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# "Linearized" dynamical mean-field theory for the Mott-Hubbard transition

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**Abstract.** The Mott-Hubbard metal-insulator transition is studied within a simplified version of the Dynamical Mean-Field Theory (DMFT) in which the coupling between the impurity level and the conduction band is approximated by a single pole at the Fermi energy. In this approach, the DMFT equations are linearized, and the value for the critical Coulomb repulsion $U_c$ can be calculated analytically. For the symmetric single-band Hubbard model at zero temperature, the critical value is found to be given by 6 times the square root of the second moment of the free ($U = 0$) density of states. This result is in good agreement with the numerical value obtained from the Projective Selfconsistent Method and recent Numerical Renormalization Group calculations for the Bethe and the hypercubic lattice in infinite dimensions. The generalization to more complicated lattices is discussed. The "linearized DMFT" yields plausible results for the complete geometry dependence of the critical interaction.

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## 1 introduction

The correlation-induced transition from a paramagnetic metal to a paramagnetic insulator (the Mott-Hubbard transition [1,2]) has been intensively studied within the single-band Hubbard model [3–5]:

$$H = \sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}. \qquad (1)$$

The model describes conduction electrons with spin $\sigma$ on a lattice with nearest-neighbor hopping matrix element $t_{ij}$ and a local Coulomb repulsion $U$. One of the first approaches to describe the metal-insulator transition in the half-filled Hubbard model has been the Hubbard-III approximation [6]. The alloy-analogy solution predicts a splitting of the density of states in upper and lower Hubbard bands for large values of $U$. On decreasing $U$, the insulator-to-metal transition occurs when the Hubbard bands start to overlap. The critical interaction is approximately given by the free bandwidth: $U_c \approx W$. The Hubbard-III approximation, however, fails to describe the Fermi-liquid properties in the metallic phase.

Later, the Mott-Hubbard transition has been described within the Gutzwiller variational approach by Brinkman and Rice [7]. Starting from the metallic side, the transition is marked by a diverging effective mass. The critical interaction is found to be $U_c = 8|e_0|$ where $e_0$ is the kinetic energy of the half-filled band per particle for $U = 0$. The Brinkman-Rice approach, however, fails to describe the insulating phase above $U_c$.

A Dynamical Mean Field Theory (DMFT), which becomes exact in the limit of infinite spatial dimensions, has been developed for the Hubbard model [8–10]. The DMFT is able to yield a consistent description of the metallic Fermi liquid for weak coupling as well as of the Mott-Hubbard insulator for strong coupling. In practice, however, the solution of the mean-field equations is by no means a trivial task. In particular, for $U \mapsto U_c$ problems may arise since the "mean field" $\Delta(\omega)$ which has to be determined self-consistently, develops a strong frequency dependence on a vanishingly small energy scale.

The first calculations for temperature $T = 0$ were performed using the so-called Iterated Perturbation Theory (IPT) [10]. Within the IPT the highly correlated Fermi liquid for $U \mapsto U_c$ is characterized by a narrow quasiparticle peak that is well isolated from the Hubbard bands. As a consequence the insulating gap appears to open discontinuously at the metal-insulator transition. These characteristics of the transition have been questioned by various authors [11–13] so that the issue of the metal-insulator transition for $T = 0$ (and also for $T > 0$ [10,14]) cannot be regarded as settled at the moment.

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Qualitatively, the IPT scenario for $T = 0$ is corroborated by recent non-perturbative calculations using the Numerical Renormalization Group (NRG) method [15, 16]. However, the critical value for the transition is found to be significantly lower as compared to the IPT result. On the other hand, the NRG value for $U_c$ is in remarkable agreement with the result of the Projective Self-consistent Method (PSCM) [17].

The value of the critical interaction for the Mott-Hubbard transition is of great interest. Using the methods mentioned above, an approximate calculation of $U_c$ is possible. This, however, represents a rather difficult numerical problem, the solution of which still depends on the approximation used. Within the framework of DMFT, an exact *analytical* result for the precise value of $U_c$ is still missing. Even an approximate analytical expression is not available up to now.

With the present paper we propose a simplified treatment of the mean-field equations ("linearized" DMFT) which allows to obtain an explicit expression for $U_c$ at zero temperature. A fully numerical treatment of the DMFT would leave us with a mere number for $U_c$ and would hardly show up the characteristic trends for different geometries unless a large number of cases were studied. Contrary, the linearized DMFT is able to yield at once the complete geometry dependence of $U_c$. In our opinion this outweighs the necessity for further approximations.

The main idea of the linearized DMFT is to approximate the hybridization function for the coupling between the impurity level and the conduction band by a single pole. This is detailed in Section 2. The reliability of the new approach is estimated by comparing the analytical results for the Bethe and the hypercubic lattice in infinite dimensions with the available numerical values from the PSCM and the NRG in Section 3.1. A satisfactory agreement is found. In the following we then demonstrate the predictive power of the approach. The geometry dependence of $U_c$ is derived for a number of more complicated lattice structures: inhomogeneous Bethe lattices (3.2 and 3.3) and hypercubic films in infinite and finite dimensions (3.4). Finally, in Section 3.5 we discuss a first correction beyond the linearized theory. Section 4 summarizes the main results.

