Temperature dependence of electronic states in the t-J model

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The temperature dependence of electronic states in the t-J model is studied in the moderately doped region by use of the composite operator method. Self-energy effects are included in two-site approximation. At higher temperature, the density of states shows a two-peak structure, and the coherent peak at the Fermi level increases its intensity with decreasing temperature. The peak at the Fermi level splits into two peaks with further decreasing temperature, corresponding to the electronic excitations from spin-singlet and -triplet states of the nearest-neighbor electrons. Electronic excitations from the singlet states form a narrower band at the Fermi level. This may relate to the spin gap formation observed in high-T_c superconductors. [S0163-1829(96)02544-1]

I. INTRODUCTION

After the discovery of high-T_c superconductors, understanding the electronic states of highly correlated electron systems has become one of the central issues to clarify the mechanism of high-T_c superconductivity. Among many models, the t-J mode[1,2] is regarded as one of the simplest which describes some essential features of those materials. This model has been extensively studied,[3] and is known to be understood reasonably well by the Heisenberg model at the half-filling; at high hole doping it is most likely described by a normal Landau Fermi liquid. For the region of moderate doping relevant for superconductivity, the motion of holes and the dynamics of spins strongly interfere, and a self-consistent treatment of both effects becomes essential in order to understand the phenomena in this region. In experiments, many crossover phenomena in temperature and doping have been reported.[4–11] It has been pointed out that one of the common features in high-T_c superconductors in the low-doped region is the appearance of the so-called spin-gap phenomena[7–12] before the critical temperature of superconductivity. It is necessary to clarify whether or not a variety of crossover phenomena in doping and temperature is expected in the t-J model due to the nonlinear effects between the hole motion and spin fluctuation, and to investigate, in relation to the mechanism of superconductivity, whether or not such a crossover phenomena of the spin gap is a necessary precursor for superconductivity, at least in the low-doped region.

Many analytical approaches to treating highly correlated electron systems have been proposed, such as the Hubbard approximation,[13] the noncrossing approximation (NCA),[14–16] slave boson method,[17–19] d_∞ method,[20–23] and their combination,[24–25] as well as projection operator[26–30] and composite operator methods.[31–38] However, it is a hard problem to judge the reliability of their results due to nonlinear effects essentially involved in this problem. One way to judge the validity of approximation methods is through a comparison with recently accumulated results of numerical simulation,[39–41,3] which still are severely restricted in cluster size and temperature. Then use of approximate analytical methods can be extended to regions which the simulation cannot cover. Recently we have developed a self-consistent treatment based on the equation of motion, the composite operator method.[31–38] In this method global properties of propagation are treated by mean fields felt by electronic composite excitations, while self-energy corrections and two-site correlation of mean fields are evaluated by two-site local level transitions.[42,43] In this way we can combine local properties, especially those of the local-spin configuration and global electron propagation, self-consistently. The method was applied to the Hubbard model,[42,43] and the results produced behavior very similar to that obtained by numerical simulation. The composite operator method has the advantage of describing crossover phenomena, since the electronic excitation is described by a certain combination of composite electronic operators. There, a crossover is described as the phenomenon in which the weight of some operator is shifted to another operator. Also, the operator expansion gives an expansion scheme in terms of the weight of the operator multiplied by coupling constants. By choosing a suitable set of operators, one can reduce the weight of the residual interactions, leading to a reasonable treatment of the residual terms as perturbation. Further, from the evaluation of contributions from two-site level transitions, it is easily seen what kind of local excitations play a dominant role with doping and temperature.

In this paper we investigate the temperature dependence of the density of states in the t-J model in the moderately doped region. It will be shown that a coherent peak at the Fermi level increases its intensity with decreasing temperature, and this coherent peak splits into two peaks when temperature is further lowered. The tendency of the two-peak structure around the Fermi level at low temperature is also seen in the results of numerical simulation in Refs. 39–41. It will be shown that this crossover originates from the forma-

tion of spin-singlet states between nearest-neighbor electrons. This may relate to the spin-gap formation observed in high-T_c superconductors. A relation to superconductivity will be discussed.

The program of this paper is as follows. In Sec. II, we present the formulation of the t-J model in the composite operator method. In Sec. III, the two-site mean-field correlation and self-energy are evaluated in the two-site approximation by use of the resolvent method. In Sec. IV, the results from the self-consistent calculation is presented. Section V is devoted to concluding remarks. Some necessary formula are presented in Appendixes A, B, and C.

II. ELECTRON PROPAGATOR

We study the t-J model given by the following Hamiltonian:

$$H=\sum_{i,\sigma}\tilde{c}^{\dagger}_{\sigma}(i)\tilde{c}_{\sigma}(i)-t\sum_{\langle i,j\rangle,\sigma}(\tilde{c}^{\dagger}_{\sigma}(i)\tilde{c}_{\sigma}(j)+\tilde{c}^{\dagger}_{\sigma}(j)\tilde{c}_{\sigma}(i))$$
$$+J\sum_{\langle i,j\rangle}\mathbf{S}(i)\cdot\mathbf{S}(j). \tag{2.1}$$

Here i indicates the ith site and the summation $\langle i,j\rangle$ is over the nearest-neighbor sites. The operator $\mathbf{S}(i)$ is the spin operator of the electron, which is given, by use of creation and annihilation electron operators at the ith site $c^{\dagger}_{\sigma}(i)$ and $c_{\sigma}(i)$, as $\mathbf{S}(i)=\frac{1}{2}\Sigma_{\sigma\sigma'}c^{\dagger}_{\sigma}(i)(\boldsymbol{\sigma})_{\sigma\sigma'}c_{\sigma'}(i)$, with $(\boldsymbol{\sigma})_{\sigma\sigma'}$ being Pauli matrices. The electronic operator $\tilde{c}_{\sigma}(i)$ is an electron annihilation operator restricted to the transition $n(i)=0\leftrightarrow n(i)=1$ with $n(i)=\Sigma_{\sigma}c^{\dagger}_{\sigma}(i)c_{\sigma}(i)$, and is given by $\tilde{c}_{\sigma}(i)=c_{\sigma}(i)(1-n_{-\sigma}(i))$ with $n_{\sigma}(i)=c^{\dagger}_{\sigma}(i)c_{\sigma}(i)$. We introduce an abbreviation, for example, $\tilde{c}^{\alpha}$, which is defined by

$$\tilde{c}^{\alpha}(x)=\int d^2y\ \alpha(x,y)\tilde{c}(y), \tag{2.2}$$

$$\alpha(x,y)=\frac{a^2}{(2\pi)^2}\int d^2k\ e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\alpha(\mathbf{k}), \tag{2.3}$$

