Mott-Hubbard Scenario for the Metal-Insulator Transition in the Two Dimensional Electron Gas

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By comparing the responses to an in-plane magnetic field near the metal-insulator transition (MIT), we find that the observed MIT in Si MOSFETs can be described by the non-perturbative Mott-Hubbard scenario. Interrelations between independent measurables are uncovered and confirmed by reploting the experimental data. A universal critical energy scale vanishing at the MIT is extracted from the experimental data and the critical exponent found.

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The properties of an electron gas (EG) are controlled by the average inter-electron distance. As the electron density is tuned from high to low, the Coulomb interaction, favoring localization of the electrons, becomes dominant over the kinetic energy and the system evolves from a metal to an insulator. Puzzling magnetotransport experiments on the silicon metal-oxide-semiconductor field-effect transistors (Si MOSFETs) in the past ten years have reactivated broad interest in the subject because of possible relations to the detection of a quantum critical point (QCP), the realization of the Wigner crystal, and the interplay between correlation and disorder. By comparing the responses to an in-plane magnetic field near the metal-insulator transition (MIT), we find that the observed MIT is controlled by the non-perturbative Mott-Hubbard (M-H) critical end point at a low but non-zero temperature, instead of a QCP. This also contradicts the long-standing speculation that the non-local part of the Coulomb interaction plays an essential role in the MIT, as it does in the Wigner crystalization. The M-H scenario predicts interrelations between independent measurables which are confirmed by reploting the experimental data. The uncovered sample independent behavior indicates that the disorder does not play an active role. A critical energy scale is extracted from the experimental data and the critical exponent found.

An MIT in the two dimensional (2D) EG was first observed via the conductivity measurements in ultra clean Si MOSFETs. When the temperature is decreased below $\sim 2K$, the conductivity is observed to increase (decrease) monotonically at densities above (below) a certain non-universal critical value $n_c \sim 10^{11} cm^{-2}$. In this temperature range, the conductivity curves in a given phase can be all collapsed into a single curve by rescaling the temperature, the observation clearly points to an unidentified type of critical behavior. It was also found that the scaling behavior is sample independent down to the lowest temperatures reached experimentally ($\lesssim 100 mK$). The most likely driving force is then the interaction induced correlation, instead of the disorder.

In the subsequent experiments in Si MOSFETs, it was found that near $n_c$ applying an increasing in-plane magnetic field $H_{||}$ causes the conductivity first to decrease and then, above a certain field $H_{\sigma}$, saturate at a roughly field independent value. As the temperature is lowered, $H_{\sigma}$ first decreases linearly and then approaches a constant. This constant depends on the electron density and vanishes as the transition is approached from the metallic side. At $H_{||} > H_{\sigma}$, the conductivity is always insulating like, decreasing as the temperature is lowered, irrespective of whether the density corresponds to a metallic or an insulating phase in the absence of the field. Shubnikov-de Haas (SdH) measurements show that the oscillation period is halved when $H_{||} \gtrsim H_{\sigma}$. This has been taken as an indication that the entire EG is fully polarized when the conductivity saturates in the field. Since $H_{\sigma}$ vanishes at $n = n_c$ and $T = 0$, this could point to a Stoner instability, although it would be hard to understand the almost coincidence of the Stoner instability with the MIT. Direct and indirect measurements show that the homogeneous spin susceptibility is enhanced in the approach to the transition and is related to a mass enhancement since the g-factor changes little.

The perturbative scaling theory for non-interacting disordered electron systems shows that no true metallic phase exist in 2D due to the disorder. However, the Coulomb interaction competes with the localization and stabilizes the metallic phase. The relevance of the scaling theory to the experiments was checked. Starting from the Fermi liquid, perturbations were used to study the temperature dependence of the conductivity and the strong mass enhancement. While they describe the 2DEG to certain extent, these perturbations are not justified since the experiments on Si MOSFETs show that the transition happens when $R_S$, the average inter electron distance measured in units of the Bohr radius, is $\gtrsim 10$. The significance of this is that $R_S$ is also given by the ratio of the interaction energy, i.e. the perturbation, to the kinetic energy.

The only non-perturbative, correlation-driven MIT we understand is the M-H transition. The M-H scenario was related to the 2DEG before. However, the clear connections between the two become evident.
only through studying the magnetotransport behavior. Within this scenario, we manage to explain the experiments and uncover previously unnoticed interrelations between independent observables.

The M-H transition, driven by the ratio of the on-site interaction \( U \) to the bandwidth \( W \), is best revealed by the behavior of the local density of states (LDOS) as shown by the dynamical mean field theory (DMFT) [10]. Near the transition and on the metallic side, the LDOS has a three peak structure (Fig. 1), with a central peak at the Fermi level and two side bands separated in energy by roughly \( U \). The former consists of extended quasiparticle states; its width is proportional to the quasiparticle weight. The latter, the upper and lower Hubbard bands, consist of localized states. In between the peaks, the LDOS is featureless, corresponding to an incoherent background. As one moves towards the insulating side by increasing \( U/W \), the width of the central peak decreases to zero. DMFT found [10] that, irrespective of the bare dispersion details, the MIT happens at \( U/(W/2) \sim 3 \) and is first-order at zero temperature. The first-order transition line extends to non-zero temperatures and ends in a critical point at \( T_c \sim 0.05 \cdot (W/2) \) beyond which the transition becomes a crossover. This picture was confirmed experimentally only recently, e.g. in the photoemission studies of V$_2$O$_3$ at \( T \gg T_c \). At \( T < T_c \), the physics is usually non-universal and depends on the system details.

