Disorder- and correlation-driven metal–insulator transitions

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Abstract

Metal–insulator transitions driven by disorder ($D$) and/or by electron correlations ($U$) are investigated within the Anderson–Hubbard model with local binary-alloy disorder using a simple but consistent mean-field approach. The $D$–$U$ phase diagram is derived and discussed for $T = 0$ and finite temperatures. © 2005 Elsevier B.V. All rights reserved.

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If spontaneous symmetry breaking is excluded, a system of electrons in a non-degenerate half-filled valence band may undergo a transition from a normal Fermi liquid to an insulator either due to Coulomb interaction or due to disorder. Metal–insulator transitions (MIT) in the presence of strong electron correlations (Mott) MIT and disorder are not well understood—even on the mean-field level. For the purely correlation-induced (Mott) MIT, the dynamical mean-field theory (DMFT) has uncovered a rather complex phase diagram [1]. The MIT to an (alloy) insulator in case of non-interacting electrons and strong diagonal binary-alloy disorder is described by the coherent-potential approximation (CPA) [2]. While spatial correlations are neglected in both cases (including effects of Anderson localization), the residual mean-field physics at low temperatures $T$ is non-trivial. The combined problem can be studied within the half-filled ($n = 1$) Anderson–Hubbard model (AHM):

$$
H = - t \sum_{\langle ij \rangle, \sigma} c_{i \sigma}^{\dagger} c_{j \sigma} + \sum_{i \sigma} (\epsilon_{i} - \mu) n_{i \sigma} + U \sum_{i} n_{i \uparrow} n_{i \downarrow}.
$$

Here the n.n. hopping is set to $t = 1$, $U$ is the on-site interaction, $\mu = U/2$ is the chemical potential, and $\epsilon_{i} = \pm \Delta/2$ with equal probabilities $x = \frac{1}{2}$ a random on-site energy at site $i$. $\Delta$ measures the disorder strength. We consider the paramagnetic phase of the AHM in $D = 3$ dimensions.
“DMFT + CPA” [3] can be regarded as the optimum mean-field approach to this model. This, however, must be supplemented by stochastic [3] or renormalization-group techniques [4] or by further approximations, e.g., weak-coupling perturbation theory [5]. While parts of the phase diagram in the $U$–$T$ space are known [3,5], a comprehensive study is still missing.

Here we employ the self-energy-functional approach (SFA) [6] and the $n_t$ = 2-site dynamical-impurity approximation (2S-DIA) which nicely reproduces the phase diagram for $\Delta = 0$ [6]. In case of disorder, a proper generalization of the formalism has to be applied [7]. Within the generalized framework, the 2S-DIA can be regarded as a strongly simplified but consistent DMFT + CPA approach. In the limit $n_t \to \infty$, one recovers the DMFT for $\Delta = 0$, the CPA for $U = 0$ and the DMFT + CPA for $U, \Delta \neq 0$.

Operationally, the Green’s function $G^\prime$ of a single-impurity Anderson model $H'$ with two sites and impurity on-site energies $\varepsilon = \pm \Delta$ is obtained by exact diagonalization and averaged, $\Gamma^\prime = \langle G^\prime \rangle$, to get the configuration-independent self-energy $\Sigma = G^{-1}_0 - \Gamma^{-1}$ where $G_0^\prime$ is the free $(U, \Delta = 0)$ Green’s function. $\Sigma = S(i\varepsilon_n)$ depends on the one-particle parameters of $H'$ and is used as a trial self-energy in a general variational principle, $\delta \mathcal{O}[\Sigma] = 0$, which gives the exact averaged grand potential of the AHM at the physical $S$. On the subspace given by $S(i\varepsilon_n)$, the functional can be evaluated rigorously (see Ref. [7]). We consider the AHM on a $D = 3$ s.c. lattice consisting of $10^3$ sites. Phase boundaries are obtained from the resulting $\Omega$ as a function of $\Delta$, $U$ and $T$. The averaged interacting local density of states (DOS) of the AHM can be calculated via $\rho(\omega) = -\text{Im} \Gamma(\omega + i\eta)/\pi$ and $\Gamma = (G_0^{-1} - S)^{-1}$, where $G_0$ is the free $(U, \Delta = 0)$ lattice Green’s function. Within the mean-field approach, $\rho(\omega = 0)$ distinguishes between metallic and insulating behavior.

