A New Iterative Perturbation Scheme for Lattice Models with Arbitrary Filling

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We derive a new perturbation scheme for treating the large d limit of lattice models at arbitrary filling. The results are compared with exact diagonalization data for the Hubbard model and found to be in good agreement.

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1. INTRODUCTION

In recent years there has been a renewed interest in the study of doped transition metal oxides like $La_{1-x}Ti_xO_2$. These materials exhibit interesting phenomena like the correlation induced metal insulator transition. Although there are several experimental data available right now [1] it is still quite difficult to tackle these substances theoretically. Realistic models have to take into account several bands and are to be explored at finite doping.

The most promising way towards a theoretical description, perhaps, is the limit of large spatial dimensions [4], which defines a dynamical mean field theory for the problem. This limit can be mapped onto an impurity model together with a selfconsistency condition which is characteristic for the specific model under consideration [1]. The mapping allows to apply several numerical and analytical techniques which have been developed to analyse impurity models over the years. There are different approaches which have been used for this purpose: qualitative analysis of the mean field equations [3], quantum Monte Carlo methods [4], iterative perturbation theory (IPT) [4], exact diagonalization methods [4], and the projective self-consistent method, a renormalization technique [1]. However, each of these methods has its shortfalls. While quantum Monte Carlo calculations are not applicable in the zero temperature limit, the exact diagonalization methods and the projective self consistent method yield only a discrete number of poles for the density of states. Moreover, the computational requirements of the exact diagonalization and the quantum Monte Carlo methods are such that they can only be implemented for the simplest Hamiltonians. To carry out realistic calculations it is necessary to have an accurate but fast algorithm for solving the Impurity model.

In this context iterative perturbation theory has turned out to be a useful and reliable tool for the case of half filling [3,4]. However, for finite doping the naive extension of the IPT scheme is known to give unphysical results. There is still no method which can be applied away from half filling and which at the same time is powerful enough to treat more complicated models involving several bands.

The aim of this paper is to close this gap by introducing a new iterative perturbation scheme which is applicable at arbitrary filling. For simplicity, we treat the single band case here. But we believe that the ideas can be generalized to more complicated models involving several bands.

The (asymmetric) Anderson impurity model

$$\begin{align*}
H_{imp} &= \epsilon_f \sum_{\sigma} f_{\sigma}^+ f_{\sigma} + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} \\
&+ \sum_{k} V_k (c_{k\sigma}^+ f_{\sigma} + f_{\sigma}^+ c_{k\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} 
\end{align*}$$

(1)

describes an impurity ($f_{\sigma}$) coupled to a bath of conduction electrons ($c_{k\sigma}$). The hybridization function is given by $\Delta(\omega) := \sum_{k} \frac{V_k^2}{\omega - \epsilon_k}$. Once a solution is known for arbitrary parameters a large number of lattice models can be solved by iteration. An example is the Hubbard Hamiltonian:

$$H = -\frac{t}{\sqrt{2}} \sum_{\langle ij \rangle,\sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

(2)

which can actually serve as an effective Hamiltonian for the description of doped transition metal oxides [2]. On a Bethe lattice with infinite coordination number $z$ the Hubbard model is connected to the impurity model by the following selfconsistency condition:

$$\Delta(\omega) = t^2 G(\omega)$$

(3)

and $\epsilon_f = -\mu$. The mapping requires that the propagator of the lattice problem is given by the impurity Green function ($G = G_f$). Below we set $D := 2t = 1$.

In the next section we will derive the perturbation scheme for the impurity model. Afterwards the scheme is applied to the Hubbard model (section III). Some results for the doped system are presented and the accuracy of our scheme is discussed. We conclude with a summary and an outlook on further extensions (section IV).

II. DERIVATION OF THE APPROXIMATION SCHEME FOR THE SINGLE IMPURITY MODEL

In this section, we derive the approximate scheme which, given the hybridization function $\Delta(\omega)$ and the impurity level $\epsilon_f$, provides a solution of model (1). For simplicity, we assume that there is no magnetic symmetry breaking ($n_\sigma = n_{-\sigma} = n$). We also restrict us to zero temperature. The procedure is an extension of the ordinary IPT scheme to finite doping. The success of IPT at half filling can be explained by that it becomes exact not only in the weak but also in the strong coupling limit [13]. Moreover, this approach captures the right low and high frequency behavior so that we are dealing with an interpolation scheme between correct limits.