where

$$\alpha(\mathbf{k})=\tfrac{1}{2}(\cos k_x a+\cos k_y a), \tag{2.4}$$

and a is the lattice length. We introduce level operators[43] $B(i)$ and $F_{\sigma}(i)$ which describe the creation of $n=0$ and 1 levels at the ith site, respectively. The operator $B(i)$ is bosonic and $F_{\sigma}(i)$ is fermionic. By use of them, the spin operator $S_i(i)$, the number operator $n(i)$ and electron operator $\tilde{c}_{\sigma}(i)$ are expressed as

$$S_i(i)=\tfrac{1}{2}F^{\dagger}(i)\sigma_i F(i), \tag{2.5}$$

$$n(i)=F^{\dagger}(i)\cdot F(i), \tag{2.6}$$

and

$$\tilde{c}_{\sigma}(i)=B^{\dagger}(i)F_{\sigma}(i). \tag{2.7}$$

Here σ_i is the Pauli matrix. Note that we have

$$1=B^{\dagger}(i)B(i)+\sum_{\sigma}F^{\dagger}_{\sigma}(i)F_{\sigma}(i). \tag{2.8}$$

The equation of motion for the electron operator $\tilde{c}$ is given by

$$i\frac{\partial}{\partial t}\tilde{c}_{\sigma}=\epsilon\tilde{c}_{\sigma}-t_R(B^{\dagger}B\tilde{c}^{\alpha}_{\sigma}+F^{\dagger}_{s}F_{\sigma}\tilde{c}^{\alpha}_{s})+2J\mathbf{S}^{\alpha}(\boldsymbol{\sigma}\tilde{c})_{\sigma}$$
$$=\epsilon\tilde{c}_{\sigma}-t_R(1-\tfrac{1}{2}n+\boldsymbol{\sigma}\mathbf{S})\tilde{c}^{\alpha}+2J\mathbf{S}^{\alpha}(\boldsymbol{\sigma}\tilde{c})_{\sigma}, \tag{2.9}$$

where

$$t_R=4t. \tag{2.10}$$

The level operators satisfy the equations

$$i\frac{\partial}{\partial t}B=\epsilon_B B-t_R\tilde{c}^{\dagger\alpha}_{s}F_s \tag{2.11}$$

and

$$i\frac{\partial}{\partial t}F_{\sigma}=\epsilon_{F_{\sigma}}F_{\sigma}-t_R B\tilde{c}^{\alpha}_{\sigma}+2J\mathbf{S}^{\alpha}(\boldsymbol{\sigma}F)_{\sigma}, \tag{2.12}$$

where the summation over the spin index s is understood and the level energies ϵ_B and ϵ_F are parametrized as

$$\epsilon_B=-\epsilon \tag{2.13}$$

and

$$\epsilon_{F_{\sigma}}=0. \tag{2.14}$$

The equations for two-site level operators are presented in Appendix A.

In the composite operator method, the electron propagator $S(\omega,\mathbf{k})$ is expressed as[31–32]

$$S(\omega,\mathbf{k})=P(\mathbf{k})\frac{1}{\omega P(\mathbf{k})-m(\mathbf{k})-\delta m(\omega,\mathbf{k})}P(\mathbf{k}). \tag{2.15}$$

The normalization matrix $P(\mathbf{k})$ is given by

$$P(\mathbf{k})=\text{F.T.}\langle\{\psi(\mathbf{x}),\psi^{\dagger}(\mathbf{y})\}\rangle, \tag{2.16}$$

with ψ being concerned electron operators and F.T. indicating the Fourier transform, the mean field $m(\mathbf{k})$ by

$$m(\mathbf{k})=\text{F.T.}\left\langle\left\{i\frac{\partial}{\partial t}\psi(\mathbf{x}),\psi^{\dagger}(\mathbf{y})\right\}\right\rangle \tag{2.17}$$

and the self-energy $\delta m(\omega,\mathbf{k})$ by

$$\delta m(\omega,\mathbf{k})=-i\,\text{F.T.}\left\langle R\left(i\frac{\partial}{\partial t}\psi\right)\left(i\frac{\partial}{\partial t}\psi\right)^{\dagger}\right\rangle_I, \tag{2.18}$$

with the subscript ''I'' indicating an irreducible part. It should be noted that expression (2.15) guarantees the sum rules

$$\int d\omega\left(-\frac{1}{\pi}\right)\text{Im}S(\omega,\mathbf{k})=P(\mathbf{k}) \tag{2.19}$$

and

$$\int d\omega\ \omega\left(-\frac{1}{\pi}\right)\mathrm{Im}S(\omega,\mathbf{k})=m(\mathbf{k}) \tag{2.20}$$

under the condition $\delta m(\omega,\mathbf{k})\to 0$ as $|\omega|\to\infty$.

We consider the paramagnetic phase, and choose $\tilde{c}$ as ψ in Eqs. (2.16)–(2.18). In the t-J model given by the Hamiltonian (2.1), the normalization P is given by

$$P=\langle 1-\tfrac{1}{2}n\rangle, \tag{2.21}$$

and the mean-field $m(\mathbf{k})$ is expressed as

$$m(\mathbf{k})=m_0+m_1\alpha(\mathbf{k}), \tag{2.22}$$

where

$$m_0=\epsilon P-m_{\tilde{c}} \tag{2.23}$$

and

$$m_1=-t_R(P^2+\delta P_t)+J\delta P_J, \tag{2.24}$$

with

$$m_{\tilde{c}}=t_R\langle\tilde{c}^{\alpha}\tilde{c}^{\dagger}\rangle-2J\langle\mathbf{S}^{\alpha}\cdot\mathbf{S}\rangle, \tag{2.25}$$

$$\delta P_t=\langle\tfrac{1}{4}\delta n\,\delta n^{\alpha}+\mathbf{S}\cdot\mathbf{S}^{\alpha}\rangle, \tag{2.26}$$

and

$$\delta P_J=3\langle\tilde{c}^{\alpha}\tilde{c}^{\dagger}\rangle. \tag{2.27}$$

The dynamical correction of the self-energy is evaluated from

$$\delta m_{\sigma}=\langle R\,\delta j_{\sigma}\delta j_{\sigma}^{\dagger}\rangle_I, \tag{2.28}$$

where

$$\begin{aligned}\delta j_{\sigma}=&-t_R((B^{\dagger}B+F_{\sigma}^{\dagger}F_{\sigma})\tilde{c}_{\sigma}^{\alpha}+F_{-\sigma}^{\dagger}F_{\sigma}\tilde{c}_{-\sigma}^{\alpha})\\&+2J(\sigma S_3^{\alpha}\tilde{c}_{\sigma}+2S_{-\sigma}^{\alpha}\tilde{c}_{-\sigma})-a_0\tilde{c}_{\sigma}-a_1\tilde{c}_{\sigma}^{\alpha},\end{aligned} \tag{2.29}$$

with

$$a_0=-m_{\tilde{c}}/P,\quad a_1=m_1/P. \tag{2.30}$$

In the expression of the mean fields (2.25) and (2.26) there appear the thermal expectation values which are not able to be obtained from the electron propagator under consideration. Since they are related to operators in two sites, we evaluate their contribution by considering level transitions in two sites. We also evaluate the dynamical correction of the self-energy $\delta m(\omega,\mathbf{k})$ in the two-site approximation by considering the time delay of two-site level transitions. For such purpose we use the resolvent method,[14] which will be presented in Sec. III.

