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Physica B 359–361 (2005) 768–770
PHYSICA B
www.elsevier.com/locate/physb

Disorder- and correlation-driven metal–insulator transitions ☆

Matthias Balzer, Michael Potthoff*

Institut für Theoretische Physik und Astrophyik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

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.

PACS: 71.23.−k; 71.27.+a; 71.30.+h

Keywords: 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 (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):

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

Here the n.n. hopping is set to $t = 1$, U is the on-site interaction, $\mu = U/2$ is the chemical potential, and $\varepsilon_i = \pm\Delta/2$ with equal probabilities $x = \frac{1}{2}$ a random on-site energy at site i. Δ measures the disorder strength. We consider the paramagnetic phase of the AHM in $D = 3$ dimensions.

☆This work is supported by the DFG (FOR 538 and SFB 410).
*Corresponding author. Tel.: +49 931 888 5724; fax: +49 931 888 5141.
E-mail address: potthoff@physik.uni-wuerzburg.de (M. Potthoff).

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doi:10.1016/j.physb.2005.01.221

"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 $U = 0$ and the DMFT + CPA for $U, \Delta \neq 0$.

Operationally, the Green's function $\boldsymbol{G}'$ 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, $\boldsymbol{\Gamma}' = \langle \boldsymbol{G}' \rangle$, to get the configuration-independent self-energy $\boldsymbol{S}' \equiv \boldsymbol{G}_0'^{-1} - \boldsymbol{\Gamma}'^{-1}$ where $\boldsymbol{G}_0'$ is the free $(U, \Delta = 0)$ Green's function. $\boldsymbol{S}' = \boldsymbol{S}(\boldsymbol{t}')$ depends on the one-particle parameters of H' and is used as a trial self-energy in a general variational principle, $\delta\Omega[\boldsymbol{S}] = 0$, which gives the exact averaged grand potential of the AHM at the physical $\boldsymbol{S}$. On the subspace given by $\boldsymbol{S}(\boldsymbol{t}')$, 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 Ω as a function of Δ, U and T. The averaged interacting local density of states (DOS) of the AHM can be calculated via $\rho(\omega) = -\mathrm{Im}\,\Gamma_{ii}(\omega + i\eta)/\pi$ and $\boldsymbol{\Gamma} = (\boldsymbol{G}_0^{-1} - \boldsymbol{S}')^{-1}$, where $\boldsymbol{G}_0$ 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 Δ, we find the AI at weak U (and $\Delta \geqslant \Delta_c(U)$) 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 $U_{c1} \leqslant U \leqslant U_{c2}$, 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 Δ dependent coexistence region $U_{c1}(\Delta) \leqslant U \leqslant U_{c2}(\Delta)$ and $U_c(\Delta) = U_{c2}(\Delta)$. A discontinuous Mott MIT with $U_{c1}(\Delta) \leqslant U_c(\Delta) \leqslant U_{c2}(\Delta)$ is found for finite temperatures $0 < T \leqslant T_c(\Delta)$. For $T > T_c(\Delta)$ there is a smooth crossover only. For $\Delta \to \infty$, the critical interactions approach a linear dependence, $U_{c1,2}(\Delta) \to \Delta + \mathrm{const}_{1,2}$ while $T_c(\Delta) \to T_c$ saturates.

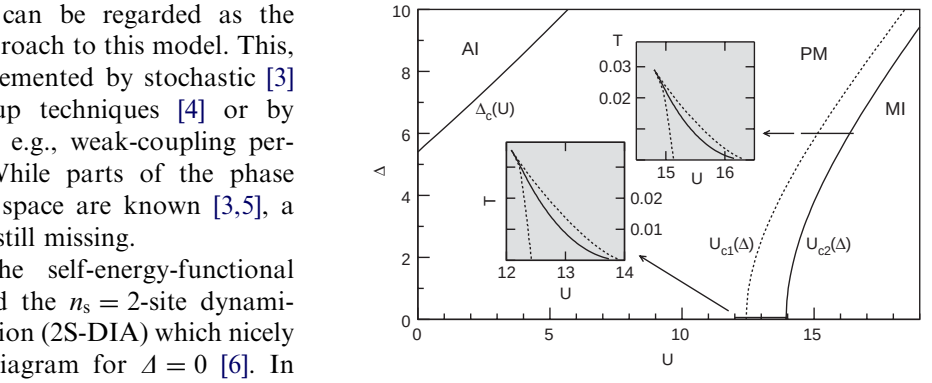

Fig. 1. U–Δ phase diagram for $T = 0$ (insets: U–T phase diagram for different Δ). Energy scale: $t = 1$.

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 Δ 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

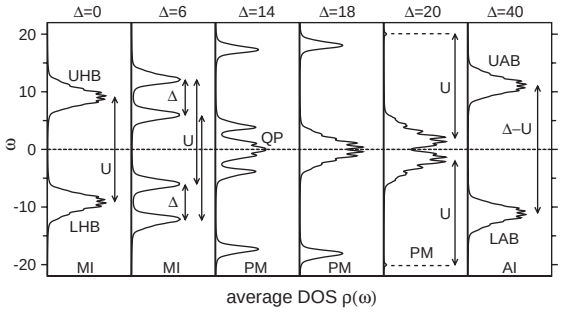

Fig. 2. Average density of states for $U = 18$ and different Δ and Lorentzian broadening with $\eta = 0.25$.

$\Delta = 20$: 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 Δ 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 $\mathrm{Im}\,\boldsymbol{S}(\omega = 0)$ which has been neglected here.

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