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Generalization of iterative perturbation theory and coherent potential approximation (ITP+CPA) to double exchange model with orbital degeneracy*

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A combination of the iterative perturbation theory (ITP) of the dynamical mean field theory (DMFT) and coherent-potential approximation (CPA) is generalized to the double exchange model with orbital degeneracy. The Hubbard interaction and the off-diagonal components for the hopping matrix $t_{ij}^{mn}(m \neq n)$ are considered in our calculation of spectrum and optical conductivity. The numerical results show that the effects of the non-diagonal hopping matrix elements are important.

Keywords: iterative perturbation theory, coherent-potential approximation, dynamical mean field theory, optical conductivity

PACC: 7540, 7530V, 7530, 7130

1. Introduction

Perovskite-type manganese oxides $T_{1-x}D_xMnO_3$, where T and D denote alkaline- earth ion and rare-earth ion respectively, are being studied intensively. These compounds show a variety of interesting phenomena such as the colossal magnetoresistance,[1−4] which is caused by several competing interactions including spin, charge, and orbital degrees of freedom. Owing to the complexity of many-body problems and the strong correlation of particles, various approximate methods are used in the theoretical calculations.

One of the important methods to deal with the strongly correlated fermion systems is the DMFT[5] and its extensions, which are based on a mapping of lattice models onto quantum impurity models subjected to a self-consistency condition. This mapping is exact in the limit of infinite spatial dimension. There are several methods to calculate the Green's function in the DMFT such as the quantum Monte Carlo simulation,[6] the exact diagonalization, the numerical renormalization group, the non-crossing approximation (NCA) and the iterative perturbation theory (ITP).[5,7,8] However the NCA and the IPT are more easily combined with other computational schemes for real materials.

It is found that the ITP combined with the CPA can be used to deal with the double exchange model in a ferromagnetic metallic phase,[9] where the ITP is applied to the Hubbard interaction and the CPA is further used to the ferromagnetic Hund coupling between conduction electrons and localized spins. Because both the ITP and the CPA are based on local approximations, the CPA procedure is properly embedded in the self-consistent equations for the DMFT. Up to now the ITP+CPA is applied only to the models without orbital degeneracy. Since the manganese oxide is a strongly correlated electron system with the orbital degeneracy, it is needed to generalize this combination method to the multi-orbital case. This is the aim of this paper. In the multi-orbital case, the off-diagonal components of the hopping matrix $t_{ij}^{\alpha\beta}(\alpha \neq \beta)$ may play an important role in the manganese oxides,[10,11] so we also investigate its effects in our calculation.

2. Model and method

We study the following multi-orbital double exchange model with the Hubbard interaction, in which

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the Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{H}_K + \hat{H}_U, \tag{1}$$

where

$$\hat{H}_0 = \sum_{\langle ij\rangle\sigma}\sum_{\alpha\beta} t_{ij}^{\alpha\beta}(c_{i\sigma\alpha}^{+}c_{j\sigma\beta} + \text{h.c.}), \tag{2}$$

$$\hat{H}_K = -J_H \sum_{i\sigma\alpha} \sigma s_i n_{i\sigma\alpha}, \tag{3}$$

$$\hat{H}_U = U\sum_i \sum_{(\sigma\alpha)\neq(\sigma'\beta)} n_{i\sigma\alpha}n_{i\sigma'\beta}, \tag{4}$$

with i (j) being site index and $\alpha(\beta) = 1, 2$ orbital index, $\sigma = \uparrow, \downarrow$, and $n_{i\sigma\alpha} = c_{i\sigma\alpha}^{+}c_{i\sigma\alpha}$. The local spins are described as classical spins because the ferromagnetic order considerably suppresses quantum effects. The transfer integral $t_{ij}^{\alpha\beta}$ depends sensitively on the orbitals. In order to exploit the effects of the multi-orbital and the off-diagonal components of $t_{ij}^{\alpha\beta}$, we suppose

