Central role of exchange-correlation hole in the 2D metal-insulator transition

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We show that the metal to insulator transition, whether generated by decreasing the electron density or by increasing the spin alignment, is determined by a universal functional form of the two-electron correlation function $g(r)$. This result provides direct evidence of the central role of the Coulomb repulsion and exchange in driving the metal-insulator transition.

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The discovery that electrons in a two-dimensional plane can switch from insulating to metallic behaviour as their density is decreased was unexpected as it had been widely believed that electrons should always remain insulating in 2D. The recent observations that a magnetic field applied parallel to the plane destabilizes the 2D metallic phase at fixed density is puzzling since a parallel field only aligns the internal spins of the electrons and does not affect their external orbital motion. Since it is widely believed that the electron interactions are a key to understanding the transition it is important to understand the role of exchange-correlations in these phenomena. We show that the two phenomena can be characterized within the single framework of a universal form for the exchange-correlation hole at the transition.

At the relatively high densities found in conventional metals and semiconductors the electron correlations resulting from mutual Coulomb repulsion are not important because the average interaction energies are much smaller than the Fermi energies. Thus the transport properties of conventional metals and semiconductors are well accounted for by the standard nearly-free-electron picture. However without electron repulsion the 2D system would always be insulating in the presence of disorder so it is clear that to treat the metal-insulator transition we must look beyond this picture.

At low electron densities the Fermi energy is small and the electron-electron correlations dominate. For extremely low electron densities the strong electron correlations drive the system to a localized state (the Wigner crystal) without the need for disorder. The metal-insulator transition is observed at significantly higher densities than the value predicted theoretically in Ref. for the Wigner transition. This has been interpreted as due to the effect of electron-defect interactions since defects reduce the mobility of the electrons, making them easier to localize.

In the Wigner crystal the strong correlations lead to near neutrality within each Wigner-
Seitz cell since each electron is surrounded by a region of near-zero electron density.\(^7\) This repulsive hard core region forms part of the electron’s exchange-correlation hole. The complete density profile of the exchange-correlation hole is known from the two-electron correlation function \(g(r)\) given in Ref.\(^7\). When the electron density is increased, the radius of the hard core in the exchange-correlation hole shrinks and the Wigner crystal melts. However the hard core persists in the delocalized state until the density increases to \(r_s \simeq 7\), a factor 25 times greater than the Wigner transition density of \(r_s \simeq 35\). \(r_s\) is the average electron spacing in effective Bohr radii.

The diffusion quantum Monte Carlo numerical simulations (DQMC) in Ref.\(^7\) also show that the exchange-correlation hole is stronger for spin polarized electrons than for unpolarized electrons. This is due to the additional exchange acting between the increased number of parallel spin electrons. In Fig. 1 we see at fixed density that polarizing the spins significantly expands the size of the hard core in \(g(r)\). At \(r_s = 7\) for the polarized system there is still a region of zero density around each electron while for the unpolarized system it has disappeared.

We propose here that the suppression of the metallic state by a parallel magnetic field is associated with the expansion of the hard core due to alignment of the electron spins by the field. We estimate the degree of electron spin polarization as a function of a parallel magnetic field \(H_{\parallel}\) using DQMC data from Rapisarda and Senateor\(^8\). At these electron densities the free energy \(E_p(r_s)\) per electron for the fully spin polarized state is close to the free energy \(E_u(r_s)\) for the unpolarized state so that the Zeeman energy gain from small magnetic fields is sufficient to fully polarize the ground state. We estimate the critical \(H_{\parallel}\) needed to fully polarize the electron spins by equating the Zeeman energy gain to the difference in free energies, \((g\mu_B/\hbar)H_c = [E_p(r_s) - E_u(r_s)]\). With \((g\sigma_z) = 1.1\) taken for GaAs\(^9\) a field \(H_{\parallel} \simeq 0.7\) T is sufficient to produce full spin polarization for \(r_s = 9\).

In Hamilton et al’s\(^5\) recent experiment the metal-insulator transition boundary in \(p\)-GaAs is shifted by a parallel field \(H_{\parallel} = 0.6\) T from hole density \(p_s = 7.5 \times 10^{10}\) cm\(^{-2}\) to \(p_s = 12.4 \times 10^{10}\) cm\(^{-2}\) that is from \(r_s = 9\) to \(r_s = 7\). If we move along the experimental transition line in the direction of decreasing \(r_s\), the critical magnetic field increases. This results in the electron spins becoming increasingly aligned. From a linear interpolation between \(H_{\parallel} = 0\) and \(H_c\) we determine at \(r_s = 7\) that a field \(H_{\parallel} = 0.6\) T induces 50% spin polarization. Figure 2 shows that as a result of the increased polarization, the \(g(r)\) on the transition boundary at \(r_s = 7\) for the polarized system is essentially identical with the \(g(r)\) on the transition boundary at \(r_s = 9\) for the unpolarized system. The hard core radius remains fixed along the entire experimental transition line. This indicates that the transition is determined by a unique functional form of the \(g(r)\), or equivalently, by a critical density profile of the exchange-correlation hole.

Because of the enhancement in the exchange, at fixed \(r_s\) the critical impurity density \(n_i\) for the polarized system is smaller than for the unpolarized system. In a separate calculation\(^10\) we have shown that fully spin polarizing the system with an \(H_{\parallel} \sim 1\) T destabilizes the metallic phase.

In conclusion, the free energy difference between the spin polarized and unpolarized states for the electron densities of relevance here, is so small that a magnetic field \(\sim 1\) T is sufficient to fully polarize the system. Using numerical simulation results we have shown that the additional gain in exchange-correlation for the polarized state is a key in
understanding the instability of the 2D metallic state. Decreasing the electron density also enhances exchange-correlation, which again destabilizes the metallic state. We show that the metal-insulator boundary is determined by a universal functional form of the two-electron correlation function $g(r)$ independent of the degree of polarization and the electron density.

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FIGURES

FIG. 1. Two-electron correlation function $g(r)$ taken from Ref. 7 at $r_s = 9$ for unpolarized system (dotted line) and fully polarized system (dashed line), showing the effect of exchange enhancement.

FIG. 2. Correlation function $g(r)$ along the metal-insulator transition boundary. Dotted line: $r_s = 9$, unpolarized. Dash-dot line: $r_s = 8$ for $H_{\parallel} = 0.4$ T. Dashed line: $r_s = 7$ for $H_{\parallel} = 0.6$ T. The three curves are essentially identical.
$g(r)$

$r_s = 9$

$\text{pol}$

$\text{unpol}$
$g(r)$ vs $k_F r$ for different $r_s$ and $H$ values:

- $r_s = 7$, $H = 0.6T$
- $r_s = 8$, $H = 0.4T$
- $r_s = 9$, $H = 0$