Numerical study of phonon spectra in strongly correlated electron systems

Kenji Tsutsui [1], Takami Tohyama, and Sadamichi Maekawa
Institute for Materials Reserch, Tohoku University, Sendai 980-8577, Japan

Abstract

We examine theoretically the phonon dynamics in the electron-phonon-coupled systems. The model Hamiltonian is a one-dimensional Hubbard model coupled with phonons. The numerically exact diagonalization of the Hamiltonian with truncations of phonon Hilbert space is performed. We calculate the phonon excitation spectra and find a deffusive feature in the spectra in the metallic region. We also calculate the charge and spin excitation spectra and find that the feature in the phonon spectra is caused by the low energy electronic excitations.

Key words: cuprate; spectral function; electron-phonon interaction

The role of the electron-phonon coupling in both electron and phonon states in high-T_c cuprates is still controversial. It has been proposed in the ARPES study [1] that the phonon plays an important role in the electronic states of the cuprates. In particular, the 'kink' dispersion and the spectral shapes in APRES spectra would be related with the anomalus behavior in longitudinal optical phonon modes exhibited in the neutron scattering experiment [2][3]. In view of theoretical study, it is neccesary to treat the electronic and phonon degrees of freedom on an equal footing for understanding both these dynamics. In this study we examine the phonon dynamics in the strongly correlated electron system. The numerically exact diagonalization technique is used to calculate the electron and phonon excitation spectra. A diffusive feature of the phonon excitation spectra is obtained in the metallic region. By comparing the energy and momentum of the phonon excitations with those of charge and spin excitations, we conclude that the feature is caused by the low energy electronic excitations.

In order to examine the momentum dependence of the phonon dynamics affected by the strongly correlated electrons, we consider the one-dimensional Hubbard model coupled with phonons defined by,

$$\begin{aligned} H = & -t\sum_{i,\sigma}\left(c^{\dagger}_{i,\sigma}c_{i+1,\sigma}+h.c.\right)+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow} \\ & +\sum_{q}\Omega_q\left(b^{\dagger}_{q}b_q+\frac{1}{2}\right) \\ & +\lambda\sum_{i,\sigma}\left(b_{i+\frac{1}{2}}+b^{\dagger}_{i+\frac{1}{2}}\right)\left(n_{i,\sigma}-n_{i+1,\sigma}\right), \end{aligned} \tag{1}$$

where $c_{i,\sigma}$ denotes the annihilation operator of electron with spin σ at site i, $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$, b_q the phonon annihilation operator with momentum q, $b_{l+\frac{1}{2}}=\frac{1}{L}\sum_q e^{iq(l+\frac{1}{2})}b_q$ (L is the system size). The parameters t, U, λ and Ω_q are the electron hopping integral between nearest neighbor sites, on-site Coulomb interaction, coupling constant between electron and phonon, and the phonon frequency, respectively. We assume that $\Omega_q=\omega_0\cos q+\Omega_0$ for simplicity. The last term in Eq. (1) denotes the interaction between phonon and electron density. We also consider another case that phonon interacts with the hopping of the electrons and discuss the differece of the couplings elsewhere [4].

[1] E-mail:tutui@imr.tohoku.ac.jp

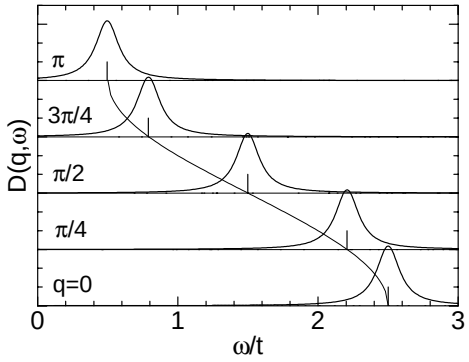

Fig. 1. The phonon excitation spectra $D(q,\omega)$ in the one-dimensional half-filled ($\rho = 8/8$) Hubbard model where phonon interacts with the electron density, obtained by exact diagonalization for the 8 site ring. The values of the parameters are $U/t = 10$, $\Omega_0/t = 1.5$, $\omega_0/t = 0.5$, and $\lambda/t = 0.25$. The thin curve denotes the dispersion of the free phonon. The δ functions (the vartical thin solid lines) are convoluted with a Lorentzian broadening of $0.1t$.

