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Effect of electron–phonon interaction on optical response in one-dimensional cuprates

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ABSTRACT

We examine the single-particle excitation and linear optical absorption spectra in the one-dimensional (1D) extended Hubbard–Holstein model. We perform dynamical density matrix renormalization group calculations with use of pseudo-site representation of phonons. We focus on the interplay among phonons and elementary excitations in 1D Mott insulators. The excitations in the Mott insulators are easily modified by the phonons. We discuss implications of the present results in light of spectroscopic measurements in 1D cuprates.

1. Introduction

Spectroscopic studies often provide important progress for understanding basic electronic properties in strongly correlated electron systems. This is because high- and low-energy physics corresponding to charge and spin dynamics, respectively, couple with each other in these systems. One of the current issues is to examine the interdependence between electron–phonon (EP) interactions and the strong electron correlation inducing the charge and spin dynamics. It is a quite general question whether EP interactions enhance the correlation effect or not.

In the ground states of strongly correlated electron systems, the on-site Coulomb repulsion suppresses charge fluctuation. Thus, the conventional Peierls instability does not occur in the Mott insulators. However, EP interactions influence mobile carriers doped into the Mott insulators chemically or by photo-excitation. Since the spin and charge degrees of freedom of these carriers strongly affect the electronic properties, it is quite important to examine the interplay among the phonons and the elementary excitations coming from these internal degrees of freedom of electrons. In this paper, we address this problem in one-dimensional (1D) cases. We believe that the study of this particular case would contribute to better understanding of electronic states in high-T_c cuprates.

Let us consider the nature of the elementary excitations in the 1D Mott insulators. They are called 'spinon', 'holon' and 'doublon' representing spin defect in the antiferromagnetic state, empty and doubly occupied sites, respectively [1]. The spinon and holon (holon and doublon) excitations can be seen in single-particle excitation (photoexcitation). A characteristic feature in 1D systems is the spin–charge separation. Thus, it is a problem whether the spin–charge separation is robust in the presence of EP interactions. In the presence of the intersite Coulomb repulsion, the holon and doublon form an excitonic bound state [2,3]. However, this exciton is different from an electron–hole pair in semiconductors, since the strong electron correlation prohibits the exchange of the holon and doublon [4]. This prohibition strongly enhances a magnitude of the third-order optical non-linear susceptibility [4–6]. Thus, it is important to understand how the exciton is modified by EP interactions.

A piece of evidence of the coupling among phonon, spinon, and holon has been seen in resent angle-resolved photoemission spectroscopy (ARPES) measurement on $SrCuO_2$ [7]. Here, the spinon and holon excitations are directly observed for the first time. However, the line widths of their spectra are much broader than temperature. Then, it is expected that these excitations are affected by EP interactions.

The effect of EP interactions on the photocarriers has been observed by the Raman spectroscopy measurements on the 1D Mott insulator $Ca_{1.8}Sr_{0.2}CuO_3$ [8]. Here, some Raman-forbidden peaks appear, and they show resonance enhancement for charge-transfer excitation. This observation indicates strong coupling

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between the phonons and the photocarriers and the selection rule is changed by EP interactions. In particular, one phonon mode is assigned to be a breathing mode that is similar to the mode intensively studied in high-T_c cuprates [9,10].

We examine the effect of the Holstein phonons on the single-particle excitation and linear optical absorption spectra in the 1D Mott insulators. For this purpose, we perform large-scale dynamical density matrix renormalization group (DMRG) calculations in the 1D Hubbard–Holstein model with the nearest-neighbor Coulomb repulsion [2,3,11–16]. In order to take account of the quantum nature of the phonons, we introduce a pseudo-site method for the phonons [16,17]. We find that the elementary excitations are very sensitive to the EP interaction. Therefore, it is necessary to take account of phonon effects in strongly correlated electron systems. We discuss implications of the present results in light of spectroscopic measurements on cuprates [7,18].

2. Formulation

The coupling between electrons and breathing phonons in the cuprates can be mapped onto the Holstein-type interaction [19]. Thus, we start with the 1D Hubbard–Holstein model with the nearest-neighbor Coulomb repulsion. The Hamiltonian is defined by

$$\begin{aligned} H = & -t\sum_{i,\sigma}(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}+\text{H.c.}) \\ & +U\sum_{i}\left(n_{i,\uparrow}-\frac{1}{2}\right)\left(n_{i,\downarrow}-\frac{1}{2}\right) \\ & +V\sum_{i}(n_i-1)(n_{i+1}-1) \\ & +\omega_0\sum_{i}b_i^{\dagger}b_i+g\sum_{i}(b_i^{\dagger}+b_i)(n_i-1), \end{aligned} \tag{1}$$

where $c_{i,\sigma}^{\dagger}$ ($c_{i,\sigma}$) is a creation (annihilation) operator of an electron with site i and spin σ, and $b_i^{\dagger}$ (b_i) is a creation (annihilation) operator of a phonon with site i. We neglect the dispersion of the phonon in order to make our discussion simple. We introduce n_i-1 instead of n_i in order to eliminate boundary effects. Hereafter we use a dimensionless electron–phonon coupling constant defined by $\lambda=g^2/4t\omega_0$. Here, we take $\omega_0=0.5t$.

