

# Mott–Hubbard and Anderson transitions in dynamical mean-field theory

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## Abstract

The Anderson–Hubbard Hamiltonian at half-filling is investigated within dynamical mean-field theory at zero temperature. The local density of states is calculated by taking the geometric and arithmetic mean, respectively. The non-magnetic ground state phase diagrams obtained within the different averaging schemes are compared.

The metal–insulator transitions (MIT) due to electronic interactions (Mott–Hubbard MIT) [1] and due to impurity scattering (Anderson localization) [2] are subtle quantum mechanical phenomena which require non-perturbative investigation schemes. In this respect, the dynamical mean-field theory (DMFT) [3] is very useful. However, it cannot describe the physics of Anderson localization if the local disorder is included by taking the arithmetic average over the disorder [4]. Recently,

it was proposed to use the geometric average over the disorder to include also the Anderson MIT [5–7]. In this contribution we compare the entire non-magnetic ground state phase diagrams of correlated, disordered electrons at half-filled lattice as obtained by taking the geometric and the arithmetic averages over the disorder within the DMFT [8].

We study the system described by a single-orbital Anderson–Hubbard model

$$H_{\text{AH}} = -t \sum_{\langle ij \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

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where  $t > 0$  is the amplitude for hopping between nearest neighbors,  $U$  is the on-site repulsion,  $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$  is the local electron number operator,  $a_{i\sigma}$  ( $a_{i\sigma}^\dagger$ ) is the annihilation (creation) operator of an electron with spin  $\sigma$ , and the local ionic energies  $\varepsilon_i$  are independent random variables. We assume a continuous probability distribution for  $\varepsilon_i$ , i.e.,  $\mathcal{P}(\varepsilon_i) = \Theta(\Delta/2 - |\varepsilon_i|)/\Delta$ , with  $\Theta$  as the step function. Here,  $\Delta$  is a measure of the disorder strength.

This model is solved within DMFT by mapping it [3] onto an ensemble of effective single-impurity Anderson Hamiltonians with different  $\varepsilon_i$ :

$$\begin{aligned} H_{\text{SIAM}} = & \sum_{\sigma} (\varepsilon_i - \mu) a_{i\sigma}^\dagger a_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} \\ & + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} a_{i\sigma}^\dagger c_{\mathbf{k}\sigma} + V_{\mathbf{k}}^* c_{\mathbf{k}\sigma}^\dagger a_{i\sigma} \\ & + \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \end{aligned} \quad (2)$$

Here  $\mu = U/2$  is the chemical potential corresponding to a half-filled band, and  $V_{\mathbf{k}}$  and  $\varepsilon_{\mathbf{k}}$  are the hybridization matrix element and the dispersion relation of the auxiliary bath fermions  $c_{\mathbf{k}\sigma}$ , respectively.

For each ionic energy  $\varepsilon_i$  we calculate the local Green function  $G(\omega, \varepsilon_i)$ , from which we can obtain either the geometrically averaged local density of states (LDOS)  $\rho_{\text{geom}}(\omega) = \exp[\langle \ln \rho_i(\omega) \rangle]$  or the arithmetically averaged LDOS  $\rho_{\text{arith}}(\omega) = \langle \rho_i(\omega) \rangle$ , where  $\rho_i(\omega) = -\text{Im} G(\omega, \varepsilon_i)/\pi$ , and  $\langle O_i \rangle = \int d\varepsilon_i \mathcal{P}(\varepsilon_i) O(\varepsilon_i)$  is the arithmetic mean of  $O_i$ . The lattice Green function is given by the corresponding Hilbert transform as  $G(\omega) = \int d\omega' \rho_{\alpha}(\omega')/(\omega - \omega')$ , where the subscript  $\alpha$  stands for either ‘‘geom’’ or ‘‘arith’’. The local self-energy  $\Sigma(\omega)$  is determined from the  $\mathbf{k}$ -integrated Dyson equation  $\Sigma(\omega) = \omega - \eta(\omega) - 1/G(\omega)$ , where the hybridization function  $\eta(\omega)$  is defined as  $\eta(\omega) = \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 / (\omega - \varepsilon_{\mathbf{k}})$ . The self-consistent DMFT equations are closed through the Hilbert transform  $G(\omega) = \int d\varepsilon N_0(\varepsilon) / [\omega - \varepsilon - \Sigma(\omega)]$ , which relates the local Green function for a given lattice to the self-energy; here  $N_0(\varepsilon)$  is the non-interacting DOS.

