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SPECTRAL FUNCTIONS OF CORRELATED ELECTRON SYSTEMS IN THE LOCAL IMPURITY SELF CONSISTENT APPROXIMATION

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Abstract—We describe the evolution of the spectral density as we dope a Mott insulator within a dynamical mean field method. After giving an intuitive description of this Local Impurity Self-Consistent Approximation (LISA) for a model with several orbitals per unit cell, we illustrate its implementation in the context of the Hubbard model in infinite dimensions. For this purpose a new iterative perturbation theory (IPT) scheme is introduced and compared with results from exact diagonalization.

1. INTRODUCTION

The evolution of spectral functions near a Mott transition is a long standing problem in the physics of strongly interacting fermions. Recently some progress has been made using a dynamical mean field method. This approach dates back to the mid seventies under names such as dynamical coherent potential approximation (CPA) or local approximation. It received substantial attention following the pioneering paper of Metzner and Vollhardt [1] pointing out the correct scaling of the hopping integrals necessary to obtain a well defined limit of large lattice coordination.

A very useful formulation of the mean field approach is based on viewing a lattice model impurity embedded in a medium obeying a self-consistency condition. For the Hubbard model, the corresponding impurity model is the Anderson model [2]. Other models of strongly correlated electrons are associated with other impurity models subject to different self-consistency conditions [3].

This method is very powerful because several numerical and analytical techniques which have been developed to analyze impurity models over the years can be implemented to solve the mean field equations. Several approaches have been used successfully for this purpose: qualitative analysis of the mean field equations [2], quantum Monte-Carlo methods [4–6], iterative perturbation theory [2,7], exact diagonalization methods [8], and the projective self-consistent method, a renormalization technique [9].

In this note we present a pedagogical discussion of the main ideas behind the mapping from lattice onto impurity models stressing the generality of the approach and its intuitive character. Then, we will review some aspects of the evolution of the spectral function of the Mott insulator at low temperatures. In this context a new scheme which allows to perform iterative perturbation theory away from half filling will be introduced and compared with results from exact diagonalization.

2. FROM LATTICE MODELS TO IMPURITY MODELS

The starting point of this section is a lattice model of strongly correlated electrons containing various orbitals per unit cell. We use a compact notation where the index $\alpha = (m, \sigma)$ combines the orbital m and the spin σ . The starting Hamiltonian, which could in principle be obtained from an *ab initio* constrained LDA calculation after a suitable folding to low energies as in Ref. [10] or from physical considerations is assumed to be of the form:

$$H_{\text{lattice}} = - \sum_{\langle ij \rangle} c_{i\alpha}^{\dagger} t_{i\alpha, j\beta} c_{j\beta} + \sum_i (E_{\alpha\beta} - \mu \delta_{\alpha\beta}) c_{i\alpha}^{\dagger} c_{i\beta} + \sum_i \Gamma_{\alpha\beta\gamma\delta} c_{i\alpha}^{\dagger} c_{i\beta} c_{i\gamma}^{\dagger} c_{i\delta} \quad (1)$$

Now we focus on a single unit cell and integrate out all degrees of freedom except for those which reside in the selected unit cell. These are described by operators c_{α} and no longer carry a site index. The dynamics of the resulting problem are described by an impurity model which describes an impurity c_{α} coupled to a bath of fermions ($a_{b\mu}$) (see Fig. 1):

$$H_{\text{imp}} = \sum_{\alpha\beta} (E_{\alpha\beta} - \mu \delta_{\alpha\beta}) c_{\alpha}^{\dagger} c_{\beta} + \sum_i \Gamma_{\alpha\beta\gamma\delta} c_{\alpha}^{\dagger} c_{\beta} c_{\gamma}^{\dagger} c_{\delta} + \sum_{b\mu} \epsilon_{b\mu} a_{b\mu}^{\dagger} a_{b\mu} + \sum_k (V_{b\mu, \alpha} a_{b\mu}^{\dagger} c_{\alpha} + h.c.) \quad (2)$$

From the impurity model we can obtain all the local correlation functions, since by construction the local lattice Green's functions are identical to the impurity Green's function $\hat{G} = (G_{\alpha, \beta})$. We use a matrix notation so that the local Green's function is given by

$$G_{\alpha, \beta}(\tau - \tau') = - \langle T_{\tau} c_{\alpha}(\tau) c_{\beta}^{\dagger}(\tau') \rangle \quad (3)$$

