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Angle-resolved photoemission spectra in one-dimensional Hubbard-Holstein model

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Abstract In order to understand the effects of electron-phonon coupling and Coulomb interactions in angle-resolved photoemission spectroscopy (ARPES), a spin-1/2 Hubbard-Holstein model at half-filling is theoretically investigated by means of the mean field theory and classical Monte Carlo simulation method. It shows that the spectral shape of the one-dimensional system is significantly modified by the electron-phonon coupling and Coulomb interactions. The suppression of charge-density wave in one-dimensional system has been ascribed to the short-range Coulomb repulsion and thermal lattice fluctuations. The competition between these interactions can induce zero energy gaps in APPES as well as complete cancellation of charge or spin ordering.

Key words ARPES, Electron-phonon coupling, Electron-electron interaction, Monte Carlo simulation

1 Introduction

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool to investigate structure of occupied electronic valence bands in solids. Being capable of measuring the binding energy as a function of given momentum, ARPES is suitable for probing electronic energy band structure of materials. Based on state-of-the-art photoemission methods on a modern synchrotron radiation light source, ARPES has become an important technique for studying electronic structure of solids. ARPES is ideal for investigating two-dimensional surface systems, with unparalleled flexibility of adjusting the incident photon energy at a high resolution of meV, i.e. the energy scale for many collective modes. At this resolution, fine electronic structures due to many-body interactions can be measured more precisely[1]. Based on high resolution ARPES experiments, novel properties have been discovered in strongly correlated systems such as superconductors and colossal magnetoresistance[2-7]. The studies show evidences that property of a complex system is governed by not only electron-electron *(e-e)* interactions but also electron-phonon (*e-ph*) couplings, as electrons near the Fermi surface are strongly scattered by the phonons, hence the importance of theoretically clarifying the main features of a complex system with *e-ph* and *e-e* interactions.

It is well known that *e-ph* coupling plays a key role in solids by modifying the electronic energy band structures[8-10]. To treat a single *e-ph* coupled system, calculations has been carried out based on the perturbation theories and unitary transformation methods. To investigate many-electron system coupled with phonons, the Migdal-Eliashberg theory has been applied to clarify the energy band structure as well as charge and spin distribution. However, these theories are not sufficient to study all features of ARPES, which spans the entire momentum region from the Fermi region to the valence band.

A path-integral theory was developed to study ARPES of many-electron systems by taking into account multiple scatterings of electrons by phonons[11]. It was found that a single Gaussian peak at band bottom evolved to a unique two-headed

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Lorentzian peak at the Fermi edge. Similar results were obtained by using adiabatic approximation and classical Monte Carlo (CMC) method[12]. In the *e-e* interacting systems, a dominant incoherent component, and a weak coherent component as well, were found in ARPES by means of quantum Monte Carlo simulation[13]. The result is quite different from those based on the widely accepted one-electron band picture indicating importance of *e-e* interaction.

Many authors have investigated ARPES in an *e-ph* coupled system or strongly correlated systems, but the competition between the *e-e* interaction and *e-ph* coupling is still an open question. In this paper, we investigate the ARPES in model systems with both interactions, and try to clarify the origin of charge-density-wave (CDW) gap and spin-density-wave (SDW) gap. A Hubbard-Holstein model is adopted to study the spectral behavior in the adiabatic limit[14], which assumes an infinite phonon mass and considers only the scattered electrons with the rigid lattice distortion. The thermal lattice fluctuations are taken into account by using CMC method[15].

2 Model and Method

To describe the *e-e* and *e-ph* interaction, we adopt a Hubbard-Holstein model as follows,

$$H=-t\sum_{l,\sigma}\left(c^{\dagger}_{l,\sigma}c_{l+1,\sigma}+c^{\dagger}_{l+1,\sigma}c_{l,\sigma}\right)-\mu\sum_{l,\sigma}c^{\dagger}_{l,\sigma}c_{l,\sigma}+U\sum_{l}n_{l,\alpha}n_{l,\beta}+g\sum_{l,\sigma}q_l\left(n_{l,\sigma}-\frac{\bar{n}}{2}\right)+\frac{K}{2}\sum_{l}q_l^2 \tag{1}$$

