Density Modulations and Addition Spectra of Interacting Electrons in Disordered Quantum Dots

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(Received 8 February 1999)

We analyze the ground state of spinless fermions on a lattice in a weakly disordered potential, interacting via a nearest-neighbor interaction, by applying the self-consistent Hartree-Fock approximation. We find that charge density modulations emerge progressively when $r_s \gtrsim 1$, even away from half-filling, with only short-range density correlations. Classical geometry-dependent *magic numbers* can show up in the addition spectrum which are remarkably robust against quantum fluctuations and disorder averaging. [S0031-9007(99)09453-3]

The interplay of disorder and interactions in two dimensional Fermi systems is currently a central problem in condensed matter physics. Mesoscopic systems provide a unique forum for analyzing ground state properties as it is possible to access the regime $kT \ll \Delta$, where Δ is the mean single particle level spacing. Examples include the study of low temperature persistent currents and magnetic response in small quantum rings and dots, and low bias measurements of the dc response [1–6] and capacitance [7] of weakly coupled quantum dots. The latter experiments made it possible to access directly the energy differences μ_N between ground states of N and $N - 1$ particles: $\mu_N = E(N) - E(N - 1)$. The addition spectrum, $\sum_i \delta(\mu - \mu_i)$, depends sensitively on the nature of the mesoscopic ground state.

Resonant tunneling measurements of the addition spectrum [1–6] have resulted in some interesting observations. While the mean peak spacings are well described by the constant interaction model, the fluctuations are not. In [3,4] the averaging was carried out over N, whereas in [5,6] the results were also averaged over sample geometry. The experimental data [3] indicate the existence of atypical addition spectrum spacings at certain values of N, suggesting that averaging over disorder may not be equivalent to averaging over N (the ergodicity principle is violated). Theoretical and numerical studies [3,8–15] attempted to address various aspects of the problem.

In the capacitance experiments of Ref. [7], the measured addition spectra display *bunching,* an indication that the Coulomb blockade becomes negative between one or more consecutive electron addition peaks; in the experiment, these peaks then coalesce. Such bunching is in direct conflict with the naive picture combining the constant interaction model with ergodic effective single-particle wave functions. It has been shown [16] that a classical charge model can reproduce many of the observed effects, but there is currently no quantum mechanical explanation as the experiments are carried out at densities considered too high to form a Wigner solid (in the case of a Coulomb

bare interaction, see Ref. [17]; for a short-ranged potential one might expect a Wigner solid to be less stable).

Motivated by these experiments, but not attempting to reproduce specific details thereof, we analyze the nature of the ground state by applying the self-consistent Hartree-Fock (SCHF) approximation [18,19]. We are thus able to go beyond the random phase approximation (RPA) with perturbation theory (valid for large dimensionless conductance g, and small r_s [9,10]), while considering larger systems than is feasible by exact methods. Experimental values of $r_s > 1$ have indeed been reported [3]. Starting from a noninteracting model, we find that as the interaction strength is increased such that $r_s \gtrsim 1$ (but still too weak to form a Wigner solid), the electron gas crosses over to a regime where (i) there are significant spatial density modulations; (ii) density-density correlation functions seem to saturate, defining only short-range order; and (iii) the addition spectrum becomes strongly N dependent, with *magic numbers* for which $\Delta_2(N) \equiv \mu_{N+1} - \mu_N$ exhibits sharp maxima that coincide with the related classical charge model.

Recent reports of exact numerical studies [3,9,20,21] have emphasized that the properties of quantum dots which are not reproduced by effective single-particle random-matrix-like theories are associated with the emergence of short-range correlations. Our results support this claim, but the main thrust here is related to (iii): some deviations from RPA behavior have a direct classical electrostatic counterpart. The signature of the latter is not totally washed out by quantum fluctuations even far from the Wigner crystallization threshold.