## 2 Linearized dynamical mean-field theory

A characteristic feature of the metal-insulator transition is that the quasiparticle peak appears to be isolated from the upper and the lower Hubbard band for $U \mapsto U_c$ and $T = 0$. Whether or not there is a real gap, *i.e.* zero spectral weight between the quasiparticle peak and the Hubbard bands, is difficult to decide with any numerical method but not very important for the present approach. Essentially, our approach is based on two approximations:

(i) We assume that in the limit $U \mapsto U_c$ the influence of the high-energy Hubbard bands on the low-energy (quasiparticle) peak is negligible. This can be specified as follows: within the DMFT the Hubbard model is self-consistently mapped onto a single-impurity Anderson model (SIAM). In the effective SIAM, we divide the conduction-electron degrees of freedom in a high-energy part $H_{\rm high}$ (the Hubbard bands) and a low-energy part $H_{\rm low}$ (the quasiparticle peak). The Hamiltonian of the effective SIAM is then written as

$$H_{\rm SIAM} = H_{\rm high} + H_{\text{high-imp}} + H_{\rm imp} + H_{\rm low} + H_{\text{low-imp}}, \tag{2}$$

where the coupling of the impurity $H_{\rm imp} \equiv \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$ to the high- (low-)energy part is denoted as $H_{\text{high-imp}}$ ($H_{\text{low-imp}}$). The first approximation is then to neglect the terms $H_{\rm high}$ and $H_{\text{high-imp}}$.

To motivate this step, consider the on-site Green function of the Hubbard model $G(\omega)$. *Via* the DMFT self-consistency condition, $G(\omega)$ defines an effective SIAM. For $U \mapsto U_c$ one indeed finds (*e.g.* within the NRG) that it makes no significant difference for the low-energy part of the solution of the resulting SIAM whether the full $G(\omega)$ is considered or the Green function with the Hubbard bands removed. This means that in the iterative solution of the DMFT equations, the low-energy peak basically reproduces itself, and the high-energy degrees of freedom are rather unimportant.

Alternatively, the first approximation can be characterized as follows: let us (for a moment) look at the insulating solution for $U = U_c$. Here the low-energy degrees of freedom are absent ($H_{\text{low-imp}}$, $H_{\rm low} = 0$) and the approximation reads: $H_{\rm high} + H_{\text{high-imp}} + H_{\rm imp} \mapsto H_{\rm imp}$. The impurity spectral function for the left-hand side is given by two Hubbard bands centered at $\pm U/2$ while it is given by two $\delta$-peaks at $\pm U/2$ for the right-hand side. So we can state that in step (i) of the approximation the finite bandwidth of the Hubbard peaks is neglected.

(ii) For $U \mapsto U_c$, the width of the quasiparticle peak vanishes. This fact is used for the second approximation: we assume that in this limit it is sufficient to describe the low-energy degrees of freedom by a single conduction-band level, *i.e.* $H_{\rm low} \mapsto \sum_\sigma \epsilon_c c_\sigma^\dagger c_\sigma$. Thereby we disregard any internal structure of the quasiparticle peak for $U \mapsto U_c$. Equivalently, this means that the hybridization function can be represented by a single pole at $\omega = 0$:

$$\Delta(\omega) = \frac{\Delta_N}{\omega} \cdot \tag{3}$$

A given hybridization function $\Delta(\omega)$ fixes the effective impurity problem. Due to

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega - (\epsilon_k - \mu)}, \tag{4}$$

the one-pole structure of $\Delta(\omega)$ corresponds to an $n_s = 2$ site single-impurity Anderson model (SIAM):

$$H_{\text{2-site}} = \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_\sigma \epsilon_c c_\sigma^\dagger c_\sigma + \sum_\sigma V (d_\sigma^\dagger c_\sigma + \text{h.c.}) \tag{5}$$

with the hybridization strength $V = \sqrt{\Delta_N}$.

Combining (i) and (ii) we obtain: $H_{\rm SIAM} \mapsto H_{\rm imp} + H_{\rm low} + H_{\text{low-imp}} \mapsto H_{\text{2-site}}$. With these two approximations we can run through the DMFT self-consistency cycle. In the one-pole ansatz (3) for the hybridization function, $\Delta_N$ is the weight of the pole. The index $N$ refers to the $N$th step in the iterative solution. Our goal is to calculate $\Delta_{N+1}$.

We restrict ourselves to the manifest particle-hole symmetric case. The chemical potential is set to $\mu = U/2$. The on-site energies in (5) are thus given by $\epsilon_d = t_{ii} = 0$ and $\epsilon_c = U/2$. For the hybridization strength we have $V = \sqrt{\Delta_N} \mapsto 0$ as $U \mapsto U_{\rm c}$. The two-site impurity model is simple enough to be solved analytically [18,19]. For small $V$ there are two peaks in the impurity spectral function at $\omega \approx \pm U/2$ as well as two peaks near $\omega = 0$ which can be considered as corresponding to the quasiparticle resonance of the infinite ($n_{\rm s} = \infty$) system. The weight of this "resonance" can be read off from the exact solution [18]; up to second order in $V/U$ and for the particle-hole symmetric case it is given by:

$$z = 2\frac{18V^2}{U^2} = \frac{36}{U^2}\Delta_N. \tag{6}$$

The two-site model equation (5) of course cannot display Fermi-liquid behaviour due to the lack of a continuum of conduction-band states near the Fermi level. The Fermi-liquid properties of the metallic phase of the Hubbard model are therefore lost within our approximation. What remains, however, and what we are focussing on, is the weight (6) of the resonances near $\omega = 0$ which we identify as the *quasiparticle* weight $z$. Therefore we still use a Fermi-liquid description for the low-energy part of the self-energy $\Sigma(\omega)$:

$$\Sigma(\omega) = U/2 + (1 - z^{-1})\omega + \mathcal{O}(\omega^2)\,. \tag{7}$$

For a homogeneous lattice and a local self-energy the on-site Green function of the Hubbard model can be written as:

$$G(\omega) = \int {\rm d}\varepsilon \frac{\rho(\varepsilon)}{\omega - (\varepsilon - \mu) - \Sigma(\omega)}, \tag{8}$$

where $\rho(\varepsilon)$ is the free ($U = 0$) density of states. Using equation (7) we obtain:

$$G(\omega) = z \int {\rm d}\varepsilon \frac{\rho(\varepsilon)}{\omega - z\varepsilon} + G^{(\text{incoh.})}(\omega), \tag{9}$$

where the first part represents the coherent part of the Green function ($G^{(\text{coh.})}(\omega)$), and the second (incoherent) part can be disregarded for small excitation energies $\omega \mapsto 0$.

