Delocalized Coulomb phase in two dimensions

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Abstract. – Extending finite size scaling theory to the many body ground state, one finds that Coulomb repulsion can drive a system of spinless fermions in a random potential from the Anderson insulator (Fermi glass of localized states) towards a new extended phase in dimension $d = 2$. The transition occurs at a Coulomb energy to Fermi energy ratio $r_s \approx 4$, where a change in the nature of the persistent currents has been previously observed. Relevance to the recently observed 2d metallic phase is suggested.

Following the scaling theory of localization [1], all 2d systems of electrons (or holes) are localized when electron-electron interaction is negligible. This absence of metals in two dimensions is nowadays questioned after the observation of a transition towards a metallic behavior in silicon based 2d electron gases [2, 3, 4] when the carrier density is varied. This unexpected phenomenon occurs also for hole gases in GaAs heterostructures [4, 5], SiGe [6] and InAs quantum wells [7]. The transition is observed at very low carrier concentrations, the charge spacing being $\geq 10^3\text{Å}$ in certain cases [7]. This suggests that Coulomb repulsion is the driving mechanism for the transition. In ref. [10], a very clean heterostructure was studied, and the transition was observed at $r_s \approx 35$, close to $r_s \approx 37$ for which Wigner crystallization is expected without disorder. In more disordered samples, the transition occurs typically around $r_s \approx 10$ and $k_F l \approx 1$, $k_F$ denoting the Fermi wave vector and $l$ the elastic mean free path. It is also at $r_s \approx 10$ that charge crystallization is numerically observed in small disordered clusters [11, 12]. This gives arguments to associate the observed transition to the quantum melting of a kind of pinned Wigner crystal. In this case, the metallic phase should cease to exist at a weaker $r_s$ also and the re-entry towards a Fermi glass of weakly interacting localized particles should occur. The re-entry has been observed in Ref. [8] at $r_s \approx 6$ (see also Ref. [9]). Those regimes are out of reach of the Landau theory of disordered metals [13, 14] valid for large $k_F l$ and small $r_s$.

The interplay between disorder and electron-electron interactions is attracting increasing theoretical interest [15], though many studies are devoted to large energy excitations [6] of a few particle states instead of the ground state properties. In Ref [12], it was shown that...
the ground state of a system of spinless fermions goes from an insulating phase (Fermi glass, \( r_s \leq r_s^F \)) towards another insulating phase (pinned Wigner crystal, \( r_s \geq r_s^W \)) through a new intermediate quantum phase. This conclusion was drawn from a study of the persistent currents supported by the ground state in small clusters. A 2d torus geometry enclosing a flux \( \phi \) around the longitudinal direction was considered. The ratio \( r_s^F \) characterizes the suppression of the transverse current \( I_t \) (not enclosing \( \phi \)). Below \( r_s^F \), the pattern of driven currents has a 2d topology and the longitudinal current \( I_l \) (enclosing \( \phi \)) can be paramagnetic or diamagnetic, depending on the sample. Above \( r_s^F \), the flow pattern has an ordered 1d topology \([12, 17]\) and the sign of \( I_l \) becomes sample independent. The higher ratio \( r_s^W \) characterizes the suppression of \( I_l \) and charge crystallization in a random substrate. For \( 0.3 < k_F l < 3 \), one obtains \( r_s^W \approx 10 \) and \( r_s^F \approx 4 \), in agreement with ratios \( r_s \approx 10 \) where the metal-insulator transition is observed, and with a ratio \( r_s \approx 6 \) where the re-entry has been reported in Ref. [1]. Though small clusters exhibit an enhancement of \( I_l \) for intermediate \( r_s \), exact diagonalization does not allow to vary system size and to establish that the intermediate phase is metallic at the thermodynamic limit.

To understand how the cooperative Coulomb behavior begins to destroy Anderson localization of weakly interacting particles, and if it drives the system towards a delocalized phase before yielding charge crystallization, we need to extend the finite size scaling method \([18, 19, 20, 21]\) successful for describing single particle delocalization to the many body ground state. We do not study in this work large Coulomb repulsions where charge crystallization sets in, but using approximations valid for weaker repulsions, one finds that the Fermi glass melts at \( r_s \approx r_s^F \approx 4 \) (in good agreement with Ref. \([12]\)) to give rise to a more fluid phase for the particles. Using a low carrier density, we characterize this melting by a suitable localization length in \( d = 2 \) a scaling behavior similar to the one body (1B) localization length in \( d = 3 \) at the mobility edge, i.e. more generally a behavior characteristic of second order phase transitions. This confirms that spinless fermions have an intermediate delocalized phase between the Fermi glass and the pinned Wigner crystal.