III. RESOLVENT FOR TWO-SITE LEVELS

In order to evaluate two-site correlations, we consider the nearest-neighbor two sites $(\mathbf{x},\mathbf{x}')$ as a representative cluster. The orthogonal basis of level operators for this subsystem are BB', FB_S', FB_A', $F_{\sigma}F_{\sigma}'$, $(F_{\uparrow}F_{\downarrow}')_S$, and $(F_{\uparrow}F_{\downarrow}')_A$ with

$$FB_S'=\frac{1}{\sqrt{2}}(FB'+BF'), \tag{3.1}$$

$$FB_A'=\frac{1}{\sqrt{2}}(FB'-BF'), \tag{3.2}$$

$$(F_{\uparrow}F_{\downarrow}')_S=\frac{1}{\sqrt{2}}(F_{\uparrow}F_{\downarrow}'+F_{\downarrow}F_{\uparrow}'), \tag{3.3}$$

and

$$(F_{\uparrow}F_{\downarrow}')_A=\frac{1}{\sqrt{2}}(F_{\uparrow}F_{\downarrow}'-F_{\downarrow}F_{\uparrow}'), \tag{3.4}$$

where operators without the prime are for the $\mathbf{x}$ point, and those with the prime are for the $\mathbf{x}'$ point. Let us denote those level operators in general as Φ_n. Modification of these levels from the surrounding system is evaluated by the resolvent[14,43] of Φ_n defined by

$$\begin{aligned}R_{nm}(t-t')&=\langle\langle 0|R\Phi_n(t)\Phi_m(t')^{\dagger}|0\rangle\rangle_R\\&=\frac{\mathrm{Tr}_R[\langle\langle 0|\Phi_n(t)\Phi_m(t')^{\dagger}|0\rangle\rangle e^{-\beta H_R}]}{\mathrm{Tr}_R[e^{-\beta H_R}]}\,\theta(t-t')\end{aligned} \tag{3.5}$$

with $|0\rangle\rangle$ being the local state vector with $n=0$ and $n'=0$ on the (x,x') site. Here H_R denotes the Hamiltonian for a system other than x and x', which we will call a reservoir system for convenience. The spectral function $\sigma_{nm}(\omega)$ of the resolvent R_{nm} is defined by

$$R_{nm}(t-t')=\frac{i}{2\pi}\int d\omega\ e^{-i\omega t}R_{nm}(\omega), \tag{3.6}$$

$$\sigma_{nm}(\omega)=-\frac{1}{\pi}\,\mathrm{Im}R_{nm}(\omega). \tag{3.7}$$

We also define $\overline{\sigma_{nm}}(\omega)$ by

$$\overline{\sigma_{nm}}(\omega)=e^{-\beta\omega}\sigma_{nm}(\omega). \tag{3.8}$$

Since Φ_n satisfies

$$\langle\langle 0|\Phi_n\Phi_m^{\dagger}|0\rangle\rangle=\delta_{nm}, \tag{3.9}$$

we have

$$R_{nm}(\omega)=\left(\frac{1}{\omega-E-\Sigma(\omega)}\right)_{nm}, \tag{3.10}$$

where E_{nm} is the energy of each level, and $\Sigma_{nm}(\omega)$ is the self-energy of the resolvent. The level energies are parametrized as

$$E_{BB}=-2\epsilon, \tag{3.11}$$

$$E_{FB_S}=-\epsilon-t, \tag{3.12}$$

$$E_{FB_A}=-\epsilon+t, \tag{3.13}$$

$$E_{FF_S}=\tfrac{1}{4}J, \tag{3.14}$$

and

$$E_{FF_A} = -\tfrac{3}{4} J, \tag{3.15}$$

where we set the energy of the F level with $J=0$ as the origin of the level energy as in Eq. (2.14).

In the evaluation of the self-energy Σ, we consider the one-loop correction arising from electron hopping and from two-site spin correlation. For example, the self-energy of FF'_A is obtained from Eq. (A6) as

$$\Sigma_{FF_A}(\omega) = \int d\kappa (1-f_F(\kappa))(\rho_{\tilde{c}R_S}(\kappa) R_{FB_S}(\omega-\kappa) + \rho_{\tilde{c}R_A}(\kappa) R_{FB_A}(\omega-\kappa) + 3J^2 \phi_A(\kappa) \times R_{FF_S}(\omega-\kappa)), \tag{3.16}$$

where $f_F(\kappa)$ is the Fermi distribution function, and $\rho_{\tilde{c}R_A}(\kappa)$ and $\rho_{\tilde{c}R_S}(\kappa)$ are spectral functions of electron propagators in the reservoir system $S_{\tilde{c}R_A}$ and $S_{\tilde{c}R_S}$ given by

$$S_{\tilde{c}R_A}(\omega) = \text{F.T.}\tfrac{1}{2}\langle R(\tilde{c}^{\tilde{\alpha}} - \tilde{c}^{\tilde{\alpha}'})(\tilde{c}^{\dagger\tilde{\alpha}} - \tilde{c}^{\dagger\tilde{\alpha}'})\rangle_R \tag{3.17}$$

and

$$S_{\tilde{c}R_S}(\omega) = \text{F.T.}\tfrac{1}{2}\langle R(\tilde{c}^{\tilde{\alpha}} + \tilde{c}^{\tilde{\alpha}'})(\tilde{c}^{\dagger\tilde{\alpha}} + \tilde{c}^{\dagger\tilde{\alpha}'})\rangle_R, \tag{3.18}$$

and ϕ_A is the spin-correlation function of the reservoir system

$$\phi_A(\omega) = 4\,\text{F.T.}\langle\{(S_i^{\tilde{\alpha}} - S_i^{\tilde{\alpha}'}),(S_i^{\tilde{\alpha}} - S_i^{\tilde{\alpha}'})\}\rangle_R, \tag{3.19}$$

where the subscript R indicates the reservoir system. The approximation used to evaluate the electron propagators and spin fluctuation in the reservoir system is presented in Appendix C. Mixture of the spin-singlet and -triplet states in the self-energies occurs through spin-flip induced by the spin interaction J in the Hamiltonian.

