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Disorder *vs.* Interaction in the Hubbard Model: Phase Diagram in Infinite Dimensions.

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Abstract. – The influence of local disorder on the thermodynamics of interacting electrons is studied within the infinite-dimensional disordered Hubbard model. Using a finite-temperature quantum Monte Carlo method, the averaged local moment and staggered susceptibility are calculated and the magnetic phase diagram at half-filling is constructed. From the averaged compressibility in the paramagnetic and antiferromagnetic phase we determine the metal-insulator transitions of the system. A rich transition scenario is revealed. Quite unexpectedly the disorder is found to *stabilize* the magnetic order in the strong-coupling limit.

Randomness can significantly influence the low-temperature behaviour of interacting systems. In particular, it may lead to new phases which have no analogue in non-random systems [1]. In the case of electrons, the simplest lattice model including both interactions and random potentials is the disordered Hubbard model. It is now known that even in the «mean-field» limit $d \to \infty$ [2,3] the Hubbard interaction remains dynamical [4] and leads to a highly non-trivial single-site problem with infinitely many coupled quantum degrees of freedom [5]. This problem is, in fact, equivalent to an Anderson impurity model complemented by a self-consistency condition [6] and is thus amenable to numerical investigations [7] within a finite-temperature quantum Monte Carlo approach [8]. In the absence of disorder this technique was already used by several groups to investigate the magnetic phase diagram [7,9], the Mott-Hubbard transition [10,11] and lately also superconductivity in a two-band version [12] of the Hubbard model in $d = \infty$; thereby important new insight was gained.

In this letter we wish to concentrate on the combined effect of disorder and interaction. We will study the effect of diagonal disorder on the low-temperature properties of the Hubbard model in $d = \infty$, in particular the competition between correlation-induced

long-range order and the disordered-induced metal-insulator transition (1). To this end, the averaged local moment, staggered susceptibility and compressibility are derived using the exact averaged free energy of the model [14] and are evaluated iteratively by quantum Monte Carlo (2). The model is given by

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

where μ is the chemical potential, ε_i are random atomic energies and d is the dimension. The thermodynamics of (1) is determined by the averaged free energy $\Omega_{\mathrm{av}} = -\beta^{-1} \cdot \langle \ln \operatorname{tr} \exp[-\beta \hat{H}] \rangle_{\mathrm{av}}$, where $\langle \ldots \rangle_{\mathrm{av}}$ is the configurational average over the random energies ε_i. In $d = \infty$ the averaging involves only a single site $\boldsymbol{R}_i$ (where the electrons encounter both a Hubbard interaction and the random energy ε_i) surrounded by a *homogeneous* effective medium described by a dynamical potential $\Sigma(\omega)$ [14]; Σ contains the full information about the physical processes taking place at all other sites. These processes may, for example, lead to antiferromagnetic (AF) long-range order in the system as in the non-random model. Hence, we must allow for breaking of translational symmetry in $\Sigma(\omega)$. For simplicity, we only consider bipartite lattices, in which case the symmetry breaking is caused by a staggered field αh, with $\alpha = \pm 1$ on A- and B-sites, respectively, with h as a magnetic field. In $d = \infty$, Ω_{av} then takes the form [14]

$$2\beta \Omega_{\mathrm{av}}/L = -\sum_{\sigma, n} \int \mathrm{d}E\, N(E) \ln[(i\omega_n + \mu_A - \Sigma_{A\sigma n})(i\omega_n + \mu_B - \Sigma_{B\sigma n}) - E^2] +$$

$$+ \sum_{\alpha, \sigma, n} \ln G_{\alpha\sigma n}^{-1} - \sum_{\alpha} \langle \ln \mathcal{Z}_{\alpha}\{G, \Sigma, \varepsilon_i\} \rangle_{\mathrm{av}} , \tag{2}$$

where L is the number of lattice sites, $N(E)$ is the density of states of the non-interacting electrons, $\mu_{\alpha} \equiv \mu + \alpha h$, and $\omega_n = (2n+1)\pi T$ are Matsubara frequencies. The quantities $\Sigma_{\alpha\sigma n} \equiv \Sigma_{\alpha\sigma}(i\omega_n)$ and $G_{\alpha\sigma n}$ specify the potential of the medium and the local part of the averaged propagator of the (non-interacting!) electrons moving in this potential, respectively (3). Here

