2D-MIT as self-doping of a Wigner-Mott insulator

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Abstract

We consider an interaction-driven scenario for the two-dimensional metal-insulator transition in zero magnetic field (2D-MIT), based on melting the Wigner crystal through vacancy-interstitial pair formation. We show that the transition from the Wigner-Mott insulator to a heavy Fermi liquid emerges as an instability to self-doping, resembling conceptually the solid to normal liquid transition in He3. The resulting physical picture naturally explains many puzzling features of the 2D-MIT.

A series of fascinating experiments, as first performed some ten years ago by Kravchenko and co-workers [1], have deeply changed our thinking about the two dimensional electron gas (2DEG). These and many later experiments demonstrated convincingly that the 2DEG can exhibit typical metallic behavior [2] above a well defined critical density n_c. One of the most prominent features of this metallic phase is an unprecedented resistivity drop, which is found only in the low density regime $n \gtrsim n_c$ close to the transition. These findings suggested that a well-defined metal-insulator transition (MIT) may exist even in two dimensions, in contrast to long held-beliefs based on the theories for noninteracting disordered electrons.

These experiments are typically performed at such low electron density where the relative strength of the Coulomb interaction is so large ($r_s \gtrsim 10$), that the localization processes could conceivably be suppressed by interaction effects. A diffusion-mode theory describing such interaction renormalizations at weak disorder has been developed by Finkelshtein and Punnoose [3], suggesting that sufficiently strong interactions may indeed stabilize the metallic phase. However, this theory can provide guidance only within a narrow diffusive regime restricted to very low temperatures.

In contrast, the most striking experimental results have been established in a broad parameter range well outside this regime, and are most pronounced *in the cleanest samples* [2]. In particular, the *best* established experimental signature of the transition relies on careful effective mass measurements, which is found to diverges as $m^* \propto (n - n_c)^{-1}$,
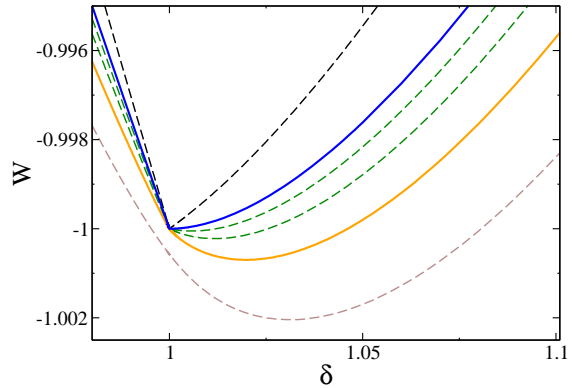

Fig. 1. Evolution of the free energy profile $W[\delta]$, as the electron density is increased across the MIT (from top to bottom). The cusp corresponds to the Wigner solid. The self-doped transition (blue line) takes place before the instability emerges at half-filling ($\delta = 0$, orange line) and the Wigner insulating state is replaced by a heavy Fermi liquid.

while the Lande g^*-factor remains largely unrenormalized. Such phenomena cannot be understood within a low-energy diffusion mode theory, which relies on Anderson localization to produce an insulating phase.

A fundamental question is thus posed by these experiments: what is the basic mechanism that drives the metal-insulator transition in these systems? Does one have to rely on disorder effects at all in the zero-th order approximation, or can one understand the most important experimental features by interaction effects alone? In this work, we concentrate solely on the effects of strong Coulomb interactions in the clean limit, and try to establish which experimental

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features can be explained by entirely ignoring the disorder.

We approach the transition from the insulating side, starting with the Wigner-Mott insulator, and examine its melting by quantum fluctuations as density increases. These are believed to be dominated [4] by the vacancy-interstitial pair excitations on top of the classical triangular lattice configuration. Within the Wigner crystal, the electrons are tightly bound, and the vacancy-interstitial excitations can be well represented by a mapping to a two-band Hubbard (i.e. charge-transfer) model, respectively corresponding to the lattice and the interstitial electrons. As the density increases, the charge-transfer gap eventually closes, and a metal-insulator transition assumes the character of a Mott-metal-insulator transition, leading to a strongly correlated metallic state on the metallic side.