We calculate the phonon excitation spectrum defined by,

$$D(q,\omega) = \frac{1}{\pi}\mathrm{Im}\left\langle 0 \left| b_q \frac{1}{\omega - i\eta - H + E_0} b_q^\dagger \right| 0 \right\rangle, \qquad (2)$$

where $|0\rangle$ denotes the ground state with energy E_0 and η is infinitesimal quantity. Note that $D(q,\omega) = \delta(\omega - \Omega_q)$ in case of the free phonon system.

We employ the numerically exact diagonalization method to examine the ground state and the excitation spectra. The infinite-dimensional phonon Hilbert space requires some further approximation even for finite-size systems. In this study we truncate the total number of phonons (~ 4) in the system. We will show the results in the case that the system size $L = 8$ throughout.

Figure 1 shows $D(q,\omega)$ for half-filling of electrons in the Hubbard model. The parameter values are $U/t = 10$, $\Omega_0/t = 1.5$, $\omega_0/t = 0.5$, and $\lambda/t = 0.25$. Parameter values for the phonon system are set to be larger than those in real transition metal oxides, because we qualitatively examine the effect of electron-phonon interaction on the phonon spectra. The thin curve in Fig. 1 denotes the dispersion of the free phonon. In Fig. 1, there is a single peak for each momentum, and the energy position of the peak remains unchanged from that of the free phonon dispersion within this figure scales. Since the charge fluctuation is much supressed, the dynamics of the phonons which couple with the charge density is less affected in case of the half-filling of electrons. Thus the feature of the spectra is the same as that of the free phonon system.

In Fig. 2, we show $D(q,\omega)$ in the hole-doped case, where the number of electrons per site ρ is 6/8. The values of the other parameters are the same as in Fig. 1. The spectrum at $q = \pi/2$ splits into some peaks, which

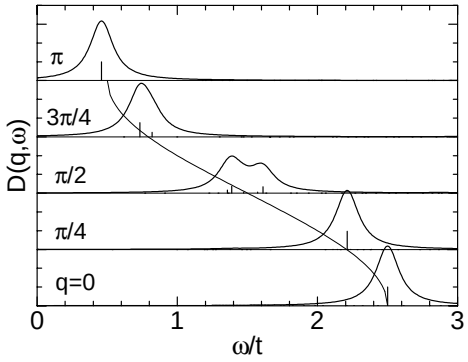

Fig. 2. The phonon excitation spectra $D(q,\omega)$ in the one-dimensional hole-doped ($\rho = 6/8$) Hubbard model where phonon interacts with the electron density. The values of the parameters are the same as in Fig. 1.

means that the diffusive feature appears with electron-phonon coupling. In order to examine the relation with the electronic excitations, we calculate the dynamical charge correlation functions (not shown here). In the charge excitation spectrum at $\pi/2$, a peak appears in the energy region of the phonon excitation. Therefore the diffusive feature in Fig. 2 is caused by the charge excitations at the same energy and momentum regions.

In summary, we have examined theoretically the phonon dynamics in the one-dimensional Hubbard model coupled with phonons. We have adopted the numerically the exact diagonalization method with truncation of phonon Hilbert space to calculate the phonon excitation spectra as well as the charge and spin excitation ones. We have found a diffusive feature in the phonon spectra in the hole-doped system and that the feature is caused by the low energy electronic excitations.

This work was supported by a Grant-in-Aid for scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan, and CREST. One of the authors (S. M.) acknowledges support of the Humboldt Foundation. The numerical calculations were performed in the supercomputing facilities in ISSP, University of Tokyo, and IMR, Tohoku University.

References

[1] A. Lanzara, et al., Nature **412** (2001) 510.

[2] R. J. McQueeney, et al. Phys. Rev. Lett. **82** (1999) 628.

[3] L. Pintschovius and M. Braden, Phys. Rev. B **60** (1999) R15039.

[4] K. Tsutsui, et al., to be published, Proceedings of MOS2002.