Anderson 1B localization is a complex phenomenon which is analytically tractable in a few limits: quasi-one dimension \([22, 23]\) and Bethe lattice \([24]\). For dimensions \( d = 2 \) and 3, our knowledge of 1B localization is mainly based on numerical works \([18, 19, 20, 21]\). The successful method consists in evaluating the 1B localization length \( L \) of a system of finite size \( L \) and to verify a scaling ansatz inspired \([18]\) from the theory of second order phase transitions:

\[
\frac{L_1(L)}{L} = F_d \left( \frac{L}{L_1(d)} \right). 
\] (1)

The lengths \( L_1(L) \) calculated for different system parameters can be mapped onto a universal curve \( F_d \) assuming a single scaling length \( L_1(d) \) which characterizes the \( d \)-dimensional lattice. For the 1B problem, it was convenient to consider \( d \)-dimensional strips of finite transverse section \( L^{d-1} \). \( L_1(d) \) was defined as the inverse of the smallest positive Lyapunov exponent of the appropriate product of transfer matrices, which is a self averaging quantity. The ansatz \([1]\) was verified in dimensions \( d \geq 1 \), and a metal-insulator transition was obtained \([18, 19, 20, 21]\) for \( d = 3 \) with \( L_1(3d) \) diverging at the mobility edge. In two dimensions, large \( L \) studies \([20]\) led to the conclusion that \( L_1(2d) \) diverges only in the clean limit, in agreement with Ref. \([1]\).

We extend this finite size scaling method to the ground state of \( N \) spinless fermions with Coulomb repulsion in a random potential defined on a square lattice with \( L^2 \) sites. The Hamiltonian reads:

\[
H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_i v_i n_i + U \sum_{i<j} n_i n_j / 2 r_{ij}. 
\] (2)

\( c_i^\dagger (c_i) \) creates (destroys) a particle in the site \( i = (i_x, i_y) \), \( t \) is the strength of the hopping terms
between nearest neighbors (kinetic energy) and \( r_{ij} \) is the inter-particle distance for a 2d torus (periodic boundary conditions). The random potential \( v_i \) of the site \( i \) with occupation number \( n_i = c_i^\dagger c_i \) is taken from a box distribution of width \( W \). The interaction strength \( U \) yields a Coulomb energy to Fermi energy ratio \( r_s = U/(2t\sqrt{n_e}) \) for a filling factor \( n_e = N/L^2 \).

To investigate the melting of the Fermi glass by Coulomb repulsions, one begins with a low density of occupied 1B states such that the charge spacing is larger than \( L_1 \) without interaction. The size \( L \) varies from \( L = 24 \) (\( N = 3 \)) to \( L = 31 \) (\( N = 5 \)), \( N \) being chosen to keep \( n_e = 1/192 \). An intermediate size \( L = 28 \) (\( N = 4 \)) with almost the same density (1/196) is also considered.

Let us first discuss some features of the 1B spectrum. If we take a small value for \( W \), strong lattice effects remain for \( L = 31 \), complicating the extrapolation towards the thermodynamic limit. The lattice effects disappear at larger \( W \), but another difficulty remains, due to the low density \( n_e \) numerically accessible. The low energy tail of the 1B spectrum is made of impurity
states where the particles are simply trapped at some site \( i \) of exceptionally low \( v_i \). Their energies are below the band [-4\( t \), 4\( t \)] of the clean system. This is a trivial localization with \( L_1 \leq 1 \) and irregular energy spacings given by the tails of the distribution of the \( v_i \). We are not interested to study the detrapping of those impurity states by Coulomb repulsions, but by the delocalization of genuine Anderson localized states, of energy \( E > -4t \). The localization of those states results from the multiple scattering of plane waves, while the impurity states involve mainly a few evanescent waves. With a higher density, it would be easy to fill the tail of 1B band and to put the Fermi energy inside the band of Anderson levels of energy \( > -4t \), having regular energy spacings \( \Delta_1 \propto 1/L^2 \) and similar \( L_1 \) (see Fig. 1 A). With a low density, in order to observe nevertheless a delocalization resulting from the mixing by the interaction of SD built out from Anderson localized states (say with \( L_1 \approx 4 \)), we calculate the \( L^2 \) 1B levels for \( W = 10 \) and we ignore the \( L^2/2 \) first 1B levels, considering only as possible 1B states the \( L^2/2 \) remaining ones. Doing so, the states near the Fermi energy of the non interacting system are not simple impurity states. We have checked that all the results presented hereafter are identical if we get rid of a smaller fraction of 1B states, as far as the Fermi energy at \( U = 0 \) is located in the constant part of the 1B density of states (Fig.1 A). For \( W = 10 \) and 1B states around the 1B band center, one can roughly estimate that \( k_F l \approx 1 \). From this restricted subset of 1B Anderson localized states, the \( N_H \) first SD ordered by increasing energy are calculated. We assume that such a procedure captures genuine 2d ground state physics, since the low energy excitations begin with a (large) 1B energy spacing \( \Delta_1 \), and not with a (very small) NB energy spacing \( \Delta_N \propto L^{-2N} \).

