

THE 2D MOTT–HUBBARD TRANSITION IN PRESENCE OF A PARALLEL MAGNETIC FIELD*

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The half-filled two-dimensional Hubbard model in presence of a uniform and static parallel magnetic field has been studied by means of the Composite Operator Method. A fully self-consistent solution, fulfilling all the constraints coming from the Pauli principle, has been found. The relevant features of a metal-insulator transition in presence of a magnetic field have been analyzed. The results qualitatively agree with the ones recently obtained by means of experimental investigations.

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The response of a two-dimensional (2D) electronic system to a parallel magnetic field is very intriguing and several anomalous properties have been observed. There is a general agreement that the observed behavior is related to the spin polarization, but further studies, both theoretical and experimental, are needed. In this paper we concentrate on the metal-insulator transition (MIT) driven by a in-plane magnetic field. Recent experiments on Si-MOSFET [1] and GaAs [2] have shown that by increasing field the spin system polarizes and the system undergoes a MIT before reaching the full polarization. Apparently, an important role is played by the electron–electron interaction, being $r_s = U/K$ (the ratio of Coulomb interaction energy to the mean kinetic energy) very large.

In order to make a qualitative and preliminary study of this phenomenon we consider the 2D Hubbard model in presence of a parallel external magnetic field. Since a parallel field does not couple to the orbital motion of electrons, the Hamiltonian is given by

$$H = \sum_{ij} (-4t \alpha_{ij} - \mu \delta_{ij}) c^\dagger(i) c(j) + U \sum_i n_\uparrow(i) n_\downarrow(i) - \frac{1}{2} h \sum_i n_3(i), \quad (1)$$

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where $c(i)$ and $c^\dagger(i)$ are the annihilation and creation operators of electrons in spinorial notation; $i = (\mathbf{i}, t)$ where \mathbf{i} are vectors of a 2D Bravais lattice; μ is the chemical potential; α_{ij} denotes the projector on first-neighbor sites; U is the local Coulomb interaction, $n_\sigma(i) = c_\sigma^\dagger(i) c_\sigma(i)$ is the charge density of the electrons with spin σ ; $n_3(i)$ is the third component of the spin density operator; h is proportional to the intensity of the external magnetic field. In the framework of the Composite Operator Method (COM) [3], we introduce the basis $\psi^\dagger(i) = (\xi^\dagger(i), \eta^\dagger(i))$ where $\xi(i) = (1 - n(i)) c(i)$ and $\eta(i) = n(i) c(i)$ are the Hubbard operators responsible for the transitions $|0\rangle \leftrightarrow |\sigma\rangle$ and $|\sigma\rangle \leftrightarrow |\uparrow\downarrow\rangle$, respectively. The composite operator $\psi(i)$ satisfies the equation of motion

$$i \frac{\partial}{\partial t} \psi(i) = (\frac{1}{2} h \sigma_3 - \mu) \psi(i) - 2t(1 + \tau_3) c^\alpha(i) + \frac{1}{2} U (1 - \tau_3) \eta(i) - 4t \tau_3 \pi(i) \quad (2)$$

where $\vec{\sigma}$ acts on the spin degree of freedom $\sigma = \uparrow, \downarrow$ and $\vec{\tau}$ on the internal degree of freedom $\psi = \xi, \eta$. $\vec{\sigma}$ and $\vec{\tau}$ are Pauli matrices. We also use the notation $\phi^\alpha(\mathbf{i}, t) = \sum_{\mathbf{j}} \alpha_{ij} \phi(\mathbf{j}, t)$. Moreover, we have $\pi(i) = \frac{1}{2} \sigma^\mu n_\mu(i) c^\alpha(i) + \xi(i) [c^{\dagger\alpha}(i) \eta(i)]$ where $\sigma_\mu = (1, \vec{\sigma})$, $\sigma^\mu = (-1, \vec{\sigma})$ and $n_\mu(i) = c^\dagger(i) \sigma_\mu c(i)$ describe the total charge- ($\mu = 0$) and spin- ($\mu = 1, 2, 3$) density operators.