$$\mathcal{Z}_{\alpha}\{G, \Sigma, \varepsilon_i\} =$$

$$= \int \mathscr{D}\psi\, \mathscr{D}\psi^* \exp\left[\sum_{\sigma, n} \tilde{\psi}_{\alpha\sigma n}^* (G_{\alpha\sigma n}^{-1} + \Sigma_{\alpha\sigma n} - \varepsilon_i) \tilde{\psi}_{\alpha\sigma n} - U \int_0^{\beta} \mathrm{d}\tau \psi_{\alpha\uparrow}^*(\tau) \psi_{\alpha\uparrow}(\tau) \psi_{\alpha\downarrow}^*(\tau) \psi_{\alpha\downarrow}(\tau) \right] \tag{3}$$

is the partition function for electrons from the medium which encounter a Hubbard interaction U and a random energy ε_i at $\boldsymbol{R}_i$. The fields $\psi_{\alpha\sigma}(\tau)$ and $\tilde{\psi}_{\alpha\sigma n}$ are Grassmann variables in imaginary times and frequency, respectively. The previously unspecified potential, $\Sigma_{\alpha\sigma n}$, is determined by the thermodynamic consistency condition $\delta \Omega_{\mathrm{av}}/\delta \Sigma_{\alpha\sigma n} = 0$ [5, 14].

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(1) In the limit $d = \infty$ the metal-insulator transition occurs only by band splitting, since there is no Anderson localization (cf. [13, 14]).

(2) The Hubbard model with separable *off-diagonal* disorder was recently examined by V. Dobrosavljević and G. Kotliar (preprint) for a Bethe lattice with infinite connectivity. They studied the one-electron spectral function within a renormalized perturbation scheme from which they deduced a scenario for local-moment formation and Mott transition.

(3) Note that $\Sigma_{\alpha\sigma n}$ plays the role of the self-energy for the electrons, but is *not* the averaged self-energy of the random, interacting system (see ref. [14]).

To determine the thermodynamic stability of various phases, we calculate the susceptibilities $X_{\mathrm{av}} = -L^{-1}\,\partial^2\Omega_{\mathrm{av}}/\partial x^2$, which correspond to the averaged compressibility κ_{av} and staggered susceptibility χ_{av} for $x = \mu, h$, respectively. In the paramagnetic phase the number of independent parameters can be reduced by setting $\Sigma_{An} \equiv \Sigma_{A\uparrow n} = \Sigma_{B\downarrow n}$, $\Sigma_{Bn} \equiv \Sigma_{B\uparrow n} = \Sigma_{A\downarrow n}$ and similarly for $G_{\alpha\sigma n}$ and $\psi_{\alpha\sigma}$. Using (2) X_{av} may be expressed in terms of a two-particle irreducible vertex function Γ as

$$X_{\mathrm{av}} = \beta^{-2} \sum_{\alpha\alpha'} \sum_{nn'} f_\alpha^x \Gamma^{\alpha\alpha'}_{nn',\,n'n} \gamma^x_{\alpha' n'} \,, \tag{4}$$

where $f_\alpha^\mu = 1$, $f_\alpha^h = \alpha$, $\gamma^x_{\alpha n} = (\partial/\partial x)(G^{-1}_{\alpha n} + \Sigma_{\alpha n})$ and

$$\Gamma^{\alpha\alpha'}_{n_1 n_1',\,n_2' n_2} = \int_0^\beta \mathrm{d}\tau_1\, \mathrm{d}\tau_1'\, \mathrm{d}\tau_2\, \mathrm{d}\tau_2' \exp\left[i(\omega_{n_1}\tau_1 + \omega_{n_1'}\tau_1' - \omega_{n_2'}\tau_2' - \omega_{n_2}\tau_2)\right] \cdot$$

$$\cdot \left\langle \left\langle \psi_\alpha(\tau_1)\psi^*_\alpha(\tau_2)\psi_{\alpha'}(\tau_1')\psi^*_{\alpha'}(\tau_2') \right\rangle_{\mathrm{T}} \right\rangle_{\mathrm{av}} \,, \tag{5}$$

with $\langle \ldots \rangle_{\mathrm{T}}$ as thermal average defined by the partition function $\mathcal{Z}_\alpha$, (3) ([4]). The dynamical response function $\gamma^x_{\alpha n}$ obeys the integral equation

$$\beta^{-1} \sum_{\alpha'} \sum_{n'} (\beta\delta_{\alpha\alpha'}\delta_{nn'} R^x_{\alpha n} + \Gamma^{\alpha\alpha'}_{nn',\,n'n})\,\gamma^x_{\alpha' n'} = f^x_\alpha R^x_{\alpha n} \,, \tag{6}$$