where, $c^{\dagger}_{l,\sigma}(c_{l,\sigma})$ is the creation (annihilation) operator of a conduction electron with spin $\sigma(=\alpha$ or $\beta)$ at site l; and $n_{l,\sigma}(\equiv c^{\dagger}_{l,\sigma}c_{l,\sigma})$ is the electron number operator; t is the transfer energy assumed for the nearest-neighbor hopping; μ is the chemical potential of electrons; the electrons are coupled to the dimensionless lattice deformation q_l with an elastic constant K; the average electron number per site is $\bar{n}(\equiv N_e/N)$, where N_e is the total electron number and N is the total number of lattice sites; g is the *e-ph* coupling constant; and U is the on-site Coulomb repulsion.

The average of a physical quantity at finite temperature can be written as

$$\langle\cdots\rangle=\frac{1}{Z}\int Dq e^{-\theta\Omega(q)}\langle\cdots\rangle_q \tag{2}$$

where $\theta\equiv 1/(k_BT)$ is the inverse temperature, and partition function is given as

$$Z=\int Dq\, e^{-\theta\Omega(q)} \tag{3}$$

The operator average $\langle\cdots\rangle$ is calculated on a given lattice configuration,

$$\langle\cdots\rangle_q=\frac{\mathrm{T_r}\left[e^{-\theta H_e(q)}\cdots\right]}{\mathrm{T_r}\left[e^{-\theta H_e(q)}\right]} \tag{4}$$

where

$$H_e(q)=-t\sum_{l,\sigma}\left(c^{\dagger}_{l,\sigma}c_{l+1,\sigma}+c^{\dagger}_{l+1,\sigma}c_{l,\sigma}\right)-\mu\sum_{l,\sigma}c^{\dagger}_{l,\sigma}c_{l,\sigma}+U\sum_{l}n_{l,\alpha}n_{l,\beta}+g\sum_{l,\sigma}q_l n_{l,\sigma} \tag{5}$$

is the electronic Hamiltonian corresponding to a given lattice configuration. Assuming eigen wavefunction $O_{lr}(q)$ and eigen energy $\varepsilon_r(q)$ for H_e, one obtains the spectral function as

$$A_\sigma(\boldsymbol{k},\omega)=-\frac{1}{\pi}\mathrm{Im}\,G^{\mathrm{R}}_{\sigma}(\boldsymbol{k},\omega)=\left\langle\frac{1}{N}\sum_{i,j}e^{i\vec{k}\bullet(\vec{R}_i-\vec{R}_j)}\sum_{r}O_{i,r}O^{*}_{j,r}\delta(\omega-\varepsilon_r)\right\rangle_q \tag{6}$$

where the delta function is

$$\delta(\omega-\varepsilon_r(q))\to\frac{1}{\pi}\frac{\eta}{(\omega-\varepsilon_r(q))^2+\eta^2} \tag{7}$$

Details of the calculation have been given in a previous paper[12]. ARPES intensity is related to the Fermi function $f(\omega)=1/(e^{\theta\omega}+1)$ as follows

$$I(\boldsymbol{k},\omega)=\sum_{\sigma}A_\sigma(\boldsymbol{k},\omega)f(\omega) \tag{8}$$

Using Eq.(6), ARPES of the systems can be calculated by the CMC method. The probability distribution of phonon configuration is created randomly. By the Metropolis method, each Monte Carlo step consists of a proposed move and an accept/reject procedure.

At each randomly samples, the total energy of electronic part is calculated by using mean-field theory, which decouples the Coulomb repulsion term as follows,

$$\sum_l n_{l,\alpha}n_{l,\beta} = \sum_l [\langle n_{l,\alpha}\rangle n_{l,\beta} + \langle n_{l,\beta}\rangle n_{l,\alpha} - \langle n_{l,\alpha}\rangle\langle n_{l,\beta}\rangle + (n_{l,\alpha} - \langle n_{l,\alpha}\rangle)(n_{l,\beta} - \langle n_{l,\beta}\rangle)] \quad (9)$$

where $\langle n_{l,\sigma}\rangle$ shows the electronic density at l^{th} site with spin σ. Ignore the last item of fluctuation, we can get the H_e as

