Metal-Insulator Transitions in the Disordered Hubbard Model

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Quantum Monte-Carlo methods are used to study the disordered Hubbard model in infinite dimensions. The averaged local moment and thermodynamic compressibility are calculated at half filling to determine the metal-insulator transitions in the paramagnetic phase. Two transitions of different physical origin are found: one driven by disorder, the other one by interactions. Taking into account the additional paramagnet-antiferromagnet transition this simple model of interacting electrons in a random potential is found to have a rich phase diagram.

One of the most fascinating physical features of disordered electronic systems is the appearence of a metal-insulator transition (MIT). It is well known that, in a tight-binding description, a system of non-interacting electrons in a random potential may exhibit a MIT either due to Anderson localization or due to band-splitting [1]. Furthermore, for a half-filled band of interacting electrons in the paramagnetic phase without disorder a MIT should occur at some critical interaction strength ("Mott-Hubbard transition"). However, for the paramagnetic state to be stable the lattice has to be non-bipartite and/or some kind of randomness must be introduced after all. Hence the simultaneous presence of disorder and electronic interaction leads to particularly interesting, albeit subtle, questions. Progress in the systematic investigation of this problem has recently been made by using the limit of infinite dimensions for fermionic lattice models [2]. Here we will employ this approach to investigate the Hubbard model with local disorder

$$\hat{H}=\frac{-t^*}{\sqrt{2d}}\sum_{\langle ij\rangle,\sigma}\hat{c}^+_{i\sigma}\hat{c}_{j\sigma}+U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}+\sum_{i,\sigma}(\epsilon_i-\mu)\hat{n}_{i\sigma} \quad (1)$$

where ϵ_i are random atomic energies and d is the dimension; in the following all energies are measured in units of $t^* \equiv 1$. In the non-interacting case, $U = 0$, (1) reduces to Anderson's disorder model [3] for which the coherent-potential approximation becomes exact in $d = \infty$ [4] (hence a MIT due to Anderson localization does not occur in this limit). On the other hand, in the non-random case, $\epsilon_i \equiv 0$, the exact solution for $d = \infty$ is analytically untractrable since the on-site Hubbard-interaction remains dynamical, leading to a non-trivial single-site problem [5].

The thermodynamics of (1) is determined by $\Omega_{av} = -\beta^{-1}\langle \ln tr \exp(-\beta\hat{H})\rangle_{av}$, the averaged free energy, where $\langle\ldots\rangle_{av}$ is the configurational average over the random energies ϵ_i. In $d = \infty$ the averaging involves only a single site $\mathbf{R}_i$ (where the electrons encounter both the Hubbard interaction and the random energy ϵ_i) surrounded by a *homogeneous* effective medium [6]. This medium is described by a dynamical potential $\Sigma(\omega)$ which contains the full information about the physical processes taking place at sites $\mathbf{R}_j \neq \mathbf{R}_i$. It must be determined self-consistently in such a way that the average scattering at site $\mathbf{R}_i$ of the electrons moving in the averaged medium is zero. The potential $\Sigma(\omega)$ then plays the rôle of the single-particle self-energy of the electrons. – Here we use a quantum Monte-Carlo method, used previously in the absence of disorder [7], to calculate the averaged compressibility $\kappa_{av} = -L^{-1}\partial^2\Omega_{av}/\partial\mu^2$ and the square of the averaged local magnetic moment $m^2_{av} = 1 - 2L^{-1}d\Omega_{av}/dU \equiv 1 - 2d_{av}$, where L is the number of lattice sites and d_{av} is the average double occupancy. These quantities provide information about the disorder-induced "split-band" and interaction-induced ("Mott") MITs. In particular, $\kappa_{av} = 0$ is a convenient thermodynamic criterion for an insulating state.