Our model Hamiltonian reads:

$$H = \sum_{i\sigma} e_f f_{i\sigma}^{\dagger} f_{i\sigma} + e_c c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$$
$$+ \sum_{i\sigma} V(f_{i\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} f_{i\sigma}) + \sum_i U f_{i\uparrow}^{\dagger} f_{i\uparrow} f_{i\downarrow}^{\dagger} f_{i\downarrow} \quad (1)$$

where $f^{\dagger}$, f and $c^{\dagger}$, c are creation and annihilation operators for site and interstitial electrons respectively. It is assumed that the inter-cell hopping t_{ij} exists only between interstitial orbitals, while only the site electrons are subject to onsite Coulomb repulsion U, and the interstitial orbitals are coupled to the site orbitals via hybridization V. The local electrostatic potentials for the two bands are denoted by e_f and e_c.

We model the strong onsite repulsion by exclusion of double ocupancy, using the standard slave-boson mean-field formalism. The free energy per electron then reads:

$$W[\lambda, Z, \mu, \delta] =$$
$$- \frac{2T}{1-\delta} \sum_{lk} \ln\left(1 + \exp\left(-(\tilde{\varepsilon}_{lk} - \mu)/T\right)\right)$$
$$+ \frac{\lambda}{1-\delta}(Z - 1) + \mu \quad (2)$$

where ε_{lk} are renormalized band energies, λ is the Lagrange multiplier enforcing the slave-boson constraint, Z is the quasiparticle weight, μ is the chemical potential. The chemical potential μ is an internal parameter here, arising similarly to λ, from constraining the electron density per unit area. The self-doping δ measures deviation in the number of electrons (per elementary cell) from the half filling. In the classical limit of low electron density $\delta = 0$, but it becomes $\delta \neq 0$ at higher density, where quantum effects are important. This is reminiscent of the liquid solid transition in He3 [5]. The equations of the state are given by the saddle point of the free energy $W[\lambda, Z, \mu, \delta]$.

A peculiarity of this model is that the band energies are not fixed, but are self-consistently determined through their dependence on the occupation of the site and interstitial orbitals. It immediately follows that the system is unstable to the self-doping at the MIT. Indeed, by carefully accounting for the electrostatic energy balance due to such charge transfer, we find that the free energy takes a lower value (relative to the classical value at $\delta = 0$) on one of the branches at $\delta \neq 0$ *before* the transition at half filling is found (see Fig. 1).

With appropriately chosen model parameters we can explain the basic experimental results, which otherwise cannot be captured by the diffusion mode theory. Similarly to what is seen experimentally, we observe strong renormalization of the effective mass near the transition $m^* \sim (n - n_c)^{-1}$. In this strongly correlated regime any extrinsic disorder is very effectively screened by interaction effects [7], providing a plausible scenario for the large resistivity drop [8]. The magneto-resistance data are also naturally explained by our two band model. The experiment [9] has shown that in high parallel magnetic fields the transport takes place by activated processes, with an activation gap that vanishes linearly at some density $n_1 > n_c$. In the strong field our model reduces to a trivial model of non-interacting spinless electrons. For the density $n < n_1$ the system is a band insulator with the lower band completely filled. The bands broaden as the density increases, and the insulating gap closes linearly at some density $n_1 > n_c$.

Our static lattice model does not capture the collective charge density fluctuations – the phonons of the Wigner crystal. Because the Coulomb interaction is long ranged, these collective modes are very soft, and play an important role in renormalizing the model parameters. It is this strong renormalization of the charge transfer gap $e_c - e_f$ that pushes the transition to such low density [6] ($r_s \gg 1$)), in a fashion that is conceptually very similar to the formation of the Coulomb gap [10]. At present, these effects are incorporated in through the choice of the electrostatic parameters of our model. In future work, we would like to systematically incorporate these soft collective modes, the effects of which are currently included in a semi-phenomenological fashion. This program can be achieved by a variety of methods, including extended dynamical mean field approaches (EDMFT), by exploiting unique properties of the Coulomb potential, and by employing the techniques recently developed in the Coulomb glass context [10].

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