Now we can evaluate two-site mean fields and the dynamical correction of the electron self-energy in the two-site approximation. First, we define the quantity Z_{Φ_n} by

$$Z_{\Phi_n} = \int d\omega\ \overline{\sigma_{\Phi_n}}(\omega). \tag{3.20}$$

Then we have

$$Z = Z_{BB} + 2(Z_{FB_S} + Z_{FB_A}) + 3Z_{FF_S} + Z_{FF_A}. \tag{3.21}$$

The two-site occupation number for each state is given by

$$n_{BB} = Z_{BB} Z^{-1}, \tag{3.22}$$

$$n_{FB_S} = 2Z_{FB_S} Z^{-1}, \tag{3.23}$$

$$n_{FB_A} = 2Z_{FB_A} Z^{-1}, \tag{3.24}$$

$$n_{FF_S} = 3Z_{FF_S} Z^{-1}, \tag{3.25}$$

and

$$n_{FF_A} = Z_{FF_A} Z^{-1}. \tag{3.26}$$

With these two-site occupation numbers, the one-site occupation number n_B ($=\langle B^\dagger B\rangle$) and n_F ($=\langle F^\dagger F\rangle$) are obtained from

$$n_B = \langle B^\dagger B 1'\rangle = \tfrac{1}{2}(n_{FB_S} + n_{FB_A}) + n_{BB} \tag{3.27}$$

and

$$n_F = \tfrac{1}{2}(n_{FF_S} + n_{FF_A} + \tfrac{1}{2}(n_{FB_S} + n_{FB_A})). \tag{3.28}$$

The electron filling number is given by

$$\langle n\rangle = 2n_F. \tag{3.29}$$

Quantities related to two sites are obtained as

$$4\langle \mathbf{S}\mathbf{S}^\alpha\rangle = n_{FF_S} - 3n_{FF_A}, \tag{3.30}$$

$$\langle n n^\alpha\rangle = n_{FF_S} + n_{FF_A}, \tag{3.31}$$

$$\delta P_t = \tfrac{1}{2}(n_{FF_S} - n_{FF_A} - \tfrac{1}{2}\langle n\rangle^2), \tag{3.32}$$

and

$$\delta P_J = \tfrac{3}{2}\langle (FB'_A)^\dagger FB'_A - (FB'_S)^\dagger FB'_S\rangle. \tag{3.33}$$

The correction term $\delta m(\boldsymbol{\omega},\mathbf{k})$ is evaluated in the two-site approximation as

$$\delta m(\omega,\mathbf{k}) = \delta m_0(\omega) + \delta m_1(\omega)\alpha(\mathbf{k}), \tag{3.34}$$

where δm_0 is related to level transitions on the equal site, while δm_1 is related to transitions across the two sites. They are evaluated by extracting the concerned two sites $\mathbf{x}$ and $\mathbf{x}'$, and by expressing δj in Eq. (2.29) in terms of transition among two-site levels. Let us rewrite δj_σ in Eq. (2.29) as

$$\delta j_\sigma = \sum_{nm} a_{nm} \Phi_n^\dagger \Phi_m \tag{3.35}$$

and

$$\delta j'_\sigma = \sum_{nm} a'_{nm} \Phi_n^\dagger \Phi_m, \tag{3.36}$$

where Φ_n is the complete set of operators for two-site levels, and the coefficients a_{nm} and a'_{nm} are given in Appendix B. In the noncrossing approximation, we have

$$\delta m_0(\omega) = Z^{-1} \int d\kappa\ d\kappa' \sum_{nmn'm'} a_{nm} a^*_{n'm'} \times \frac{\sigma_{mm'}(\kappa)\overline{\sigma_{n'n}}(\kappa') + \overline{\sigma_{mm'}}(\kappa)\sigma_{n'n}(\kappa')}{\omega - \kappa + \kappa' + i\delta} \tag{3.37}$$

and

$$\delta m_1(\omega) = Z^{-1} \int d\kappa\ d\kappa' \sum_{nmn'm'} a_{nm} a^{*\prime}_{n'm'} \times \frac{\sigma_{mm'}(\kappa)\overline{\sigma_{n'n}}(\kappa') + \overline{\sigma_{mm'}}(\kappa)\sigma_{n'n}(\kappa')}{\omega - \kappa + \kappa' + i\delta}. \tag{3.38}$$

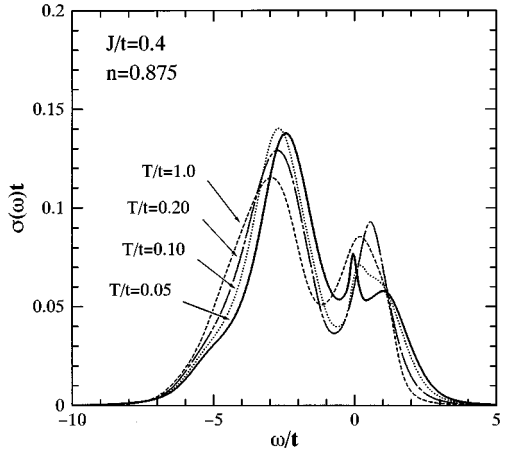

FIG. 1. Temperature dependence of the density of states.

We have fixed all functions appearing in the composite operator method within the two-site approximation.

In the present approximation, the propagation of electronic excitations in the system is expressed by the propagator $S(\omega,\mathbf{k})$, which is a function of the occupation number $\langle n\rangle$, mean fields $m_{\tilde{c}}$, δP_t, and δP_J, and dynamically corrected two-site self-energies $\delta m_0(\omega)$ and $\delta m_1(\omega)$. For given $\langle n\rangle$, δP_t, δP_J, $\delta m_0(\omega)$, and $\delta m_1(\omega)$, we can self-consistently determine ϵ and $m_{\tilde{c}}$ from

$$\langle n\rangle = \langle \tilde{c}^{\dagger}\tilde{c}\rangle \tag{3.39}$$

and

$$m_{\tilde{c}} = t_R \langle \tilde{c}^{\alpha}\tilde{c}^{\dagger}\rangle. \tag{3.40}$$

When the propagator is obtained, we can evaluate the irreducible propagator, $S_{\tilde{c}R_S}(\omega)$ and $S_{\tilde{c}R_A}(\omega)$, with respect to the nearest-neighbor two sites. Then two-site resolvents are self-consistently obtained, from which δP_t, δP_J and $\delta m_0(\omega)$, $\delta m_1(\omega)$ and two-site spin fluctuation in the noncrossing approximation are evaluated. This gives a totally self-consistent scheme. We determine ϵ in the resolvent and ϵ in the propagator independently for a given $\langle n\rangle$ in order to guarantee that $\langle n\rangle$ has the same value both in the calculation of the propagator and resolvent. We regard that such a difference appears due to the difference of the approximation scheme between local and itinerant values. The result shows that both values are very close.

