Fluctuation-driven insulator-to-metal transition in an external magnetic field

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We consider a model for a metal-insulator transition of correlated electrons in an external magnetic field. We find a broad region in interaction and magnetic field where metallic and insulating (fully magnetized) solutions coexist and the system undergoes a first-order metal-insulator transition. A global instability of the magnetically saturated solution precedes the local ones and is caused by collective fluctuations due to poles in electron-hole vertex functions.

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Metal-insulator together with magnetic transitions belong to the most important collective phenomena caused by the (screened) Coulomb electron repulsion. Particularly the correlation-driven Mott-Hubbard transition from a paramagnetic metal to a paramagnetic insulator, i.e. with no apparent symmetry breaking, has been studied intensively in an effort to explain qualitatively the experimental findings in vanadium oxides doped with chromium. Although observed only at finite temperatures, the Mott-Hubbard transition is theoretically studied mostly as an extrapolation to zero temperature and in the mean-field limit with only local dynamical fluctuations. Antiferromagnetic long-range order is supposed to be suppressed at low temperatures by a frustration destroying the perfect-nesting property.

But even in this maximally simplified situation one is unable to solve the problem exactly. A scenario for the Mott-Hubbard transition in the spin-symmetric case was initially deduced from the so-called iterated perturbation theory (IPT), but it was later supported by analytical and numerical renormalization-group arguments. The detailed transition behavior remains, however, still controversial.

Unfortunately we do not have many cogent methods for the description of the critical behavior at the metal-insulator transition. The existing solutions are extrapolations. There is not a reliable interpolation between the Fermi-liquid regime and the strong-coupling, atomic like solution. IPT seems the only technique based on perturbation theory being able to cover the desired features of the weak and strong coupling limits and to describe qualitatively the Mott-Hubbard transition.

The description of the Mott-Hubbard transition in the spin-symmetric phase is further plagued with the nonexistence of a parameter controlling the critical behavior. Nozières recently suggested to extend the $d = \infty$ description of the Mott-Hubbard transition to the magnetic case. The density of states (DOS) is no longer pinned at the Fermi energy and IPT does not reproduce correctly the strong-coupling limit. New methods are to be used to examine the magnetic case.

On the other hand, magnetic field and spin polarization offer a natural parameter, magnetization, with the aid of which we can control the transition behavior. Moreover, the exact insulating fully spin-polarized state is explicitly known, namely the Hartree solution with well separated bands for up and down spins. The question whether the saturated magnet decays to a metallic state or whether the insulating phase remains stable for non-saturated magnetizations at intermediate and strong coupling can be studied as an extension of the Mott metal-insulator transition.

A picture for the Mott transition near the fully saturated magnetic state in finite dimensions was suggested in [9]. It was shown that the fully saturated ferromagnet decays at $B = B_s(U)$ differently at weak and strong coupling. While in the former it is noncritical, a two-particle function gets critical at the ferromagnetic boundary in the latter. Recently this analysis was extended to the mean-field limit of a simplified Hubbard model with one spin species static [10].

Unlike the spin-symmetric case, it is the metallic side of the transition that is difficult to describe in the magnetic case. There is no complete solution below the ferromagnetic boundary at intermediate and strong coupling. Only recently it has been shown that for $B > B_s(U)$ the parquet approximation reproduces the exact asymptotics of the Bethe ansatz solution in $d = 1$ [11]. However, a closed solution beyond weak-coupling [12,13] has not yet been constructed.

The aim of this work is to investigate the existence and kind of the fluctuation-driven insulator-to-metal transition in an applied magnetic field within the exact limit of high spatial dimensions. We concentrate on nearly ferromagnetic states at intermediate coupling.

Using field-theoretic, diagrammatic techniques we show that at weak coupling, $U < U_{c0} \approx 1.38w$ (for a semi-elliptic density of states with the bandwidth $2w$), the insulating, fully magnetized solution goes continuously over to a metallic one by merging the bands of the up- and down-spin electrons at $B_s(U) = w - U/2$. The behavior is controlled by one-particle functions. At intermediate and strong coupling, $U > U_{c0}$, however, the magnetically saturated solution gets globally unstable along $B_0(U) > w - U/2$. A second critical point $U_{c1} \approx 1.65$ is found from which the saturated magnet gets also locally
unstable with a diverging electron-hole vertex function at \( B_s > w - U/2 \) but \( B_s < B_0 \).