We argue that the magnetotransport experiments on the 2DEG can be explained by the evolution in a magnetic field of the three peak LDOS. On the metallic side, an increasing in-plane magnetic field first splits the quasiparticle peak while reducing its height. This reduces the LDOS near the Fermi surface and thus the conductivity. When the field is strong enough so that the quasiparticle peak is either entirely split apart or suppressed, the LDOS left over near the Fermi surface derives only from the incoherent background. Consequently the conductivity saturates at a value determined by the short mean free time of those states and its temperature dependence becomes insulating-like. The field at which this saturation appears is \( H_s \propto (1/g\mu_B) \cdot \max((ZW,k_BT)) \), meaning the Zeeman energy should be strong enough to split or suppress the quasiparticle peak and overcome the thermal excitations. So as \( T \) is reduced, \( H_s \) first decreases linearly and then saturates to a constant \( \propto Z \). Since \( Z \) reduces to zero as the transition is reached from the metallic side, \( H_s(T=0) \) vanishes accordingly. Meanwhile, the effective mass (\( \propto 1/Z \)) gets enhanced and diverges.

To support the above explanation, we have computed the evolution in an in-plane magnetic field of the LDOS near the M-H transition using a half-filled lattice Hubbard model,

\[
H = \sum_{\sigma = \pm} \int_{|k| \leq \Lambda} \frac{d^2k}{(2\pi)^2} \left( \epsilon_k + \sigma H_0 \right) C_{k,\sigma}^\dagger C_{k,\sigma} + U \sum_i N_{i\uparrow} N_{i\downarrow}
\]

where we used \( N_{i,\sigma} = C_{i,\sigma}^\dagger C_{i,\sigma} \) and set the \( g \)-factor = 2. We approximate the first Brillouin zone by a disk. The momentum cut-off \( \Lambda = 2\sqrt{\pi} \) ensures the normalization of the momentum integral and sets the lattice constant to be \( 2\pi/\Lambda \). We use the free dispersion \( \epsilon_k = k^2/2 \) specific to the EG. The bandwidth is thus \( W = 2\pi \). This effective model is valid when the thermal and Zeeman energies are small comparing to the bandwidth. We mention, though, even at low temperatures there is a non-zero possibility that an electron jumps to a higher energy state. In terms of the one-band lattice model, this is like an electron hopping away from the lattice sites and into the interstitials.

In this dimensionless model for the 2DEG, the energy is measured in units of \( E_0 = 2eB R_f^{-2} \), with the electron band mass \( m_0 \sim 0.2m_e \) and the dielectric constant for the Si MOSFET \( \epsilon \sim 7.7 \). Since in the experiments, the MIT is observed around \( R_c \sim 10 \), we estimate \( E_0 \) to be \( \sim 10.6 K \). The corresponding magnetic field unit is, using \( g = 2, H_0 = E_0/(\mu_B m_e/m_0) \sim 3.17 \). A rough estimation of the non-universal \( T_c \) for the M-H critical end point is possible at this stage. Applying the DMFT estimation in the current model, we obtain \( T_c \sim 1.7 K \). The mean field estimation is about one order of magnitude higher than the experimental value \( T_c \lesssim 100 mK \).

To compute the conductivity, we use the Kubo formula [10]. In the EG, the current operator is given by \( j(\vec{q}) = \sum_{\vec{k},\sigma} \hat{C}_{\vec{k},\sigma}^\dagger \hat{C}_{\vec{k}+\vec{q},\sigma} \). Only the particle-hole bubble survives in the current-current correlation in DMFT [10]. The conductivity, in unit of \( e^2/(kT) \),

\[
\sigma = \lim_{\omega \to 0} \frac{1}{\omega} \sum_{\sigma = \pm} \int_{|k| \leq \Lambda} \frac{d^2k}{(2\pi)^2} \frac{\beta}{\theta} \sum_{ip_n} k^2 G_{\sigma}(\vec{k}, ip_n)G_{\sigma}(\vec{k}, ip_n + i\omega),
\]

with \( p_n = (2n + 1)\pi/\beta \).

We solve this model numerically via DMFT, using quantum Monte Carlo (QMC) as the impurity solver [10]. In Fig. 1 the evolution of the LDOS is presented at an inverse temperature \( \beta = 5.0 \) and an on-site interaction \( U = 7.0 \). The latter is chosen so that the system is on the metallic side and close to the MIT. The conductivity saturation behavior is shown in the inset of Fig. 2. The \( T \) vs \( H_s \) relation is shown in the main plot. In the temperature region solved, \( H_s \) depends linearly on \( T \), similar to that observed experimentally [13].