IV. RESULTS

The propagator and resolvent are self-consistently solved by use of the formulas presented in previous sections. In this paper we investigate the moderately doped region, and parameters are fixed as $n=0.875$ and $J/t=0.4$. In Fig. 1, the temperature behavior of the density of states (DOS), $\sigma(\omega)$, is presented, where

$$\sigma(\omega) = \frac{a^2}{(2\pi)^2}\int d^2k\left(-\frac{1}{\pi}\right)\mathrm{Im}S(\omega,\mathbf{k}). \tag{4.1}$$

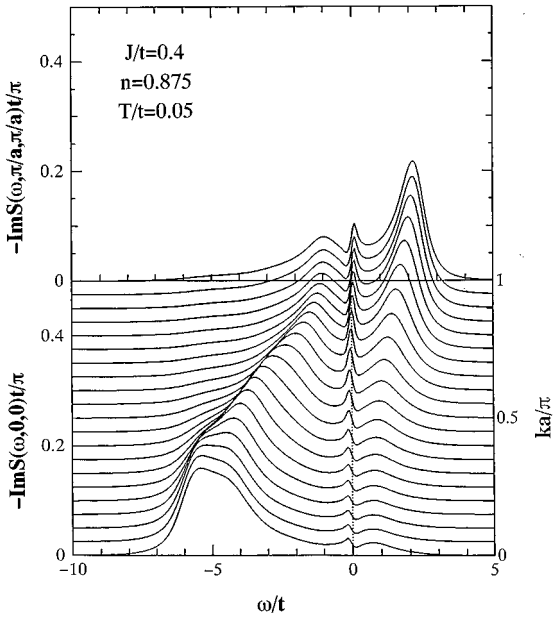

FIG. 2. Spectral intensity at $T/t=0.05$.

The Fermi level (FL) is chosen at $\omega=0$. Temperature is changed as $T/t=1.0$, 0.2, 0.1, 0.05. At $T/t=1.0$ and 0.2, the DOS has a two-peak structure, a large peak around $\omega/t=-2.5$ and a narrow peak around the Fermi level. The former peak originates from the Van Hove singularity in the two-dimensional model with the nearest-neighbor hopping. The narrow peak at the FL increases its intensity with decreasing temperature. Further decreasing the temperature ($T/t=0.1$ and 0.05) causes an additional narrower peak to develop at the FL. This narrower band (coherent band) ranges between $\omega/t=-1.0$ and 1.0, and corresponds to the band near the Fermi level reported in Ref. 39. In Fig. 2 we present the spectral function $-(1/\pi)\mathrm{Im}S(\omega,\mathbf{k})$ in the Γ-M direction [i.e., the $(0,0)-(\pi/a,\pi/a)$ direction] for $T/t=0.05$. The bandwidth of the coherent band identified from the peak dispersion is about $0.3t$, while Ref. 39 gives about $2.0t$. The slave boson method[44] gives $8t\delta/2+O(J\delta)\sim 0.5t$ ($\delta=1-n=0.125$), close to the present result. The smaller dispersion and less intensity of the coherent band and a larger intensity for the high-energy incoherent contribution may be due to a stronger local nature of the NCA in the present approximation.

In order to understand the above crossover of the DOS at the FL, we show the spectral functions of various resolvents for temperature $T/t=0.2$ in Fig. 3 and $T/t=0.05$ in Fig. 4. The electron self-energy receives contributions from transitions among those levels, and it can be seen from Fig. 3 that a nearly zero-energy transition, which is the origin of the narrow peak at the FL, is induced by the transitions between FB_S and (FF_A, FF_S). In this calculation we have a bare transition energy in the resolvent $\epsilon=-1.89$ ($\epsilon=-1.83$ in the propagator), and a lowering of the level energy for FB_S is induced by the continuum contribution formed by the (FF_A, FF_S) level and the $\tilde{c}$-hole excitation. Recalling the noncrossing approximation[14–16] in the Kondo problem, we can say that the appearance of the coherent peak at high temperature is very similar to the case that occurs in the Kondo effect.

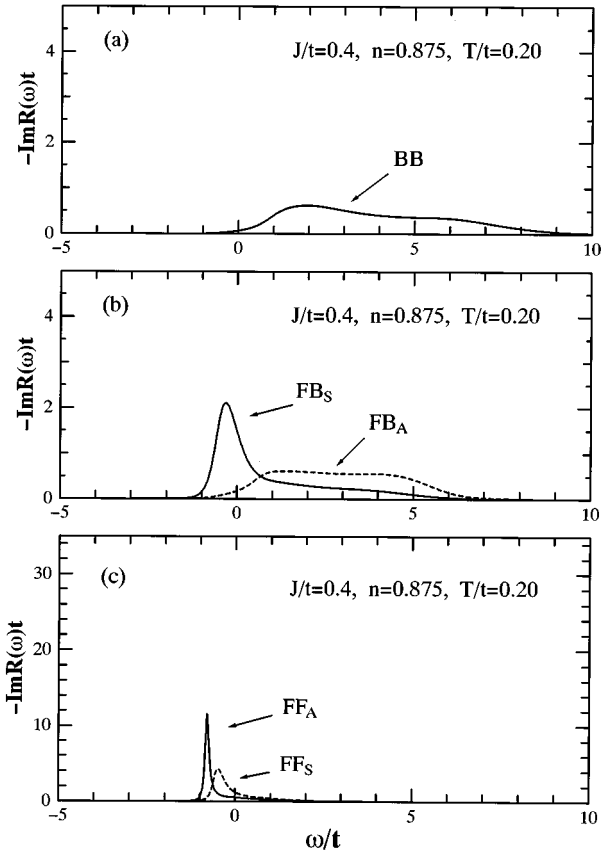

FIG. 3. Various spectral functions for resolvents for two-site levels at $T/t=0.2$.

