Fast impurity solver for dynamical mean field theory based on second order perturbation around the atomic limit*

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This paper proposes an impurity solver for the dynamical mean field theory (DMFT) study of the Mott insulators, which is based on the second order perturbation of the hybridization function. After careful benchmarking with quantum Monte Carlo results on the anti-ferromagnetic phase of the Hubbard model, it concludes that this impurity solver can capture the main physical features in the strong coupling regime and can be a very useful tool for the LDA (local density approximation) + DMFT studies of the Mott insulators with long range order.

Keywords: dynamical mean field theory, impurity solver, Mott insulator, antiferromagnetic order

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1. Introduction

Mott insulators are insulators which are caused by electron–electron interaction rather than the crystal structure. In sufficient low temperatures, long range spin or orbital order will be established to get rid of the remaining entropy induced by the unfrozen spin or orbital degree of freedoms. Various types of interesting long range order may appear in different systems, i.e. the anti-ferromagnetic (AF) order, the non-collinear spin order as well as the orbital ordering states. The fruitfulness of the long range orders in the Mott insulator phases is a consequence of the detailed balance among electron kinetic energy, interaction energy and the spin–orbital coupling in the solid. Therefore the *ab initio* study of the Mott insulators is very crucial to achieve quantitative understanding about these materials.

While the first principle calculations for the Mott insulators based on local density approximation (LDA) always encounter problems generated by the strong correlation effect among those partially occupied localized orbitals in these materials. For example, the LDA calculation incorrectly predicts two typical Mott insulators NiO and FeO to be metallic. This is due to the fact that the non-interacting form of the LDA type wave function cannot capture the electron correlation effect, especially the strong on-site correlation effect in the relatively local orbitals such as 3d or 4f orbitals. Although LDA underestimates the strong correlation effects in these materials, it still describes quite well the long range Coulomb interaction and those less correlated s p bands. Therefore a very efficient way to solve this problem is to implement the LDA with some many-body techniques which can treat the correlation effect better. The first example of such a scheme is the LDA+U (Hubbard parameter U) method,[1] in which the Hartree–Fock mean-field (MF) treatment is adopted to capture the orbital physics. The LDA+U method can correctly describe many Mott insulators, i.e. the YVO_3 and $LaVO_3$.[2] Since the wave function in LDA+U is still the single Slater determinant, it can only capture the static orbital or spin correlation but not the dynamical correlation effect. Another attempt is the LDA+ G (Gutzwiller) method proposed very recently by two of the authors, where the Gutzwiller variational approach[3,4] is used to take into account the correlation effect. The LDA+ G is superior to LDA+U in the sense that the dynamical correlation effect can be taken into account by the multi-configuration nature of the Gutzwiller trial wave function. However, LDA+ G is still very difficult to be used in the finite temperate problems because it is a variational

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method.

In the past twenty years, the dynamical mean-field theory (DMFT)[5] has been quickly developed to be a powerful method to solve the strongly correlated models on the lattice. The DMFT maps the lattice models to the corresponding quantum impurity models with the environment to be determined self-consistently by the DFMT self-consistent equations. The DMFT keeps the full local dynamics induced by the local interaction and has been successfully applied to various correlation systems, such as the Mott transition in Hubbard model,[6,7] the pseudo gap behaviour in high T_c cuperates[8] as well as the heavy fermion system.[9,10] Combined with LDA, the LDA+DMFT has quickly become a very useful numerical tool for the first principle studies of strongly correlated materials, which has been successfully applied to many strongly correlated materials.

The nuclei of DMFT is to solve the Anderson impurity model introduced by the DMFT self-consistent procedure. The solver could be either numerical and analytical. The most popular two numerical solvers are exact diagonalization[11,12] method and Hirsh–Fye quantum Monte Carlo.[13−15] Besides, the continuous-time quantum Monte Carlo (CTQMC) solver[16−19] has also been developed recently and greatly boosted the progress in this field. However, the numerical methods are often very time-consuming and for large systems it is better to use some analytical solver which is much faster and can capture the basic physics as well. The analytical solvers include Hubbard-I approximation,[20,21] the equation of motion (EOM) method,[22] the iterative perturbation theory,[23,24] the fluctuation exchange approximation (FEA)[25,26] and the non-crossing approximation.[27−29] Among them the Hubbard-I solver, which simply takes the atomic self-energy, is very convenient and easy to be implemented in the existing *ab initio* codes. Since it can capture the atomic multiplet effect (Hubbard bands) in a very efficient way, the Hubbard-I solver has been widely used to study the paramagnetic Mott insulators. While the Hubbard-I solver cannot be directly applied to the Mott insulator states with long range order, simply because the atomic self-energy does not contain any information about the long range order in the system. The way to solve this problem is to go beyond the atomic approximation and include the leading order corrections from the heat bath as well.

