklovskii to Mott hopping conductivity is expected not only increasing temperature but also increasing carrier density, as observed in [4].

To measure possible delocalization effects, we have calculated the number of occupied sites per particle $\xi_s = N/\sum_i \rho_i^2$ where $\rho_i = \langle \Psi_0 | n_i | \Psi_0 \rangle$ is the charge density of the ground state at the site $i$. Around $r_s \approx 1.2$ and after ensemble average, the maximum increase of $\xi_s$ compared to $r_s = 0$ is negligibly small (2%). These are mainly the distribution and the average value of the first excitation energy which exhibit noticeable effects. This matters for the hopping conductivity. The usual argument is to consider the length $L(T)$ where $\exp[-(2L/\xi(r_s) + \Delta_0(r_s)/kT)]$ is maximum with the localization length $\xi(r_s) \approx \xi(0)$. If one takes for $\Delta_0(r_s)$ its average value $\approx (A + Br_s)/L^\alpha(r_s)$ (see Fig. 1) one obtains for the hopping resistivity a smooth and continuous crossover from Mott to Efros-Shklovskii hopping, given by:

$$\rho(T) \propto \exp \left(\frac{T(r_s)}{T}\right)^{1/(\alpha+1)},$$

where

$$T(r_s) \approx \frac{A + Br_s}{kT^\alpha}.$$  \hspace{1cm} (8)

This prediction neglects the sharp transition in the distribution of $\Delta_0$ at $r_s^C$, which could be better included by considering a more typical value for $\Delta_0(r_s)$ than its average, for instance obtained from the value $s_0$ for which $\int_0^{s_0} \rho(s)ds = b$, with $b = 1/2$ for instance. This will introduce a sharp discontinuity at $r_s^C$ in $T(r_s)$.

In summary, we have analyzed the Coulomb gap statistics for spinless fermions in a strongly disordered squared lattice when $r_s < 3$. On one hand, we have found a sharp interaction-induced transition at $r_s^C \approx 1.2$, characterized by a scale invariant distribution. Around the critical point, the gap distribution tends to Poisson or to Wigner-like distributions respectively at the thermodynamic limit. This effect is present at the HF mean field level, the residual interaction weakly shifts $r_s^C$ and improves the Wigner-like character of one of the limits. On the other hand, the exponent $\alpha$ characterizing the average gap smoothly decays from 2 to 1 in this range of $r_s$ values. The average gap is substantially reduced from its HF value by the residual interaction. We associate this transition to a crossover in the hopping resistivity inside an insulating phase.

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