$$t_{ij}^{\alpha\beta} = -t\begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}, \quad -t\begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}, \quad -t\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{5}$$

for $\boldsymbol{r}_j = \boldsymbol{r}_i \pm \hat{x}$, $\boldsymbol{r}_j = \boldsymbol{r}_i \pm \hat{y}$, $\boldsymbol{r}_j = \boldsymbol{r}_i \pm \hat{z}$, respectively, where $\hat{x}$, $\hat{y}$ and $\hat{z}$ are the nearest-neighbouring distances along x, y and z directions, respectively. This form of $t_{ij}^{\alpha\beta}$ corresponds to that of double-exchange ferromagnet $La_{1-x}Sr_xMnO_3$.[12] The Fourier transform of $t_{ij}^{\alpha\beta}$ is

$$t_{\alpha\beta}^{\mathrm{H}}(k) = \begin{pmatrix} \varepsilon_0 + \varepsilon_1 & \varepsilon_2 \\ \varepsilon_2 & \varepsilon_0 - \varepsilon_1 \end{pmatrix}, \tag{6}$$

where

$$\begin{aligned} k &= (k_x, k_y, k_z), \\ \varepsilon_0 &= t(\cos k_x + \cos k_y + \cos k_z), \\ \varepsilon_1 &= \frac{t}{2}(\cos k_x + \cos k_y - 2\cos k_z), \\ \varepsilon_2 &= -\frac{\sqrt{3}t}{2}(\cos k_x - \cos k_y). \end{aligned} \tag{7}$$

The lattice constants as well as $\hbar$ are taken to be unity.

First, we consider $\hat{H}_0 + \hat{H}_U$ and treat the electron correlations due to the Hubbard interaction by making use of the ITP within the DMFT. The Green's function in an effective medium is defined as

$$G_{\sigma\alpha\beta}^{0\,-1}(\mathrm{i}\omega_n) = [\mathrm{i}\omega_n + \mu - \Delta_\sigma(\mathrm{i}\omega_n)]\delta_{\alpha\beta}. \tag{8}$$

The local Green's function is expressed as

$$G_{\sigma\alpha\beta}(\mathrm{i}\omega_n) = \left[G_{\sigma\alpha\beta}^{0\,-1}(\mathrm{i}\omega_n) - \sum\nolimits_{\sigma}^{U}(\mathrm{i}\omega_n)\right]_{\alpha\beta}, \tag{9}$$

where the self-energy $\sum_{\sigma\alpha\beta}(\mathrm{i}\omega_n)$ can be expressed as the following form that is a simple extension of Ref.[13]:

$$\sum\nolimits_{\sigma\alpha\beta}^{U}(\mathrm{i}\omega_n) = Un_{\bar{\sigma}\alpha}(N_{\deg}-1)\delta_{\alpha\beta} + \frac{A_{\sigma\alpha}\sum_{\sigma\alpha\beta}^{U(2)}(\mathrm{i}\omega_n)}{1 - B_{\sigma\alpha}(\mathrm{i}\omega_n)\sum_{\sigma\alpha\beta}^{(2)}(\mathrm{i}\omega_n)}, \tag{10}$$

where $N_{\deg} = 4$ is the degeneracy with respect to spins and orbitals,

$$A_{\sigma\alpha} = \frac{n_{\bar{\sigma}\alpha}(1-n_{\bar{\sigma}\alpha})}{n_{0\bar{\sigma}\alpha}(1-n_{0\bar{\sigma}\alpha})}, \tag{11}$$

$$B_{\sigma\alpha}(\mathrm{i}\omega_n) = \frac{\mathrm{i}\omega_n - \varepsilon_d^0 + \mu}{U^2(N_{\deg}-1)n_{0\bar{\sigma}\alpha}(1-n_{0\bar{\sigma}\alpha})} + \frac{A_{\sigma\alpha}(X-a)(X-b)}{X\{(a+b)^2 - ab - U^2\} - (a+b)ab}, \tag{12}$$