The metallic solution at intermediate coupling is stabilized by correlations and the spectral function shows two satellite bands and a Kondo-like narrow quasiparticle peak around the Fermi energy. The metallic remains stable also for \( B > B_4(U) \) where already the fully spin polarized solution exists. It is destroyed at an upper critical filed \( B_5(U) \) with a jump in magnetization to the fully magnetically saturated state. We hence find a rather broad area of parameters \( U, B \) for which the metallic and insulating solutions coexist as local minima of the free-energy functional and within which a first-order metal-insulator transition takes place. We have a situation with magnetic hysteresis and discontinuities in magnetization as known from metamagnetic transitions \([14,15]\).

Unlike weak coupling, the insulator-to-metal transition at intermediate and strong coupling is controlled by two-particle vertex functions and their singularities (poles). No weak-coupling theory suppressing vertex corrections is able to describe this fluctuation-driven metal-insulator transition and the metallic solution with a narrow quasiparticle resonance correctly. Only self-consistent theories containing at least infinite series of multiple singlet and triplet electron-hole scatterings can offer an appropriate qualitative picture of the behavior of correlated electrons near the metal-insulator transition at intermediate coupling.

We start with the Hubbard Hamiltonian in an external magnetic field \( B \)

\[
\hat{H} = \sum_{k\sigma} \left( \epsilon(k) - \mu + \sigma B \right) c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i \tilde{n}_{\uparrow i} \tilde{n}_{\downarrow i},
\]

with \( \sigma = \pm 1 \) denoting the spin direction and \( \mu \) the chemical potential. We are interested in half filling at which \( \mu = U/2 \) due to the electron-hole symmetry. The one-particle propagator can be represented as

\[
G_\sigma(k, z) = \left[ z + \sigma \left( B + \frac{U}{2} \right) - \epsilon(k) - \Sigma_\sigma(k, z) \right]^{-1}
\]

where \( \Sigma_\sigma \) is a dynamical correction to the Hartree static self-energy absorbed in the magnetization \( m \). The dynamical self-energy is determined from the Schwinger-Dyson equation of motion

\[
\Sigma_\sigma(k) = \frac{U}{2\pi N^2} \sum_{k'q} \Gamma_{\sigma-\sigma}(k, k'; q) G_\sigma(k + q) G_{-\sigma}(k' + q) G_{-\sigma}(k').
\]

where \( \Gamma_{\sigma-\sigma} \) is the full two-particle vertex. We use a four-vector notation \( k = (k, i\omega_n) \), \( q = (q_i, i\nu_m) \) for fermionic and bosonic variables, respectively.

The vertex function \( \Gamma_{\sigma-\sigma} \) has to be determined from a diagrammatic skeleton expansion. To allow for multiple electron-hole scatterings we must take into considerations at least the FLEX-type approximations with singlet and triplet electron-hole channels \([1,2]\). The electron-hole vertices are for the singlet and triplet channels, respectively:

\[
\Gamma_{\sigma-\sigma}(k, k'; q) = \frac{U}{1 - X_{\sigma\sigma}(k - k')},
\]

\[
K_{\sigma-\sigma}(k, k'; q) = \frac{U}{1 - X_{\uparrow\uparrow}(q) X_{\downarrow\downarrow}(q)}
\]

with dimensionless electron-hole bubbles

\[
X_{\sigma\sigma'}(q) = \frac{U}{\beta N} \sum_k G_\sigma(k) G_{\sigma'}(k + q).
\]

In this and the other FLEX approximations, the vertex at the two-particle scattering events remains unrenormalized. These approximations are hence reliable only at weak or moderate interaction strengths. At strong coupling we have to pass to a higher level, the parquet approximation with renormalized vertices at scattering events. At intermediate coupling, for \( U \approx 2w \), the FLEX and the two-channel parquet approximations deliver qualitatively similar pictures in the spin-symmetric situation \([17]\).

The electron-hole bubble functions from \([16]\), \( X_{\sigma\sigma'}(q) \), are real and negative at the Fermi energy and the vertex functions get singular and negative if

\[
1 + X_{\sigma\sigma'}(q, 0) \leq 0.
\]

Equality indicates the existence of a pole at the Fermi energy and negativity an instability of the solution, i.e. a local energy minimum turns into a local maximum.

Bipartite lattices with perfect nesting and one electron per lattice site get usually first unstable in the singlet channel at the antiferromagnetic point \( q = (\pi, \pi, \ldots) \). Frustration due to the inclusion of next-to-nearest or random hopping destroys this instability and a fully frustrated model is expected to have no preference for a particular low-temperature long-range order \([18]\).

