Three-Orbital Spin-Fermion Model for CuO_2 Planes

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High-T_c Cuprates became important materials when their superconducting properties were discovered in the 1980s. They form a complex three-dimensional structure that is hard to study, and this is why researches have focused on the study of the more basic Copper-Oxygen planes. The CuO_2 plane consists of copper ions at the sites of a square lattice and oxygen ions at the links. The orbitals of significance are the $3d_{x^2-y^2}$ and the p_σ orbitals. This results in a three-orbital model which is still difficult to study accurately. As a result, researches effectively used a one-orbital model such as the t-J model where only the $3d_{x^2-y^2}$ is considered.

Single-orbital models are often used to study the cuprates, since Angle Resolved Photoemission Spectroscopy (ARPES) results show one single band at the Fermi surface and the Zhang-Rice singlet transforms the three-orbital model to a t-J model. The orbital at the Fermi surface is a *d*-orbital that is split at the chemical potential due to the Hubbard interaction which is less than the energy difference between the *d* and *p* orbitals. This results in a Mott-Hubbard type insulator. Nevertheless, the cuprates are charge-transfer insulators with the hybridized *p*-orbital in between the upper and lower Hubbard bands. In our study we ask the questions: do oxygen p_σ orbitals play an important role and is the Zhang-Rice picture correct? Therefore, we need a three-orbital model that can be studied numerically in large lattices and at all temperatures.

The phenomenological Spin-Fermion (SF) model consists of a tight binding Hamiltonian,

$$H_{\mathrm{TB}} = \sum_{\mathbf{k},\alpha,\beta,\sigma} T^{\alpha,\beta}(\mathbf{k}) c^{\dagger}_{\mathbf{k},\alpha,\sigma} c_{\mathbf{k},\beta,\sigma}$$

where $T^{\alpha,\beta}$ is a matrix that takes the hopping signs into consideration. The interaction part, consists of the *d*-orbital term, that prevents its double occupancy, via the interaction of the quantum spin with the phenomenological localized spins,

$$H_p = J_d \sum_{\mathbf{i}} S_{\mathbf{i}} \cdot s^{d}_{\mathbf{i}}$$

the *p*-orbital term, that introduces frustration,

$$H_p = J_p \sum_{\mathbf{i},\boldsymbol{\mu}} S_{\mathbf{i}} \cdot s^{p}_{\mathbf{i}+\boldsymbol{\mu}/\mathbf{2}}$$

and a Heisenberg term that encourages an antiferromagnetic order via the localized spin interaction,

$$H_{\mathrm{Heis}} = J_{\mathrm{NN}} \sum_{<\mathbf{i},\mathbf{j}>} S_{\mathbf{i}} \cdot S_{\mathbf{j}}$$

A similar model has been used for the pnictides [1], one-orbital cuprates [2] and manganites [3]. The simplification in this model is the use of classical localized spins that renders the Hamiltonian bilinear in its operators and allows it to be studied using Monte Carlo. The studied cluster sizes we analyzed cannot be accessed with Density Matrix Renormalization Group (DMRG), Lanczos nor with Quantum Monte Carlo.

From the three-band Hubbard model, using the variational cluster approach [4], we found that the density of states for the Zhang-Rice Band (ZRB) should consist of equal contributions from the *d* and *p* orbitals. Thus, we were able to determine the appropriate parameters in our model to reflect the properties of the cuprates,

$$J_d = 3.0, \qquad J_p = 1.0 \quad \& \quad J_{\mathrm{NN}} = 0.1$$

In our results, for the undoped case, five electrons per unit cell, we can observe the ZRB as seen in Figure 1. Its dispersion is about 0.5-0.8 eV, close to the experimental results. Moreover, a spontaneously developed dispersion which is symmetric about $(\pi/2, \pi/2)$ can be seen, as in experiments, that is not captured by the single-orbital t-J model [5].

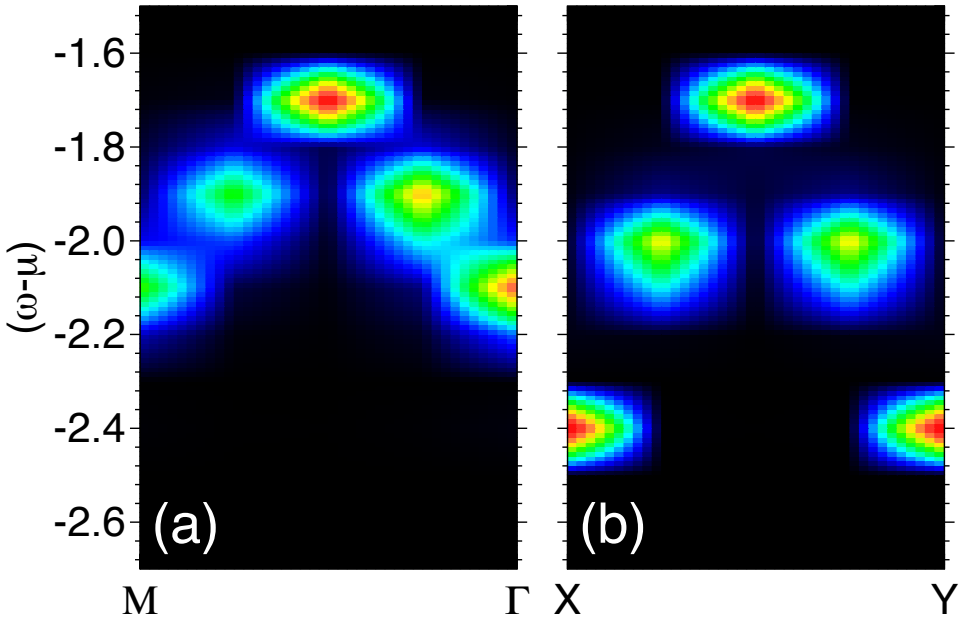

Figure 1: The Zhang-Rice Band for the undoped case in (a) the M-Γ direction and (b) the X-Y direction, which shows a dispersion that is symmetric about $(\pi/2, \pi/2)$, that is not captured by the t-J model.