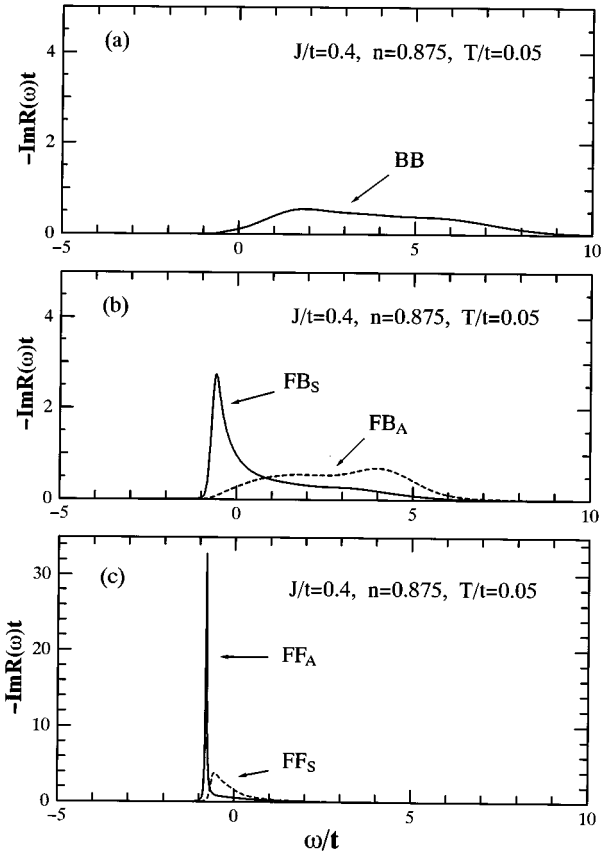

FIG. 4. Various spectral functions for resolvents for two-site levels at $T/t=0.05$.

Electron spins of occupied states are thermally fluctuating, and the spin of a hole is shielded by the surrounding spins; that is, the narrow peak is due to the spin-dressed hole propagation. When temperature is decreased as $T/t=0.05$, the weight of FF_A, which is the singlet state, increases, while the FF_S state (the triplet state) continues to have a broad spectrum. The spectrum of FB_S is also sharpened, which is due to mixing with the continuum formed with FF_A. Because of this dominance of the singlet states, the two-site transition produces a two-peak structure: one originates from the transition $FF_A \leftrightarrow FB_S$, and the other from $FB_S \rightarrow FF_S$. The former is the origin of the sharp peak at the FL in Fig. 1, and the latter produces a broad peak at about energy scale 4 J above the FL, which is the energy necessary to break the singlet bonds. This tendency of the two-peak structure at the Fermi level at low temperature is also seen in results of numerical simulations in Refs. 39–41; the bandwidth and the positions of the peaks are roughly equal, though the strength of the intensity is different. At low temperature, occupied electron spins start to form spin-singlet states, and the hole motion is changed to the excitation from such states.

From the analysis of this paper we conclude that, in the moderately doped region of the t-J model, the hole motion near the FL shows a crossover from a spin-dressed hole state to excitation from the spin-singlet state with decreasing temperature.

V. CONCLUDING REMARKS

In this paper we studied the temperature dependence of the density of states in the t-J model in the moderately doped region. There appears a crossover of the density of states near the Fermi level with decreasing temperature, and the coherent peak at high temperature splits into two peaks with lowering temperature. From the analysis of two-site level transition, we may be able to interpret this coherent peak as the result of holes dressing with spin fluctuation. The narrower peak developing at lower temperature originates from the formation of spin-singlet states in nearest-neighbor electrons. The splitting energy of the spin singlet and triplet is of order J, and the band near the Fermi level is formed mainly from the transition from the spin-singlet state. This may relate to an observation of the spin gap in a high-T_c superconductor, since it naturally relates to a diminishing of spin freedom in the local sense. If the essential scenario of superconductivity is hidden in the t-J model, this result gives an interesting indication in the mechanism of high-T_c superconductivity. In the present analysis, the formation of the nearest-neighbor spin-singlet state is related to the antiferromagnetic interaction. Local properties of two-site systems are affected by the surrounding system, while the total system is controlled by properties of the transition among local levels. The difference between effects from the surrounding normal state and the superconducting system appears in the contribution from the nondiagonal electron propagator, which induces mixing among levels with a two-electron number difference in the superconducting state. Such mixing occurs between the blank level BB' and the

spin-singlet level FF'_A of two-site systems in the t-J model. Therefore the appearance of the spin-singlet formation is a necessary precursor to allow further lowering of the ground-state energy by a possible mixing of the spinless blank state. The present formalism can be extended straightforwardly to investigate a superconducting phase in the same approximation scheme. Such an analysis will be a future problem.

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APPENDIX A: EQUATIONS FOR TWO-SITELEVEL OPERATORS

The orthonormalized basis of a two-site level operator is given by BB', FB'_S, FB'_A, FF'_S, and FF'_A. The equation of motion for these level operators are given as follows:

$$i\frac{\partial}{\partial t}BB'=2\epsilon_B BB'-\frac{t_R}{\sqrt{2}}(\tilde{c}_s^{\dagger\tilde{\alpha}}+\tilde{c}_s^{\dagger\tilde{\alpha}'})(F_sB')_S-\frac{t_R}{\sqrt{2}}(\tilde{c}_s^{\dagger\tilde{\alpha}}-\tilde{c}_s^{\dagger\tilde{\alpha}'})(F_sB')_A, \tag{A1}$$

$$i\frac{\partial}{\partial t}(F_\sigma B')_S=(\epsilon_{FB}-\tfrac{1}{4}t_R)(F_\sigma B')_S-\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\tilde{\alpha}}+\tilde{c}_\sigma^{\tilde{\alpha}'})BB'-\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\dagger\tilde{\alpha}}-\tilde{c}_\sigma^{\dagger\tilde{\alpha}'})F_\sigma F'_\sigma-\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}}-\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_S$$
$$+\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}}+\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_A+2J(\mathbf{S}^{\tilde{\alpha}}+\mathbf{S}^{\tilde{\alpha}'})(\boldsymbol{\sigma})_{\sigma s}(F_sB')_S+2J(\mathbf{S}^{\tilde{\alpha}}-\mathbf{S}^{\tilde{\alpha}'})(\boldsymbol{\sigma})_{\sigma s}(F_sB')_A, \tag{A2}$$

$$i\frac{\partial}{\partial t}(F_\sigma B')_A=(\epsilon_{FB}+\tfrac{1}{4}t_R)(F_\sigma B')_A-\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\tilde{\alpha}}-\tilde{c}_\sigma^{\tilde{\alpha}'})BB'+\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\dagger\tilde{\alpha}}+\tilde{c}_\sigma^{\dagger\tilde{\alpha}'})F_\sigma F'_\sigma+\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}}+\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_S$$
$$-\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}}-\tilde{c}_{-\sigma}^{\dagger\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_A+2J(\mathbf{S}^{\tilde{\alpha}}-\mathbf{S}^{\tilde{\alpha}'})(\boldsymbol{\sigma})_{\sigma s}(F_sB')_S+2J(\mathbf{S}^{\tilde{\alpha}}+\mathbf{S}^{\tilde{\alpha}'})(\boldsymbol{\sigma})_{\sigma s}(F_sB')_A, \tag{A3}$$