In the next steps we use this idealization of a fully frustrated system within the dynamical mean-field theory where the four-momenta are substituted by Matsubara frequencies. Further on, we use a semi-elliptic model density of states of the \( d = \infty \) Bethe lattice \( \rho_\beta(E) = \frac{2}{\beta \pi} \sqrt{w^2 - E^2} \), with \( w = 1 \), approximating a three-dimensional DOS with a finite bandwidth and sharp edges.

As a first step we investigate a local instability of the Hartree solution that can occur only in the singlet channel, since the triplet bubbles vanish in the saturated state. It is easy to find the explicit representation for the singlet electron-hole bubble

\[
X_{\uparrow\uparrow}(0) = -4U \left\{ \frac{2}{3\pi} \left[ 1 - B_{m1}^{3/2} \right] + B_{m1} \right\}
\]

\[
+ 4U \int_{-1}^{1} \frac{dx}{\pi} \frac{1}{\sqrt{1 - x^2 \sqrt{\left(2B_m - x\right)^2 - 1}}}
\]

(6a)
with the equilibrium magnetization

\[ m = \frac{2}{\pi} \left[ \arcsin(B_m) + B_m \sqrt{1 - B_m^2} \right]. \]  

(6b)

Here \( B_m = B + \frac{U}{2} m \). The saturated magnetic solution \((m = 1)\) gets unstable if either \( B + U/2 < 1 \) or \( X_{\uparrow \downarrow}(0) < -1 \). The former condition follows from (6a), i.e. from the one-particle magnetization. The latter is the existence criterion for a pole in the vertex function \( \Gamma_{\uparrow \downarrow} \).

The one-particle instability is realized at weak coupling for \( U < U_{\text{c1}} \). The magnetization decreases and the DOS at the Fermi energy increases continuously upon decreasing the applied field \( B \), Fig. 1.

![FIG. 1. DOS of \( \uparrow \)-electrons at weak coupling for different applied fields.](image1)

At a critical point \( U_{\text{c1}} \approx 1.65 \) both conditions (6a) are fulfilled simultaneously and for \( U > U_{\text{c1}} \) the two-particle spin-flip instability (6a) at \( B_s(U) > 1 - U/2 \) causes the saturated magnet to get locally unstable and to decay to a magnetically non-saturated solution.

We use the FLEX approximation with all three channels for the quantitative description of the non-saturated solution at intermediate coupling. The self-energy from the most important electron-hole singlet channel has the explicit analytic representation

\[ \Sigma_{\sigma}^{\text{el}}(\omega^\nu) = U \int_{-\infty}^{0} \frac{d\omega'}{\pi} \left\{ G_{-\sigma}(\omega' + \omega^\nu) \text{Im} \frac{X_{\sigma,-\sigma}(\omega^\nu)}{1 + X_{\sigma,-\sigma}(\omega^\nu)} + X_{\sigma,-\sigma}(\omega' - \omega^\nu) \text{Im} G_{-\sigma}(\omega^\nu) \right\} \]

(7)

where \( \omega^\nu = \omega + i\delta^\nu \). Analogous formulae hold for the other channels where only second-order contribution must correctly be subtracted.

We find that the saturated solution at \( B = B_s(U) \) for \( U > U_{\text{c1}} \) decays discontinuously, with a jump in the magnetization and energy, to a metallic solution with pronounced side bands and a sharp maximum in DOS at the Fermi energy accompanied by a narrow, correlation-induced Kondo resonance. Upon increasing the magnetic field, the metallic solution remains locally stable and preserves the three-peak structure of the spectral function. The side bands get more pronounced and the central resonance narrower with a decrease in maximum, Fig. 2. The metallic solution gets locally unstable at an upper critical field \( B_u(U) \) at which it again discontinuously goes over to the saturated magnetic insulator. The upper critical field is determined by a one-sided \((B \searrow B_u)\) divergence in the longitudinal (local) magnetic susceptibility determined by the triplet electron-hole vertex \( K \). The central Kondo resonance develops from a maximum to a sharp edge for the side bands with a jump in the Fermi-level occupation at the transition point.

![FIG. 2. DOS of \( \uparrow \)-electrons at intermediate coupling for different applied fields. The local instability for the saturated solution lies at \( B \approx 0.135 \).](image2)
for a non-equilibrium magnetization. A first instability appears for $m = 0$, but for the triplet channel with $X_{1T}$. For the semi-elliptic DOS we then have an equation $\pi/4U = 2(1 - B^2)^{3/2}$ defining an upper bound, $B_0(U)$, for a global instability of the Hartree solution. The fully saturated magnetic state is hence globally stable only for $B > B_0(U)$ and $B > B_s(U)$.

