Dynamical Stripe Correlation in the d-p Model at 1/8-filling

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Abstract

We investigate the dynamical stripe correlation in the two-dimensional d-p model near 1/8-filling on the basis of the dynamical cluster approximation combined with the unrestricted fluctuation exchange approximation. We obtain the fully self-consistent solutions near 1/8-filling. The spin correlation function near 1/8-filling reflects the existence of the quasi-one-dimensional fluctuation.

Key words: dynamical stripe correlation ; two-dimensional d-p model ; 1/8-filling

1. Introduction

The quasi-one-dimensional (Q1D) charge order in high-Tc cuprates (HTC), which is known as a striped state, has been one of the significant issues for the last years [1]. Considering the various experimental results, it seems natural that this order originates from the strong on-site Coulomb repulsion. By the many numerical and analytical studies it has been clarified that the stripe state can be the ground state of the two-dimensional (2D) Hubbard or d-p model near 1/8-filling [2–6,8,9]. Although at finite temperature strong fluctuations can destroy long-ranged order, short-ranged Q1D fluctuations will persist. Thus, we should consider both antiferromagnetic (AF) spin fluctuation and Q1D charge fluctuation in a self-consistent manner in order to see their influences on the electronic property. In this work we investigate the electronic correlation function in 2D d-p model on the basis of the dynamical cluster approximation (DCA) combined with the unrestricted fluctuation exchange approximation (UFEA). We calculate the dynamical spin correlation functions at finite temperature.

2. Dynamical stripe correlation

We consider only the on-site Coulomb repulsion $U$ among d-electrons at each Cu site, and divide our model Hamiltonian into the non-interacting part $H_0$ and the interacting part $H_1$ as

$$ H = H_0 + H_1 = - \mu \sum_{k, \sigma} \left[ d_{k, \sigma}^{\dagger} d_{k, \sigma} + p_{k, \sigma}^{x} p_{k, \sigma}^{x} + p_{k, \sigma}^{y} p_{k, \sigma}^{y} \right]. $$ (1)

Here $d_{k, \sigma}$ and $p_{k, \sigma}^{x(y)}$ are the annihilation (creation) operator for d- and p-electrons of momentum $k$ and spin $\sigma$, respectively. $\mu$ is the chemical potential. The non-interacting part $H_0$ is represented by

$$ H_0 = \sum_{k, \sigma} \left[ \begin{array}{c} d_{k, \sigma}^{\dagger} \\ p_{k, \sigma}^{x} \\ p_{k, \sigma}^{y} \end{array} \right] \left[ \begin{array}{ccc} \Delta_{dp} & \zeta_{k}^{x} & \zeta_{k}^{y} \\ -\zeta_{k}^{x} & 0 & \zeta_{k}^{y} \\ -\zeta_{k}^{y} & 0 & 0 \end{array} \right] \left[ \begin{array}{c} d_{k, \sigma} \\ p_{k, \sigma}^{x} \\ p_{k, \sigma}^{y} \end{array} \right], $$ (2)

where $\Delta_{dp}$ is the hybridization gap energy between d- and p-orbitals. We take the lattice constant of the square lattice formed of Cu sites as the unit of length, and we can represent $\zeta_{k}^{(y)} = 2t_{dp} \sin \frac{a_{k}^{(y)}}{2}$ and $\zeta_{k}^{x} = -4t_{pp} \sin \frac{a_{k}^{x}}{2} \sin \frac{a_{k}^{y}}{2}$, where $t_{dp}$ is the transfer energy be-
between d-orbital and its neighboring p\(^{(y)}\)-orbital and
\(t_{pp}\) is that between p\(^{x}\)-orbital and p\(^{y}\)-orbital. In this
study, we take \(t_{dp}\) as the unit of energy. The residual
part, \(H_1\), is described as

\[
H_1 = \frac{U}{N} \sum_{k \ell} \sum_q d_{kq}^\dagger d_{k+\ell q}^\dagger 
\]

where \(N\) is the number of \(k\)-space lattice points in the
first Brillouin zone (FBZ).