A second order strong coupling expansion solver has been developed by one of the authors.[30] Although the long range ordering temperature can be correctly calculated by using this solver, it also suffers from the following facts. i) Because the strong coupling expansion is based on the atomic limit without long range order, it is not valid to treat the systems with large order parameter, i.e. the AF phase in low temperature with the fully developed AF order. ii) Due to the multiple summation over the configuration space, the calculation is still quite heavy for the multi-orbital system especially the f-electron system.

In order to overcome the above two problems, in this paper we propose a new scheme to include leading order corrections from the heat bath. The idea is quite simple, we use the second order perturbation theory to correct the energy level of each atomic eigen-states, then we construct the "atomic" Green's function and the corresponding self-energy on a single site based on the re-normalized atomic eigen-energy. With the above procedure, we can obtain the main contribution of the heat bath to the self-energy in the Mott insulator case, which is the re-normalization of the eigen-energy of the atomic configurations. Because only the eigen-energy not the occupation of the atomic configurations is treated by second order perturbation, the present method can be applied to very low temperature with quite large order parameters. With the present impurity solver the static inter-site spin or orbital correlation, such as the super-exchange process, can be taken into account. Compared with the previous atomic expansion solver, this solver does not have multiple summations over the atomic configurations, which make it very fast and is more suitable for the study of the f-electron systems.

The paper is organized as follows. We will present the detailed formalism of the impurity solver in Section 2. After that in Section 3, we will do benchmark on both paramagnetic and anti-ferromagnetic Mott insulator phases in the Hubbard model. And finally we will carefully discuss the results and make the conclusion.

2. Derivations

2.1. General formalism

The crucial part of the DMFT is to solve the quantum impurity model with the following Hamiltonian:

$$H_{\rm imp} = \sum_l \epsilon_l c_l^\dagger c_l + \sum_{lm}(V_{lm} f_m^\dagger c_l + {\rm h.c.}) + \sum_{mm'} t_{mm'} f_m^\dagger f_{m'} + \frac{1}{2}\sum_{mnpq} U_{mnpq} f_m^\dagger f_n^\dagger f_q f_p. \quad (1)$$

The above expression is a general form of the multi-orbital Anderson impurity model with arbitrary local interactions as well as the heat bath introduced by DMFT self-consistent procedure. In this Hamiltonian, m, m' and n, p, q are the combined spin and orbital indices respectively, while l denotes the energy levels in the heat bath.

In the LDA+DMFT study, we often need a fast impurity solver which can capture the most important features of the impurity problem. For the Mott insulators, such a fast solver can be constructed by doing perturbation around the atomic limit. In the present paper, we apply the "contour integral" technique to obtain the electron Green's function.[27,28] The retarded form of the electron Green's function on the impurity site can be written as

$$G_f^{mm'}(\omega+{\rm i}\eta) = \frac{1}{\mathcal{Z}}\oint_c \frac{{\rm d}z}{2\pi{\rm i}} {\rm e}^{-\beta z}\sum_{\alpha\beta}(F^m)_{\alpha\beta}(F^{m'\dagger})_{\beta\alpha} \times P_\beta(z)\Pi_{\beta,\alpha}(z, z+\omega+{\rm i}\eta) \times P_\alpha(z+\omega+{\rm i}\eta), \quad (2)$$

$$\mathcal{Z} = \oint_c \frac{{\rm d}z}{2\pi{\rm i}} {\rm e}^{-\beta z}\sum_\alpha P_\alpha(z). \quad (3)$$