Three different phases are identified at $T = 0$ (see Fig. 1): a paramagnetic metallic phase (PM), a Mott insulator (MI), and an alloy insulator (AI). For any disorder strength $\Delta$, we find the AI at weak $U$ (and $\Delta \geq \Delta_c(U)$) to be well separated from the MI at strong $U$ by the PM in between. For $\Delta = 0$ the critical interaction for the Mott MIT is found to be $U_c = 13.9 \approx 1.16W$ (with $W = 12$ the free bandwidth) while $\Delta_c \approx 5.4 = 0.46W$ for the MIT at $U = 0$. This agrees well with full DMFT and CPA estimates, respectively [1,2,6]. For $U_{c1} \leq U \leq U_{c2}$, a coexistence of the stable PM phase with the metastable MI phase is observed ($U_{c1} = 12.4$). This scenario for the Mott MIT is well known for $\Delta = 0$ [1] and is shown here to survive for any finite disorder strength with a $\Delta$ dependent coexistence region $U_{c1}(\Delta) \leq U \leq U_{c2}(\Delta)$ and $U_c(\Delta) = U_{c2}(\Delta)$. A discontinuous Mott MIT with $U_{c1}(\Delta) \leq U_c(\Delta) \leq U_{c2}(\Delta)$ is found for finite temperatures $0 < T < T_c(\Delta)$. For $T > T_c(\Delta)$ there is a smooth crossover only. For $\Delta \to \infty$, the critical interactions approach a linear dependence, $U_{c1,2}(\Delta) \to \Delta + \text{const}_{1,2}$ while $T_c(\Delta) \to T_c$ saturates.

The topology of the phase diagram can be understood by looking at the DOS, see Fig. 2. Characteristic for the MI at $\Delta = 0$ and $U > U_c$ is the insulating gap between the lower and upper Hubbard band (LHB, UHB). For finite $\Delta$ the gap decreases due to a broadening and, eventually, a splitting of each of the Hubbard bands (Fig. 2, $\Delta = 6$). The closure of the gap is preempted by the occurrence of a quasi-particle peak (QP) at $\omega = 0$ which marks the transition to the PM (see $\Delta = 14$). Apart from the QP, the spectrum can be understood as being composed of two Hubbard bands at $\omega \approx \pm \Delta/2 \pm U/2$ for each of the two atomic configurations $\varepsilon = \pm \Delta/2$. This explains the strong spectral-weight transfer when increasing $\Delta = 18$ to

![Fig. 1. $U$–$T$ phase diagram for $T = 0$ (insets: $U$–$T$ phase diagram for different $\Delta$). Energy scale: $t = 1$.](image-url)
As the $\varepsilon = +\Delta/2$-DOS ($\varepsilon = -\Delta/2$-DOS) becomes almost completely unoccupied (occupied), the weight of the UHB (LHB) must disappear. Finally, a further increase of $\Delta$ induces a splitting into an upper and lower alloy band (UAB, LAB) and a MIT to the AI. Recently, Byczuk et al. [4] have shown that DMFT+CPA predicts the AHM to exhibit a Mott MIT also for fillings $n \neq 1$ if $x = n$. Similar to the presently considered case $n = 1 = 2x$, a sharp QP at $\omega = 0$ (even for strong disorder) as well as a coexistence of the PM and the MI is found close to the MIT. We like to point out that the phase diagram for $n = x \neq 1$ [4] can be understood by an analysis of the DOS completely analogous to the $n = 1 = 2x$ case discussed above—although its topology is quite different.

Concluding, we have proposed a mean-field scenario for the MIT in the AHM at half-filling $n = 1 = 2x$ on the basis of a simplified DMFT+CPA approach. The phase diagram can be understood by a quasi-atomic interpretation of the DOS in combination with the Mott MIT scenario of the pure system. This should be contrasted with full DMFT+CPA calculations in the future which may also clarify the importance of disorder scattering due to a finite self-energy $\text{Im} S(\omega = 0)$ which has been neglected here.

References