where $R^\mu_{\alpha n} = [G^{-2}_{\alpha n} - \langle G^2_{\alpha n}\rangle^{-1}]^{-1}$, with $\langle G^2_{\alpha n}\rangle \equiv \int \mathrm{d}E\, N(E)[i\omega_n + \mu - \Sigma_{\alpha n} - E]^{-2}$, and $R^h_{\alpha n} = [G^{-2}_{\alpha n} - (i\omega_n + \mu - \Sigma_{\alpha n})\,G^{-1}_{\alpha n}]^{-1}$. Since Γ is a purely local quantity, the information about long-range correlations in the system is contained in γ. Physically speaking, γ measures the response of the effective medium to an infinitesimal change of the field x. In the antiferromagnetic phase (4) and (5) do not change, but (6) acquires a more complicated dependence on the index α.

Equations (4)-(6) form the basis for the numerical evaluation of κ_{av} and χ_{av}. The numerical calculations were performed with a semi-elliptic density of states (DOS) ([5]) with bandwidth $W = 4t^*$, *i.e.* $N(E) = (2/\pi t^*)[1 - (E/2t^*)^2]^{1/2}$ (in the following $t^* \equiv 1$). Due to its finite, algebraic band edges, this DOS resembles the DOS of lattices in $d = 3$ better than does the Gaussian DOS [2] for a hypercubic lattice in $d = \infty$. We now have to specify the local randomness in the model. Here we choose the distribution of a binary alloy. To be able to study the competition between magnetic order caused by the electronic interactions and the disordering effects due to the random potential, we work with an average band filling $n = 1$. To this end we put $\varepsilon_i = \pm \Delta/2$ with equal probability. We can then fix the chemical potential at $\mu = U/2$. We are thus left with three energy scales: the interaction U, the disorder strength Δ and the temperature T (here $k_{\mathrm{B}} \equiv 1$). For the numerical evaluation of the functional integral (3) we employ the algorithm of Hirsch and Fye [8]. We discretize the time variable, *i.e.* $\beta = \Lambda\,\Delta\tau$, with $0.125 \leqslant \Delta\tau \leqslant 0.5$, and then extrapolate the quantities under investigation to $\Delta\tau \to 0$ ([6]). Exact summations over spin variables in the discrete Hubbard-Stratonovich transformation were used whenever possible, *i.e.* for $\Lambda \leqslant 22$. We note that in $d = \infty$ and for a binary alloy the number of independent random configurations is reduced to

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([4]) Note that, for $x = h$, X_{av} corresponds to the averaged *longitudinal* staggered susceptibility which, in the case of spin-rotation invariance, yields the same results as the transverse quantity used in ref. [7].

([5]) This DOS is exact for a Bethe lattice with infinite connectivity.

([6]) For all relevant two-particle quantities $X(\Delta\tau)$ we observed $\delta X(\Delta\tau) := X(0) - X(\Delta\tau) \propto \Delta\tau$ for small $\Delta\tau$; hence we extrapolated with a linear fit.

two. After 4-6 iterations an accuracy of 10^{-6} and 10^{-3} was reached in the exact summations and in the Monte Carlo sampling with 10^4 sweeps per iteration, respectively.

We first study the influence of disorder on the formation of AF order. The latter arises from correlations between local magnetic moments whose static average, m_{av}, is defined by $m_{\mathrm{av}}^2 \equiv L^{-1} \sum_i \langle\langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rangle_{\mathrm{T}} \rangle_{\mathrm{av}} = 1 - 2d_{\mathrm{av}}$. Here $d_{\mathrm{av}} = L^{-1}\, \mathrm{d}\Omega_{\mathrm{av}}/\mathrm{d}U$ is the average double occupancy of lattice sites. The results for m_{av}^2 as a function of U are shown in fig. 1 for $\Delta = 0, 2, 4, 8$ at $T = 1/8$. The disorder is seen to have two main effects: 1) at small U the moments are reduced as the disorder is increased. For a discrete spectrum of random energies and lattices with a finite bandwidth there always exists a critical value $U_{\mathrm{c}}^{\mathrm{MI},1}(\Delta) \geqslant 0$ where, at $T = 0$ and for sufficiently large Δ, the moments disappear completely ([7]). At this point a metal-insulator transition (MIT) occurs. 2) For increasing U the moments grow monotonically and start to saturate at $U \gtrsim \Delta$.