In the hole-doped case of sixteen holes in the 8x8 cluster, we can see a pseudogap at the chemical potential. Its dispersion is about 1 eV, close to experiments. Additionally, we can see the "waterfall" feature along the M-Γ direction, Figure 2, as seen in Dynamical Mean-Field Theory calculations [6].

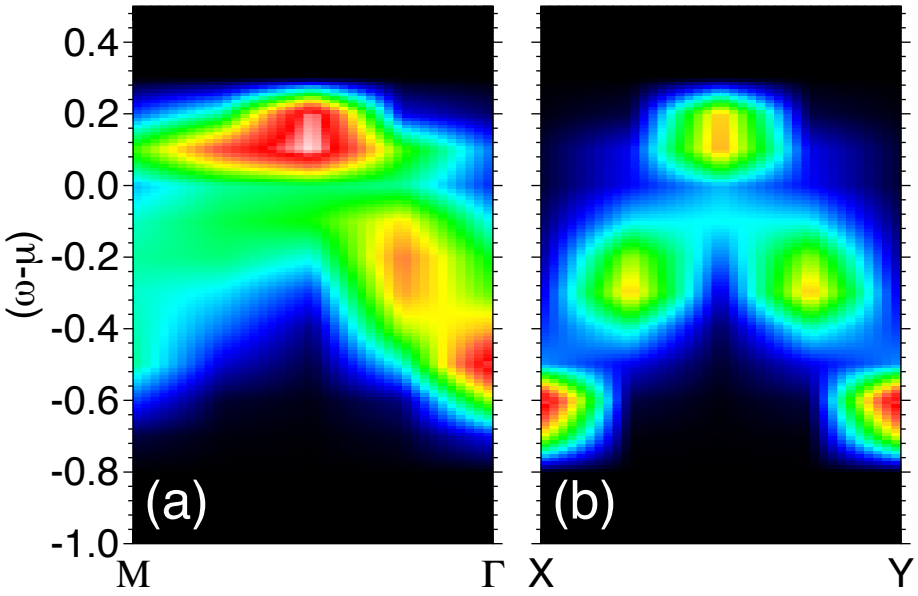

Figure 2: The pseudogap can be seen for the case of sixteen holes doping in (a) the M-Γ direction, which shows the "waterfall" feature and (b) the X-Y direction.

For the magnetic structure, Figure 3, we can observe a tendency towards antiferromagnetic long-range order, which stabilizes in the undoped limit at a temperature about 300K.

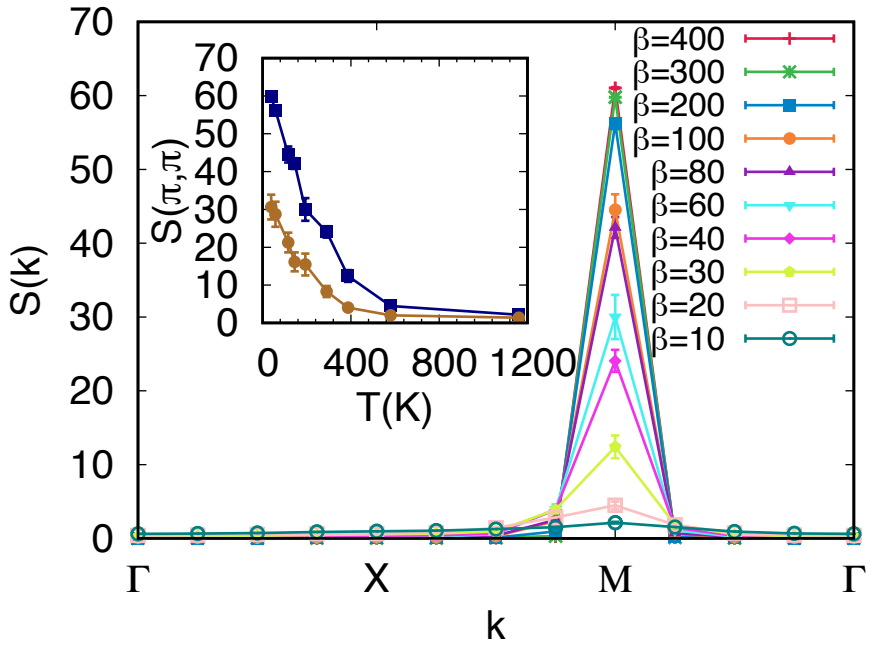

Figure 3: for the undoped case, there is a tendency towards antiferromagnetic long-range order. The peak at **M** can be seen decreasing with increasing temperature, decreasing β. In the inset, for $\mathbf{k} = (\pi, \pi)$, we can see that the quantum copper spin (green), multiplied by five, follows the same trend as the classical localized spins (blue).

As a next step, we will study charge-spin structures such as stripes, Zhang-Rice singlets, high spin polarons and intertwined orders. Preliminary results are already submitted for publication [7].

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