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The metal–insulator transition in the paramagnetic Hubbard Model

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Abstract

We study the Mott transition in the Hubbard Model within the dynamical mean field theory (DMFT) approach. The DMFT equations are solved using the density matrix renormalization group technique. The densities of states for the half-filled and heavily doped cases are shown. The full phase diagram is also presented.
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1. Introduction

The Mott metal–insulator transition still poses a great theoretical challenge, and the process of doping the Mott insulator is thought to be a source of many interesting phenomena, such as high-temperature superconductivity or colossal magnetoresistance. Particularly difficult is the regime in which the electronic kinetic and Coulomb energies are of the same order. In this case, analytical tools based on perturbative approximations usually fail and direct numerical studies are limited to low-dimensional systems. An alternative approach known as the dynamical mean field theory (DMFT) is an approximation that allows the study of both the weakly and the strongly interacting limits and the transition between them within a single theoretical framework [1]. Currently, a large effort is being made to incorporate the DMFT method as the local correlation physics "engine" for first-principle calculations of realistic compounds [2,3].

For the paramagnetic Hubbard Model in a Bethe lattice in the limit of infinite dimensions,

$$H = \frac{t}{\sqrt{2d}} \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right) - \mu \sum_{i,\sigma} n_{i,\sigma}, \quad (1)$$

the DMFT method maps the original lattice problem on an Anderson impurity embedded in a self-consistently determined bath [1]. In order to solve this impurity problem with exact diagonalization or the density matrix renormalization group (DMRG), it is convenient to use a bath consisting of two chains attached to the impurity [4,5]. The energy and hoppings of the non-interacting sites are determined by the requirement that the hybridization function $\Delta(\omega)$ is related to the impurity Green's function $G(\omega)$ by $\Delta(\omega) = t^2 G(\omega)$. We take the half bandwidth of the non-interacting model as the unit of energy, thus $D = 2t = 1$.

Here, we will show the solutions of the DMFT equations obtained with DMRG in chains of up to 101 sites (50 sites on each side chain plus the impurity) and using up to 256 states to describe each DMRG block.

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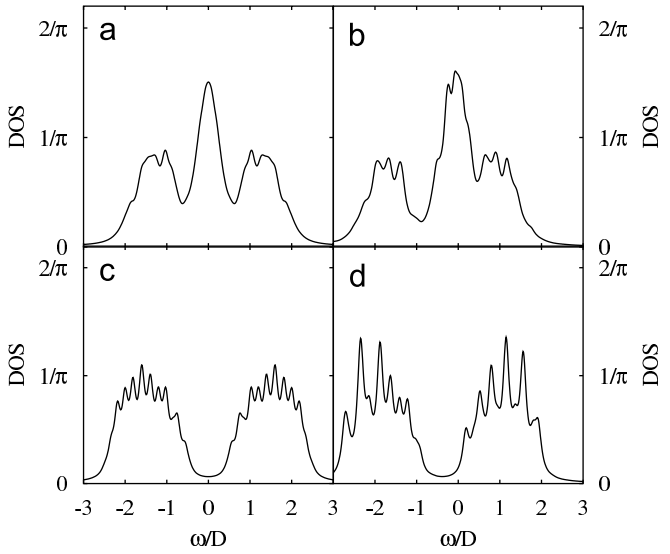

Fig. 1. Density of states for the doped Hubbard Model: (a) $U/D=2.0$, $\mu/D=0$; (b) $U/D=2.0$, $\mu/D=0.4$; (c) $U/D=3.0$, $\mu/D=0$; (d) $U/D=3.0$, $\mu/D=0.4$. The structure seen in the DOS comes from finite size effects.

2. Results

The density of states (DOS, Fig. 1a) for small U/D and $\mu/D=0$ is particle–hole symmetric and metallic. The DOS exhibits the usual quasiparticle peak around $\omega=0$ with the lower and upper Hubbard bands at $\omega\sim\pm U/2$ [1]. When μ is increased (Fig. 1b) the quasiparticle peak moves and merges with the upper Hubbard band, while the lower Hubbard band loses weight and remains at energies $\omega\sim -U$. For the insulating solution, at $\mu=0$, a clear gap is seen between the lower and upper Hubbard bands (Fig. 1c). In contrast to the metallic case, as the chemical potential is increased no distortion is seen in the DOS, but a rigid shift of the bands instead (Fig. 1d).

The boundary of the metallic phase U_{c2} can be obtained following either the doping (defined as the deviation of the charge with respect to one electron per site) or the Drude weight. In the doped case (Fig. 2) the optical conductivity has a Lorentzian shape at low frequencies, from which the Drude weight can be obtained [6]. At larger frequencies $\omega\sim U$ interband contributions from transitions to the lower Hubbard band enhance the optical conductivity. The boundary of the insulating solution U_{c1} can be obtained for $\mu=0$ as the value of U for which the gap closes. For $\mu\neq 0$ U_{c1} can be obtained following the first excited state and finding where it touches the Fermi level. The full phase diagram obtained in this way is shown in Fig. 3. There is a finite region where metallic and insulating solutions coexist. A more detailed description of the transition region can be found in Ref. [6]. The phase diagram shows a reasonable agreement with the one obtained with exact diagonalization [7].

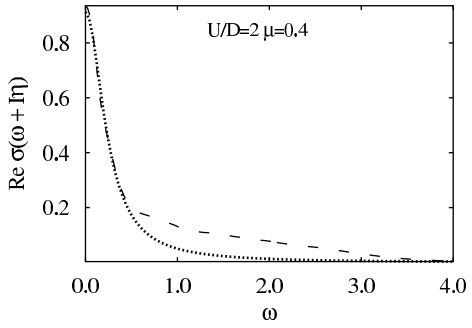

Fig. 2. Real part of the optical conductivity $\sigma(\omega)$ for $U/D=2$ and $\mu/D=0.4$. A small imaginary part $\eta=0.1$ has been used to compute σ. The dotted line corresponds to the low-frequency Lorentzian fit.

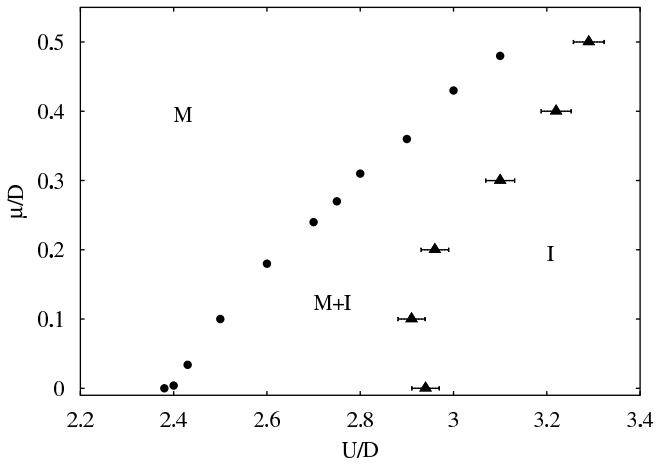

Fig. 3. Phase diagram of the paramagnetic Hubbard Model. M (I) stands for a metallic (insulating) state. Triangles (circles) show the boundary of the metallic (insulating) phase.

3. Conclusions

The DMRG method, in its various forms [5,6,8,9], has been shown to be a reliable method to obtain the phase diagram and the DOS of the single band Hubbard Model at zero temperature. These results open the way for the DMFT solution of more complex problems such as the multi-orbital case.

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