with $X = \mathrm{i}\omega_n - \varepsilon_d^0 - Ur + \mu$, $q = n_d - r$, $a + b = U\{-q(N_{\deg}-1) + r\}/N_{\deg}$, $ab = -U^2\{N_{\deg}(1-q) - r + 2rq + q\}/N_{\deg}$, integer r satisfying $r < n_d < r + 1$. $n_{0\sigma\alpha} = T\sum_n G_{\sigma\alpha\alpha}^0(\mathrm{i}\omega_n)\mathrm{e}^{\mathrm{i}\omega_n 0^+}$, $n_{\sigma\alpha} = T\sum_n G_{\sigma\alpha\alpha}(\mathrm{i}\omega_n)\mathrm{e}^{\mathrm{i}\omega_n 0^+}$, and $T = 1/\beta$ being the temperature. The second-order self-energy $\sum_{\sigma\alpha\beta}^{U(2)}(\mathrm{i}\omega_n)$ is the Fourier transformation of $\sum_{\sigma\alpha\beta}^{(2)}(\tau)$ which satisfies

$$\sum\nolimits_{\sigma\alpha\beta}^{(2)}(\tau) = -U^2(N_{\deg}-1)G_{\sigma\alpha\beta}^0(\tau)^2 G_{\sigma\alpha\beta}^0(-\tau). \tag{13}$$

We now incorporate the effect of the Hund coupling by introducing an additional self-energy $\sum_{\sigma\alpha\beta}^{\mathrm{H}}$ into the local Green's function as follows:

$$G_{\sigma\alpha\beta}^{-1}(k, \mathrm{i}\omega_n) = (\mathrm{i}\omega_n + \mu)\delta_{\alpha\beta} - t_{\alpha\beta}^{H}(k) - \sum\nolimits_{\sigma\alpha\beta}^{U}(\mathrm{i}\omega_n) - \sum\nolimits_{\sigma\alpha\beta}^{H}(\mathrm{i}\omega_n). \tag{14}$$

For this Ising-like Hound coupling, we expect that $\sum_{\sigma\alpha\beta}^{H}(\mathrm{i}\omega_n) = \sum_{\sigma\alpha}^{H}(\mathrm{i}\omega_n)\delta_{\alpha\beta}$. According to the CPA,[11] $-J_{\mathrm{H}}S_{\mathrm{i}}\sigma$ in expression (3) can be viewed as a random potential, leading to

$$\left\langle \frac{-J_H S_{\rm i}\sigma - \sum_\sigma^H}{1 - G_\sigma\left(-J_H S_{\rm i}\sigma - \sum_\sigma^H\right)} \right\rangle_{S_{\rm i}} = 0, \tag{15}$$

which can be rewritten as

$$G_{\sigma\alpha\beta}(\mathrm{i}\omega_n)\left[(J_H S)^2 - \sum\nolimits_{\sigma\alpha}^H (\mathrm{i}\omega_n)^2\right] = \left[\sum\nolimits_{\sigma\alpha}^H (\mathrm{i}\omega_n) - \sigma J_H M\right]\delta_{\alpha\beta}, \tag{16}$$

where M is the magnetization of localized spins.

The chemical potential μ is determined by the Friedel sum rule.[14] The following self-consistency condition

$$G_{\sigma\alpha\beta}(\mathrm{i}\omega_n) = \frac{1}{N}\sum_k G_{\sigma\alpha\beta}(k, \mathrm{i}\omega_n) \tag{17}$$

is required such that we can complete the self-consistent loop.