Although it provides us with some essential features regarding the MIT in 2DEG, this effective model contains certain limitations. These include the lack of the incoherent hopping of the electrons into the interstitial space. This should be responsible for the observed saturated conductivity being non-zero at \( T > 0 \), instead of vanishing as shown in the inset of Fig. 2. Actually it was found experimentally that the saturated conductivity increases with the temperature and at \( T \gtrsim 1K \) it can reach the same order of magnitude as that measured at
FIG. 1: The evolution of the LDOS in an external in-plane magnetic field $H_{\parallel}$. At zero field, the LDOS shows a quasiparticle peak at the Fermi energy ($E = 0$) together with two side bands. An increasing $H_{\parallel}$ causes the peak to split and finally get suppressed. At $H_{\parallel} \sim 0.7$ when the quasiparticle peak is fully split, the LDOS shows that the localized spins are still not entirely polarized. In this model calculation, the strongly incoherent background as observed experimentally in the M-H systems is absent from the LDOS.

...a metallic density and with no external field. SdH measurements then become possible even at $H_{\parallel} \gtrsim H_{\sigma}$. The observed halving of the SdH oscillation period when $H_{\parallel} > H_{\sigma}$ is thus due to the full polarization of the itinerant electrons, including those within the quasiparticle peak and those involved in the interstitial hopping. The electrons localized in the lower Hubbard band do not contribute to the transport.

While only one energy scale ($Z$) controls the critical transport behavior, two distinct energy scales are responsible for the spin polarization, the super exchange ($\propto 1/U$) for the local moments and the quasiparticle peak width ($\propto Z$) the itinerant electrons. Near the transition, $Z \rightarrow 0$ and it costs almost no energy to polarize the itinerant electrons. Meanwhile, a non-zero exchange energy must be overcome to polarize the local moments. This behavior can be seen in the LDOS at $H \sim 0.7$ in Fig. 1, where the quasiparticle peak is already fully split while the local moments are only partially polarized. A direct proof of the two-energy-scale behavior could be found from a measurement of the magnetization and a study of its saturation behavior in a magnetic field. For the 2DEG, no consensus has been reached experimentally, although indications favoring the existence of the local moment band were reported. This convincing experiment would allow to discern the M-H scenario from the Stoner picture. In the latter there is only one magnetic energy scale and all the electrons are polarized simultaneously by a vanishing field near the transition.

According to the M-H scenario, all the critical behaviors are related to $Z$. The saturation magnetic field, $H_{\sigma}(T = 0) \propto Z$ should vanish and the effective mass $m^* \propto 1/Z$ diverge in approaching the transition from the metallic side. Besides, it is also responsible for the vanishing energy scale $T_0$ as revealed by the universal...
scaling of the conductivity \[\sigma\] so \[T_0 \propto Z^n\]. In Fig. 3, we transformed, rescaled, and replotted the experimental scaling temperature \[T_0\] data [12], the \[H_\sigma\] data [13], and the \[m^*\] data [21]. Although belonging to independent measurements on different samples, the \[H_\sigma\] and \[m^*\] data sets collapse well when their densities overlap, revealing the previously unnoticed interrelations that we derived from the M-H scenario. From Fig. 3, we find that \[Z \propto \delta n^{0.64}\] for \[\delta n \lesssim 2\]. This universal relation can be used to calibrate the critical behaviors. Note that, the DMFT solution gives \[Z \propto \delta n\], since \[Z \propto U_c - U\] and the mapping from the density to \[U\] is expected to be analytic even around the transition. The deviation of the critical exponent is not unexpected for a mean field theory.

The M-H picture captures the universal critical behavior when \[T_r \lesssim T \lesssim 2K\], where the conductivity scaling was achieved [12] and all the other above-mentioned behaviors were observed [2, 3]. The non-universal properties specific to the 2DEG at \[T \ll T_r\] were previously studied. Monte Carlo simulations [24] showed, in between the paramagnetic metallic and the Wigner crystal phases, there lies at least one other phase, the polarized liquid phase. A similar result was obtained by studying the free energy. It was shown that a direct transition is forbidden and various intermediate phases are present [24]. At \[T \gtrsim 2K\] the system crosses over to another different behavior. It was observed that the conductivity as a function of temperature is insulating like \[\sigma\] irrespective of the density being above or below \[n_c\]. This is likely due to the Anderson localization behavior [4] before the correlation sets in and the M-H critical point takes over at lower temperatures.

We have managed to establish that the non-perturbative M-H critical point describe the observed MIT in 2DEG. Our theory provides a framework for understanding the interrelations between the independent measurables, which is confirmed by reploting the experimental data. A universal energy scale vanishing at the transition is uncovered. In the light of the M-H scenario, we suggest further experiments on the 2DEG of measuring the magnetization saturation behavior in an in-plane magnetic field. This will allow to reveal the predicted two-energy-scale behavior near the transition. Subjects remain to be clarified including the proper descriptions of the incoherent hopping into the interstitials and the ineffectiveness of the non-local part of the partially screened Coulomb interaction. To fulfill these purposes, a controlled derivation of an effective low energy lattice model for the EG will be helpful.

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