Local lattice distortion in high-T_c cuprates

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The dynamical local lattice distortion in the CuO_2 plane of the cuprate high-temperature superconductors is investigated with the numerical diagonalization study for finite clusters of *t*-*J* model. It is found that the in-plane vibrations of the oxygens play an important role in the formation of some static orders like CDW and SDW through the polaronic self localization effect. The 1/8 problem is also discussed based on the present result.

Keywords: high-T_c cuprate, electron-phonon interaction, polaron, charge ordering, 1/8 problem

1. Introduction

The x-ray spectroscopy is one of the most useful method to detect some static charge orderings and lattice distortions in the strongly correlated electron systems. In fact the Cu *K*-edge x-ray absorption has also used to investigate local distortions in the CuO_2 plane of the $La_{1.85}Sr_{0.15}CuO_4$. (Saini *et al*., 1997) The 1/8 problem has attracted much current interest, since the charge stripe order was observed in some high-T_c cuprates near the special value of the hole concentration $x = 1/8$. (Tranquada *et al*., 1995) The x-ray diffraction (Kakinuma *et al*., 1999) revealed that the stripe order is not related with the structural phase transition between the tetragonal high-temperature phase and the orthorhonbic midtemperature one. However, the *dynamical* lattice distortion can still contribute to the charge ordering. Then it would be interesting to investigate the interplay of the electron-phonon interaction and the charge density wave (CDW) and spin density wave (SDW) correlations in the strongly correlated electron systems.

The finite-cluster calculation study on the 2D Hubbard and *t*-*J* model in nearly half-filled case with on-site electron-phonon coupling in the static limit indicated an evidence of the polaronic self-localization effect. (Zhong & Schüttler, 1992) At quarter filling, the adiabatic *t*-*J*-Holstein model leads to ordering of polarons into a commensurate CDW (Röder *et al*., 1994), proposed as an explanation of the observed superlattice in $La_{2-x}Sr_xNiO_{4+y}$. (Chen *et al*., 1993) The 20-site cluster study on the planer *t*-*J* model including a few coherent modes of the dynamical displacements of the in-plane oxygens revealed that a sufficiently large electron-phonon coupling yields the self-localization of the holes and the enhancement of the SDW and CDW instabilities at nearly half filling. (Poilblanc *et al*., 1996) On the other hand, there is experimental evidence that those phonon modes have a small dispersion in the Brillouin zone for the cuprates. (Weber *et al*., 1988) In other words, the oxygen vibrational modes are very localized and can be considered independent. In this paper, we consider a generalized *t*-*J*-Holstein model for which every local breathing vibration of the in-plane oxygen is taken into account as an independent phonon mode. Using the exact diagonalization of finite clusters of the CuO_2 plane, we investigate the role of the dynamical local lattice distortion in the high-T_c cuprates. Out-of-plane buckling vibrations are neglected, because they were revealed to have almost no effect on the static ordering. (Sakai *et al*., 1997)

2. Model and Method

The Hamiltonian is a generalization of the *t*-*J*-Holstein Hamiltonian,

$$H = -t\sum_{<\mathbf{i},\mathbf{j}>,\sigma}(\tilde{c}^{\dagger}_{\mathbf{j},\sigma}\tilde{c}_{\mathbf{i},\sigma} + \tilde{c}^{\dagger}_{\mathbf{i},\sigma}\tilde{c}_{\mathbf{j},\sigma}) + J\sum_{<\mathbf{i},\mathbf{j}>}(\mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{j}} - \tfrac{1}{4}n_{\mathbf{i}}n_{\mathbf{j}}) + \sum_{\mathbf{i},\delta}(\frac{p^2_{\mathbf{i},\delta}}{2m} + \frac{1}{2}m\Omega^2 u^2_{\mathbf{i},\delta}) + g\sum_{\mathbf{i},\delta}u_{\mathbf{i},\delta}\,(n^h_{\mathbf{i}} - n^h_{\mathbf{i}+\delta}) \quad (1)$$