The integration can formally be carried out by means of a continued-fraction expansion which for a symmetric density of states $\rho(\varepsilon)$ reads:

$$\begin{aligned} G^{(\text{coh.})}(\omega) &\equiv z \int {\rm d}\varepsilon \frac{\rho(\varepsilon)}{\omega - z\varepsilon} = G^{(U=0)}(z^{-1}\omega) \\ &= 1/(z^{-1}\omega - b_1^2/(z^{-1}\omega - b_2^2/\ldots)). \end{aligned} \tag{10}$$

The expansion coefficients $b_n$ are related to the moments $M_n$ of the $U = 0$ density of states. The first coefficient $b_1$ is given by:

$$b_1^2 = M_2 = \int {\rm d}\varepsilon\ \varepsilon^2 \rho(\varepsilon). \tag{11}$$

The second moment $M_2$ is easily calculated by evaluating an (anti-)commutator of the form $\langle [\,[[c, H_0]_-, H_0]_-, c^\dagger]_+ \rangle$ which yields:

$$M_2 = \sum_j t_{ij}^2. \tag{12}$$

Thus we obtain:

$$G^{(\text{coh.})}(\omega) = \frac{z}{\omega - z^2 M_2 F(\omega)}, \tag{13}$$

where we have $F(\omega) = 1/\omega + \mathcal{O}(\omega^{-2})$ for the remainder.

Starting from equation (3) in the $N$th step, the DMFT self-consistency equation,

$$\Delta(\omega) = \omega - (\epsilon_d - \mu) - \Sigma(\omega) - G(\omega)^{-1}, \tag{14}$$

yields a new hybridization function $\Delta(\omega)$ for the $(N+1)$th step. With equations (7, 13) we get:

$$\Delta(\omega) = z M_2 F(\omega) \tag{15}$$

for low frequencies $\omega \mapsto 0$. Insisting on the one-pole structure,

$$\Delta(\omega) \stackrel{!}{=} \frac{\Delta_{N+1}}{\omega}, \tag{16}$$

for $U \mapsto U_{\rm c}$, we must have $F(\omega) = 1/\omega$. This amounts to replacing the coherent part of the on-site Green function by the simplest Green function with the same moments up to the second one.

From equations (6, 13) we thus have:

$$\Delta_{N+1} = \frac{36}{U^2} M_2 \Delta_N. \tag{17}$$

The coefficient of the $(N+1)$th iteration step is thereby expressed in terms of the coefficient of the $N$th step. This is our main result. For $U = U_{\rm c}$ the DMFT equations are linearized, they are reduced to a simple linear algebraic equation which determines the evolution of a single parameter ($\Delta_N$) under subsequent iterations.

The linearized mean-field equation (17) has only one non-trivial solution with $\Delta_{N+1} = \Delta_N$ which occurs for $U = U_{\rm c}$ with $U_{\rm c}^2 = 36 M_2$. Any $U < U_{\rm c}$ gives $\Delta_{N+1}/\Delta_N > 1$, so that $\Delta_N$ increases exponentially with iteration number. This indicates the breakdown of the one-pole approximation. For any $U > U_{\rm c}$ the weight $\Delta_N$ decreases exponentially with increasing iteration number. This corresponds to the vanishing of the quasiparticle peak in the insulating regime. Consequently, $U_{\rm c}$ has the meaning of the critical interaction for the Mott-Hubbard transition and its value is given by:

$$U_{\rm c} = 6\sqrt{\int {\rm d}\varepsilon\ \varepsilon^2 \rho(\varepsilon)} = 6\sqrt{\sum_j t_{ij}^2}. \tag{18}$$

For a lattice with nearest-neighbor coordination number $q$ and hopping integral $t = |t_{ij}|$ between nearest-neighbors $i$ and $j$, we have: $U_c = 6t\sqrt{q}$.

The result (18) has been derived within the DMFT which becomes exact in the limit $q \mapsto \infty$. With the usual scaling for the hopping integral, $t = t^*/\sqrt{q}$ and $t^* = \text{const.}$ [8], we have:

$$U_c = 6t^*. \tag{19}$$

However, equation (18) may also be used for finite-dimensional systems where the DMFT is effectively the approximation of a purely local self-energy functional.

## 3 Discussion

### 3.1 Bethe and hypercubic lattice

For the Bethe lattice with infinite coordination number and scaling $t = t^*/\sqrt{q}$, the free bandwidth is given by $W = 4t^*$. So we expect from equation (19) the Mott-Hubbard metal-insulator transition to occur at $U_c = 1.5W$. This result is in very good agreement with the result from the Projective Self-consistent Method (PSCM) [10,17] $U_{c,\mathrm{PSCM}} \approx 1.46W$ and with recent calculations using the Numerical Renormalization Group (NRG) method [16] which yield $U_{c,\mathrm{NRG}} \approx 1.47W$. It also agrees well with the value of $U_c \approx 1.51W$ obtained in the NRG calculations of Shimizu and Sakai [20]. The earlier IPT result $U_{c,\mathrm{IPT}} \approx 1.65W$ [10] overestimates the critical $U$ as compared to the other, non-perturbative methods. The Random Dispersion Approximation (RDA) [13] predicts a considerably lower critical value $U_{c,\mathrm{RDA}} \approx W$. The origin of this discrepancy, however, is presently not clear.

