# 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-$\mathrm{T_c}$ 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.

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## 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

$$H = H_0 + H_1 - \mu \sum_{\boldsymbol{k}\sigma} \left[ d^\dagger_{\boldsymbol{k}\sigma} d_{\boldsymbol{k}\sigma} + p^{x\dagger}_{\boldsymbol{k}\sigma} p^x_{\boldsymbol{k}\sigma} + p^{y\dagger}_{\boldsymbol{k}\sigma} p^y_{\boldsymbol{k}\sigma} \right]. \tag{1}$$

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

$$H_0 = \sum_{\boldsymbol{k}\sigma} \begin{pmatrix} d_{\boldsymbol{k}\sigma} \\ p^x_{\boldsymbol{k}\sigma} \\ p^y_{\boldsymbol{k}\sigma} \end{pmatrix}^{T\,\dagger} \begin{pmatrix} \Delta_{dp} & \zeta^x_{\boldsymbol{k}} & \zeta^y_{\boldsymbol{k}} \\ -\zeta^x_{\boldsymbol{k}} & 0 & \zeta^p_{\boldsymbol{k}} \\ -\zeta^y_{\boldsymbol{k}} & \zeta^p_{\boldsymbol{k}} & 0 \end{pmatrix} \begin{pmatrix} d_{\boldsymbol{k}\sigma} \\ p^x_{\boldsymbol{k}\sigma} \\ p^y_{\boldsymbol{k}\sigma} \end{pmatrix}, \tag{2}$$

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 $\zeta^{x(y)}_{\boldsymbol{k}} = 2\mathrm{i}\, t_{dp} \sin\frac{k_{x(y)}}{2}$ and $\zeta^p_{\boldsymbol{k}} = -4t_{pp} \sin\frac{k_x}{2} \sin\frac{k_y}{2}$, where $t_{dp}$ is the transfer energy between d-orbital and its neighboring $\mathrm{p}^{x(y)}$-orbital and $t_{pp}$ is that between $\mathrm{p}^x$-orbital and $\mathrm{p}^y$-orbital. In this study, we take $t_{dp}$ as the unit of energy. The residual part, $H_1$, is described as

$$H_1 = \frac{U}{N} \sum_{\boldsymbol{kl}} \sum_{\boldsymbol{q}} d^\dagger_{\boldsymbol{k}+\boldsymbol{q}\uparrow} d^\dagger_{\boldsymbol{l}-\boldsymbol{q}\downarrow} d_{\boldsymbol{l}\downarrow} d_{\boldsymbol{k}\uparrow}, \tag{3}$$

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

We diagonalize $H - H_1$ and derive unperturbed Green function, $g^\sigma_d(\boldsymbol{k}, \mathrm{i}\epsilon_n)$. With the help of the DCA concept [10], our unrestricted perturbed Green function is approximated as $G^\sigma_d(\boldsymbol{k}, \boldsymbol{k}'; \mathrm{i}\epsilon_n) \simeq G^\sigma_{d\boldsymbol{K}}(\boldsymbol{k}, \mathrm{i}\epsilon_n)$ if $\boldsymbol{k}' - \boldsymbol{k} \in \{\boldsymbol{K}\}$. Here we use an abbreviation, $\epsilon_n = \pi T(2n+1)$ with $n = 0, \pm 1, \pm 2, \ldots$. $T$ represents the temperature, and $\{\boldsymbol{K}\}$ does a cell in the FBZ represented by a cluster momentum $\boldsymbol{K}$ in the center of the cell. This perturbed Green function and the unperturbed one are combined by the Dyson equation :

$$\left[G^\sigma_{d\boldsymbol{K}}(\boldsymbol{k}, \mathrm{i}\epsilon_n)\right]^{-1} = \{g^\sigma_d(\boldsymbol{k}, \mathrm{i}\epsilon_n)\}^{-1} \delta_{\boldsymbol{K}} - \Sigma^\sigma_{\boldsymbol{K}}(\boldsymbol{k}, \mathrm{i}\epsilon_n). \tag{4}$$

We adopt the UFEA in order to compute our unrestricted self-energy [11], $\Sigma^\sigma_{\boldsymbol{K}}(\boldsymbol{k}, \mathrm{i}\epsilon_n)$. In eq. (4) we use an abbreviation for the inverse operation, $[\cdots]^{-1}$, defined so that the identities :

$$\delta_{\boldsymbol{K}} = \sum_{\boldsymbol{L}} G^\sigma_{d\boldsymbol{K}-\boldsymbol{L}}(\boldsymbol{k} + \boldsymbol{L} - \boldsymbol{K}, \mathrm{i}\epsilon_n) \left[G^\sigma_{d\boldsymbol{L}}(\boldsymbol{k}, \mathrm{i}\epsilon_n)\right]^{-1} \tag{5}$$

are satisfied for all $\boldsymbol{k}$ and $n$. $\delta_{\boldsymbol{K}}$ is Kronecker's delta. We have to solve all equations for the fully self-consistent solution, $G^\sigma_{d\boldsymbol{K}}(\boldsymbol{k}, \mathrm{i}\epsilon_n)$.

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

$$I(\boldsymbol{q}, E) = \mathrm{Im} \sum_{\boldsymbol{K}} \chi^{+-}_{-\boldsymbol{K}}(\boldsymbol{q}, \mathrm{i}\omega_m) \times \left[\delta_{\boldsymbol{K}} - U\chi^{+-}_{\boldsymbol{K}}(\boldsymbol{q} - \boldsymbol{K}, \mathrm{i}\omega_m)\right]^{-1}\Big|_{\mathrm{i}\omega_m \to E}, \tag{6}$$

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

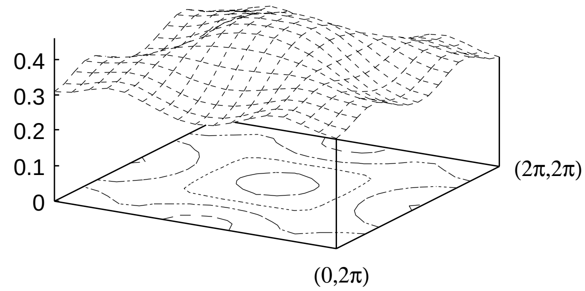


Fig. 1. $I(\boldsymbol{q}, E)$ at $E = 0.24 \sim 192\mathrm{meV}$

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 experiment in $\mathrm{La_{2-x}Sr_xCuO_4}$ [12].

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