![Image of graph showing $B_s$ and $B_0$ instabilities](image)

**FIG. 3.** Local ($B_s$) and global ($B_0$) instabilities of the magnetically saturated solution with two critical points $U_{c0}$ (■) and $U_{c1}$ (●). The dashed lines below the critical points show the respective instabilities of the non-saturated Hartree solution.

However, the actual insulator-to-metal transition does not occur at the instability of either the insulating or the metallic solution. It is the energy that decides which solution is at global minimum. The line of the first-order metal-insulator transition, $B_c(u)$, depends on the approximation and lies in the coexistence region between the boundaries defined by local instabilities of the insulating and metallic solutions $B_s < B_c < B_u \leq B_0$, respectively [13]. The line of first-order transitions ends up at a critical point $U_{c0}$, where the line of the global, $B_0(U)$, and of the local, $B_s(U)$, instability meet, Fig. 3.

To conclude, we have investigated correlated electrons at zero temperature subjected to an external magnetic field and found that local instabilities of the insulating, fully saturated magnetic solution at intermediate and strong coupling are preceded by a global instability. The saturated magnetic state decays via a first-order transition with a jump in magnetization to a non-saturated, metallic solution. We explicitly demonstrated the coexistence of metallic and insulating solutions on a mean-field ($d = \infty$) model, but the same holds also for finite-dimensional systems near magnetic saturation. We have to take into consideration global fluctuations when investigating metal-insulator transitions and the stability and decay of fully polarized magnets. We further showed that the existence and shape of the metallic solution in the coexistence region is conditioned by the existence of poles in *two-particle* electron-hole vertices. To understand the metal-to-insulator transition behavior in systems with correlated electrons completely requires to match the magnetic case studied here with the spin symmetric situation and the Mott-Hubbard transition there.

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[1] F. Gebhard, *The Mott Metal-Insulator Transition*, Springer Tracts in Modern Physics, Vol. 137 (Springer, Berlin, 1997).

[2] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).

[3] X. Y. Zhang, M. J. Rozenberg, and G. Kotliar, Phys. Rev. Lett. 70, 1666 (1993).

[4] G. Moeller, Q. Si, G. Kotliar, M. Rozenberg, and D. S. Fisher, Phys. Rev. Lett. 74, 2082 (1995).

[5] R. Bulla, Phys. Rev. Lett. 83, 136 (1999).

[6] S. Kehrein, Phys. Rev. Lett. 81, 3912 (1998), J. Schlipf, M. Jarrell, P. G. J. van Dongen, N. Blümer, S. Kehrein, T. Pruschke, and D. Vollhardt, Phys. Rev. Lett. 82, 4890 (1999).

[7] P. Nozières, European Phys. J. B6, 447 (1998).

[8] The atomic limit is contained in IPT only in the spin-symmetric case. There are self-energy contributions beyond $U^2$ for $n_1 \neq n_{\uparrow}$.

[9] P. G. J. van Dongen and V. Janiš, Phys. Rev. Lett. 72, 3258 (1994).

[10] P. G. J. van Dongen and C. Leinung, Ann. Physik (Leipzig) 6, 45 (1997).

[11] V. Janiš, J. Phys.: Condens. Matter 10, 2915 (1998).

[12] K. Dichtel, R. J. Jelitto, and H. Koppe, Z. Physik. B246, 248 (1971) and R. J. Jelitto, *ibid* B258, 175 (1973).

[13] Q. P. Li and R. Joynt, Phys. Rev. B47, 3979 (1993) and *ibid* B49, 1632 (1994).

[14] H. Yamada, Phys. Rev. B47, 11211 (1993), G. S. Tripathi, Phys. Rev. B52, 6522 (1995).

[15] Metamagnetic behavior at a transition to an antiferromagnetically ordered state in an external magnetic field was recently studied by D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, and M. Ulmke, Z. Phys. B 103, 283 (1997) and K. Held, M. Ulmke, N. Blümer, and D. Vollhardt, Phys. Rev. B56, 14469 (1997).

[16] N. E. Bickers and D. J. Scalapino, Ann. Phys. (NY) 193, 206 (1989), S. Wermester, Phys. Rev. B53, 10569 (1996).

[17] V. Janiš, preprint cond-mat/9904069, to appear Phys. Rev. B.

[18] We found numerically within FLEX that $B_u < B_0$ for $U > U_{c0}$, but we were unable to exclude the equality for the exact theory.