On the infinite-dimensional hypercubic lattice with the scaling $t = t^*/\sqrt{q}$, we expect the metal-insulator transition to occur at $U_c = 6t^*$. Again, this agrees well with the NRG calculations [16] where the value $U_c \approx 5.80t^*$ has been found.

The existence of a metal-insulator transition in the hypercubic lattice at a finite $U_c$ is not at all clear, considering the fact that the free density of states is Gaussian, *i.e.* has no cutoff. In any case, the actual bandwidth (which is infinite for a Gaussian density of states) cannot play a role for the value of $U_c$. It is much more plausible that it is the effective bandwidth (which is proportional to $\sqrt{\int \mathrm{d}\varepsilon \rho(\varepsilon)\varepsilon^2}$) that has to be taken as a measure for $U_c$.

Our analysis also shows that $U_c$ is roughly independent of the details of the lattice structure and only depends on the *local* quantity $\sum_j t_{ij}^2$. This result can quite naturally be understood when the electrons are considered as getting localized at the transition. In this case the electrons would only see their immediate surrounding which is the same for both the infinite dimensional Bethe and the hypercubic lattice.

### 3.2 Two-sublattice model

Let us now work out the predictions of the linearized DMFT for *inhomogeneous* lattices, *i.e.* lattices with reduced (translational) symmetries. The presumably simplest but non-trivial case is a Bethe lattice that consists of two non-equivalent sublattices $Q_1$ and $Q_2$ where each site of $Q_\alpha$ has $q_\alpha$ nearest neighbors that belong to $Q_{\overline{\alpha}}$ (with $\overline{\alpha} = 2$ for $\alpha = 1$ and $\overline{\alpha} = 1$ for $\alpha = 2$). We consider the limit of infinite coordination numbers $q_1, q_2 \mapsto \infty$ with $0 < q_1/q_2 < \infty$. As for the homogeneous case $q_1 = q_2$, it can be shown that the Hubbard model on the inhomogeneous lattice remains well-defined and non-trivial if the hopping integral is scaled appropriately, *e.g.* $t = t^*/\sqrt{q_1 + q_2} = t^{**}/\sqrt{q_1}$ with $t^*, t^{**} = \text{const.}$ As a consequence, the self-energy $\Sigma_\alpha(\omega)$ is local but sublattice dependent. The lattice problem can be mapped onto two impurity models that are characterized by hybridization functions $\Delta_\alpha(\omega)$. The DMFT self-consistency equations read:

$$\Delta_\alpha(\omega) = \omega - (\epsilon_d - \mu) - \Sigma_\alpha(\omega) - G_\alpha(\omega)^{-1}, \tag{20}$$

where $G_\alpha(\omega)$ is the on-site Green function for a site $i$ within the sublattice $\alpha$. One easily verifies that the free ($U = 0$) local density of states on each sublattice is symmetric and that $\mu = U/2$ at half-filling. Furthermore, with $q_1, q_2 \mapsto \infty$, we obtain from the lattice Dyson equation:

$$G_\alpha(\omega)^{-1} = \omega + \mu - \Sigma_\alpha(\omega) - q_\alpha t^2 G_{\overline{\alpha}}(\omega). \tag{21}$$

The linearized DMFT for $U \mapsto U_c$ iterates the one-pole ansatz $\Delta_\alpha(\omega) = \Delta_N^{(\alpha)}/\omega$. From equations (20, 21) we have $\Delta_\alpha(\omega) = q_\alpha t^2 G_{\overline{\alpha}}(\omega)$ for $\alpha = 1, 2$. This implies that the quasiparticle peak for the sublattice $\overline{\alpha}$ with weight $z_{\overline{\alpha}} = (36/U^2)\Delta_N^{(\overline{\alpha})}$ generates a corresponding peak in $\Delta_\alpha(\omega)$ with the weight $\Delta_{N+1}^{(\alpha)} = q_\alpha t^2 z_{\overline{\alpha}}$. Thus we get:

$$\Delta_{N+1}^{(\alpha)} = \sum_\beta K_{\alpha\beta}(U)\Delta_N^{(\beta)}, \tag{22}$$

where the $2 \times 2$ matrix $\mathbf{K}(U)$ is defined as:

$$\mathbf{K}(U) = \frac{36t^2}{U^2}\begin{pmatrix} 0 & q_1 \\ q_2 & 0 \end{pmatrix}. \tag{23}$$

A fixed point of $\mathbf{K}(U)$ corresponds to a self-consistent solution. Let $\lambda_r(U)$ denote the eigenvalues of $\mathbf{K}(U)$. We can distinguish between two cases: if $|\lambda_r(U)| < 1$ for $r = 1$ and $r = 2$, there is the trivial solution $\lim_{N\mapsto\infty} \Delta_N^{(\alpha)} = 0$ only (insulating solution for $U > U_c$). On the other hand, if there is at least one $\lambda_r(U) > 1$, $\Delta_N^{(\alpha)}$ diverges exponentially as $N \mapsto \infty$ (metallic solution for $U < U_c$). The critical interaction is thus determined *via* the maximum eigenvalue by the condition:

$$\lambda_{\max}(U_c) = 1. \tag{24}$$

This yields:

$$U_c = 6t\sqrt[4]{q_1 q_2}, \tag{25}$$

*i.e.* the geometrical mean of the critical interactions of two homogeneous Bethe lattices with coordination numbers $q_1$ and $q_2$, respectively. The result recovers the homogeneous case $q_1 = q_2$ and correctly gives $U_c = 0$ for the atomic limit $q_1 \mapsto 0$ or $q_2 \mapsto 0$.