We consider the following tight binding Hamiltonian for spinless fermions with periodic boundary conditions:

$$H = \sum_i w_i c_i^+ c_i - t \sum_{\langle ij \rangle} c_i^+ c_j + \frac{U}{2} \sum_{\langle ij \rangle} c_i^+ c_j^+ c_j c_i, \quad (1)$$

where $\langle ij \rangle$ denotes pairs of nearest neighbors, w_i is the random on-site energy in the range $[-W/2, W/2]$, and t the hopping matrix element. All lengths are measured

in units of the lattice constant a, so that $U = e^2/a$ and $t = \hbar^2/2ma^2$. For low filling (i.e., a parabolic band) we find $r_s = U/t\sqrt{4\pi\nu}$ [22], where $\nu = N/A$ is the filling factor, for N electrons in an area A. For the noninteracting system we find $g = k_F l/2 = 96\pi\nu(t/W)^2$ by applying the Born approximation (valid for $1 \ll g \ll A$); $k_F = \sqrt{4\pi\nu}$ and l is the elastic mean free path. In the capacitance measurements [7], the 2D quantum dots were sandwiched between a metallic source (heavily doped n^+ GaAs) and drain (Cr/Au), separated, at distances comparable with the mean particle separation, by tunnel barriers. To account for external sources of screening (taken as half planes), one can insert a bare interaction between electrons in the dot that is dipolar ($1/r^3$) at distances greater than the dot to gate separation when there is only one close gate, and in the case of two close gates with exponentially small long-range interactions [23]. Here we model such interactions with a nearest-neighbor pair potential.

The ground state is obtained in the SCHF approximation, over a range of densities and disorder strengths at zero magnetic field. The generalized inverse participation ratio (GIPR) is then calculated according to the following definition:

$$I \equiv \frac{1}{\nu^2 A} \sum_i \langle \rho(\mathbf{r}_i)^2 \rangle, \qquad (2)$$

where $\rho(\mathbf{r}_i)$ denotes the expectation value of the total density at the lattice site i. The angle brackets correspond to an average over the disorder ensemble. The GIPR provides a convenient measure of the degree of density modulation: in the limit of a perfectly flat density profile it takes the value unity, and increases for a modulated density. The maximal value that can be obtained for the GIPR occurs when all the charge is concentrated on only N sites, in which case $I = 1/\nu$.

The GIPR is plotted for a range of disorder strengths in Fig. 1. For $\nu = 1/4$ it increases rapidly between $U \approx t$ and $U \approx 5t$ depending on the disorder strength, then gives way to a weaker interaction dependence for $U \gtrsim 5t$. For comparison we also plot results for an identical system but with bare Coulomb interactions, such that the interaction potentials are both equal to U between nearest-neighbor sites: the relative rapidity of the increase of I for nearest-neighbor interactions is clear. The increase in the GIPR signals an increase in the spatial modulation of the total electron density; we shall refer to the increased density modulation at finite U as a charge density modulation (CDM) [24].

At zero interaction we find $I - 1 \sim 1/g$ for large g (not shown). Within our numerical accuracy we were unable to find a consistent size dependence in the GIPR, suggesting that disorder is the dominant mechanism controlling the small to large U crossover, as seen in Fig. 1 [25].

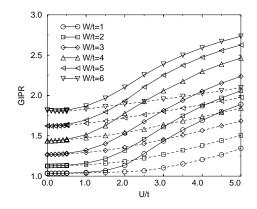The GIPR yields no information on the spatial structure of the ground state, for which we evaluate the density-

FIG. 1. The GIPR is plotted for a range of disorder values as a function of the relative interaction strength U/t. The system is a 16×16 lattice with nearest-neighbor (solid) and Coulomb (dashed) interactions. We do not average over disorder, but remark that the GIPR is self-averaging. Here $\nu = 1/4$, implying $r_s \approx 0.56 U/t$.