We calculate the single-particle excitation spectrum

$$A(k,\omega)=-\frac{1}{\pi}\text{Im}\left\langle 0\left|c_{k,\uparrow}^{\dagger}\frac{1}{E_0-\omega-H+i\gamma}c_{k,\uparrow}\right|0\right\rangle, \tag{2}$$

and the current–current correlation function

$$\chi(\omega)=-\frac{1}{\pi L}\text{Im}\left\langle 0\left|j\frac{1}{\omega+E_0-H+i\gamma}j^{\dagger}\right|0\right\rangle, \tag{3}$$

where $|0\rangle$ is the ground state with energy E_0, the current operator j is defined by

$$j=-it\sum_{i,\sigma}(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}-\text{H.c.}) \tag{4}$$

and γ is a small positive number. In the following calculation, the open boundary condition is used. Then, $c_{k,\uparrow}$ is described by

$$c_{k,\uparrow}=\sqrt{\frac{2}{L+1}}\sum_{l}\sin(kl)c_{k,\uparrow}, \tag{5}$$

where $k=n\pi/(L+1)$ and $n=1,2,\ldots,L$. In this paper, we take $L=20$.

In order to calculate these quantities, the DMRG method is applied [11,12]. In order to treat excited states in a framework of the DMRG, we introduce the mixed-state density matrix that is composed of the following four target states [2,3,13–16]:

$$|0\rangle=|\psi_1\rangle, \tag{6}$$

$$O^{\dagger}|0\rangle=|\psi_2\rangle, \tag{7}$$

$$\frac{1}{z-H}O^{\dagger}|0\rangle=|\psi_3\rangle+i|\psi_4\rangle, \tag{8}$$

$$\frac{1}{z+2\gamma-H}O^{\dagger}|0\rangle=|\psi_5\rangle+i|\psi_6\rangle, \tag{9}$$

where $z=\varepsilon+E_0+i\gamma$ for $O=j$ and $z=E_0-\varepsilon+i\gamma$ for $c_{k,\uparrow}^{\dagger}$. The density matrix is given by

$$\rho=\sum_{\alpha=1}^{6}p_{\alpha}\text{Tr}|\psi_{\alpha}\rangle\langle\psi_{\alpha}|/\langle\psi_{\alpha}|\psi_{\alpha}\rangle, \tag{10}$$

where we take $\sum_{\alpha}p_{\alpha}=1$, and the trace is taken for the states of the environment block. Then, the spectrum for $O=j$ and $\varepsilon<\omega<\varepsilon+2\gamma$ ($O=c_{k,\uparrow}^{\dagger}$ and $\varepsilon-2\gamma<\omega<\varepsilon$) is calculated after one-DMRG run. The number of the eigenstates in density matrix are taken up to 400 for renormalization. In order to correctly deal with the phononic degrees of freedom, we use the pseudo-boson method [17]. In this method, a boson operator with a restricted Hilbert space is exactly transformed into a set of hard-core bosons. For instance, the boson operator with four states is given by

$$b^{\dagger}=a_1^{\dagger}+\sqrt{2}a_2^{\dagger}a_1+(\sqrt{3}-1)a_1^{\dagger}a_2^{\dagger}a_2, \tag{11}$$

with use of the hard-core boson operators $a_1^{\dagger}$ and $a_2^{\dagger}$. Then, step-by-step renormalization of each bosons are carried out. It strongly depends on the magnitude of g whether the restriction is better or not. Thus, we systematically increase the number of the hard-core bosons up to 16 states per site.

3. Single-particle excitation spectra

In this section, we examine how the spinon and holon excitations are modified by the phonons. Fig. 1 shows $A(k,\omega)$ for $U=8t$ and $V=0$. There are two pronounced branches. One at high-binding energy side is the holon branch, and the other is the spinon branch. The singularity of the holon branch is smeared out even for the relatively weak EP interaction. The singularity of the spinon branch is still robust, although the 'peak-dip-hump' structure appears just below the spinon branch. The result seems to show the spin–charge separation in the presence of the EP interaction, since the roles of the EP interaction on the holon and spinon branches are different. The effect of the relatively strong EP interaction on the spinon branch is shown in the inset of Fig. 1. In this case, the spinon branch is also smeared out. This modification is quite anomalous, since the Holstein phonons directly couple with the holon excitation. Furthermore, a tiny peak appears at $\omega\sim-2t$, and this peak is located at lower-binding energy side of the zero-phonon line at $\omega\sim-2.4t$. However, these results are also understood by using an effective model based on the spin–charge separation scenario. The model is defined by superposition of the spectra without spin degrees of freedom:

$$A_{\text{eff}}(k,\omega)=\sum_{q=-\pi/2}^{\pi/2}A_h\left(k-q,\omega+2t+\varepsilon_s\left(q+\frac{\pi}{2}\right)\right), \tag{12}$$

where $\varepsilon_s(q)=-(\pi J/2)|\sin q|$ and $A_h(k,\omega)$ is the spectrum for the Holstein model. We think it interesting to examine whether this relation is generally satisfied for the other phonon modes.