where $\tilde{c}^{\dagger}_{\mathbf{i},\sigma}$ is the usual hole creation operator, $n_{\mathbf{i}}$ and $n^h_{\mathbf{i}}$ are the electron and hole local densities respectively, m is the oxygen ion mass, Ω is the phonon frequency and $\delta = \mathbf{x}, \mathbf{y}$ differentiates the bonds along the x- and y-direction respectively. Throughout, energies are measured in unit of the hopping integral t. The electron-phonon g-term involves the coupling of each copper hole with the in-plane breathing displacements of the four neighboring oxygens $u_{\mathbf{i},\delta}$ and $u_{\mathbf{i}-\delta,\delta}$ in the CuO_2 plane. Note that the displacements $u_{\mathbf{i},\delta}$ are considered throughout as *independent* variables. We rewrite the electron-phonon interaction in the boson representation of the phonons,

$$H_{e-ph} = \Omega\sum_{\mathbf{i},\delta}(b^{\dagger}_{\mathbf{i},\delta}b_{\mathbf{i},\delta} + \frac{1}{2}) + \lambda_0\sum_{\mathbf{i},\delta}(b_{\mathbf{i},\delta} + b^{\dagger}_{\mathbf{i},\delta})(n^h_{\mathbf{i}} - n^h_{\mathbf{i}+\delta}) \quad (2)$$

where $\lambda_0 = g\sqrt{\frac{1}{2m\Omega}}$. Since the phononic Hilbert space has an infinite dimension, we truncate it to a finite number of bosonic states i.e. $b^{\dagger}_{\mathbf{i},\delta}b_{\mathbf{i},\delta} \leq n_{ph}$ at each oxygen site. To test the validity of the approximation, the one-hole GS energy of the 2×2 (Cu_4O_8) cluster for $J = 0.3$ and $\Omega = 0.2$ is plotted versus lattice with n_{ph} up to 5, in Fig. 1. The converging behavior for $n_{ph} \geq 2$ suggests that even the one-phonon calculation is a good approximation in the weak-coupling region ($\lambda \leq 0.3$). Thus we will also show the result of the $\sqrt{8}\times\sqrt{8}$ (Cu_8O_{16}) cluster with $n_{ph} = 1$ in the following analyses. This is the largest system size available for the present computer systems. Throughout the paper we fix the phonon frequency as $\Omega = 0.2$.

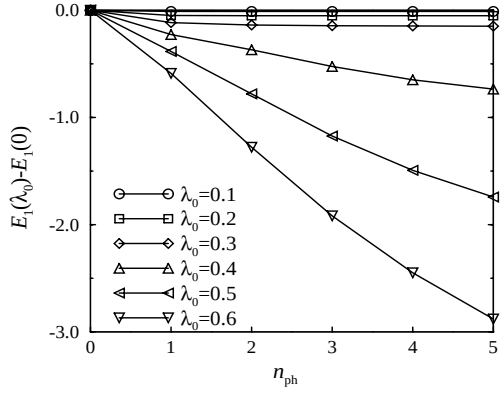

Figure 1
One-hole ground state energy vs truncated phonon number n_{ph} at each oxygen site on 2×2 cluster.

3. Polaronic Self-Localization

The breathing lattice deformations around the hole lower the potential at the hole site, while they raise that at the nearest neighbor Cu sites. Thus it is expected that they make the effective mass of the hole larger and the effect can lead to self-localization of the hole. The absolute value of the kinetic energy in the one-hole ground state

$$E_{kin} = \Big\langle -t \sum_{<\mathbf{i},\mathbf{j}>,\sigma} (\tilde{c}^{\dagger}_{\mathbf{j},\sigma}\tilde{c}_{\mathbf{i},\sigma} + \tilde{c}^{\dagger}_{\mathbf{i},\sigma}\tilde{c}_{\mathbf{j},\sigma})\Big\rangle, \tag{3}$$

of the 4-site cluster (the hole concentration is $x = 1/4$) for $n_{ph} \leq 5$ and $J = 0.3$ is shown in Fig. 2. $|E_{kin}|$ decreases significantly with increasing λ_0, which indicates an evidence of the self-trapping of the hole. Larger n_{ph} approximations make such a mass renormalization clearer and specify a crossover point as $\lambda_{0c} \sim 0.3$. $|E_{kin}|$ in the one-hole ground state of the 8-site cluster (x=1/8) with the one-phonon approximation for J =0.3, 0.4 and 0.5 is also shown in Fig. 3. Although the crossover point of the self-localization is not so clear as the larger-phonon approximations, it indicates that the polaron effect occurs even for much smaller λ_0 ($\sim$ 0.1) than the case of $x = 1/4$.