In the polar approximation [3] we linearize the equation of motion by projecting the source on the basis $\psi(i)$. Then, the retarded Green's function $S(\mathbf{k}, \omega) = \mathcal{F} \langle \mathcal{R} [\psi(i) \psi^\dagger(j)] \rangle$, where \mathcal{F} and \mathcal{R} are the Fourier transform and the usual retarded operators, respectively, has the following expression

$$S(\mathbf{k}, \omega) = \sum_{l=1}^4 \frac{\sigma^{(l)}(\mathbf{k})}{\omega - E^{(l)}(\mathbf{k}) + i\delta}, \quad (3)$$

where the energy spectra $E^{(l)}(\mathbf{k})$ are the eigenvalues of the energy matrix $\varepsilon(\mathbf{k}) = \mathcal{F} \langle \{J(\mathbf{i}, t), \psi^\dagger(\mathbf{j}, t)\} \rangle I^{-1}(\mathbf{k})$ and the spectral density matrices $\sigma^{(l)}(\mathbf{k})$ are calculated by means of the formula $\sigma_{\alpha\beta}^{(l)}(\mathbf{k}) = \Omega_{\alpha l}(\mathbf{k}) \sum_\gamma \Omega_{l\gamma}^{-1}(\mathbf{k}) I_{\gamma\beta}(\mathbf{k})$ where $\Omega(\mathbf{k})$ is the matrix whose columns are the eigenvectors of the energy matrix $\varepsilon(\mathbf{k})$ and $I(\mathbf{k}) = \mathcal{F} \langle \{ \psi(\mathbf{i}, t), \psi^\dagger(\mathbf{j}, t) \} \rangle$ is the normalization matrix. The explicit expressions of $E^{(l)}(\mathbf{k})$ and $\sigma^{(l)}(\mathbf{k})$ will be given elsewhere. Calculations show that the Green's function depends on the following set of parameters: $\mu, m, \Delta_\sigma, p_\sigma$. $m = \frac{1}{2} \langle n_3(i) \rangle$ is the magnetization per site. The parameters Δ_σ and p_σ describe a constant shift of the bands and a band width renormalization, respectively, and are defined as

$$\begin{aligned} \Delta_\sigma &= \left\langle \xi_\sigma^\alpha(i) \xi_\sigma^\dagger(i) \right\rangle - \left\langle \eta_\sigma^\alpha(i) \eta_\sigma^\dagger(i) \right\rangle \\ p_\sigma &= \frac{1}{4} \left[\langle n_\mu^\alpha(i) n_\mu(i) \rangle + 2(-)^\sigma \langle n^\alpha(i) n_3(i) \rangle \right] \\ &\quad - \left\langle [\xi_\uparrow(i) \eta_\downarrow(i)]^\alpha \eta_\downarrow^\dagger(i) \xi_\uparrow^\dagger(i) \right\rangle. \end{aligned} \quad (4)$$

The determination of these parameters is very crucial and wrong results are easily obtained as shown in Ref. [4]. The parameters m and Δ_σ are expressed in terms of the Green’s function as $m = \frac{1}{2}(C_{44} - C_{22})$, $\Delta_\uparrow = C_{11}^\alpha - C_{22}^\alpha$ and $\Delta_\downarrow = C_{33}^\alpha - C_{44}^\alpha$. We have defined the correlation matrices $C = \langle \psi(i) \psi^\dagger(i) \rangle$ and $C^\alpha = \langle \psi^\alpha(i) \psi^\dagger(i) \rangle$. The other parameters μ and p_σ are not determined by the equation of motion and are fixed by choice of the representation where the Green’s functions are realized [5]. In the COM we choose the representation by requiring that all the relations among the operators dictated by the algebra (Pauli principle) are conserved also at the level of expectation values. In the present study, this requirement leads to $C_{11} = C_{33}$ and $C_{12} = C_{34} = 0$. Because we are interested in the study of the MIT, we consider the special case of half filling ($n = \langle n(i) \rangle = 1$) where: $\mu = \frac{U}{2}$, $\Delta_\uparrow = -\Delta_\downarrow$, $p_\uparrow = p_\downarrow - 2m$ and $C_{12} \equiv C_{34} \equiv 0$. It is worth to note that these latter relations are a manifestation of the particle-hole symmetry which is conserved owing to the choice of the representation. Any other choice of the representation will lead, in the context of the pole-approximation, to a violation of the symmetry [4]. Finally, we have a set of three coupled self-consistent equations which determine the three parameters which are left: m , $\Delta = \Delta_\uparrow$, $p = p_\uparrow$.