In the above equations, c is a contour in the complex plane, oriented counterclockwise, and surrounding all singularities of the resolvent $(z-H_{\rm loc})^{-1}$, where $H_{\rm loc}$ is the local part of $H_{\rm imp}$; α denotes the α-th eigen-state of $H_{\rm loc}$ with the eigenvalue of E_α; $(F^m)_{\alpha\beta}$ is the matrix element of local fermion operator f_m; $\Pi_{\beta,\alpha}(z, z+\omega+{\rm i}\eta)$ is a proper vertex function to be discussed below; $\mathcal{Z}$ is the partition function of the impurity problem and $P_\alpha(z)$ can be viewed as the "propagator" of the atomic eigen-states. In the absence of hybridization $P_\alpha(z)$ takes the simple form of $P_{\alpha,0}(z) = 1/(z-E_\alpha)$. Taking the hybridization part into account, we can express $P_\alpha(z)$ as

$$P_\alpha(z) = 1/(z - E_\alpha - \Sigma_\alpha(z)), \quad (4)$$

where $\Sigma_\alpha(z)$ can be viewed as the self-energy of the α-th local configuration that comes from the hybridization between the impurity site and the bath.

In order to evaluate $\Sigma_\alpha(z)$, we use the heuristic method from the techniques in the large-N expansion. The self-energy can be expressed in a diagrammatic way as it is introduced in detail in the review of Bickers.[31] In this paper, we focus on the Mott insulator system, which only requires the lowest order diagram as shown in Fig. 1.

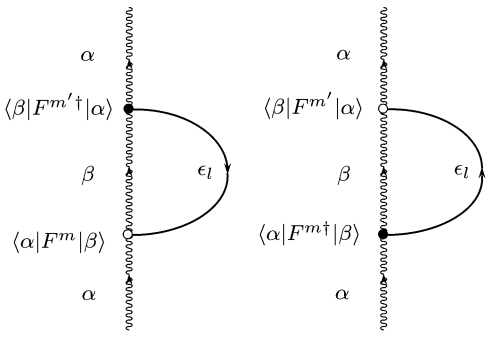


Fig. 1. The diagrams of the lowest order contribution to the self-energy of local atomic states. The wave lines denote the propagators of atomic states, the continuous lines the propagator of electrons in the heat bath, and each vertex corresponds to an element of a local Fermion operator with the coupling strength V.

The expression of self-energy corresponding to the above diagram is

$$\Sigma_\alpha(z) = \sum_\beta\sum_l\sum_{mm'}\frac{(F^m)_{\alpha\beta}(F^{m'\dagger})_{\beta\alpha}V^*_{lm'}V_{lm}}{z-E_\beta+\epsilon_l}f(\epsilon_l) + \sum_\beta\sum_l\sum_{mm'}\frac{(F^{m\dagger})_{\alpha\beta}(F^{m'})_{\beta\alpha}V^*_{lm}V_{lm'}}{z-E_\beta-\epsilon_l}f(-\epsilon_l)$$
$$= \left(-\frac{1}{\pi}\right)\sum_\beta\sum_{mm'}\left[(F^m)_{\alpha\beta}(F^{m'\dagger})_{\beta\alpha}\int\frac{\Delta''_{m'm}(-\epsilon)f(-\epsilon)}{z-E_\beta-\epsilon}{\rm d}\epsilon + (F^{m\dagger})_{\alpha\beta}(F^{m'})_{\beta\alpha}\int\frac{\Delta''_{mm'}(\epsilon)f(-\epsilon)}{z-E_\beta-\epsilon}{\rm d}\epsilon\right], \quad (5)$$

where $f(\epsilon_l)$ is the fermi distribution function, while

$$\Delta_{mm'}(\omega+{\rm i}\eta) = \sum_l\frac{V^*_{lm}V_{lm'}}{\omega+{\rm i}\eta-\epsilon_l} \quad (6)$$

is the hybridization function in the DMFT and its imaginary part is denoted as

$$\Delta''_{mm'}(\epsilon) = \mathrm{Im}[\Delta_{mm'}(\epsilon + \mathrm{i}\eta)] \tag{7}$$

in Eq. (5).

Afterwards, for the sake of a simplest self-consistent approximation that provides a soluble set of equations, the vertex function in Eq. (2) could be set

$$\Pi_{\alpha,\alpha'}(z, z') \equiv \mathbf{1}, \tag{8}$$

and we get the final expression of $G_f^{mm'}(\omega + \mathrm{i}\eta)$ in Eq. (2).

The local electrons' quasi-particle spectrum functions are the direct result of the retarded form of the Green's functions.

For a given Hamiltonian as Eq. (2), one may use the equations above to evaluate the Green's function. Implemented with the DMFT self-consistent condition described in Ref. [5], this method can be used as an impurity solver in the DMFT study of the multi-orbital systems with complicated local interactions.