The idea of our approach is to construct a self energy expression which retains these features at arbitrary doping and reduces at half filling to the ordinary IPT result.

Ordinary IPT approximates the self energy by its second order contribution: $\Sigma(\omega) \approx U n + \Sigma_0^{(2)}(\omega)$ where

$$\begin{align*}
\Sigma_0^{(2)}(\omega) := U^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\rho^{(0)}(\epsilon_1) \rho^{(0)}(\epsilon_2) \rho^{(0)}(\epsilon_3)}{\omega + \epsilon_1 - \epsilon_2 - \epsilon_3 - i\eta} \\
+ U^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\rho^{(0)}(\epsilon_1) \rho^{(0)}(\epsilon_2) \rho^{(0)}(\epsilon_3)}{\omega + \epsilon_1 - \epsilon_2 - \epsilon_3 - i\eta}
\end{align*}$$

(4)

with $\rho^{(0)} = \frac{1}{\pi} \text{Im} G^{(0)}$. Here, the (advanced) Green function $G_0^{(0)}(\omega)$ is defined by...
\[ G_0(\omega) := \frac{1}{\omega + \tilde{\mu}_0 - \Delta(\omega)} \]

The parameter \(\tilde{\mu}_0\) is given by \(-\epsilon_f - Un\). In particular it vanishes at half filling. The full Green function follows from

\[ G_f(\omega) = \frac{1}{G_0^{-1} - \tilde{\mu}_0 - \epsilon_f - \Sigma(\omega)} \]

To ensure the correctness of this approximation scheme in different limits, we modify the self energy functional as well as the definition of the parameter \(\tilde{\mu}_0\).

We start with an ansatz for the self energy:

\[ \Sigma_{int}(\omega) = Un + \frac{A\tilde{\Sigma}_0^{(2)}(\omega)}{1 - B\tilde{\Sigma}_0^{(2)}(\omega)} \]

Here, \(\tilde{\Sigma}_0^{(2)}(\omega)\) is the normal second order contribution defined in equation (4). We determine the parameter \(A\) from the condition that the self energy has the exact behavior at high frequencies. Afterwards, \(B\) is determined from the atomic limit.

The leading behavior for large \(\omega\) can be obtained by expanding the Green function into a continuous fraction (15): \(G_f(k, \omega) = 1/(\omega - \epsilon_f - \alpha_1 - \frac{\alpha_2 - \alpha_1}{\omega + i\eta})\). Here, \(\alpha_1\) marks the \(i\)th order moment of the density of states. One can compute these quantities by evaluating a commutator (see [16]). We obtain for our model \(\tilde{\Sigma}(\omega)\) defined in equation (4). We determine the parameter \(A\) (see [16]). We obtain for our model \(\tilde{\Sigma}(\omega)\) defined in equation (4). We determine the parameter \(A\) (see [16]).

We introduce the Friedel sum rule (16):

\[ \frac{1}{2} \arctg \left( \frac{-\epsilon_f - \Sigma_{int}(0) - \Re\Delta(0)}{\Im\Delta(0)} \right) \]

\[ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \epsilon^{i\omega+0+G_f(\omega)} \frac{\partial\Delta(\omega)}{\partial\omega} \]

This statement, which is equivalent to the Luttinger theorem, \(\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \epsilon^{i\omega+0+G_f(\omega)} \frac{\partial\Delta(\omega)}{\partial\omega} = 0\), should be viewed as a condition on the zero frequency value of the self energy to obtain the correct low energy behavior. The use of the Friedel sum rule is the main difference to an earlier approximation scheme [14] and is essential to obtain a good agreement with the exact diagonalization method.

So far, we considered three different limits: strong coupling, zero frequency and large frequency. It remains to check the weak coupling limit. Taking into account that \(n = n_0\) and \(\tilde{\mu}_0 = -\epsilon_f\) for \(U = 0\), it follows that (14) is indeed exact to order \(U^2\).