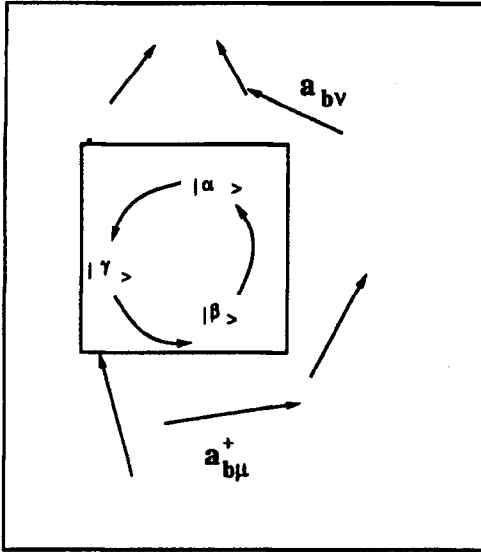


Fig. 1. Illustration of the unit cell containing the local degrees of freedom and the rest of the crystal treated as a bath. In the selected unit cell, different correlated configurations are fluctuating. Non interacting electrons describe the effective medium.

This should be viewed as a functional of the parameters $\epsilon_{b\mu}$ and $V_{b\mu,\alpha}$. To determine these parameters we construct the “Weiss field” which describes the effect of the rest of the electrons on the selected cell, $\hat{G}_0^{-1}(i\omega_n) = (i\omega_n + \mu)\hat{I} - \hat{E} - (\sum_{b\mu} \frac{V_{b\mu,\alpha}V_{b\mu,\beta}}{i\omega_n - \epsilon_{b\mu}})$, and the self energy of the impurity, $\hat{\Sigma}(i\omega_n) = \hat{G}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$, viewed as a functional of $\epsilon_{b\mu}$ and $V_{b\mu}$. These parameters are determined by requiring that the bath and the local degrees of freedom describe the electrons in the original lattice problem. Namely we can construct the local Green’s function from the lattice Green’s function obtained by adding a k independent self energy to the non interacting lattice Green’s function (obtained from eqn (1) by setting the interaction terms to zero) or from the impurity model.

$$\hat{G}(i\omega_n) = \sum_k \left((i\omega_n + \mu)\hat{I} - \hat{t}(k) - \hat{\Sigma}(i\omega_n) - \hat{E} \right)^{-1} \quad (4)$$

Notice that the mean field equations for all the models in [3] are particular cases of eqns (2) and (4).

3. IPT AWAY FROM HALF FILLING

To make progress one needs a practical and accurate technique for solving the system of eqn (4). The computational requirements of the exact diagonalization and the quantum Monte-Carlo methods are such that they can only be implemented for very simple Hamiltonians. To carry out realistic calculations it is necessary to have an accurate but fast algorithm for solving the Anderson impurity model. Here we introduce a new perturbative method and illustrate it by

applying it to the Hubbard model (one band per unit cell) away from half filling.

The approach is in the spirit of the iterative perturbation theory approach introduced in [7,12]. The key idea is to search for a self energy as a functional of the “Weiss field” such that the self energy expression becomes exact both in the weak and in the strong coupling limit. Moreover, it should have the correct behavior both at small and at large frequencies. The naive extension of the method originally proposed for half filling fails to give reasonable results for finite doping. However, we propose a generalization to arbitrary filling by constructing a self energy expression which has the correct behavior in the limits discussed above:

$$\sum^{(2)}(\omega) = \frac{\frac{n(1-n)}{n_0(1-n_0)} \sum_0^{(2)}(\omega)}{1 - \frac{(1-n)U - \mu + \tilde{\mu}_0}{n_0(1-n_0)U^2} \sum_0^{(2)}(\omega)} \quad (5)$$

Here $\sum_0^{(2)}(\omega)$ is the normal second order contribution to the self energy evaluated by the bare Green’s function $G_0(\omega) = \frac{1}{\omega - \tilde{\mu}_0 - \tilde{\rho}G(\omega)}$ (Bethe lattice). The parameter $\tilde{\mu}_0$ is determined such that the Luttinger theorem is fulfilled ($\mu_0 = \mu - Un - \sum^{(2)}[\tilde{\mu}_0](\omega=0)$, $\mu_0 = \mu|_{U=0}$). The particle number is given by $n = \frac{1}{\pi} \int_{-\infty}^0 \text{Im}G(\omega)d\omega$. In analogy, n_0 is a fictitious particle number computed from G_0 . The self-consistency condition becomes

$$G^{-1}(\omega) = G_0^{-1}(\omega) - \tilde{\mu}_0 + \mu - Un - \sum^{(2)}(\omega). \quad (6)$$

For the numerical implementation, it is more convenient to fix $\tilde{\mu}_0$ (rather than μ). Then, starting with a guess for G and μ , one can compute G_0 , n_0 and n . Afterwards eqn (5) yields $\sum^{(2)}(\omega)$, and we obtain a new μ from the Luttinger theorem. The loop is closed by eqn (6).