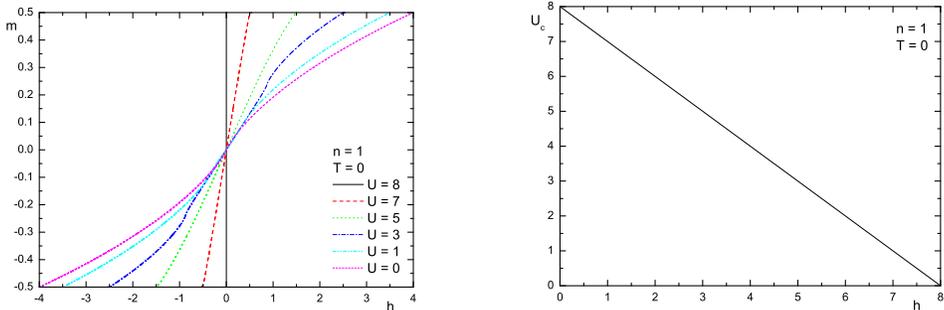


Fig. 1. (left) The magnetization m as a function of the external magnetic field h for $T = 0$, $n = 1$ and various values of the Coulomb repulsion U ; (right) The critical value U_c of the Coulomb repulsion U for the MIT as a function of the external magnetic field h for $T = 0$ and $n = 1$. t is taken as unity.

In Fig. 1 (left panel) we plot the magnetization m versus the magnetic field h . The magnetization is an increasing function of both the applied magnetic field and the Coulomb interaction U . It reaches the saturation value (*i.e.*, $1/2$) at a critical value of the magnetic field, which depends on the intensity of the Coulomb interaction. At zero temperature $T = 0$, when U approaches the bandwidth $W_{2D} = 8t$, the magnetization experiments a discontinuous jump from zero up to the saturation value. We have also

inspected the analytical behavior of the static susceptibility by analyzing the self-consistent equations in the limit of very low magnetic fields. Results show a divergence when the Hubbard repulsion approaches the bandwidth at zero temperature. The double occupancy decreases when increasing both the interaction and the magnetic field. The latter provides the spins of the electrons with an orientation and, due to the Pauli principle, reduces the double occupancy. There is a quite good agreement between COM results and Gutzwiller ones [6].

The MIT can be studied by looking at the density of states (DOS): the opening of a gap in the DOS is a signal of the transition from metallic to insulating phase. In Ref. [7] we have studied the MIT exhibited by the Hubbard model in absence of magnetic field for the 2D and 3D cases. It was found that the transition is driven by the Coulomb interaction: there is a critical value U_c where the MIT occurs. In particular, the value $U_c = 1.68W$ ($W_{2D} = 8t$ and $W_{3D} = 12t$ for the 2D and 3D system, respectively) was reported. In presence of a magnetic field the value of U_c is drastically influenced. In Fig. 1 (right panel) we plot the critical value versus the magnetic field at zero temperature. As we turn on a rather small magnetic field, the critical value U_c suddenly jumps from $U_c = 1.68W$ to $U_c = W$. This discontinuity at zero field is related to the discontinuity of the magnetization, as shown in Fig. 1 (left panel). By increasing h , U_c decreases and vanishes when the field equates the bandwidth at zero temperature (*i.e.*, $U_c(h, T = 0) = W - h$), in qualitative agreement with the experimental findings.

In conclusion, our study shows that the 2D Hubbard model in presence of a parallel magnetic field can describe the experimental evidence of a field-driven MIT. The transition is controlled by the field and disappears for some critical value of it. A more detailed discussion of the MIT and of the order parameter controlling the transition will be reported elsewhere.

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