density correlation function defined as

$$C(r) = \langle \rho(r)\rho(0) \rangle_c / \langle \rho(0)^2 \rangle_c . \qquad (3)$$

The subscript c indicates that only connected averages are included, and here, due to the homogeneity of the disorder averaged potential, the correlation function depends only on the vector separation $\mathbf{r}$. We only consider $\mathbf{r}$ to be directed along a lattice vector $(1, 0)$. A typical result for the correlation function is plotted in Fig. 2. As the interaction strength is increased, short-range correlations develop, and then saturate. The underlying square lattice excludes the possibility of observing incipient Wigner crystal fluctuations, which possess the symmetry of a triangular lattice.
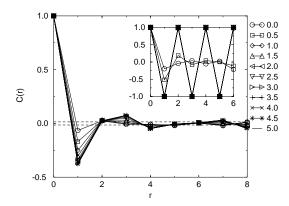

FIG. 2. The density-density correlation function (see text) shows increasing short-ranged correlations as U/t is increased; the values of U/t are given in the legend. Here $W = 4t$; the lattice is 16×16. Here $\nu = 1/4$, implying $r_s \approx 0.56 U/t$. The results are averaged over 20 samples and each lattice site. The dashed lines show approximately 1 standard deviation due to sampling, assuming that all correlations have vanished. Inset: at half-filling we find no decay of the correlation function with distance for $U/t \gtrsim 1$.

Comparing Figs. 1 and 2, one can see that the short-ranged correlations develop over the same range of interaction strength as the rapid increase in I. We did find that on rare occasions a further rearrangement occurs at larger interaction values, but it is not clear whether this is a genuine effect which for larger systems would become correspondingly less rare, or a manifestation of metastable configurations.

Let us now look at the longer-range behavior of $C(r)$. At half-filling it has been claimed that in clean infinite lattice systems a second order transition to a crystalline state occurs at strong interactions [26]. In disordered systems, evidence of at least short-range order has been seen in exact calculations on small systems [9,20]. Within the SCHF approximation we find no decay of correlations. It is well known that at half-filling, nesting of the Fermi surface leads to a $2k_F$ charge density wave instability, but away from half-filling this nesting does not occur. In Fig. 2 it can be seen that, in the presence of disorder, there exists no long-range order in the SCHF ground state for $\nu = 1/4$. This, however, is also true of the related classical system [i.e., $t = 0$ and $W/U \to 0$ in the Hamiltonian (1)], where one expects the formation of a noncrystalline solid. One way to establish whether the electrons possess solid- or liquidlike correlations is to analyze the excited states of the system. However, to show that classical results can provide information on the SCHF ground state away from half-filling, at least when the particle *packing* is *compact,* we consider the appearance of geometrical frustration, where the ground state of the classical system contains line defects with respect to a pure crystal. These defects lead to the disappearance of long-ranged order, but at the same time give rise to *magic* filling factors where $\langle \Delta_2(N) \rangle$ exhibits large variations in N.

This brings us to the central observation of this study, namely, the strong geometry and filling factor dependent variations that can arise in the average addition spectrum spacing $\langle \Delta_2(N) \rangle$ as the interaction strength is increased [27]. Consider first a collection of classical charges, on a square lattice, with nearest-neighbor interactions. If the lattice is a torus with $2n \times 2m$ sites, it is possible to insert up to $2nm$ particles without incurring an energy cost. The remaining $2mn$ particles cost an additional $4U$ to add, so that $\langle \Delta_2(N) \rangle$ displays a peak, $\mathcal{O}(U)$, at $N = 2nm$. If on the other hand one of the sides (or both) of the lattice is odd [e.g., $(2n + 1) \times (2m + 1)$] the maximum number of particles that can be added without nearest neighbors is reduced. It is not difficult to see that such a maximally filled configuration contains a line defect and long-range order is lost. In other words, the lattice of sites without nearest neighbors is incommensurate with the underlying lattice. In the commensurate case, the quantum system also shows a peak in $\Delta_2(N)$ at half-filling, but the nesting of the Fermi surface in the noninteracting system also makes this filling special. We show below that in the incommensurate case we find that within the SCHF approximation, remnants of the peaks at the *magic* filling factors in the related classical model are visible far from the classical limit, despite the lack of nesting.