Next, we study the spatial correlations between the local moments. For this we evaluate the staggered susceptibility χ_{av}, (4). In particular, to detect the instability of the paramagnetic phase with respect to AF fluctuations, we look for a divergence of χ_{av}. To determine T_{c} we plotted $[\chi_{\mathrm{av}}(T; \Delta\tau)]^{-1}$ *vs.* T for different time slicing $\Delta\tau \leqslant 0.5$. At sufficiently large U a Curie law with a mean-field critical exponent $\nu = 1.0$ is observed to fit the data very well, in agreement with ref. [7, 9] (fig. 2). For these values of U one may safely extrapolate $[\chi_{\mathrm{av}}(T; \Delta\tau)]^{-1}$ to zero to determine the critical temperature $T_{\mathrm{c}}(\Delta\tau)$. However, for values $U \lesssim \Delta$, the low-temperature behaviour of χ_{av}^{-1} no longer follows a Curie law and hence an extrapolation to $\chi_{\mathrm{av}}^{-1} = 0$ becomes ambiguous. For the temperatures investigated here ($T \geqslant 1/8$) we observe two regimes: i) $U \sim \Delta$: here χ_{av}^{-1} still decreases monotonically for decreasing T, but an extrapolation would suggest $T_{\mathrm{c}}(\Delta\tau) < 0$, *i.e.* a paramagnetic state; ii) $U \lesssim \Delta$: here χ_{av}^{-1} begins to *increase* again (fig. 2). The latter behaviour is a direct

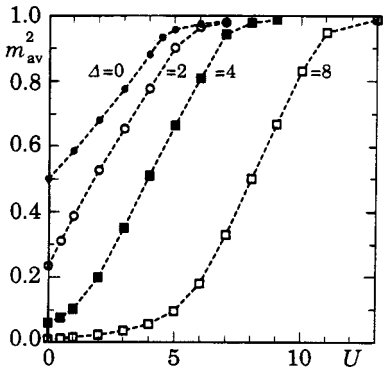

Fig. 1.

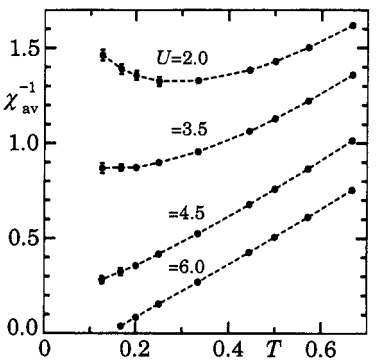

Fig. 2.

Fig. 1. – Averaged quadratic local moment, m_{av}^2, *vs.* interaction U for disorder strengths $\Delta = 0$ (●), 2 (○), 4 (■), 8 (□) at temperature $T = 1/8$; all energies in units of t^*. Here and in the following figures the dashed lines are guides for the eye only. Error bars are of the size of the plotting symbols unless shown explicitly.

Fig. 2. – Inverse averaged staggered susceptibility, χ_{av}^{-1}, *vs.* T for $U = 2, 3.5, 4.5, 6$ at $\Delta = 4$ and $\Delta\tau = 0.125$.

([7]) For the binary-alloy distribution of disorder used here, a metal-insulator transition due to band splitting occurs at $\Delta_{\mathrm{c}}(U) \geqslant 2$ for $T = 0$. Indeed, $\Delta_{\mathrm{c}}(0) = 2$ follows from the exact analytic result for $d = \infty$ provided by the coherent potential approximation; cf. ref. [13].

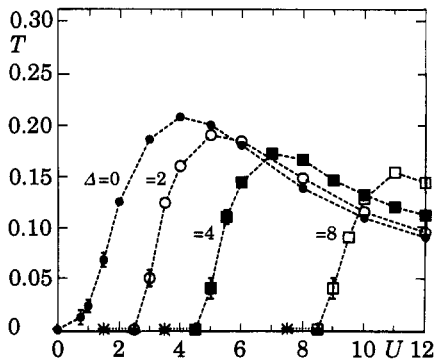

Fig. 3

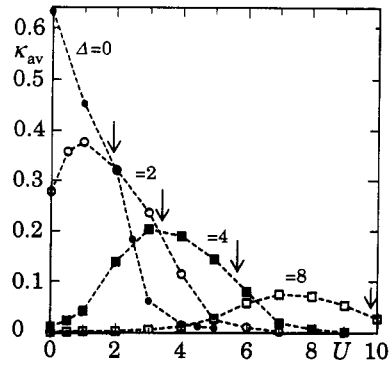

Fig. 4.

Fig. 3. – T-U phase diagram for disorder strengths $\Delta = 0, 2, 4, 8$. Paramagnetic (antiferromagnetic) phase stable above (below) curves. Data points at $T = 0$ were obtained from the Curie law but were the *first* points where $\chi_{\rm av}^{-1} > 0$ at $T = 0$. Dotted lines to the left of these points indicate the regime where deviations from the Curie law become noticeable (see fig. 2). Below the crosses $\chi_{\rm av}^{-1}$ begins to increase with decreasing T and an AF phase can no longer be expected to form.