$$H_e = -t\sum_{l,\sigma}(c^{\dagger}_{l,\sigma}c_{l+1,\sigma} + c^{\dagger}_{l+1,\sigma}c_{l,\sigma}) - \mu\sum_{l,\sigma}c^{\dagger}_{l,\sigma}c_{l,\sigma} + g\sum_{l,\sigma}q_l n_{l,\sigma} + U\sum_l [\langle n_{l,\alpha}\rangle n_{l,\beta} + \langle n_{l,\beta}\rangle n_{l,\alpha} - \langle n_{l,\alpha}\rangle\langle n_{l,\beta}\rangle] \quad (10)$$

where, $\langle n_{l,\sigma}\rangle$ can be determined self-consistently by iteration method. In each step, the density of electron can be calculated by

$$\langle n_{l,\alpha}\rangle = \sum_{j=1}^{N}\langle\psi_{j,\alpha}(l)|c^{+}_{l,\alpha}c_{l,\alpha}|\psi_{j,\alpha}(l)\rangle\frac{1}{e^{(E_{j,\alpha}-\mu)/K_BT}+1}$$
$$\langle n_{l,\beta}\rangle = \sum_{j=1}^{N}\langle\psi_{j,\beta}(l)|c^{+}_{l,\beta}c_{l,\beta}|\psi_{j,\beta}(l)\rangle\frac{1}{e^{(E_{j,\beta}-\mu)/K_BT}+1} \quad (11)$$

where $\{E_{l,\sigma}\}$ are eigen energies and $\{\Psi_{l,\sigma}\}$ are eigen wavefunctions of H_e. The chemical potential is numerically determined by conservation of electrons,

$$N_e = \sum_{l=1}^{N}(n_{l,\alpha} + n_{l,\beta})$$

3 Results and discussion

The periodic boundary condition is imposed on a one-dimensional chain system at half-filling. The transfer integral t is defined as the unit of energy, and phonon frequency is fixed at K=0.2. In the previous paper[12], discussions were restricted to non half-filling systems with weakly and intermediately *e-ph* coupling. Since half-filled low-dimensional systems are subject to Peierls instability accompanied by a CDW gap at low temperatures, such a gap may cause extra complexity in ARPES near the Fermi surface. In this paper, a 1D chain model at half-filling is studied to investigate the competition between CDW and SDW orders in the system, where *e-e* and *e-ph* interactions coexist.

To clarify the mechanism of ARPES alteration due to the two interactions at finite temperature, a 1D system with 64 sites is numerically investigated by Monte Carlo simulation with 10^5 sampling and 100 iterations mean-filed calculation at each step to ensure the precision.

Figure 1 shows ARPES intensity $I(\boldsymbol{k},\omega)$ as function of energy with respect to different *e-ph* coupling strengths. To examine the effect of *e-ph* coupling, the on-site coulomb interaction is switched off, *i.e.* U=0. The temperature is fixed at θ=10.0. In the case of weak coupling g=0.4, the spectrum at $\boldsymbol{k}=\boldsymbol{k}_{\mathbf{F}}$ has a strong peak at the Fermi energy (Fig.1a). It indicates that the system is in the metallic phase with zero gap. In the case of intermediate coupling g=0.5, the peak at $\boldsymbol{k}=\boldsymbol{k}_{\mathbf{F}}$ becomes broad and red-shifted (Fig.1b). A CDW gap has been opened at the Fermi surface with lattice dimerization induced by Peierls phase transition in 1D system. The CDW gap is enhanced as *e-ph* coupling increases (Fig.1c). It shall be noted that a CDW gap exists even in infinitesimal *e-ph* coupling in 1D system at zero temperature. At finite temperature, thermal lattice fluctuation tends to destroy CDW order and stabilize a metallic phase.