2.2. Single pole approximation

The method shown above works well for the Mott insulator phase, and a few results will be shown in the next section. However, here we introduce a further approximation which makes the impurity solver much faster and more convenient. The main idea of this approximation can be interpreted as follows. For a Mott insulator solution in DMFT with long range order, the most important effect of the heat bath is to modify the effective energy level of the atomic configurations. Therefore in the present paper, we only consider the effect of heat bath in the renormalization of the atomic levels, but neglect the possible broadening of the atomic levels.

With the above consideration, equation (4) can be approximated as

$$\begin{aligned} P_\alpha(z) &= 1/(z - E_\alpha - \Sigma_\alpha(z)) \\ &\approx 1/(z - E_\alpha - \mathrm{Re}[\Sigma_\alpha(E_\alpha)]) \\ &\equiv 1/(z - \tilde{E}_\alpha), \end{aligned} \tag{9}$$

where $\tilde{E}_\alpha \equiv E_\alpha + \mathrm{Re}[\Sigma_\alpha(E_\alpha)]$ is the renormalized atomic level containing the second order correction of the hybridization function. Because the Green's function $P_\alpha(z)$ contains only one pole at $\tilde{E}_\alpha$, as the same form in unperturbed case, we call it "single pole approximation". Thus the electron Green's function can be written in a similar form as the atomic Green's function

$$\begin{aligned} G_f^{mm'}(\omega + \mathrm{i}\eta) = \frac{1}{Z_f} \sum_{\alpha\beta} (F^m)_{\beta\alpha} (F^{m'\dagger})_{\alpha\beta} \\ \times \frac{1}{\omega + \mathrm{i}\eta + \tilde{E}_\beta - \tilde{E}_\alpha} \\ \times \left[\mathrm{e}^{-\beta\tilde{E}_\beta} + \mathrm{e}^{-\beta\tilde{E}_\alpha}\right], \end{aligned} \tag{10}$$

where the partition function is $Z_f = \sum_\alpha \mathrm{e}^{-\beta\tilde{E}_\alpha}$. Correspondingly, the self-energy that comes from local two-particle interactions becomes

$$\Sigma(\omega + \mathrm{i}\eta) = \omega + \mathrm{i}\eta + \mu - \hat{t} - G_f^{-1}. \tag{11}$$

This self-energy can be implemented in the DMFT self-consistent loop and we obtained a fast impurity solver for the Mott insulators with the long range order fully developed. With the current approximation, the DMFT here is equivalent to a generalized static mean field approximation using the local many-body bases. The spontaneous symmetry breaking can be well described by the difference in energy and occupation for atomic configurations which can be connected by symmetry, i.e. the singly occupied spin-up and spin-down states in the one-band Hubbard model. Therefore the super-exchange process can be thus captured through the self-consistent determination of the hybridization function in the DMFT loop.

3. Results and discussion

3.1. Single band, paramagnetic phase

The spectral function of one-band Hubbard model with various local repulsive energy U at half filling is plotted in Fig. 2. It works on the Bethe lattice with the semicircular density of states

$$D(\epsilon) = \frac{1}{2\pi t^2}\sqrt{4t^2 - \epsilon^2}, \quad |\epsilon| < 2t, \tag{12}$$

where $t = 0.5$ as usual. Here we do not use the "single pole approximation", which means that equation (5) is implemented. As a perturbation method around atomic limit, we echo the fact that this kind of solver is limited to integer filling and large U,[30] that is, the present solver is just good to study in the regime of Mott insulating state.