$$i\frac{\partial}{\partial t}F_\sigma F'_\sigma=(2\epsilon_F+\tfrac{1}{4}J)F_\sigma F'_\sigma-\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\tilde{\alpha}}-\tilde{c}_\sigma^{\tilde{\alpha}'})(F_\sigma B')_S+\frac{t_R}{\sqrt{2}}(\tilde{c}_\sigma^{\tilde{\alpha}}+\tilde{c}_\sigma^{\tilde{\alpha}'})(F_\sigma B')_A$$
$$+2J(\sigma(S_3^{\tilde{\alpha}}+S_3^{\tilde{\alpha}'})F_\sigma F'_\sigma+\sqrt{2}(S_{-\sigma}^{\tilde{\alpha}}+S_{-\sigma}^{\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_S-\sqrt{2}(S_{-\sigma}^{\tilde{\alpha}}-S_{-\sigma}^{\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_A), \tag{A4}$$

$$i\frac{\partial}{\partial t}(F_\sigma F'_{-\sigma})_S=(2\epsilon_F+\tfrac{1}{4}J)(F_\sigma F'_{-\sigma})_S-\frac{t_R}{2}(\tilde{c}_\sigma^{\tilde{\alpha}}-\tilde{c}_\sigma^{\tilde{\alpha}'})(F_{-\sigma}B')_S+\frac{t_R}{2}(\tilde{c}_\sigma^{\tilde{\alpha}}+\tilde{c}_\sigma^{\tilde{\alpha}'})(F_{-\sigma}B')_A-\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\tilde{\alpha}}-\tilde{c}_{-\sigma}^{\tilde{\alpha}'})(F_\sigma B')_S$$
$$+\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\tilde{\alpha}}+\tilde{c}_{-\sigma}^{\tilde{\alpha}'})(F_\sigma B')_A+2J(\sigma(S_3^{\tilde{\alpha}}-S_3^{\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_A+\sqrt{2}(S_{-\sigma}^{\tilde{\alpha}}+S_{-\sigma}^{\tilde{\alpha}'})F_{-\sigma}F'_{-\sigma}+\sqrt{2}(S_\sigma^{\tilde{\alpha}}+S_\sigma^{\tilde{\alpha}'})F_\sigma F'_\sigma), \tag{A5}$$

$$i\frac{\partial}{\partial t}(F_\sigma F'_{-\sigma})_A=(2\epsilon_F-\tfrac{3}{4}J)(F_\sigma F'_{-\sigma})_A-\frac{t_R}{2}(\tilde{c}_\sigma^{\tilde{\alpha}}+\tilde{c}_\sigma^{\tilde{\alpha}'})(F_{-\sigma}B')_S+\frac{t_R}{2}(\tilde{c}_\sigma^{\tilde{\alpha}}-\tilde{c}_\sigma^{\tilde{\alpha}'})(F_{-\sigma}B')_A+\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\tilde{\alpha}}+\tilde{c}_{-\sigma}^{\tilde{\alpha}'})(F_\sigma B')_S$$
$$-\frac{t_R}{2}(\tilde{c}_{-\sigma}^{\tilde{\alpha}}-\tilde{c}_{-\sigma}^{\tilde{\alpha}'})(F_\sigma B')_A+2J(\sigma(S_3^{\tilde{\alpha}}-S_3^{\tilde{\alpha}'})(F_\sigma F'_{-\sigma})_S+\sqrt{2}(S_{-\sigma}^{\tilde{\alpha}}-S_{-\sigma}^{\tilde{\alpha}'})F_{-\sigma}F'_{-\sigma}-\sqrt{2}(S_\sigma^{\tilde{\alpha}}-S_\sigma^{\tilde{\alpha}'})F_\sigma F'_\sigma). \tag{A6}$$

APPENDIX B: TWO-SITE DYNAMICAL CORRECTION

The self-energy is obtained by evaluating the correction arising from δj given in Eq. (2.29). By choosing a representative lattice $(\mathbf{x},\mathbf{x}')$, from $\delta j_\sigma(x)$ we have

$$\begin{aligned}\delta j_\sigma(x,x') &= -t_R(B^\dagger BB^{\dagger\prime}F'_\sigma + F^\dagger_\sigma F_\sigma B^{\dagger\prime}F'_\sigma + F^\dagger_{-\sigma}F_\sigma B^{\dagger\prime}F'_{-\sigma}) + J(B^\dagger F_\sigma F^{\dagger\prime}_\sigma F'_\sigma - B^\dagger F_\sigma F^{\dagger\prime}_{-\sigma}F'_{-\sigma} + 2B^\dagger F_{-\sigma}F^{\dagger\prime}_{-\sigma}F'_\sigma) \\ &\quad - a_0 B^\dagger F_\sigma (B^{\dagger\prime}B' + F^{\dagger\prime}_\sigma F'_\sigma + F^{\dagger\prime}_{-\sigma}F'_{-\sigma}) - a_1(B^\dagger B + F^\dagger_\sigma F_\sigma + F^\dagger_{-\sigma}F_{-\sigma})B^{\dagger\prime}F'_\sigma \\ &= a_{BBFB_S}(BB')^\dagger (FB'_S)_\sigma + a_{BBFB_A}(BB')^\dagger (FB'_A)_\sigma + a_{FB_SFF_S}(FB'_S)^\dagger_\sigma FF'_{2\sigma} + a_{FB_AFF_S}(FB'_A)^\dagger_\sigma FF'_{2\sigma} \\ &\quad + \frac{1}{\sqrt{2}}\, a_{FB_SFF_S}(FB'_S)^\dagger_{-\sigma}(FF'_S)_0 + \frac{1}{\sqrt{2}}\, a_{FB_AFF_S}(FB'_A)^\dagger_{-\sigma}(FF'_S)_0 + a_{FB_AFF_A}(FB_A)^\dagger_{-\sigma}\sigma FF'_A \\ &\quad + a_{FB_SFF_A}(FB_S)^\dagger_{-\sigma}\sigma FF'_A, \end{aligned} \tag{B1}$$