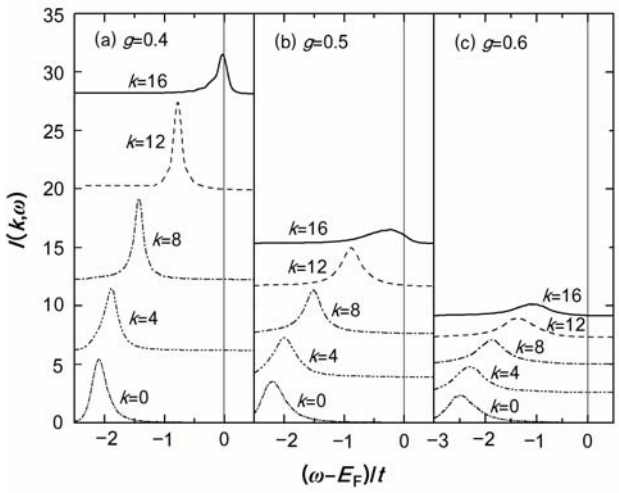

Fig.1 ARPES intensity of 1D Hubbard-Holstein model at half-filling (N=64) for (a)weak, (b) intermediate, and (c) strong *e-ph* coupling. Other parameters are given as follows, θ=10, K=0.2, U=0.0.

For the effect of *e-e* interaction, ARPESs at different U with strong *e-ph* coupling of g=0.6 are shown in Fig.2. As on-site Coulomb interaction U increases from 0.0 to 1.0, the spectrum peak at $\boldsymbol{k}_{\mathbf{F}}$ is blue-shifted, indicating a decreased gap that approaches to zero at U =2.0 (Fig.2c). It is evident that the CDW order has been destroyed by Coulomb interaction. Furthermore, the gap appears again in

spectrum indicating a SDW order at U=3.0 (even larger U is not discussed because the mean-field theory is not suitable for strongly correlated systems).

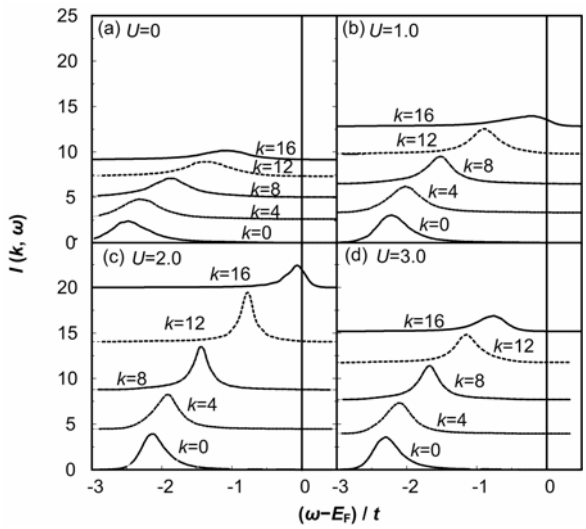

Fig.2 ARPES intensity of 1D Hubbard-Holstein model at half-filling (N=64) for Coulomb repulsions (a) U=*0* , (b) U=1.0 (c) U=2.0 (d) U=3.0. Other parameters are given as follows, θ=10, K=0.2, g=0.6.

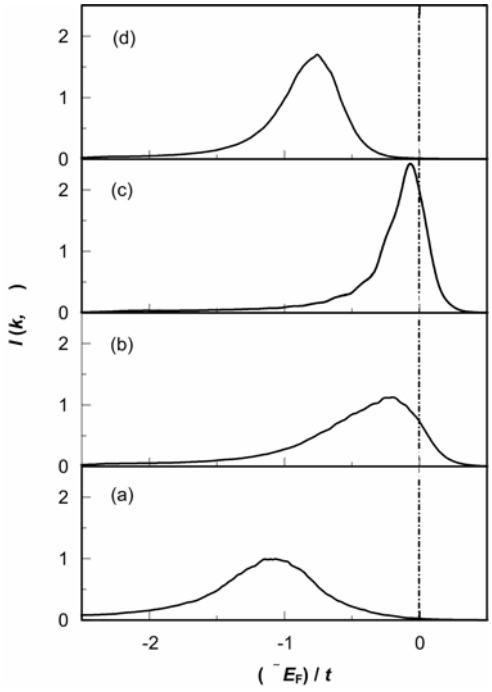

Fig.3 ARPES intensity at the Fermi surface ($\boldsymbol{k}$=$\boldsymbol{k}_{\mathrm{F}}$) of 1D Hubbard-Holstein model at half-filling (N=64) for Coulomb repulsions at θ=10, K=0.2 and g=0.6.. (a) U=0.0, (b) U=1.0, (c) U=2.0, (d) U=3.0.