The analysis can be generalized straightforwardly to an arbitrary number of $s$ sublattices $Q_1, \ldots, Q_s$. We consider a Bethe lattice where each site of the sublattice $Q_\alpha$ has $(q_\alpha - 1)$ nearest neighbors belonging to the sublattice $Q_{\alpha_+}$ and one nearest neighbor in the sublattice $Q_{\alpha_-}$ where $\alpha_\pm \equiv \alpha \pm 1$ except for $\alpha = s$ (here $\alpha_+ \equiv 1$) and $\alpha = 1$ ($\alpha_- \equiv s$). In the limit $q_\alpha \mapsto \infty$ with fixed pairwise ratios $0 < q_\alpha/q_\beta < \infty$, we have:

$$G_\alpha(\omega)^{-1} = \omega + \mu - \Sigma_\alpha(\omega) - q_\alpha t^2 G_{\alpha_+}(\omega), \tag{26}$$

and the argument proceeds as above. We finally arrive at the mean-field equation (22) with $\mathbf{K}(U)$ being an $s$-dimensional matrix with $s$ non-zero elements:

$$\mathbf{K}(U) = \frac{36t^2}{U^2} \begin{pmatrix} 0 & q_1 & & & \\ & 0 & q_2 & & \\ & & 0 & .. & \\ & & & .. & q_{s-1} \\ q_s & & & & 0 \end{pmatrix}. \tag{27}$$

This implies:

$$U_c = 6t \left( \prod_{\alpha=1}^{s} q_\alpha \right)^{1/2s}. \tag{28}$$

Again, this is plausible since $q_\alpha = 0$ for any $\alpha$ would mean to cut the lattice into unconnected pieces of finite size, and the Mott transition becomes impossible ($U_c = 0$).

Also the $s \mapsto \infty$ limit of equation (28) is meaningful: consider *e.g.* $q_{\alpha=1} \neq q \equiv q_2 = q_3 = \ldots$. This describes a Bethe lattice with coordination number $q$ for all sites except for one distinguished impurity site with coordination number $q_1$. As expected physically, $U_c$ is unaffected by the presence of the impurity. Furthermore, in any case where one changes the number of nearest neighbors of a *finite* number of sites only, the value for $U_c$ remains unchanged.

### 3.3 General inhomogeneous Bethe lattice

We finally tackle the "inverse" problem: given a matrix $\mathbf{K}$, is there a realization of a (Bethe) lattice such that the critical interaction is determined by the maximum eigenvalue of $\mathbf{K}$? For this purpose we consider the Hubbard model with nearest-neighbor hopping on a *general* inhomogeneous Bethe lattice where each site $i$ may have a different coordination number. Remaining spatial symmetries are accounted for by classifying the lattice sites into sublattices $Q_\alpha$ that consist of equivalent sites only. By $q_{\alpha\beta}$ we denote the number of nearest neighbors of a site $i \in Q_\alpha$ that belong to the sublattice $Q_\beta$. We are interested in the limit $q_{\alpha\beta} \mapsto \infty$ with $0 < q_{\alpha\beta}/q_{\gamma\delta} < \infty$ since this implies a local but $\alpha$-dependent self-energy $\Sigma_\alpha(\omega)$. Within the DMFT this Hubbard model is mapped onto impurity models which are labeled by the sublattice index $\alpha$. The self-consistency conditions are given by equation (20).

Let $G^{(0)}_\alpha(\omega) \equiv G_\alpha(\omega)$ be the on-site Green function for a site $i$ in $Q_\alpha$, and $G^{(n)}_{\alpha_n\alpha_{n-1}\cdots\alpha_1\alpha}(\omega) = \langle\langle c_{i\sigma}; c^\dagger_{j\sigma}\rangle\rangle_\omega$ the off-site Green function for $n$th nearest-neighbor sites $i \in Q_{\alpha_n}$ and $j \in Q_\alpha$. $G^{(n)}$ depends on the sublattice indices that are met along the (unique) path from $j$ to $i$. *Via* its equation of motion, $G^{(0)}_\alpha$ couples to the nearest-neighbor off-site Green function $G^{(1)}_{\alpha_1\alpha}$:

$$(\omega + \mu - \Sigma_\alpha(\omega)) G^{(0)}_\alpha(\omega) = 1 + t \sum_{\alpha_1} q_{\alpha\alpha_1} G^{(1)}_{\alpha_1\alpha}(\omega). \tag{29}$$

For a Bethe lattice the nearest-neighbor Green function $G^{(1)}_{\alpha_1\alpha}$ can only couple to $G^{(2)}_{\alpha_2\alpha_1\alpha}$ and to $G^{(0)}_\alpha$ again. More generally, the equation of motion for the $n$th nearest-neighbor off-site Green function reads:

$$\begin{aligned}(\omega + \mu - \Sigma_{\alpha_n}(\omega)) G^{(n)}_{\alpha_n\cdots\alpha_1\alpha}(\omega) = \\ t G^{(n-1)}_{\alpha_{n-1}\cdots\alpha_1\alpha}(\omega) + t \sum_{\alpha_{n+1}} q_{\alpha_n\alpha_{n+1}} G^{(n+1)}_{\alpha_{n+1}\cdots\alpha_1\alpha}(\omega),\end{aligned} \tag{30}$$

where in the second term on the r.h.s. we have used the approximation $q_{\alpha\beta} - 1 \approx q_{\alpha\beta}$ which becomes exact in the limit of infinite coordination numbers. The infinite series defined by equations (29, 30) can formally be summed up. This yields:

$$G_\alpha(\omega)^{-1} = \omega + \mu - \Sigma_\alpha(\omega) - t^2 \sum_\beta q_{\alpha\beta} G_\beta(\omega). \tag{31}$$

