Mott Transition in the Multi-Band Hubbard Model in Infinite Dimensions

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Abstract

The Mott metal-insulator transition in the multi-band Hubbard model in infinite dimensions is studied by using the linearized dynamical mean-field theory. The critical interaction U_c is obtained analytically. For the symmetric case and for orbital degeneracy M we find $U_c = (4M + 2)\sqrt{L_2}$ where L_2 is the second moment of the non-interacting density of states. We also derive an analytical expression for the discontinuity of the chemical potential $\mu = \mu(n)$ at the filling $n = M$ for $U > U_c$. The findings are in good agreement with numerical results obtained from the exact diagonalization method.

Key words: Mott transition; Metal-insulator transition; multi-band Hubbard model; orbital degrees of freedom

The Mott metal-insulator transition (MIT) driven by electron correlations has received intensive experimental and theoretical attention. It is observed in various transition-metal oxides [1] as well as in fullerenes [2]. The minimal model to describe the Mott MIT is the single-band Hubbard model. However, a consistent description of the above mentioned systems certainly requires more realistic models including orbital degrees of freedom.

Theoretical advances in the past decade – mainly due to the development of the dynamical mean-field theory (DMFT) [3,4] – have led to an increased understanding of multi-orbital Hubbard models [5–13]. Nevertheless, a number of questions still need to be clarified. Even within the DMFT reliable results for the $T = 0$ Mott MIT in multi-band models are still missing. Furthermore, results for the M-dependence of the critical U seem controversial, i.e. both a $\propto \sqrt{M}$ [11] and a $\propto M$ [5,8,12] dependence have been reported in the literature. To clarify these issues, a simple but reliable method is needed – such as the linearized DMFT for which we present an extension to the multi-orbital case in this paper.

The linearized DMFT (L-DMFT) [14] maps the lattice problem onto an Anderson impurity model with a single bath site only by considering a simplified self-consistency condition just at the critical point. This allows for extremely fast numerical calculations or even analytical results to estimate the critical parameters. The L-DMFT has been tested extensively by comparing with numerical results from the full DMFT. For the standard Hubbard model [14,15] but also for different thin-film and semi-infinite surface geometries [16] as well as for the *d-p* model [17,18] a remarkable agreement has been found. For quantitative estimates, errors of the order of a few per cent have to be tolerated. We can thus expect the L-DMFT to be a fast but reliable tool for multi-band systems as well.

Here we consider a multi-band Hubbard model without exchange Coulomb interaction [19]:

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$$H = \sum_{ij\alpha\sigma} t_{ij} c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} + \frac{U}{2} \sum_{i(\alpha\sigma)\neq(\alpha'\sigma')} \hat{n}_{i\alpha\sigma}\hat{n}_{i\alpha'\sigma'}, \quad (1)$$

where i is a site index and $\sigma = \uparrow, \downarrow$. The different orbitals labeled by $\alpha = 1, ..., M$ are considered to be equivalent, M is the orbital degeneracy.

In the limit of infinite dimensions, the self-energy becomes local, and the local Green's function is given by the impurity Green's function of an effective Anderson impurity model,

$$H = \sum_{\alpha\sigma,k=2}^{n_s} \epsilon_k \, a^\dagger_{k\alpha\sigma} a_{k\alpha\sigma} + \sum_{\alpha\sigma,k=2}^{n_s} V_k \, (f^\dagger_{\alpha\sigma} a_{k\alpha\sigma} + \text{h.c.}) + \sum_{\alpha\sigma} \epsilon_f \, f^\dagger_{\alpha\sigma} f_{\alpha\sigma} + \frac{U}{2} \sum_{\alpha\alpha'\sigma\sigma'} f^\dagger_{\alpha\sigma} f^\dagger_{\alpha'\sigma'} f_{\alpha'\sigma'} f_{\alpha\sigma}. \quad (2)$$

In the model eq.(2), the hybridization function $\Delta(\omega) = \sum_k V_k^2/(\omega - \epsilon_k)$ includes the effects of the interaction at all the sites except for the impurity site and is determined self-consistently so as to satisfy the DMFT self-consistency equation [4].

The L-DMFT assumes that the MIT is characterized by a vanishing weight of a low-energy quasi-particle resonance. Close to the MIT, the quasi-particle peak is approximated by a single pole at the Fermi energy. Correspondingly, the hybridization function is a one-pole function $\Delta(\omega) = \frac{V^2}{\omega}$. This effectively represents an approximate mapping of the model (1) onto an Anderson model (2) with $n_s = 2, V \equiv V_{k=2}, \epsilon_c \equiv \epsilon_{k=2} = 0$ and $\epsilon_f = -\mu$. The DMFT self-consistency equation is simply written by $V^2 = zL_2$ [14]. Here L_2 is the second moment of the non-interacting density of states $L_2 = \int \mathrm{d}\omega \, \omega^2 \rho^{(0)}(\omega) = \sum_j t_{ij}^2$. The quasi-particle weight z can be calculated from the impurity spectral function of the two-site Anderson model and is given by $z = z(V, \epsilon_c, \epsilon_f, U, M) = V^2 F(\mu, U, M) + O(V^4)$. Using the standard (Brillouin-Wigner) degenerate perturbation theory we find $F(\mu, U, M) = \frac{1}{2}(\frac{M+1}{MU-\mu} + \frac{M}{\mu-(M-1)U})^2 + \frac{1}{2}(\frac{M}{MU-\mu} + \frac{M+1}{\mu-(M-1)U})^2$. Hence, we obtain

$$L_2 F(\mu, U, M) = 1 \quad (3)$$

as a condition for the MIT. This depends on the filling $n = 1, ..., 2M-1$ through the chemical potential μ.

For $U < U_c$ and half-filling $n = M$ [19] in the symmetric model, the chemical potential is fixed to $\mu = (M - \frac{1}{2})U$ due to particle-hole symmetry. Substituting this into eq.(3), we obtain for the critical interaction

$$U_c(M) = (4M + 2)\sqrt{L_2} \, . \quad (4)$$

For $U > U_c$, the system is a Mott insulator at $n = M$. As a function of the filling the chemical potential shows a jump $\Delta\mu = \mu_+ - \mu_-$, where $\mu_\pm$ is obtained by solving eq.(3) for $U > U_c$ [15]. $\Delta\mu$ thus obtained is

$$\Delta\mu(U, M) = U\big(B - \sqrt{B^2 - 1 + 1/u^2}\big)^{\frac{1}{2}}, \quad (5)$$

where $B \equiv 1 + 1/(2(2M+1)^2 u^2)$ and $u = U/U_c$.

We have also calculated $\Delta\mu$ numerically by using the NRG method for $M = 1$ and the ED method for $M = 1, 2$. The analytical results of the L-DMFT eqs.(4) and (5) agree very well with the numerical results both for $M = 1$ [15] and $M = 2$ [20].

Remarkably, our findings show that $U_c(M)$ depends linearly on M. This is in agreement with previous results from the Gutzwiller method [5] and slave boson calculations [8]. There have been reports on a $\sqrt{M}$ dependence as well [11], a result which has not been reproduced by other methods. The quantum Monte-Carlo calculations of Han et al. [10], for instance, are not conclusive, in particular due to the fairly large T used in the calculations.

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