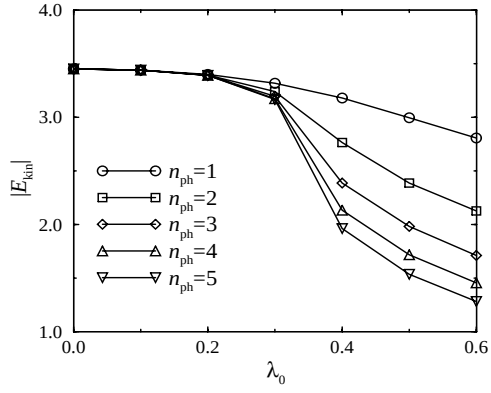

Figure 2
Absolute value of kinetic energy $|E_{kin}|$ in the one-hole ground state of the 2×2 cluster (x=1/4) plotted vs the electron-phonon coupling λ_0 for various truncated phonon numbers n_{ph}. ($J = 0.3$).

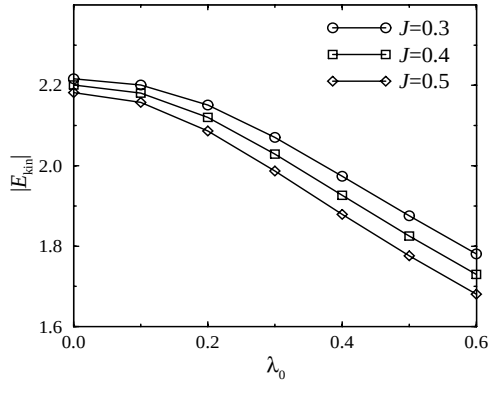

Figure 3
Absolute value of kinetic energy $|E_{kin}|$ in the one-hole ground state of the 8-site cluster Cu_8O_{16} (x=1/8) plotted vs the electron-phonon coupling λ_0 for J =0.3, 0.4 and 0.5.

4. SDW and CDW Instabilities

In order to investigate the enhancement of the SDW and CDW instabilities, we consider the (π, π) component of the spin and charge structure factors defined as

$$S_s(\pi,\pi) = \Big\langle \big(\sum_{\mathbf{i}} (-1)^{(i_x+i_y)} S^z_{\mathbf{i}}\big)^2 \Big\rangle, \tag{4}$$

$$S_c(\pi,\pi) = \Big\langle \big(\sum_{\mathbf{i}} (-1)^{(i_x+i_y)} n^h_{\mathbf{i}}\big)^2 \Big\rangle, \tag{5}$$

respectively. We calculate them in the ground state for several hole concentrations. The spin structure factor of the 4-site cluster with one hole (x=1/4) for various truncated phonon numbers ($J = 0.3$) is shown in Fig. 4. It suggests that the enhancement of the SDW instability begins to occur around the same crossover point $\lambda_{0c} \sim 0.3$ as the self-localization in Fig. 2. $S_s(\pi,\pi)$ of 8-site cluster with one hole (x=1/8) in Fig. 5 also indicates an evidence of the growth of the antiferromagnetic correlation accompanied with the mass renormalization in Fig. 3 for $\lambda_0 \geq 0.1$.

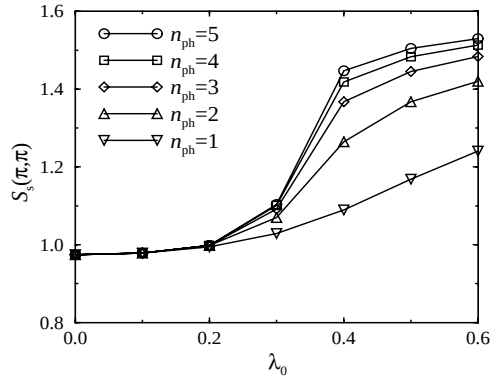

Figure 4
Spin structure factor $S_s(\pi,\pi)$ of Cu_4O_8 with a single hole (x=1/4) for various truncated phonon numbers n_{ph}. ($J = 0.3$).

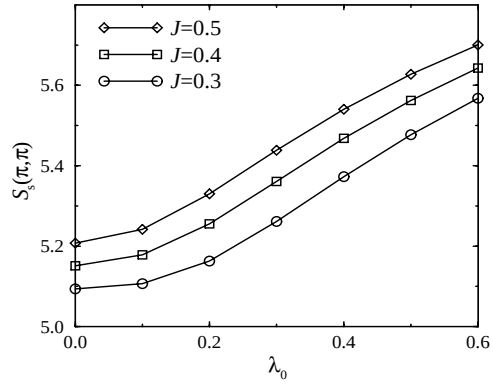

Figure 5
Spin structure factor $S_s(\pi,\pi)$ of Cu_8O_{16} with a single hole (x=1/8).