The actual solution of the impurity model is determined by a pair \((\tilde{\mu}_0, n)\) which satisfies equations (4), (6), (8), (9), and (14). For the numerical implementation Broyden’s method [24], a generalization of Newton’s method, has been turned out to be very powerful. Defining two functions \(f_1(n, \tilde{\mu}_0) := n - \int_{-\infty}^{\infty} d\omega \Im G_0^{(2)}(\omega)\) and \(f_2(n, \tilde{\mu}_0) := n - n_{Friedel}\) the impurity problem can be solved by searching for the zeros of \(f_1\) and \(f_2\) \((n_{Friedel}\) is the particle number determined from the Friedel sum rule). The algorithm is very efficient as in most cases a solution is found within 4 to 10 iterations.

**III. APPLICATION TO THE HUBBARD MODEL**

After treating the Anderson impurity model, we now apply the perturbation scheme to the solution of the Hubbard model. Starting with a guess for \(\Delta(\omega)\) one can solve...
the impurity model using the scheme described above. This yields a propagator $G_f = G$, which can be used to determine a new hybridization function $\Delta(\omega)$ according to (3). The iteration is continued until convergence is attained. It is most accurate to perform the calculation first on the imaginary axis. Once the constants $A$ and $B$ in the interpolating self energy are determined in this way, they can be used to perform the iteration on the real axis.

In the case of the Hubbard model, the Luttinger theorem takes the simple form [21]

$$\mu_0 = \mu - \Sigma_{int}(\omega = 0), \quad \mu_0 := \mu|_{U=0}$$

This can be used to simplify the selfconsistency procedure if $\mu_0$ rather than $\mu$ is fixed. Starting with a guess for $G$ and $\mu$, one can compute $G_0$, $n$, and $n_0$. Afterwards (14) yields $\Sigma_{int}(\omega)$ and a new $\mu$ is obtained from (16).

To illustrate the accuracy of our method we compare it with results obtained using the exact diagonalization algorithm of Caffarel and Krauth [10]. Both methods are in close agreement when used on the imaginary axis (see figure 1). The real advantage of our perturbation scheme compared to the exact diagonalization is disclosed when we display the spectral functions obtained by these two methods on the real axis (figure 2).

$$\text{FIG. 1. Im } G(i\omega) \text{ at } T = 0 \text{ for } U = 4D \text{ and hole doping } \delta = 0.14: \text{ iterative perturbation scheme (full line) vs. exact diagonalization (dashed line)}$$

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

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.

Figure 3 shows the evolution of the spectral density of the doped Mott insulator ($U = 4D$) with increasing hole doping $\delta$. The qualitative features are those expected from the spectra of the single impurity [5] and are in agreement with the quantum Montecarlo calculations [22]. For small doping there is a clear resonance peak at the fermi level. As $\delta$ 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 density 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 [23] 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 Montecarlo techniques [22] at higher temperatures, and is also not easily seen in exact diagonalization algorithms [13].
FIG. 3. Evolution of the spectral function for $U = 4 D$ and $T = 0$ with increasing hole doping $\delta$

IV. DISCUSSION AND OUTLOOK

In this paper we introduced a new perturbation scheme for the solution of lattice models away from half filling. The basic idea is to construct an expression for the self energy which interpolates between correct limits. In the weak coupling limit our approximate self energy is exact to order $U^2$, and it is also exact in the atomic limit. The proper low frequency behavior is ensured by the Friedel sum rule (or, equivalently, the Luttinger theorem). This is important to obtain the right low energy features in the spectral density. The overall distribution of the density of states on the other hand is determined by the spectral moments, which are reproduced exactly up to second order by satisfying the proper large frequency behavior. In the light of these features it might not be too astonishing that we obtain a good agreement with the exact diagonalization method.

Since the algorithm described here is accurate and very fast (a typical run to solve the Hubbard model takes 60 seconds on a DEC alpha station 200 4/233) it has a wide range of applications. Two examples that come to mind are the effects of disorder on the Hubbard model away from half filling and the study of realistic models with orbital degeneracy. The latter is very important to make contact with realistic three dimensional transition metal oxides.

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