The Anderson–Hubbard model (1) is solved for a semi-elliptic DOS,  $N_0(\varepsilon) = 4\sqrt{1 - 4\varepsilon^2}/\pi$ . Then  $\eta(\omega) = G(\omega)/16$ . The DMFT equations are solved at zero temperature by the numerical renormalization group technique [9]. For numerical integra-

tions we use discrete values of  $\varepsilon_i$  selected according to the Gauss–Legendre algorithm. The number of  $\varepsilon_i$  levels depends on  $\Delta$  and is adjusted to obtain smooth spectral functions [4].

The main results are presented in Figs. 1 and 2, where the non-magnetic ground state phase diagrams of the Anderson–Hubbard model (1) are plotted. At weak disorder, both averaging schemes are seen to lead to very similar results for the Mott–Hubbard transition from the paramagnetic correlated, disordered metal (I) to the paramagnetic, disordered Mott insulator (IV). For  $\Delta \lesssim 2$  we find hysteresis and a coexistence regime (II). Above  $\Delta \approx 2$  there is a crossover regime (III). At strong disorder the DMFT with geometrically averaged LDOS describes an Anderson transition between a correlated, disordered metallic and insulating phase, respectively (V) [10]. Since neither the paramagnetic Mott nor the Anderson insulator is characterized by a broken symmetry they are continuously connected, i.e., the phases IV and V in Fig. 1 are connected by a continuous line which does not cross a metallic phase. Obviously, the Anderson transition is missed

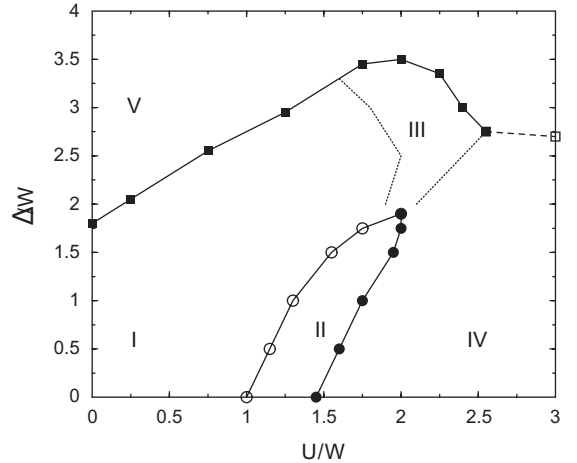


Fig. 1. Non-magnetic ground state phase diagram of the Anderson–Hubbard model at half-filling as calculated by DMFT with the geometrically averaged local density of states. I—correlated, disordered metal, II—coexistence regime, III—crossover regime, IV—Mott insulator, V—Anderson insulator. At the dashed line all states within the Hubbard subbands become localized.  $W$  is a bare energy band-width.

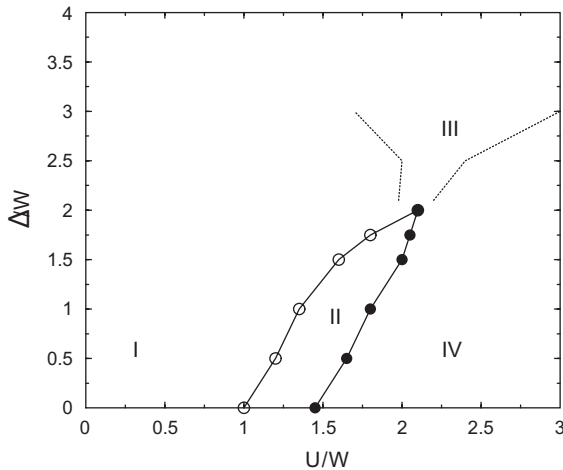


Fig. 2. Non-magnetic ground state phase diagram of the Anderson–Hubbard model at half-filling as calculated by DMFT with the arithmetically averaged local density of states. Labels I–IV are the same as in Fig. 1.

within the DMFT supplied by the arithmetic averaging.

In summary, although the geometric averaging procedure does not capture all aspects of Anderson localization [6,11] it provides valuable new insights into MITs in correlated and disordered electron systems, which are not obtained by taking the arithmetic disorder average [4].

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