Disorder- and correlation-driven metal-insulator transitions
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Abstract
Metal-insulator transitions driven by disorder (Δ) 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 Δ–U phase diagram is derived and discussed for T = 0 and finite temperatures.

Key words: metal-insulator transitions, dynamical mean-field theory, Anderson-Hubbard model

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 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 (Anderson) insulator in case of non-interacting electrons and strong diagonal binary-alloy disorder can be described by the coherent-potential approximation (CPA) [2]. While spatial correlations are neglected in both cases, the residual mean-field physics at low temperatures T is non-trivial and relevant for three-dimensional transition-metal oxides, for example. The combined problem can be studied within the half-filled (n = 1) Anderson-Hubbard model (AHM): $H = -t \sum_{(i,j),\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (\epsilon_i - \mu) n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$. Here the n.n. hopping is set to \( t = 1 \), \( U \) is the on-site interaction, \( \mu = U/2 \) the chemical potential, and \( \epsilon_i = \pm \Delta/2 \) with equal probabilities \( x = 1/2 \) a random on-site energy at site \( i \). \( \Delta \) measures the disorder strength.

“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-Δ-T space are known [3,5], a comprehensive study is still missing. Here we employ the self-energy-functional approach (SFA) [6] and the \( n_s = 2 \)-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 \( n_s \to \infty \) one recovers the DMFT for \( \Delta = 0 \), the CPA for \( U = 0 \).

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and the DMFT-CPA for \( U, \Delta \neq 0 \).

Operationally, the Green’s function \( G' \) of a single-impurity Anderson model \( H' \) with two sites and impurity on-site energies \( \epsilon = \pm \Delta \) is obtained by exact diagonalization and averaged, \( \Gamma' = \langle G' \rangle \), to get the configuration-independent self-energy \( S' = G_0^{-1} - \Gamma' \), where \( G_0 \) is the free \((U, \Delta = 0)\) Green’s function. \( S' = S(t') \) depends on the one-particle parameters of \( H' \) and is used as a trial self-energy in a general variational principle, \( \delta \Omega[S] = 0 \), which gives the exact averaged grand potential of the AHM at the physical \( S \).

On the subspace given by \( S(t') \), the functional can be evaluated rigorously (see [7]). We consider the paramagnetic phase of the AHM on a three-dimensional 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.

Three different phases are identified at \( T = 0 \) (see Fig. 1): a paramagnetic metallic phase (PM), a Mott insulator (MI), and an Anderson 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 band width) while \( \Delta_c = 5.4 = 0.46W \) 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 \( 0 < T \leq T_c(\Delta) \). For \( T \geq T_c(\Delta) \) 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 \( \omega \approx \pm \Delta/2 \) for each of the two atomic configurations \( \epsilon = \pm \Delta/2 \). This explains the strong spectral-weight transfer when increasing \( \Delta = 18 \) to \( \Delta = 20 \):

Fig. 2. Average density of states for \( U = 18 \) and different \( \Delta \) and Lorentzian broadening with \( \eta = 0.25 \).

As the \( \epsilon = \pm \Delta/2 \)-DOS (\( \epsilon = -\Delta/2 \)-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 \( n = x = 1 \) [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

[1] A. Georges, G. Kotliar, W. Krauth and M.J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
[2] B. Velický, S. Kirkpatrick and H. Ehrenreich, Phys. Rev. 175, 747 (1968).
[3] M. Ulmke and V. Janiš and D. Vollhardt, Phys. Rev. B 69, 045112 (2004).
[4] K. Byczuk, W. Hofstetter and D. Vollhardt, Phys. Rev. B 51, 10411 (1995).
[5] M. S. Laad, L. Craco and E. Müller-Hartmann, Phys. Rev. B 64, 195114 (2001).
[6] M. Potthoff, Eur. Phys. J. B 32, 429 (2003); Eur. Phys. J. B 36, 335 (2004); M. Potthoff, M. Aichhorn and C. Dahnken, Phys. Rev. Lett. 91, 206402 (2003).
[7] M. Potthoff and M. Balzer, to be published.