The mean-field equation of the linearized DMFT thus has again the form (22) where the $K$-matrix is given by:

$$K_{\alpha\beta}(U) = \frac{36t^2}{U^2} q_{\alpha\beta}. \tag{32}$$

The critical interaction is given by $6t$ times the maximum eigenvalue of the coordination-number matrix $\mathbf{q}$. Note that for a general (non-symmetric), irreducible matrix with non-negative elements, the eigenvalue with maximum absolute value is real and non-negative (Perron-Frobenius theorem [21]). Thus we conclude that any quadratic matrix $\mathbf{K}$ with non-negative elements can be related to the Mott transition on a Bethe lattice with certain (infinite) coordination numbers.

### 3.4 Hypercubic films

As a more realistic example for the Mott transition on an inhomogeneous lattice we consider a hypercubic Hubbard film. A $D$-dimensional film is built up from a number $d$ of $(D-1)$-dimensional "layers". For a hypercubic film these layers are cut out of the usual $D$-dimensional hypercubic lattice. A set of Miller indices $[x_1, x_2, \ldots, x_D]$ characterizes the film-surface normal direction. The most simple films are those with low-index surfaces given by $x_1 = \cdots = x_r = 1$ and $x_{r+1} = \cdots = x_D = 0$. For any site

in the film except for sites at the film surfaces there are $q_1 = 2D - 2r$ nearest neighbors within the same layer and $q_2 = r$ nearest neighbors in each of the adjacent layers; the total coordination number is $q = q_1 + 2q_2 = 2D$.

For $D \mapsto \infty$ the Hubbard model is well defined with the usual scaling of the hopping $t = t^*/\sqrt{2D}$, the self-energy becomes local but layer dependent and dynamical mean-field theory is exact [22]. The lattice problem is mapped onto a set of $d$ impurity problems. The DMFT self-consistency conditions are given by equation (20) where the index $\alpha$ now has to be interpreted as the layer index: $\alpha = 1, \ldots, d$.

The linearized DMFT can be developed as in Section 2. Equation (8), however, is no longer valid and must be replaced by the Dyson equation corresponding to the given film geometry. The coherent part of the on-site Green function for a site in the layer $\alpha$ is given by:

$$G_\alpha(\omega) = z_\alpha \widetilde{G}_\alpha(\omega) = \frac{z_\alpha}{\omega - \widetilde{M}_2^{(\alpha)} F_\alpha(\omega)} \tag{33}$$

where $z_\alpha$ is the layer-dependent quasiparticle weight, $z_\alpha = (1 - \partial \Sigma_\alpha(i0^+)/\partial\omega)^{-1}$ and $\widetilde{G}_\alpha(\omega)$ is the on-site element of the free ($U = 0$) Green function but calculated for the renormalized hopping $t_{ij} \mapsto \sqrt{z_i}\, t_{ij} \sqrt{z_j}$ with $z_i = z_\alpha$ for a site $i$ in the layer $\alpha$. In the expression on the right, $\widetilde{M}_2^{(\alpha)}$ denotes the corresponding second moment which is calculated as $\widetilde{M}_2^{(\alpha)} = z_\alpha(q_1 z_\alpha + q_2 z_{\alpha-1} + q_2 z_{\alpha+1})t^2$. This means that the linearized mean-field equation has again the form (22) with the following $d$-dimensional tridiagonal matrix:

$$\mathbf{K}(U) = \frac{36t^2}{U^2} \begin{pmatrix} q_1 & q_2 & & \\ q_2 & q_1 & q_2 & \\ & q_2 & q_1 & .. \\ & & .. & .. \end{pmatrix}. \tag{34}$$

Its eigenvalues are the zeros of the $d$th degree Chebyshev polynomial of the second kind [23]. From the maximum eigenvalue we obtain:

$$U_\mathrm{c} = 6t \sqrt{q_1 + 2q_2 \cos\left(\frac{\pi}{d+1}\right)}. \tag{35}$$

Equation (35) describes the complete thickness and geometry dependence of the critical interaction for the Mott-Hubbard transition in hypercubic Hubbard films.

In the limit of thick films $d \mapsto \infty$ one recovers the bulk value $U_\mathrm{c} = 6t\sqrt{q_1 + 2q_2}$. For $d < \infty$ the critical interaction not only depends on the film thickness $d$ but also on the geometry of the film surface which is characterized by $r$. Varying $r$ we can pass continuously from the most closed ($r = 1$) to the most open ($r = D$) surface geometry. For $r = 1$, *i.e.* a (1000...) film surface, a site in the topmost layer has $q_\mathrm{S} = q_1 + q_2 = 2D - 1$ nearest neighbors to be compared with $q = 2D$ in the bulk. For $D \mapsto \infty$ the local environment of the surface sites is essentially the same as in the bulk, *i.e.* surface effects become meaningless. Consequently, we get $U_\mathrm{c} = 6t^*$, *i.e.* the bulk value irrespective of $d$. For $r = D$ one obtains the open (1111...) film surface. The surface coordination number is reduced to $q_\mathrm{S} = q_2 = D$. The critical interaction is $U_\mathrm{c} = 6t^* \sqrt{\cos(\pi/(d+1))}$ which is smaller than $6t^*$ for any $d$.