The sizes \( N_H = (L^2)!/(N!(L^2 - N)!)) \) of the corresponding Hilbert space are huge and only the projection of the Hamiltonian \( \hat{H} \) onto smaller subspaces can be diagonalized (Lanczos method). For weak \( U \), we consider the subspace spanned by the \( N_H \) Slater determinants (SD) corresponding to the first low energy states of the non interacting problem. The \( N \) body (NB) ground state \( |\Psi_0> \) is obtained after diagonalizing the truncated Hamiltonian, \( |\Psi_0> = \sum_i C_i |SD_i> \) is typically extended in the SD basis over \( N_{SD} = <\sum_i |C_i|^2>^{-1} \) SD, the brackets denoting the average over 5 \( \times \) 10^3 disordered samples. In Figs. 1 B-C, one can see that \( N_{SD} \) remains stable when \( N_H \geq 500 \) at a value negligible compared to \( N_H = 1000 \) (value for \( N_H \) assumed hereafter). Though the stability of our results have been checked when \( N_H \) varies inside a range negligible compared to \( N_H \), making difficult to rule out the existence of a slow variation which cannot be detected inside a too narrow range, we assume that \( |\Psi_0> \) has a negligible chance to have a significant projection outside the 1000 first SD when \( L \leq 31 \) and \( U \leq 1.5 \).

Figure 1 D gives the number \( M_s = N <\sum_i \rho_i^2>^{-1} \) of occupied sites per particle in the ground state, \( \rho_i = <\Psi_0|n_i|\Psi_0> \) denoting the charge density of the ground state at site \( i \). For \( U = 0 \), \( M_s \) is obviously smaller than \( L_1^2 \), a limit where the \( N \) occupied 1B states do not overlap. When one goes towards the thermodynamic limit, \( M_s \) is almost size independent for the Fermi glass \( (U \leq 1) \), but varies as a function of \( L \) when \( U \geq 1 \). This provides a first evidence that one has a delocalization effect at an interaction threshold \( U \approx 1 \). The glassy ground state melts towards a more fluid phase which fills a larger fraction of the sample. This observed delocalization cannot be related to charge crystallization, since \( M_s \) increases while \( M_s \to 1 \) when \( U \to \infty \).

To characterize the NB ground state by an appropriate localization length, we consider the change \( \delta \rho_j \) of the charge density induced by a small change \( \delta v_i \) of the random potential \( v_i \) located at a distance \( r = |i - j| \). For a Slater determinant made with \( N \) occupied 1B
Fig. 2. – A: $<\ln|\delta\rho(r)|>$ as a function of $r$ for $L = 31$ at $U = 0$ (circle), 0.25 (square), 0.5 (diamond), 0.75 (triangle up), 1 (triangle left), 1.25 (triangle down) and 1.5 (triangle right). The lengths $\xi_L(U)$ are given by the slopes of the thick lines. B: $\xi_L$ as a function of $U$ for $L = 24$ (circle), 28 (square) and 31 (diamond).

eigenfunctions ($\psi_\alpha$), first order perturbation theory gives:

$$\delta\rho_j = 2\delta v_i \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha} \frac{\psi_\alpha(i)\psi_\beta(i)\psi_\alpha(j)\psi_\beta(j)}{E_\beta - E_\alpha} \propto \exp \frac{-2r}{L_1},$$

the index $\beta$ varying over the 1B spectrum. Therefore, the change $\delta\rho$ remains localized on a scale $\xi_L \approx L_1/2$ without interaction. We study how $\xi_L$ depends on $U$ for different values of $L$. To improve the statistical convergence, we calculate more precisely the change $\delta\rho(r) = \sum_j \delta\rho_{r,j}$ of the charge density on the $L$ sites of coordinate $j = r$ yielded by the change $v_{0,i_x} \rightarrow v_{0,i_x}(1+1/100)$ for the $L$ random potentials of coordinate $i_x = 0$. The quantity $\delta\rho(r)$ for $W = 10$ has a broad symmetric distribution of amplitude $|\delta\rho(r)|$ which is almost log-normal for $U = 0$. There is no underlying law of large numbers which tells us what is the right self-averaging scaling variable, as Oseledec’s theorem for the quasi-1d 1B problem [18]. Though the log-normal character of the distribution becomes less pronounced when $U$ increases, it still makes sense to characterize the typical strength of the fluctuations by

$$|\delta\rho(r)|_{\text{typ}} = \exp <\ln|\delta\rho(r)|> \propto \exp \frac{-r}{\xi_L},$$

where the brackets denote the average over 5 $\times$ 10$^3$ disordered samples. We extract the range $\xi_L$ of the perturbation from the $r$ dependence of this typical value inside a square of size $L$.