Although the charge structure factor $S_c(\pi,\pi)$ is meaningless for the one-hole system on such finite lattices, the bulk system is expected to exhibit the enhancement of the CDW instability due to the polaron ordering at the same crossover point as that of the self-localization and SDW. In fact the charge structure factor $S_c(\pi,\pi)$ of 4-site cluster with two holes (x=1/2 and $J = 0.3$), shown in Fig. 6, indicates that the CDW instability begins to grow at $\lambda_0 \sim 0.3$. $S_c(\pi,\pi)$ of 8-site cluster with two holes (x=1/4) in Fig. 7 also exhibits a significant increase for $\lambda_0 \geq 0.4$. (A gradual decrease of $S_c(\pi,\pi)$ for $\lambda_0 \leq 0.4$ in Fig. 7 is due to the finite size effect; the spin and charge correlations with the momentum (π,π) compete with each other on the 8-site cluster under the periodic boundary condition.) The crossover point ($\lambda_{0c} \sim 0.4$) is a little larger than that for the 4-site cluster with the same hole concentration (x=1/4), obtained above. This is because the one-phonon approximation tends to overestimate the crossover point, as shown in Figs. 4 and 6.

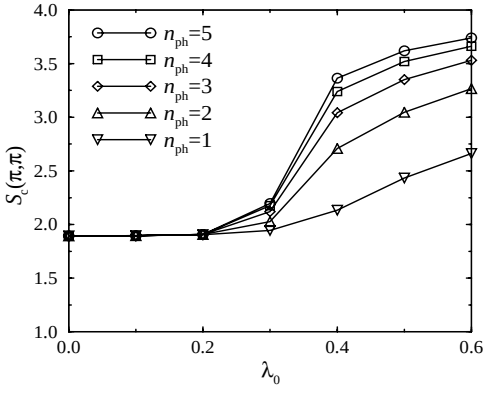

Figure 6
Charge structure factor $S_c(\pi,\pi)$ of Cu_4O_8 with two holes (x=1/2) for various truncated phonon numbers n_{ph}. ($J = 0.3$).

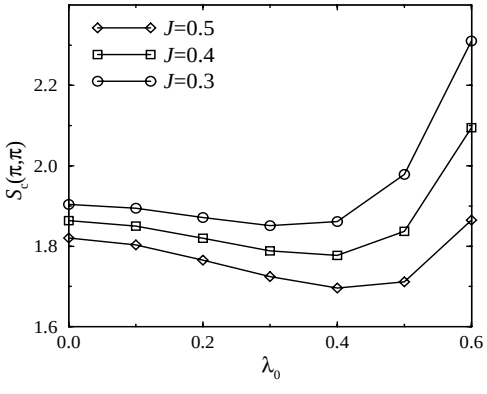

Figure 7
Charge structure factor $S_c(\pi,\pi)$ of Cu_8O_{16} with two holes (x=1/4).

5. Concluding Remarks

The results in the previous sections lead to the conclusion that the SDW and CDW instabilities increase significantly due to the polaroinc self-localization effect when the electron-phonon interaction exceeds some critical value λ_{0c}. In order to consider the 1/8 problem, we list the crossover point λ_{0c} for $\Omega = 0.2$ and $J = 0.3$ together with the hole concentrations obtained in the present work: $\lambda_{0c} \sim 0.1$ for x=1/8 (8 site with one hole), $\lambda_{0c} \sim 0.3$ for x=1/4 (4 site with one hole), $\lambda_{0c} \sim 0.3$ for x=1/2 (4 site with two holes). In addition the two-coherent-phonon approximation for the 20-site cluster with two holes with the same parameters ($\Omega = 0.2$ and $J = 0.3$) gave the result $\lambda_{0c} \sim 0.4$ for x=1/10. (Poilblanc *et al*., 1996) Those results indicate that x=1/8 is a quite special case when the SDW and CDW instabilities are enhanced by the polaronic mass renomalization even for much smaller electron-phonon coupling than other cases. It implies that the structure of possible charge or spin orderings for x=1/8 is very sensitive to the local breathing vibrations of the in-plane oxygen. Further study on the system with some other values of x near 1/8 would be desirable.

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