Equation (35) can also be applied to finite-dimensional films ($D < \infty$) if one additionally assumes the local approximation for the self-energy functional to hold. For $D = 3$ simple-cubic films with a thickness ranging from $d = 1$ up to $d = 8$ and for sc(100), sc(110) and sc(111) film surfaces, the prediction (35) of the linearized DMFT has been tested in reference [22] by comparing with the results for $U_\mathrm{c}$ of a fully numerical evaluation of the DMFT equations using the exact diagonalization of small impurity models ($n_\mathrm{s} = 8$). It is found that the linearized DMFT qualitatively and – as far as can be judged from the numerical evaluation – also quantitatively predicts the correct geometry and thickness dependence of $U_\mathrm{c}$ [22].

### 3.5 Critical exponent and critical profiles

So far the discussion was restricted to the calculation of the critical value $U_\mathrm{c}$ which is derived from a *linear* homogeneous mean-field equation (Eqs. (17, 22)). To determine the critical behaviour of the quasiparticle weight $z$ for $U \mapsto U_\mathrm{c}$, one has to go beyond the linearized DMFT. For this purpose a simple generalization of the arguments in Section 2 is necessary.

We replace the second-order result for the quasiparticle weight $z = 36V^2/U^2$ (Eq. (6)) by the result up to fourth order in $V/U$:

$$z = 36\frac{V^2}{U^2}\left(1 - 44\frac{V^2}{U^2}\right). \tag{36}$$

With the same steps as before, one arrives at:

$$\Delta_{N+1} = \left(1 - 44\frac{\Delta_N}{U^2}\right)\frac{36}{U^2} M_2 \Delta_N, \tag{37}$$

which is a non-linear equation for the "mean field" $\Delta$. The self-consistency requires $\Delta_{N+1} = \Delta_N = \Delta$. Solving for $\Delta$ yields:

$$\Delta = \frac{1}{22} U_\mathrm{c}\,(U_\mathrm{c} - U)\,, \tag{38}$$

where we have already expanded the right hand side in powers of $(U_\mathrm{c} - U)$. The result for the quasiparticle weight near $U_\mathrm{c}$ is

$$z = \frac{18}{11}\frac{U_\mathrm{c} - U}{U_\mathrm{c}}\,. \tag{39}$$

This equation is, of course, only valid for $U < U_\mathrm{c}$. We obtain a linear vanishing of the quasiparticle weight near the metal-insulator transition. The equation that determines the quasiparticle weight near the critical interaction can be put into the form $z = (\alpha/2)(1 - (U/U_\mathrm{c})^2)$. This is reminiscent of the Brinkman-Rice result [7]. The difference consists in the value for the coefficient $\alpha$ which is $\alpha = 2$

within the Brinkman-Rice approach and $\alpha = 18/11$ within the simplified DMFT. Compared with numerical results, however, $\alpha = 18/11$ still seems to be too large. Exact-diagonalization results for $n_s = 8$ sites [10] yield a similar or a significantly smaller value depending on the details of the method [24,25]. A smaller value is also found within the PSCM which yields $\alpha = 0.9 \pm 0.15$ [10]. The NRG [16] gives a value $\alpha \ll 1$, but a precise determination is not possible.

For the Hubbard model on an inhomogeneous lattice, the self-energy and thus the quasiparticle weight is site or sublattice dependent: $z_\alpha = (1 - \partial\Sigma_\alpha(i0^+)/\partial\omega)^{-1}$. Within the linearized DMFT (Eq. (22)), the critical interaction is determined from the largest eigenvalue $\lambda_{\max}(U_c) = 1$ in the eigenvalue problem

$$z_\alpha = \sum_\beta K_{\alpha\beta}(U_c) z_\beta. \tag{40}$$

The corresponding eigenvector $z_\alpha = z_\alpha(U_c)$ describes the critical *profile* of the quasiparticle weight. The profile is uniquely determined up to a normalization constant. While $z_\alpha(U) \mapsto 0$ for each $\alpha$ as $U \mapsto U_c$, the ratios $z_\alpha(U_c)/z_\beta(U_c)$ remain to be non-trivial. For example, in the two-sublattice model characterized by equation (23), the critical profile is given by $z_1(U_c)/z_2(U_c) = \sqrt{q_1/q_2}$.

To determine the critical behaviour of the $\alpha$-dependent quasiparticle weight for $U \mapsto U_c$ but $U < U_c$, we again have to expand up to fourth order in $V_\alpha/U$. This yields the following mean-field equation:

$$z_\alpha(U) = \sum_\beta K_{\alpha\beta}(U)\ z_\beta(U) - \frac{11}{9} z_\alpha^2(U). \tag{41}$$

For the two-sublattice model we obtain:

$$z_{1,2}(U) = \frac{36}{11} \frac{\sqrt{q_{1,2}}}{\sqrt{q_1} + \sqrt{q_2}}\ \frac{U_c - U}{U_c}\,. \tag{42}$$

For $q_1 = q_2$ this result reduces to equation (39).

## 4 Conclusions

We have discussed a "linearized" version of the Dynamical Mean-Field Theory which allows for the analytical calculation of the critical interaction for the Mott-Hubbard metal-insulator transition at $T = 0$. The main result is:

$$U_c = 6\sqrt{\int \mathrm{d}\varepsilon\, \varepsilon^2 \rho(\varepsilon)} = 6\sqrt{\sum_j t_{ij}^2}, \tag{43}$$

which shows that it is the second moment of the non-interacting density of states which determines $U_c$. The values for $U_c$ obtained with the linearized DMFT have been compared with the available results from numerical solutions of the full DMFT equations, and a good agreement is found.