An exponential decay of $|\delta\rho(r)|_{\text{typ}}$ occurs only over a scale $r << L/2$ since the boundary conditions are periodic. In Fig. 2 A, one can see how the length $\xi_L$ are obtained from the slope of the linear parts of the curves (thick straight lines). Fig. 2 B gives how $\xi_L$ depends on $U$ for the three considered sizes. This figure conveys a very different information than Fig. 1 C. The number $N_{SD}$ of SD over which the NB ground state has important projections linearly increases as a function of $U$, without exhibiting a change of behavior. This rules out that $U$ can induce a sharp localized-delocalized transition in Hilbert space of the type suggested in
Fig. 3. – **A**: Localization lengths $\xi_L(U)$ as a function of $L$ for $U \leq 1$ (filled symbols): 0 (triangle up), 0.25 (triangle left), 0.5 (triangle down), 0.75 (triangle right), 0.85 (circle) and 1 (square) and $U > 1$ (empty symbols): 1.15 (square), 1.25 (triangle), 1.35 (diamond) and 1.5 (circle). **B**: Ratios $\xi_L(U)/L$ mapped onto the scaling curve $F_2$ as a function of $\xi(2d)/L$. The two dimensional scaling length $\xi(2d)$ is given in the insert.

Ref. [25] for metallic quantum dots. The behavior of $\xi_L(U)$ is much more interesting. When $L = 31$ and $U \geq 1$, the range of a local perturbation has a sharper increase which can only be due to the nature of the last SD participating to the NB ground state, and not to their number $N_{SD}$. The last SD participating to the ground state when $U \geq 1$ should not be made of 1B states localized in the vicinity of those playing a role when $U \leq 1$. This may indicate that the underlying delocalization mechanism is related to variable range hopping between localized 1B states yielded by Coulomb repulsions. This possibility was discussed in Refs. [26, 27, 28].

The scaling analysis is shown in Fig. 3. The size dependence of $\xi_L$ is presented in Fig. 3 A for increasing Coulomb repulsions. One finds the behavior typical of a transition: $\xi_L$ converges towards a finite value when $U < U_c$ (localized Fermi glass); diverges linearly as a function of $L$ at $U = U_c \approx 1$ (critical point) and diverges faster than linearly when $U > U_c$ (extended phase). This is exactly the behavior [15] which characterizes the Anderson transition at $d = 3$ for the 1B spectrum. In Fig. 3 B, one verifies the scaling ansatz (1), where $\xi_L$ and $\xi(2d)$ play the role of $L_1(L)$ and $L_1(d)$ respectively. All the data of Fig. 3 A can be mapped onto a universal curve $F_2$ shown in Fig. 3 B, assuming the scaling length $\xi(2d)$ given in the insert. When $U < U_c$, this length characterizes the localization of the effect of a local perturbation of the substrate in the two dimensional thermodynamic limit. Considering that the delocalization threshold is located at $U_c \approx 1$, a power fit of $\xi(2d) \propto |U - U_c|^{-\nu}$ yields a rough estimate for the critical exponent $\nu \approx 4$. More detailed and accurate studies of the vicinity of the delocalization threshold are necessary for confirming this value for $\nu$. Very often, additional corrections $\propto L^{-\alpha}$ to the scaling ansatz occurs for small sizes. We point out that our results can be fitted by a simple linear law $\xi_L = 0.17L$ for $U = U_c$. This is a further indication that the simple ansatz (1) describes scaling for $L \geq 24$, without noticeable additional $L^{-\alpha}$ corrections. The obtained interaction threshold $U_c \approx 1$ gives $r_s \approx 4$, which agrees with the $r_s^F$ given in Ref. [12] for similar values of $k_Fl$ and is consistent with the threshold $r_s \approx 6$ where
the re-entry is reported in Ref. [4].

In summary, we have shown that there is a melting of the Fermi glass towards a new delocalized phase at \( r_s = r_s^F \approx 4 \) and \( k_F f \approx 1 \). In the glassy state, the particles occupy a tiny fraction \( \leq n_s L_s^2 \) of the sample and the effect of a local perturbation remains localized. Above \( r_s^F \), the ground state becomes extended over the whole sample, as shown by the divergence of the range \( \xi(2d) \) characterizing the two dimensional thermodynamic limit when \( r_s \to r_s^F \). The range \( \xi_L \) calculated in a square of size \( L \) satisfies a finite size scaling ansatz consistent with a second order quantum phase transition and a power law divergence of \( \xi(2d) \) at \( r_s^F \). The effect of a local perturbation (motion of a single atom) have interesting implications for \( 1/f \) noise in the metallic [29] and localized [30] regimes. Therefore, the implications of our numerical results might be checked by suitable noise measurements in low density 2d gases of electrons or holes.

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