For our calculations we chose a semi-elliptic density of states with bandwidth $W = 4$ for the non-interacting electrons, and a binary alloy distribution for the random energies, i e. $\epsilon_i = \pm\Delta/2$ with equal probability such that the average band filling $n_{av} = 1$ and $\mu = U/2$. The Monte-Carlo

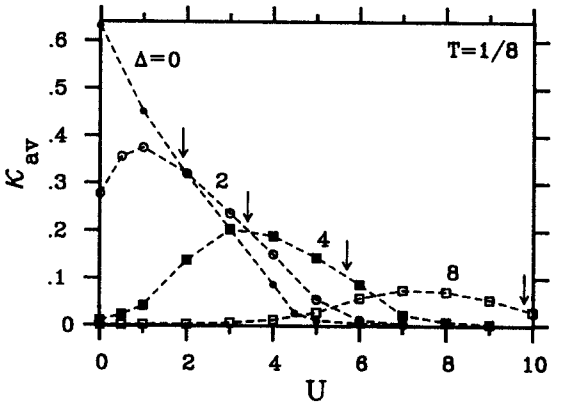

Fig. 1: Averaged conpressiblity vs. U for disorder strengths $\Delta = 0, 2, 4, 8$ at $T = 1/8$. Error bars are of the size of the symbols.

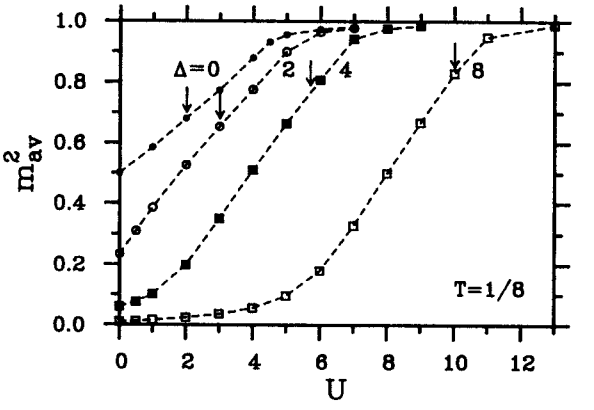

Fig. 2: Averaged quadratic local moment vs. U for $\Delta = 0, 2, 4, 8$ at $T = 1/8$.

evaluations were performed for temperatures between $1/32 \leq T \leq 1/4$; they did not lead to substantial differences. The time slices $\Delta\tau$ were chosen as $1/8 \leq \Delta\tau \leq 1/2$ and the results were extrapolated to $\Delta\tau = 0$. The results for $\kappa_{av}(U)$ for disorder strengths $\Delta = 0, 2, 4, 8$ and $T = 1/8$ are shown in Fig. 1. While for $\Delta = 0$ κ_{av} is a monotonic function it develops a peak at $U \simeq \Delta$ for $\Delta > 0$. For sufficiently large Δ (here $\Delta > 2$) κ_{av} vanishes both at weak and strong coupling. Thus there exist *two* MITs, at $U_c^{MI,1}$ and $U_c^{MI,2}$, due to band splitting – the first induced by disorder, the second by interactions. The difference in origin of these MITs is also apparent from the results for the averaged local magnetic moment shown in Fig. 2: the MIT at weak coupling is characterized by $m_{av} \to 0$, i. e. by a saturation of double occupancy at its maximum value ($d_{av} \to \frac{1}{2}$) and that at strong coupling by $m_{av} \to 1$, i. e. the disappearance of d_{av}. In the regime $U_c^{MI,1} < U < U_c^{MI,2}$ the system is metallic; its width increases with increasing disorder. In this regime m_{av} is an increasing function of U and hence one may expect that the moments begin to order antiferromagnetically at some critical value U_c^{AF}. By calculating the staggered susceptibility one can show that this is indeed the case; the positions of $U_c^{AF}(\Delta)$ are indicated in Figs. 1,2 by arrows; details of the calculation will be reported elsewhere [8]. Hence we found that *even in the presence of disorder* there is no MIT from a paramagnetic metal to a paramagnetic insulator at $T = 0$. We also see that the paramagnetic $\to$ antiferromagnetic transition occurs in the metallic phase so that, close to U_c^{AF}, *the ordered phase is a metal.* As U is further increased the DOS at the Fermi level is emptied and the Mott-MIT at $U_c^{MI,2}$ finally occurs in the magnetically ordered phase.

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