The linearized DMFT is of course not able to answer detailed questions about the nature of the Mott-Hubbard transition, such as the existence or absence of a hysteresis, the order of the transition, etc. Its advantage is that it can be easily generalized to a variety of geometries. To obtain the critical interaction, it is sufficient to find the maximum eigenvalue of the respective coordination-number matrix, the dimension of which is determined by the remaining spatial symmetries (see *e.g.* Eq. (32)). The analytical results for *e.g.* the metal-insulator transition in thin Hubbard films have been checked against numerical solutions of the full DMFT equations, and the geometry dependence has been found to be essentially the same, in the DMFT and in the linearized DMFT.

The results from the linearized DMFT show some similarities (but also differences) to the Brinkman-Rice scenario. Both methods give an analytical expression for $U_c$ but the dependence on the non-interacting density of states is quite different: $U_{c,\mathrm{BR}} \propto \int_{-\infty}^{0} \mathrm{d}\varepsilon\ \varepsilon\rho(\varepsilon)$ and $U_{c,\mathrm{LDMFT}}^2 \propto \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\ \varepsilon^2\rho(\varepsilon)$. The behaviour of the quasiparticle weight near $U_c$ is linear in both methods with a difference, however, in the slope: $z_{\mathrm{BR}} = 2(1 - U/U_c)$ and $z_{\mathrm{LDMFT}} = \frac{18}{11}(1 - U/U_c)$. Conceptually, both approaches project the full onto an effective low-energy problem that is characterized by a single parameter $z$ only. The starting point, the necessary assumptions and the realization of the respective approach are, however, quite different.

The linearized DMFT might be considered as a realization of the Exact-Diagonalization (ED) technique [24,25] with a minimum number of sites: $n_s = 2$ (one impurity and one bath site). The difference to such a lowest-order ED is, however, that in the linearized DMFT a special criterion is used to define the parameters of the effective (two-site) Anderson model, namely only the low-energy peaks in the spectral functions are used (see Sect. 2). On the other hand, the fit procedure of Caffarel and Krauth [25] partly involves the high-energy degrees of freedom as well – even for $n_s = 2$. The same holds for the ED approach of Rozenberg *et al.* [24] which becomes identical with the latter for $n_s = 2$. However, since only the low-energy spectral function is relevant for the determination of the low-energy part of the hybridization function *via* the DMFT self-consistency equation, the linearized DMFT is conceptually superior compared with a simple $n_s = 2$-site ED.

The linearized DMFT is best characterized as being the lowest-order realization of the projective self-consistent method [10,17] which in general can only be evaluated numerically. Assuming the separation of low- and high-energy scales for $U \mapsto U_c$, the PSCM exactly maps the full onto an effective (low-energy) Kondo problem by a generalized Schrieffer-Wolff canonical transformation. If we adopt the same two approximations described in Section 2, namely (i) neglecting the high-energy conduction-band states and (ii) ignoring any internal structure of the quasi-particle peak, one obtains within the PSCM a Kondo problem in the atomic limit with a coupling $J_{\mathrm{spin}} = -4D/U$ (using the notations of Ref. [10], $D$ is the half band width of the Bethe DOS). This can be solved analytically and eventually yields a critical interaction of $U_c = 3D$ for the Bethe lattice which

coincides with the value of the linearized DMFT (see Sect. 3.1).

Obviously, the linearized DMFT could be improved by taking into account more states for the effective conduction band (in the Hubbard bands and/or the quasiparticle peak). However, its main advantage – the possibility to obtain analytical results for $U_c$ – would then be immediately lost, and one would essentially recover the PSCM which must be evaluated numerically.

To estimate to what extent an improved description of the low- or high-energy degrees of freedom would affect the value for the critical interaction, let us consider the equation that determines $U_c$ within the PSCM [10]: $1 = (1/2)J_{\rm spin}^2(3/8 - \langle \mathbf{S} \cdot \mathbf{s}_{\rm low} \rangle)$. Using approximation (ii), one obtains an atomic-limit Kondo problem which implies $\langle \mathbf{S} \cdot \mathbf{s}_{\rm low} \rangle = -3/4$ for the spin-spin correlation function. This may be compared with the numerical value $\langle \mathbf{S} \cdot \mathbf{s}_{\rm low} \rangle \approx -0.46$ [17]. Together with $J_{\rm spin} = -4D/U$ (using (i)) the above PSCM equation implies a *decrease* of $U_c$ by about 14% when starting from the linearized theory and then including all low-energy degrees of freedom ($U_c = 3D \mapsto U_c = 2.585D$). This decrease must be compensated almost perfectly by a corresponding *increase* of $U_c$ when including all high-energy degrees of freedom additionally, because the linearized-DMFT result $U_c = 3D$ is very close to the numerically exact value (Sect. 3.1). In fact, the influence of the Hubbard bands is not completely negligible. Within the NRG approach [26], the iteration of the DMFT equations without the Hubbard peaks but including the full low-energy information yields a critical interaction of $U_c \approx 2.5D$. We conclude that the excellent agreement between the results of the linearized and the full theory (Sect. 3.1) is partly due to error cancellation.

Finally, we like to emphasize once more the main advantage of the present approach: the possibility to calculate a reliable estimate for the critical interaction analytically and for *arbitrary* geometries. It would be very interesting to see whether experiments on Mott-Hubbard systems in different geometries will show similar trends as predicted by the linearized DMFT.

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