3. Optical conductivity

As an example of the applications of the method mentioned above, we calculate the optical conductivity[13]

$$\mathrm{Re}\sigma_{\mu\mu'}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \frac{f(\varepsilon) - f(\varepsilon+\omega)}{\omega} \times \sum_{\sigma,k,\alpha,\alpha'} I^\sigma_{\alpha\alpha'}(k,\varepsilon,\varepsilon+\omega) \times \sum_\beta [A^\alpha(k) j^\mu k) A^{\alpha'}(k) j^{\mu'}(k)]_{\beta\beta}, \tag{18}$$

where $A^\alpha_{\beta\beta}(k) = U_{\beta\alpha}(k)U^{-1}_{\alpha\beta}(k)$, $I^\sigma_{\alpha\alpha'}(k,\varepsilon_1,\varepsilon_2) = D^\sigma_\alpha(k,\varepsilon_1)D^\sigma_{\alpha'}(k,\varepsilon_2)$, $D^\sigma_\alpha(k,\omega) = -\dfrac{\mathrm{Im}G_{\sigma\alpha}(k,\omega)}{\pi}$ and $j^{\mu'}_{\beta\beta}(k) = -\mathrm{e}\dfrac{\partial t^{\rm H}_{\beta\beta}(k)}{\partial k_\mu}$. $f(x)$ is Fermi function, and $U_{\alpha\beta}(k)$ is the unitary matrix which diagonalizes the matrix $t^{\rm H}_{\alpha\beta}(k)$, and it is expressed as

$$U_{\alpha\beta}(k) = \begin{pmatrix} \dfrac{-\varepsilon_2}{\sqrt{2\Delta(\Delta+\varepsilon_1)}} & \dfrac{\varepsilon_2}{\sqrt{2\Delta(\Delta-\varepsilon_1)}} \\ \sqrt{\dfrac{\Delta+\varepsilon_1}{2\Delta}} & \sqrt{\dfrac{\Delta-\varepsilon_1}{2\Delta}} \end{pmatrix},$$

with $\Delta = \sqrt{\varepsilon_1^2 + \varepsilon_2^2}$. (19)

In Fig.1 we show the values of optical conductivity $\sigma_{xx}(\omega)$ calculated for different values of Hubbard interaction U. There are two peaks that originate from the intraband and the interband excitations. The peaks are around $\omega \approx 0$ and $\omega \approx 0.6$. These peaks become higher and their widths turn narrower with the value of U increasing. These behaviours are qualitatively similar to those obtained by using the combination of the slave-boson approach with the CPA [15] (but with different input data and units in calculation). In Fig.2, we make a comparison between conductivities $\sigma_{xx}(\omega)$ and $\sigma_{zz}(\omega)$ calculated at $M = 0.2$, $U = 2$ and $\beta = 50$. It can be seen that the peaks of $\sigma_{zz}(\omega)$ are higher than of $\sigma_{xx}(\omega)$, but the widths are narrower.

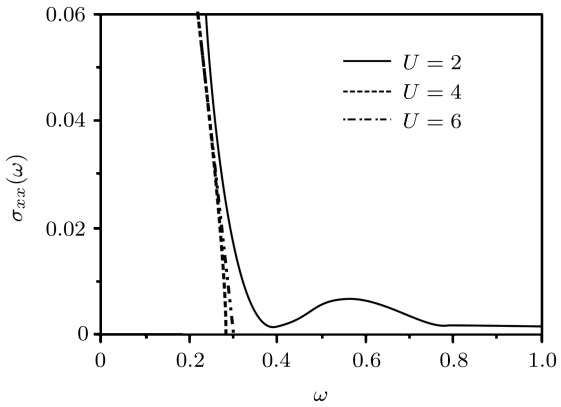


Fig.1. The values of optical conductivity $\sigma_{xx}(\omega)$ for different values of U, with $\beta = 30$ and M(Magnetization) $= 0.2$.