where

$$a_{BBFB_S} = \frac{1}{\sqrt{2}}\,(-t_R - a_1 - a_0), \tag{B2}$$

$$a_{BBFB_A} = \frac{1}{\sqrt{2}}\,(t_R + a_1 - a_0), \tag{B3}$$

$$a_{FB_SFF_S} = \frac{1}{\sqrt{2}}\,(-t_R - a_1 - J + a_0), \tag{B4}$$

$$a_{FB_AFF_S} = \frac{1}{\sqrt{2}}\,(-t_R - a_1 + J - a_0), \tag{B5}$$

$$a_{FB_AFF_A} = \frac{1}{2}\,(-t_R + a_1 - 3J - a_0), \tag{B6}$$

$$a_{FB_SFF_A} = \frac{1}{2}\,(-t_R + a_1 + 3J + a_0). \tag{B7}$$

We have

$$\begin{aligned}\delta j_\sigma(x,x')' &= \delta j_\sigma(x',x) \\ &= a'_{BBFB_S}(BB')^\dagger (FB'_S)_\sigma + a'_{BBFB_A}(BB')^\dagger (FB'_A)_\sigma + a'_{FB_SFF_S}(FB'_S)^\dagger_\sigma FF'_{2\sigma} + a'_{FB_AFF_S}(FB'_A)^\dagger_\sigma FF'_{2\sigma} \\ &\quad + \frac{1}{\sqrt{2}}\, a'_{FB_SFF_S}(FB'_S)^\dagger_{-\sigma}(FF'_S)_0 + \frac{1}{\sqrt{2}}\, a'_{FB_AFF_S}(FB'_A)^\dagger_{-\sigma}(FF'_S)_0 + a'_{FB_AFF_A}(FB_A)^\dagger_{-\sigma}\sigma FF'_A \\ &\quad + a'_{FB_SFF_A}(FB_S)^\dagger_{-\sigma}\sigma FF'_A, \end{aligned} \tag{B8}$$

where

$$a'_{BBFB_S} = a_{BBFB_S}, \tag{B9}$$

$$a'_{BBFB_A} = -a_{BBFB_A}, \tag{B10}$$

$$a'_{FB_SFF_S} = -a_{FB_SFF_S}, \tag{B11}$$

$$a'_{FB_AFF_S} = a_{FB_AFF_S}, \tag{B12}$$

$$a'_{FB_AFF_A} = -a_{FB_AFF_A}, \tag{B13}$$

$$a'_{FB_SFF_A} = a_{FB_SFF_A}. \tag{B14}$$

APPENDIX C: SITE-IRREDUCIBLE PROPAGATORS

The reservoir propagators defined by Eqs. (3.17) and (3.18) are expressed as

$$S_{\tilde{c}R_A} = S_{\tilde{c}R} - S'_{\tilde{c}R}, \tag{C1}$$

$$S_{\tilde{c}R_S} = S_{\tilde{c}R} + S'_{\tilde{c}R}, \tag{C2}$$

with

$$S_{\tilde{c}R}=t_R^2\langle R\tilde{c}^{\tilde{\alpha}}\tilde{c}^{\dagger\tilde{\alpha}}\rangle_R, \tag{C3}$$

$$S'_{\tilde{c}R}=t_R^2\langle R\tilde{c}^{\tilde{\alpha}}\tilde{c}^{\dagger\tilde{\alpha}'}\rangle_R, \tag{C4}$$

where the subscript R indicates that the propagator avoids to cross the lattice point $\mathbf{x}$ and $\mathbf{x}'$. By denoting the Hamiltonians of the total system, the concerned two sites and the reservoir as H, H_S, and H_R, respectively, we have

$$H_R+H_S=H-H_{\mathrm{RS}} \tag{C5}$$

where H_{RS} is the interaction between the system and reservoir. We evaluate $S_{\tilde{c}R}$ and $S'_{\tilde{c}R}$ as an impurity scattering induced by H_{RS}. By denoting $\Psi=(\tilde{c}^{\tilde{\alpha}}/\tilde{c}^{\tilde{\alpha}'})$, we approximate as

$$\mathrm{F.T.}\langle R\Psi\Psi^{\dagger}\rangle_R\approx[\tilde{S}]+t_R^2[\tilde{S}][S_0][\tilde{S}]+\cdots, \tag{C6}$$

where

$$[\tilde{S}]=\begin{pmatrix}\tilde{S} & \tilde{S}'\\ \tilde{S}' & \tilde{S}\end{pmatrix}, \tag{C7}$$

with

$$\begin{aligned}\tilde{S}&=\mathrm{F.T.}\langle R\tilde{c}^{\tilde{\alpha}}\tilde{c}^{\dagger\tilde{\alpha}}\rangle\\ &=\mathrm{F.T.}(\tfrac{1}{2}\langle R\tilde{c}^{\alpha}\tilde{c}^{\dagger\alpha}\rangle+\tfrac{1}{16}\langle R\tilde{c}\tilde{c}^{\dagger}\rangle)\end{aligned} \tag{C8}$$

and

$$\begin{aligned}\tilde{S}'&=\mathrm{F.T.}\langle R\tilde{c}^{\tilde{\alpha}}\tilde{c}^{\dagger\tilde{\alpha}'}\rangle\\ &=\mathrm{F.T.}(\langle R\tilde{c}^{\alpha}\tilde{c}^{\dagger\alpha}\rangle-\tfrac{7}{16}\langle R\tilde{c}\tilde{c}^{\dagger}\rangle),\end{aligned} \tag{C9}$$

and $[S_0]$ is the on-site propagator for the concerned two-site systems. Since the total propagator is rewritten in the present approximation as

$$S(\omega,\mathbf{k})=\frac{1}{S_0^{-1}(\omega)+t_R\alpha(\mathbf{k})V(\omega)}, \tag{C10}$$

we have

$$[S_0]^{-1}=\begin{pmatrix}S_0^{-1} & \frac{1}{4}V\\ \frac{1}{4}V & S_0^{-1}\end{pmatrix}. \tag{C11}$$

Then we have

$$[S_R]^{-1}=\frac{1}{t^2}[\tilde{S}]^{-1}-[S_0], \tag{C12}$$

with

$$[S_R]=\begin{pmatrix}S_{\tilde{c}R} & S'_{\tilde{c}R}\\ S'_{\tilde{c}R} & S_{\tilde{c}R}\end{pmatrix}. \tag{C13}$$

To evaluate the loop correction arising from the spin fluctuation, we also need the spin-correlation functions

$$\phi(t-t')=4\langle\{S_i^{\tilde{\alpha}}(t),S_i^{\tilde{\alpha}}(t')\}\rangle_R, \tag{C14}$$

$$\phi'(t-t')=4\langle\{S_i^{\tilde{\alpha}}(t),S_i^{\tilde{\alpha}'}(t')\}\rangle_R. \tag{C15}$$

We approximate them in the two-site approximation by considering the six-site cluster including $(\mathbf{x},\mathbf{x}')$, in which each pair of sites aligns in parallel,

$$\phi(t-t')\approx\tfrac{1}{2}\langle\{S_i(t),S_i(t')\}\rangle, \tag{C16}$$

$$\phi(t-t')'\approx\tfrac{1}{2}\langle\{S_i(t),S_i(t')'\}\rangle. \tag{C17}$$

Then $\langle\{S_i(t),S_i(t')\}\rangle$, etc. is evaluated by the noncrossing approximation in the resolvent method.

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