Fig. 4. – Averaged compressibility *vs.* U for disorder strenghts $\Delta = 0, 2, 4, 8$ at $T = 1/8$. Arrows indicate the position of $U_{\rm c}^{\rm AF}$ taken from fig. 3 where the paramagnet-antiferromagnet transition occurs.

consequence of the suppression of the local moments due to the disorder as discussed above. For $U \simeq \Delta$ there is still a possibility that $\chi_{\rm av}^{-1}$ vanishes, *e.g.* non-analytically. The actual phase boundary between the paramagnetic and the AF phase is determined by extrapolating $T_{\rm c}(\Delta\tau)$ to $\Delta\tau = 0$. The resulting T-U phase diagram is shown in fig. 3 for $\Delta = 0, 2, 4, 8$. As expected, the disorder suppresses the AF order for $U \lesssim \Delta$ and reduces the maximal value of $T_{\rm c}$. However, $T_{\rm c}$ is not a monotonically decreasing function of the disorder for all $U > U_{\rm c}^{\rm AF}(\Delta)$: for $U \gtrsim 6$ the curves separating the ordered and the disordered phase are seen to cross. This implies that, quite unexpectedly, the disorder *favours* the formation of an ordered phase, *i.e.* the critical temperature $T_{\rm c}(\Delta)$ initially *increases* with Δ and reaches a maximum at some value $\Delta_{\rm max}(U)$ before it falls to zero. This raises the question about the nature of the ordered ground state in the strong-coupling limit of the Hubbard model with local disorder.

For $n = 1$ and $\Delta = 0$ the ground state of the system is an AF insulator for all $U > 0$. How does the disorder affect this property? Insight is gained from the averaged compressibility $\kappa_{\rm av}$ of the system, (4). A thermodynamic criterion for an insulating state is $\kappa_{\rm av} = 0$ in both the paramagnetic and antiferromagnetic phases. At small U, *i.e.* $U \lesssim U_{\rm c}^{\rm AF}$, the disorder will reduce $\kappa_{\rm av}$ until, at $\Delta \gtrsim U$, $d_{\rm av} \simeq 1/2$ is reached, in which case the system cannot be further compressed. As U is increased (at fixed Δ) up to $U \simeq \Delta$, $d_{\rm av}$ decreases and $\kappa_{\rm av}$ may then grow. For even larger values of U, $\kappa_{\rm av}$ must again decrease due to the repulsion between the particles. The averaged compressibility at $T = 1/8$, calculated in the paramagnetic and antiferromagnetic phases (transition points indicated by arrows), is shown in fig. 4 for various values of Δ. Below the transition the slope of $\kappa_{\rm av}$ becomes steeper compared to the result for the paramagnetic case, but this effect becomes weaker for increasing disorder. In the vicinity of the transition $\kappa_{\rm av}$ is clearly non-zero; it approaches zero only for values of U considerably larger than $U_{\rm c}^{\rm AF}$. We thus conclude that, at least close to the transition point $U_{\rm c}^{\rm AF} > 0$, the AF phase is *metallic*. For decreasing T the critical interaction $U_{\rm c}^{\rm AF}$ decreases too, but never reaches zero if $\Delta > 0$ (see fig. 3). Since at very large U (Heisenberg limit) the

ground state is insulating at $T = 0$, *another* MIT must occur at a value $U_c^{MI,2}$ where the AF metal becomes an AF insulator. There is no *a priori* reason to expect that U_c^{AF} and $U_c^{MI,2}$ ever coincide.

In summary, we investigated the influence of disorder on the low-temperature phase diagram of the Hubbard model. To do this we evaluated the averaged local moment, staggered susceptibility and compressibility in both the paramagnetic and antiferromagnetic phases in $d = \infty$ using quantum Monte Carlo. The competition between the kinetic energy, electron interaction and disorder leads to a rich scenario of phase transitions. Our results indicate that even at half-filling, for increasing U and sufficiently strong disorder, there is a sequence of transitions from a paramagnetic insulator to a paramagnetic metal at $U_c^{MI,1}$, then to an AF metal at U_c^{AF} and finally, at $U_c^{MI,2}$, to an AF insulator. This transition scenario, together with the anomalous effect of the stabilization of the ordered phase due to disorder at strong coupling, clearly shows that the simultaneous presence of disorder and strong electron- electron correlations leads to new, non-perturbative quantum many-body phenomena which deserve further investigations.

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