Coulomb Correlations and the Wigner-Mott Transition

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Strong correlation effects, such as a dramatic increase in the effective mass of the carriers of electricity, recently observed in the low density electron gas [1] have provided spectacular support for the existence of a sharp metal-insulator transitions in dilute two dimensional electron gases [2]. Here we show that strong correlations, normally expected only for narrow integer filled bands, can be effectively enhanced even far away from integer filling, due to incipient charge ordering driven by non-local Coulomb interactions. This general mechanism is illustrated by solving an extended Hubbard model using dynamical mean-field theory [3]. Our findings account for the key aspects of the experimental phase diagram, and reconcile the early view points of Wigner and Mott. The interplay of short range charge order and local correlations should result in a three peak structure in the spectral function of the electrons which should be observable in tunneling and optical spectroscopy.

First indications of a two-dimensional metal-insulator transition (2D-MIT) have emerged from transport studies, leading to a great deal of controversy and debate [2]. Long-held beliefs [4] that even small amounts of impurities can destroy a Fermi liquid at zero temperature were brought into question, triggering renewed interest and activity. Careful theoretical work [5] suggested that sufficiently strong interactions may suppress weak localization tendencies and stabilize the metal at weak disorder. More recent experiments [1, 6-8, 10] focused on higher mobility (weaker disorder) samples, where advances in experimental capabilities allowed precision measurements of the spin susceptibility $\chi$ and the effective mass $m^*$. Within experimental resolution, both quantities appear to diverge at the critical density $n_c$, while the Wison ratio $\chi/m^* = g^*$ appears to have a weaker density dependence. These findings, which have been confirmed by several complementary experimental methods [11, 12, 13], are most clearly pronounced in the cleanest samples, strongly suggesting that interaction effects [1] - and not disorder - are the dominant driving force for the 2D-MIT [14].

The divergence of the effective mass and spin susceptibility has been observed in transition metal oxides near the density driven Mott transition [13], and in $^3$He monolayers near solidification [10]. For these materials, a description in terms of an almost localized Fermi liquid, and the Brinkman-Rice theory of the Hubbard model has been very successful [17]. The similarity between the observation in oxides, $^3$He and 2D electron gases (2DEG) suggests that we should think about the physics of the 2D-MIT as yet another example of the Hubbard-Mott phenomena [18, 19]. Still, the situation relevant to the 2DEG experiments corresponds to a nearly empty conduction band - a regime very removed from near integer filling where Mott-Hubbard physics has been successfully applied to interpret experiments in $^3$He and transition metal oxides.

Another aspect of the Hubbard-Mott picture for 2D-MIT seems equally troubling. Early theories of the Mott transition, using the Gutzwiller variational approach [17], did predict an enhanced $m^*$ but a noncritical $g^*$, as seen in experiments. However more accurate calculations using dynamical mean-field theory (DMFT) [3] established that one generally should not expect $\chi$ to diverge at the transition, but should instead saturate at a finite value $\chi_c \sim 1/J$, where $J$ is the (finite) superexchange interaction characterizing the Mott insulating phase of the lattice model in question. In this case one expects $g^*$ to gradually decrease and vanish as the transition is approached - in striking contrast to the 2DEG experiments.

Should one think of 2D-MIT as a manifestation of Mott physics - a gradual conversion of the electrons into localized magnetic moments - or does the explanation require a completely different physical picture? In this paper we provide a simple answer to this important question, and present detailed and careful model calculations to support our view. We envision that near the 2D-MIT the electron gas has short range crystalline order, which we model with a tight binding Hamiltonian. The lattice sites represent the precursors, in the fluid phase, of vacancies and interstitials in the Wigner crystal phase. This is a lattice model at quarter filling where the area of a cell containing two lattice sites, corresponds to an area $\pi r_B^2$, containing one electron in the electron gas problem. Here $a_B$ is the Bohr radius and $r_s$ is the dimensional ratio between Coulomb interaction and Fermi energy. Since the system is not close to integer filling, the nonlocal (inter-site) part of the Coulomb interaction cannot be neglected, as it induces significant charge correlations. These in turn enhance the role of the short-range (on-site) part of the Coulomb force, leading to strong correlation physics even far away from integer filling. As

\[ m^* \sim \frac{g^*}{\chi} \]

\[ J \sim \frac{1}{\chi_c} \]
the ratio of the Coulomb interactions to the Fermi energy increases, the system develops short range crystalline or-
der which in turn allows the Hubbard interaction to be
effective resulting in the signatures of Mott localization.

Model. We neglect the effect of disorder and we fo-
cus on the extended Hubbard model \[20\] as an effective
Hamiltonian to describe the physics of the 2D electron
gas at low energies. This model contain in addition to the
usual on-site Hubbard \(U\), a nearest neighbor (NN) inter-
site repulsion \(V\). We envision that \(V\) and \(U\) are increas-
ing functions of \(r_s\) as described in Fig. 1 (the arrow). We
have checked that all the qualitative features discussed in
this paper do not depend on the precise trajectory taken.
The spirit of our approach is similar to that of the almost
localized Fermi liquid framework \[17, 21\] which success-
fully described key aspects of the physics of Helium near
solidification.

The extended Hubbard model has been studied in
detail using DMFT \[3\] where the nonlocal part of the
Coulomb interaction is treated at the Hartree level. To
incorporate the physics of Wigner crystallization we con-
sider a simple bipartite lattice, at quarter filling, with a
semi-circular density of states. The energy is measured in
units of the half-bandwidth \(W = 1\). To accurately solve
the DMFT equations at low temperatures (\(T = 0.01\)) we
utilize the numerically exact continuous time quantum
Monte Carlo algorithm as the impurity solver \[22\].