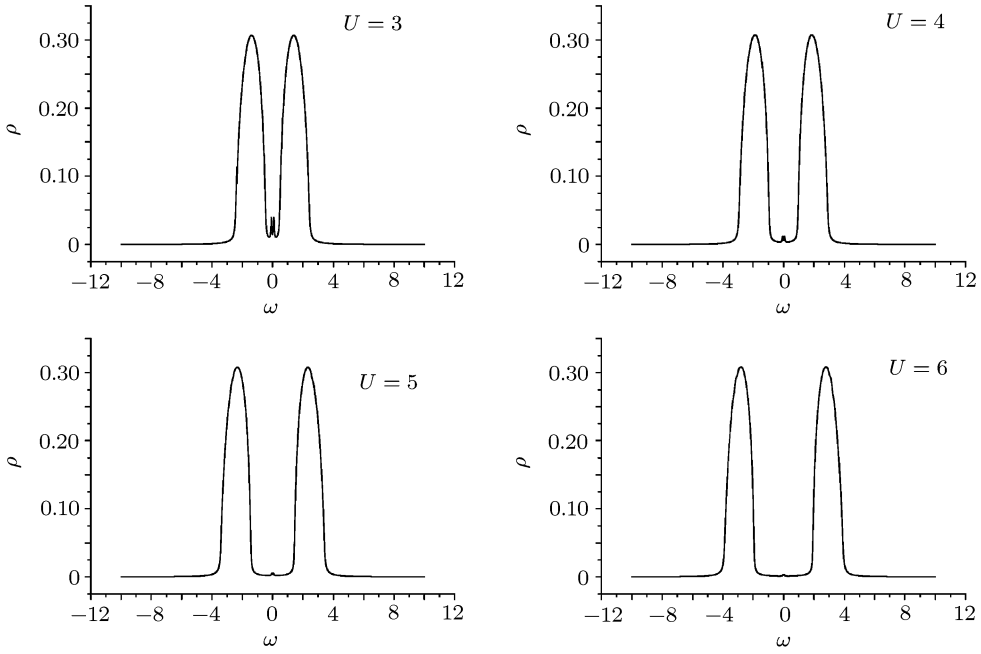


Fig. 2. The spectral function of single band Hubbard model on the Bethe lattice at half filling for various values of U, the energy unit is chosen as $D = 2t = 1$.

As a comparison, we also exhibit the result of the present solver with and without single pole approximation compared with that of DMFT+NRG (numerical renormalization group),[32] see Fig. 3. It shows that the result of present solver at large U regime agrees well with that of NRG, and the single pole approximation captures the main features of the Hubbard bands.

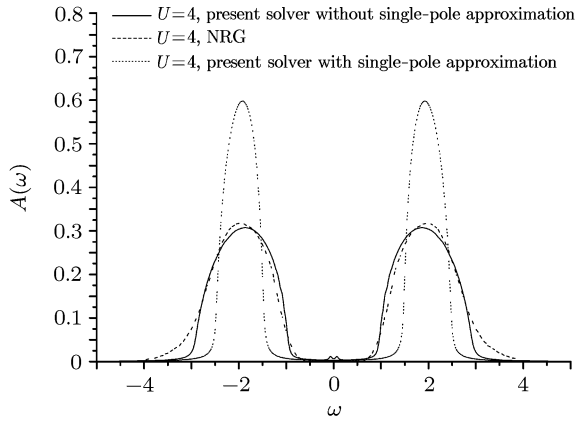


Fig. 3. The spectral function for $U = 4$ on the Bethe lattice compared with DMFT+NRG, the energy unit is chosen as $D = 2t = 1$.

3.2. Single band, antiferromagnetic–paramagnetic phase transition

In this section, we study the antiferromagnetic (AF)–paramagnetic phase transition in the single band Hubbard model at half filling. (For the case that the antiferromagnetic phase that deviates from half filling, see some DMRG results.[33–35]) We focus on the AF order parameter $m = \langle n_\uparrow - n_\downarrow \rangle$ on a given sublattice the Néel temperature. Henceforth we use the single pole approximation, with the self-energy in Eq. (11). First we study the single band Hubbard model on the Bethe lattice with the semicircular density of state.

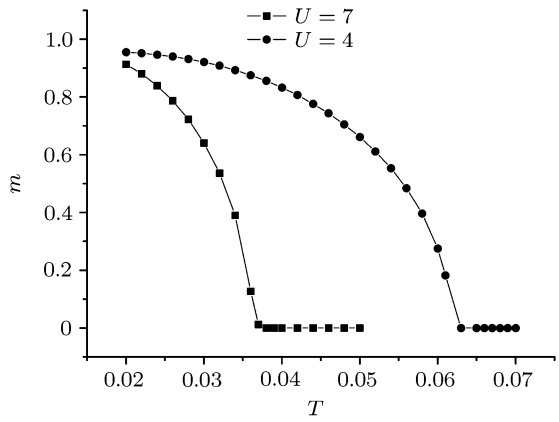


Fig. 4. The sublattice magnetization m versus temperature T for $U = 4, 7$, the energy unit is chosen as $D = 2t = 1$.