We consider a lattice of the type $(2n + 1) \times (2n + 1)$ as an example; the predictions for other incommensurate lattices are easily obtained. In the classical limit with nearest-neighbor interactions, the first $n(2n + 1)$ particles can be added with no interaction energy cost, the next $2n + 1$ particles cost an additional $2U$, and the rest cost an additional $4U$. As a result, in the classical limit, $\langle \Delta_2(n(2n + 1)) \rangle$ [as well as $\langle \Delta_2((n + 1)(2n + 1)) \rangle$] is significantly larger than all other values of $\langle \Delta_2(N) \rangle$ [28]. In our calculations we include a trivial constant interaction term to make the results easier to read. In Fig. 3, we plot some typical results for $\langle \Delta_2(N) \rangle$ for a 7×7 lattice, which shows that for $U \gtrsim 2t$ remnants of this classical effect can be seen clearly at the predicted filling $N = 21$. This magic number effect disappears as U/t vanishes, where spectral fluctuations become well described by random matrix theory [14].

Similar behavior has been observed for other sample sizes and geometries. Although these results correspond to a density regime where quantum fluctuations are predominant, the structure in $\langle \Delta_2(N) \rangle$ agrees qualitatively with that of the classical counterpart. One might expect that extending the range of the interaction will give rise to a more intricate classical structure, but with a correspondingly smaller amplitude which is thus more easily washed out by quantum fluctuations. This question is left for a future study. In previous work [16] the results of [7] were reproduced by interacting classical charges in a parabolic potential. In this case the source of magic numbers incorporated the existence of topological defects in the ground state, as well as the interplay with the confining potential. This work suggests that even if quantum fluctuations are strong enough to destabilize a
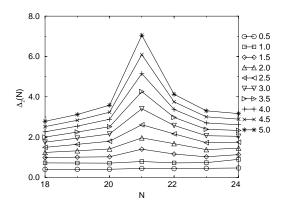

FIG. 3. The addition spectrum is shown to be strongly dependent on the number of particles in the dot, which can be understood from classical arguments. The legend denotes the values of U/t considered. The lattice is 7×7, $W = 2t$, and the results are averaged over 400 samples.

Wigner solid, they may not completely wash out such classical effects.

In summary, we show that the metallic ground state develops charge density modulations, controlled by the electron-electron interaction, at densities $r_s \gtrsim 1$ depending on disorder. The development of the CDMs with increasing r_s is more rapid for shorter-range interactions, presumably because of the large gradient of the interaction potential. We also show that away from half-filling, the CDMs are associated with short-range order only. Elsewhere [14], it has been demonstrated that the existence of these CDMs result in unusual fluctuations of Δ_2 over the disorder ensemble. Finally, we demonstrate that topological defects in the equivalent classical system occur in the CDM, and that they result in strong filling factor and geometry dependent variations in Δ_2, clearly visible for $U \gtrsim 2t$. It seems clear that the ergodicity principle fails in this case, and so disorder averaging and averaging over N are not equivalent. These results lend support to the classical analysis of Ref. [16], which suggests that the behavior seen in the experiments of Ref. [7] is due to topological defects in the classical ground state configuration. We stress, however, that bunching is not generated in the geometry that we consider.

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[28] At typical filling factors, the classical result is $\langle \Delta_2 \rangle - V \sim \mathcal{O}(W/A)$, where V is a constant interaction term that may be included. In the case considered, if N electrons fill a *shell*, $\langle \Delta_2(N) \rangle - V \sim \mathcal{O}(U)$ (for $U \gg W/A$).