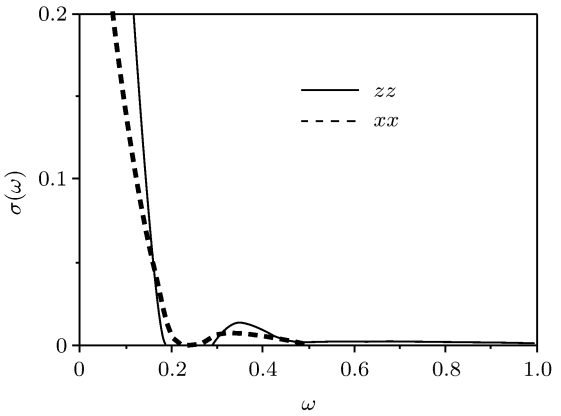


Fig.2. A comparison between optical conductivities $\sigma_{xx}(\omega)$ and $\sigma_{zz}(\omega)$, at $M = 0.2$, $U = 2$, and $\beta = 50$.

Figure 3 shows the values of $\sigma_{zz}(\omega)$ for different values of magnetization M. Increasing M leads to higher Drude-like peaks, which means that the life time of the quasiparticle is longer.[16]

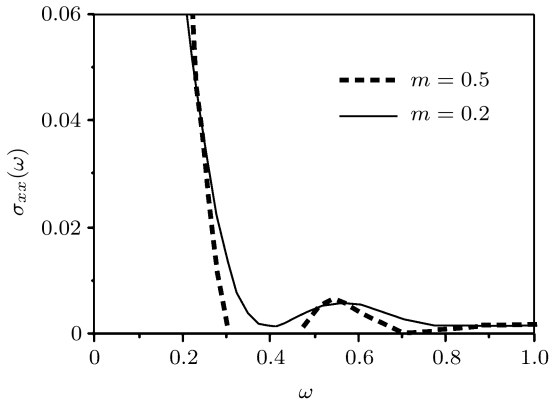


Fig.3. The values of optical conductivity $\sigma_{xx}(\omega)$ for different values of M, at $\beta = 30$ and $U = 2$.

In order to investigate the effect of the non-diagonal hopping matrix elements, we calculate the values of optical conductivity $\sigma_{xx}(\omega)$ for the cases in which $\varepsilon_2 = 0$, and $\varepsilon_2 \neq 0$ because the non-diagonal hopping matrix elements are proportional to ε_2. It is obvious from Fig.4 that this effect can be large. When $\varepsilon_2 = 0$, the curve has a third peak around $\omega \sim 1.0$. This is not true for real materials. It leads to an unreal result without considering the non-diagonal hopping matrix elements in our input data. Another effect of the non-diagonal hopping matrix elements is reducing the optical conductivity. These marked features strongly support the previous guess at which the effect of the non-diagonal hopping matrix elements may play an important role for real materials.

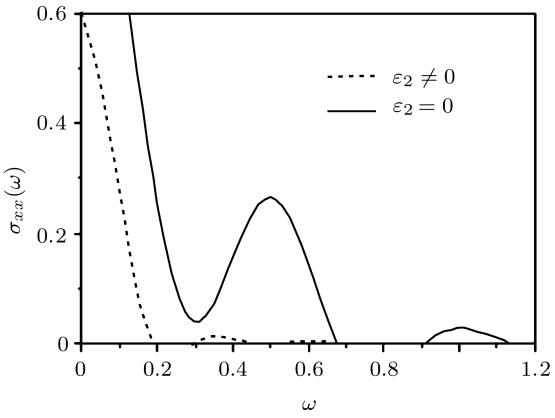


Fig.4. The values of optical conductivity $\sigma_{xx}(\omega)$ for different non-diagonal hopping matrix elements at $M = 0.2$, $\beta = 50$ and $U = 2$.

4. Conclusion

We present a scheme that generalizes ITP+CPA to the double exchange model with orbital degeneracy. To illustrate this scheme, we calculate the optical conductivity for the multi-orbital double exchange model with the Hubbard interaction. With this model, we also investigate the effect of the non-diagonal hopping matrix elements in the Hamiltonian. We find that it plays an important role in our model.

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