In order to understand change of gap nearly E_{F}, we plot spectral lines at $\boldsymbol{k}$=$\boldsymbol{k}_{\mathrm{F}}$ in Fig.3 for different the on-site Coulomb repulsions. It can be seen that the CDW gap at Fermi surface due to *e-ph* coupling is weakened by *e-e* interaction. Such a gap finally disappears and is replaced by a new one at even greater *e-e* interactions. The new SDW gap is induced by on-site Coulomb interaction, enhanced by increased U. The peak shape shows a strong dependence on *e-e* interaction. At zero Coulomb interaction, the peak takes a Gaussian shape, which is induced by thermal fluctuation of lattice at finite temperature. The peak width (FWHM) increases with temperature. At finite U, the peak evolves gradually to a Lorentzian one, which is in close relation with electron scattering at the Fermi surface.

The charge (spin) densities profiles are shown in Fig.4 for different U. The densities are the thermal averages for all lattice configurations,

$$\left\langle n_{l,\alpha} \pm n_{l,\beta} \right\rangle = \frac{1}{Z} \int Dq e^{-\theta\Omega(q)} \left\langle n_{l,\alpha} \pm n_{l,\beta} \right\rangle_q \quad (12)$$

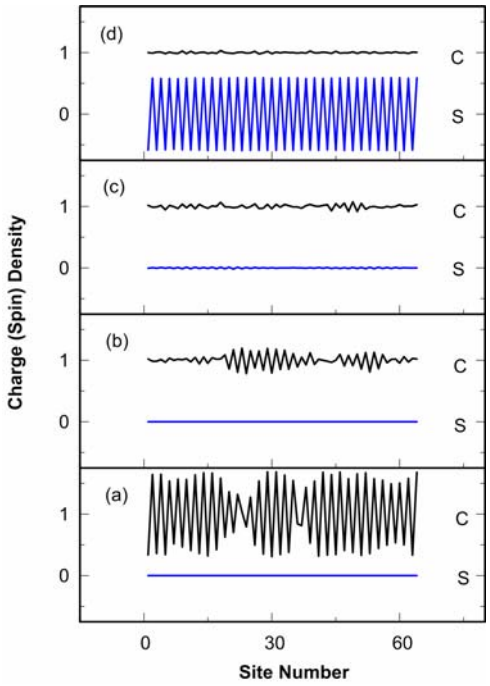

Fig.4 CMC results of the charge and spin density profiles of 1D Hubbard-Holstein model at half-filling (N=64) for Coulomb repulsions at θ=10, K=0.2 and g=0.6. (a) U=0.0, (b) U=1.0, (c) U=2.0, (d) U=3.0.

Figure 4a is characterized by strong CDW order, which is obviously induced by *e-ph* coupling as shown in Fig.3a. We noted that a perfect staggered order of charge density can exist in absolute zero temperature. The new structure in charge density in Fig.4a is induced by thermal lattice fluctuation. With increasing U, the CDW order is significantly

weakened while the SDW order is negligibly small (Fig.4b). Such a decreasing CDW order results from the completion between *e-ph* coupling and *e-e* interaction. At U=2.0, only small fluctuation can be observed in either order (Fig.4c). Lots of interesting physics may be hidden in a zero-gap ARPES due to the cancellation of CDW and SDW in the model system. We shall pay more attention to the competition between the e-e and e-ph interactions, and clarify the mechanism behind a "simple" spectrum. Fig.4(d) gives the results for even greater on-site Coulomb interaction, in which the CDW order is replaced by the SDW order.

4 Conclusion

ARPES of the half-filled 1D Hubbard-Holstein model under the adiabatic approximation has been studied by means of the CMC method and mean field theory. We clarify the role played by *e-ph* coupling and *e-e* interaction by systematic investigation of various parameters. It is found that the CDW gap due to *e-ph* coupling can be destroyed by thermal lattice fluctuation or by Coulomb interaction. The competition between these interactions can induce zero energy gaps in APPES as well as complete cancellation of charge or spin ordering. It is also observed that the shape ARPES is modified significantly as the system evolves from the CDW insulating phase to the SDW one. Since the present model is studied by using mean field theory, it is impossible to take into account spin fluctuations at finite temperature or many-electron scattering at the Fermi surface. Further studies are necessary to clarify the high-order electron correlations.

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