It is easy to check that in the case of half filling the procedure reduces to ordinary IPT. In the weak coupling limit eqn (5) is exact to order U^2 . Moreover, it can be verified that the expression becomes also exact for $U \rightarrow \infty$. The correct low frequency behavior is realized by satisfying the Luttinger theorem. This is the main difference with an earlier scheme which uses related ideas [11] and is essential to obtain good agreement with the exact diagonalization results at low temperatures.

We establish the accuracy of our method by comparing it with results obtained using the exact diagonalization algorithm to solve the impurity model, as described by Caffarel and Krauth [8]. Both methods are in close agreement when used on the imaginary axis. The real advantage of combining our perturbation scheme with the exact diagonalization is shown when we display the spectral functions obtained by these two methods on the real axis (Fig. 2).

It is clear that the exact diagonalization is doing its best in producing the correct spectral distribution. But it is unable to give a smooth density of states. Instead several sharp structures occur as a consequence of treating only a finite number of orbitals in the Anderson model.

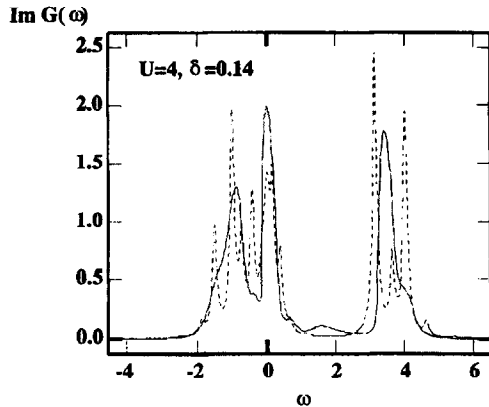


Fig. 2. $\text{Im}G(\omega)$ at $T = 0$ for $U = 4D$ and hole doping $\delta = 0.14$: iterative perturbation theory (full line) vs exact diagonalization (dashed line).

As an example, Fig. 3 shows the evolution of the spectral density of the doped Mott insulator with increasing hole doping δ . The qualitative features are those expected from the spectra of the single impurity [2] and are in agreement with the quantum Monte-Carlo calculations [13]. For small doping, there is a clear resonance peak at the fermi level. As δ is increased, the peak broadens and is shifted through the lower Hubbard band. At the same time the weight of the upper band decreases.

The most striking feature of the evolution of the spectral function as a function of doping is the finite shift of the Kondo resonance from the insulating band edge as the doping goes to zero. It was demonstrated analytically that this is a genuine property of the exact solution of the Hubbard model in infinite dimensions using the projective self-consistent method [14] and is one of the most striking properties of the Hubbard model in large dimensions. This feature did not appear in the earlier studies of Hubbard model in large dimensions using Monte-Carlo techniques [13] at high temperatures, and is also not easily seen in exact diagonalization algorithms [15].

4. CONCLUSIONS

The dynamical mean field approach is widely applicable to the one particle spectroscopy of correlated electrons. The mean field equations are tractable and contain rather rich information. A very important lesson is that it is necessary to use a combination of analytical and numerical techniques to obtain reliable results on the physical content of the mean field theory. This was illustrated in a discussion of the spectral function of the doped Mott insulator. In this context, we reported briefly a new perturbation scheme which allows to perform IPT away from half filling. This

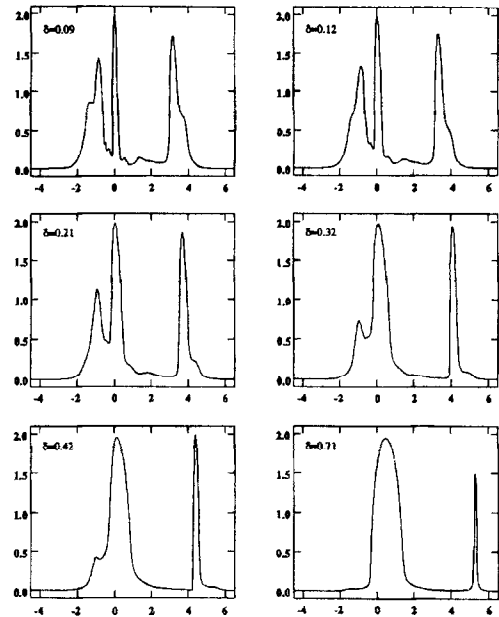


Fig. 3. Evolution of the spectral function for $U = 4$ and $T = 0$ with increasing hole doping δ .

approach is very economical and promising and has already been extended to systems with more complex units cells, as will be reported elsewhere.

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