Figure 4 shows the magnetization m on one sublattice versus temperature T for $U = 4$ and $U = 7$. The curves show that the phase transition is of second order, and the critical temperatures are about

$T_c = 0.061$ for $U = 4$ and $T_c = 0.037$ for $U = 7$ respectively. Likewise, we get T_c under different U and plot them in Fig. 5. This result is comparable to that of DMFT+QMC (quantum Monte Carlo) in large U regime, as it is expected.

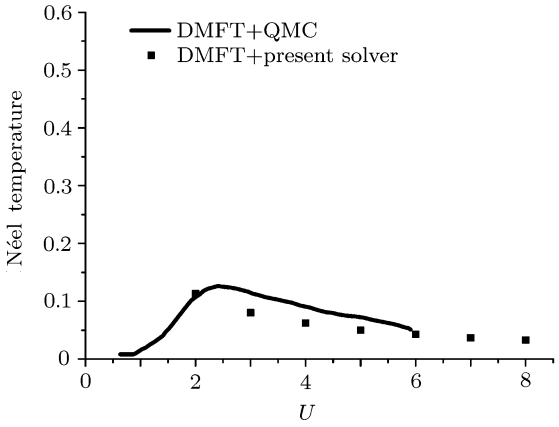


Fig. 5. The comparison of the Néel temperature obtained by DMFT+QMC (thick line) and present solver (circle dots) on the Bethe lattice at half filling. The half band width is used as the energy unit by defining $D = 2t = 1$.

We also apply this method to estimate the Néel temperature on the 3-dimensional (3D) isotropic simple cubic lattice. As the dispersion relation is $E(\boldsymbol{k}) = 2t(\cos k_x + \cos k_y + \cos k_z)$, we choose $t = 1/6$ to ensure that the half band width equals 1. It is known that, in the large U limit, on the 3D cubic lattice, the Hubbard model is equivalent to a Heisenberg model with an antiferromagnetic coupling J, and the relation between the parameters reads $J = 4t^2/U$.[36] Accordingly, the correct Néel temperature of the model is $T_N = 3.83t^2/U$,[37] while the Weiss mean field gives the result $T_N = 6t^2/U$.[38] Remember that we only take the lowest order of corrections to the local interactions, so the result should be close to the one of Weiss mean field, see Fig. 6. We have also plotted in this diagram the Hartree–Fock Neel temperature for the same model.[39] which is completely wrong in the large U limit.

It is intuitive to compare our results to that of the Heisenberg model, because the latter has been studied intensively. For example, we have compared the antiferromagnetic condensed energy. In the antiferromagnetic spin-wave theory for Heisenberg model, this condensed energy is $12.96t^2/U$ on 3D simple cubic lattice,[40] about twice as much as T_N of Weiss mean field. Here we have calculated the energy difference between antiferromagnetic and paramagnetic solutions, at a temperature of $0.002t$ which is sufficiently low and plotted it in Fig. 7 together with the condensation energy obtained by spin wave theory for the corresponding Heisenberg model. Our results are in good agreement with the spin wave theory which indicate that our method works very well even in low temperatures.

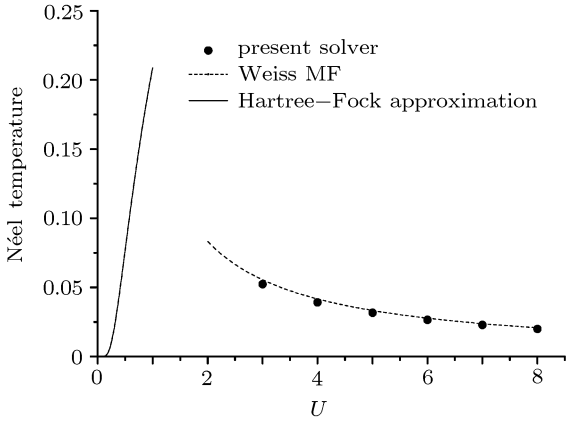


Fig. 6. The comparison of the Néel temperature obtained by Weiss MF (mean field) and present solver on the 3D cubic lattice at half filling. For cubic lattice the unit energy is chosen as the half band width $D = 6t = 1$.