We diagonalize \(H - H_1\) and derive unperturbed Green
function, \(g_d^\sigma(k, \varepsilon_n)\). With the help of the DCA
concept [10], our unrestricted perturbed Green function is approximated as \(G_{d}^\sigma(k, \varepsilon_n) \simeq G_{d}^\sigma(K, \varepsilon_n)\)
if \(k' - k \in \{K\}\). Here we use an abbreviation, \(\varepsilon_n = \pi T(2n + 1)\) with \(n = 0, \pm 1, \pm 2, \ldots\). \(T\) represents the
temperature, and \(\{K\}\) does a cell in the FBZ represented
by a cluster momentum \(K\) in the center of the

cell. This perturbed Green function and the unperturbed one are combined by the Dyson equation :

\[
\left[ G_{d}^\sigma(K, \varepsilon_n) \right]^{-1} = \left\{ g_d^\sigma(k, \varepsilon_n) \right\}^{-1} \delta_{K} = \Sigma_{\delta}^\sigma(k, \varepsilon_n).
\]

(4)

We adopt the UFEA in order to compute our unrestricted self-energy [11], \(\Sigma_{\delta}^\sigma(K, \varepsilon_n)\). In eq. (4) we use
an abbreviation for the inverse operation, \([ \cdots ]^{-1}\), defined so that the identities :

\[
\delta_{K} = \sum_L G_{d}^\sigma(L, \omega) \left[ K + L - K, \varepsilon_n \right] \left[ G_{d}^\sigma(L, \varepsilon_n) \right]^{-1}
\]

are satisfied for all \(k\) and \(n\). \(\delta_{K}\) is Kronecker’s delta. We
have to solve all equations for the fully self-consistent solution, \(G_{d}^\sigma(K, \varepsilon_n)\).

We divide the FBZ into \(16 \times 16\) meshes, and take \(8 \times 2\)
cluster momenta. We prepare \(2^{11}\) Matsubara frequencies
for temperature \(T = 0.030 \sim 270K\). Our other parameters : \(t_{dp} = 1.0 \sim 0.80eV\), \(t_{pp} = 0.60 \sim 0.48eV\),
and \(\Delta_{dp} = 0.0, U = 10.0 \sim 8.0eV\). In our results \(\delta \equiv n_k^{\hbar total} - 1 = 0.120,\) and \(n_k^{\hbar} / n_k^{\hbar total} = 1.64.\) We adopt Padé
approximating for the method of analytic continuation.

We calculate the dynamical spin correlation function :

\[
I(q, E) = \text{Im} \sum_K \left( \chi_{-}^\dagger K(q, \varepsilon_n) \right) 
\]

\[
\times \left[ \delta_{K} - U \chi_{-}^\dagger K(q - K, \varepsilon_n) \right]^{-1} \big|_{\varepsilon_n \rightarrow -E}
\]

which corresponds to the inelastic neutron scattering
intensity. In Fig. 1 we show its momentum dependence
at \(E = 0.24\). We can find that it reflects a weak Q1D
character of the electronic state. Such a Q1D character
appears around \(E = 0.22 \sim 0.25\), but in the other

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{\(I(q, E)\) at \(E = 0.24 \sim 192meV\)}
\end{figure}

energy range does not. This Q1D character originates
from the strong Coulomb repulsion.

In summary, in this work we analyze the dynamical spin
correlation in the two-dimensional d-p model near
1/8-filling. We calculate the one-particle spectral function,
the charge correlation function, and the spin correlation
function at finite temperature. We obtain the fully self-consistent solutions taking account of some
certain types of inhomogeneities in our system. The
spin correlation function reflect the existence of the
Q1D fluctuation. In three-dimensional real materials
this fluctuation tends to form the vertical stripe state,
which has been observed in the neutron scattering ex-
periment in \(La_2-xSr_xCuO_4\) [12].

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