Wigner-Mott transition at quarter filling. At quarter
filling and when the inter-site interaction \(V\) vanishes, no
insulating solution is found even if the interaction param-
eter \(U\) is arbitrarily large. For \(V > 0\) charge ordering
occurs. The DMFT phase diagram of the system as a
function of \(U\) and \(V\) is shown in Fig. 1.

The system goes from a weakly correlated Fermi liq-
uid (small \(U\) and \(V\)), to a charge ordered Fermi liquid,
to a Wigner-Mott insulator. It is well known that broken
symmetry phases in mean field theory, are sometimes in-
dicative of the onset of pronounced strong short range
order in the two dimensional system. Therefore we can-
not address with this approach the possibility of the ex-
istence of metallic charge ordered phase in the electron
gas \[23\].

Remarkably strong correlation effects only emerge in
the intermediate regime, where charge ordering sets in.
Increasing the charge occupation on one of the two sub-
lattices \(\langle n_A \rangle \lesssim 1\), boosts the effects of the on-site
Coulomb repulsion \(U\), and dramatically increases the cor-
relation effects. Hence, charge order leads to a dramatic
increase of the effective mass and the spin susceptibility,
while the system remain metallic (Fig. 2). This behavior
is strongly reminiscent of that found in the 2DEG ex-
periments, where the mass enhancement is seen only in a
narrow region preceding the metal to insulator transition,
but not at high densities, where \(m/m^* \approx 1\).

The details of the magnetic interactions very close to
the 2D-MIT, as well as the different types of magnetic
long range order in the insulator, depend to some extent
on the type of lattice used. Note however that the en-
hancement of \(\chi\) at the Wigner-Mott transition, which is
stronger at quarter filling than at half filling for the same
model, is a robust feature.

In the physical picture advocated in this approach the
enhancement of the effective mass is accompanied by the
development of a quasiparticle peak in the one particle density of states, as shown in Fig. 3. The width of the quasiparticle peak is inversely proportional to $m^*$.

FIG. 3: Evolution of the density of states. Correlations are more important as $U$ and $V$ increase along the path (see Fig. 1), and a quasiparticle peak develops near the Fermi energy.

A stringent test of our scenario is the relation between the Fermi liquid parameter $F_0^a (g^* = (1 + F_0^a)^{-1})$ and the mass enhancement. In Fig. 4 we show the behaviour of $F_0^a$ versus inverse mass $m/m^*$. Note the significant difference of this quantity when measured in the vicinity of the Mott-Hubbard transition or close to the Wigner-Mott transition at quarter filling. The latter is strikingly similar to the available experimental data on the 2DEG. The displayed experimental data was compiled from transport measurements, magnetic measurements [24, 25, 20] or both [6, 7, 12] following a previous survey [27] as a function of $r_s$.

Magnetic field. One of the most interesting features of 2D-MIT is the dramatic sensitivity of the correlated Fermi liquid regime to the Zeeman (spin) splitting introduced by applying a parallel magnetic field. Indeed, experiments demonstrated that the heavy Fermi liquid can be effectively destroyed by applying a parallel field, producing a spin-polarized insulating state above a “saturation field” $B^*(n)$ of only a few Tesla. For a heavy Fermi liquid one expects $B^* \sim 1/m^*$, and indeed experiments and our theory (see Fig. 5) show that $B^*(n) \sim (n - n_c)$, consistent with a singularly enhanced $m^*$ at the transition. Such field-induced localization is only found in the correlated regime close enough to the transition.

This behavior is very hard to understand from the point of view of a half-filled Hubbard model, since in this case sufficiently strong fields always lead to insulating behavior. The field response we find at quarter filling is dramatically different, as shown in Fig. 5. A field-driven localization transition is still found, but in contrast to the half-filled case, it is restricted to the strongly correlated charge-ordered region; the featureless Fermi liquid remains metallic even upon spin polarization. These findings find surprising agreement with the experimentally established phase diagram (Fig. 5 inset).

The dependence of the effective mass on the applied magnetic field is relatively weak, due to the presence of two competing effects. On one hand the magnetic field locks the spin fluctuations, hence reducing the entropy and the effective mass of the system. On the other hand, the magnetic field enhances the charge ordering, which in turn produces a CDW coherence peak at the band edge, enhancing the density of states.

Conclusions. We presented the solution of a simple microscopic model which correctly captures the qualita-
The characteristic spectral features as-probe the evolution of the one particle density of states to emission and scanning electron microscopy (STM) can probe the formation of a strongly correlated state on the metallic side. The magnetic field dependence proves to be dramatically different from what is expected in a one band Hubbard model at half filling but it is in excellent agreement with experiments on the 2DEG.

The current theory considers the on-site Coulomb repulsion at the single site DMFT level and the nearest neighbor repulsion at the Hartree level. A better treatment, which incorporates dynamical charge fluctuations, the long range Coulomb interactions and short range correlation effects, is possible using extensions of DMFT. We believe this treatment will replace the long-ranged neighbor repulsion at the Hartree level. A better treatment, which incorporates dynamical charge fluctuations, the long range Coulomb interactions and short range correlation effects, is possible using extensions of DMFT.

These experiments should be able to distinguish between the Wigner-Mott perspective which views disorder as the main driving force of freedom into local moments, and the alternative perspective which views disorder as the main driving force for the 2D-MIT.

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