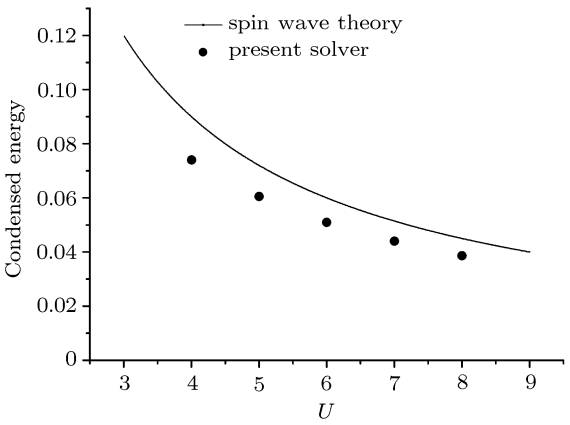


Fig. 7. The antiferromagnetic condensed energy compared with the spin-wave theory for Heisenberg model, where the unit energy is $D = 6t = 1$.

3.3. Two band, antiferromagnetic–paramagnetic phase transition

We have also studied antiferromagnetic–paramagnetic phase transition in the two-band Hubbard model at half filling, using DMFT with single pole approximation. Because there are two bands on one single site, the situation becomes much more complicated. Here we only consider the simplest case. First, we consider two-degenerate band, with semicircular density of states and the band width is set to be 1.

Second, we neglect the hopping between different orbits. Therefore the Hamiltonian can be written as[41]

$$\hat{H}_{\rm at} = U\sum_{b}\hat{n}_{b,\uparrow}\hat{n}_{b,\downarrow} + U'\sum_{\sigma,\sigma'}\hat{n}_{1,\sigma}\hat{n}_{2,\sigma'} - J\sum_{\sigma}\hat{n}_{1,\sigma}\hat{n}_{2,\sigma}. \quad (13)$$

There are three adjustable parameters above, which are U—the intra-band Coulomb repulsive energy, U'—the inter-band Coulomb energy, and J the interaction between different bands with the same spin. For $J > 0$, the third term on the right-hand side in Eq. (13) contains the Hund's coupling $-J'S_1^zS_2^z$ since $S^z = 1/2(n_\uparrow - n_\downarrow)$. The discussions below are based on this Hamiltonian.

Here we further assume $U - U' = 2J$, which is true for systems with the cubic symmetry.[42] The Néel temperatures versus various U obtained by us for $J = 0$ and $J = 1$ are shown in Fig. 8 respectively.

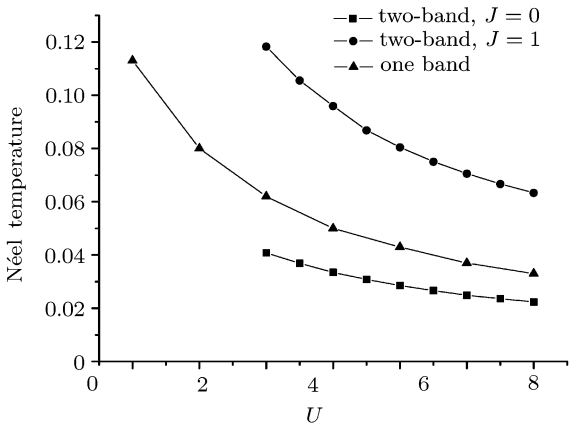


Fig. 8. Two-band model on the Bethe lattice under the condition of $U - U' = 2J$ for $J = 0$ and $J = 1$ respectively, compared with one-band result. The energy unit here for the Bethe lattice is chosen as $D = 2t = 1$.

The Néel temperature of two-band Hubbard model with $U = U'$ is lower than that of one-band model with the same U. This can be understood in the way that in a two-band system at half filling, there is AF order developed in two different orbitals. But there is no term to lock the relative fluctuation between them, which reduces its tendency to be antiferromagnetic. With non-zero Hund's rule coupling J, such relative fluctuation between AF order in different orbitals will be greatly suppressed, which results in the dramatic increment of the Néel temperature as shown in Fig. 8.

4. Conclusions

This paper presents a new impurity solver based on the perturbation theory in the hybridization around the atomic limit. For the sake of speed and convenience, we have introduced a further "single pole approximation" with which we carefully studied the antiferromagnetic–paramagnetic phase transition in one-band and two-band Hubbard model at half filling. The DMFT with the current impurity solver thus provides a way to do mean-field approximation with the atomic configurations rather than energy levels for the single particle states. Compared with the DMFT+QMC on the single band Hubbard model, the Neel temperature obtained by this new impurity solver fits quite well with the DMFT+QMC results, which indicates that LDA+DMFT studies can be very useful for Mott insulators.

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