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FINITE-TEMPERATURE SIMULATION BASED ON THE LANCZOS ALGORITHM FOR LOW-DIMENSIONAL STRONGLY CORRELATED ELECTRON SYSTEMS; HIGH-TEMPERATURE SUPERCONDUCTING CUPRATES

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ABSTRACT

The Lanczos algorithm is applied to calculate some finite-temperature physical quantities, as well as the ground-state ones. We introduce the finite-temperature Lanczos algorithm and apply it for some current problems in the low-dimensional strongly correlated electron systems; the charge stripe, the pseudogap and phonon-induced anomalous ARPES spectrum in the high-Tc superconducting cuprates.

Key Words: Lanczos algorithm, charge stripe, pseudogap, high-Tc superconducting cuprates

1. INTRODUCTION

The standard Lanczos algorithm has been one of the best numerical method to investigate the ground state and the low-lying excitations in the low-dimensional quantum systems, as well as the quantum Monte Carlo simulation. In particular, to study on the electron systems like Hubbard, Anderson and t-J models or the frustrated antiferromagnets in the ground state, the Lanczos method is much more useful, because the quantum Monte Carlo calculation suffers from the negative sign problem.

Recently Jaklic and Prelovsek [1] proposed a useful method based on the Lanczos algorithm conbined with a random sampling of the initial wave function, to calculate finite-temperature quantities without such a negative sign problem. Using the method, they investigated several dynamical properties of the high-Tc cuprates. However, the finite-temperature Lanczos algorithm has not been so widely used yet, although it is quite useful for the low-dimensional quantum systems.

In the present paper, we introduce the finite-temperature Lanczos method, as well as the standard Lanczos algorithm in the following sections. In addition we show some interesting new results from applying them for recently interesting problems in the low-dimensional quantum systems; the charge stripe [2], the pseudogap phenomena [3] and phonon-induced anomalous angle-resol ved photoemission (ARPES) spectrum [4] in the high-temperature cuprate superconductors.

2. CHARGE STRIPES

As one of the most suitable model to describe the low-temperature properties of CuO_2 supercond ucting plane of the cuprates, we consider the square lattice t-J Hamiltonian

$$H = -t \sum_{\langle i,j \rangle,\sigma} (\tilde{c}^{+}_{j,\sigma}\tilde{c}_{i,\sigma} + \tilde{c}^{+}_{i,\sigma}\tilde{c}_{j,\sigma}) + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) ,$$

where $\tilde{c}_{j,\sigma}$ and $\tilde{c}^{+}_{j,\sigma}$ are the hole operators at each Cu site. In order to explain a possible mechanis m of the charge stripes observed in the neutron scattering experiment, we introduce the cyclic rin g exchange interaction J_4 among the four spins at each plaquette. Using the standard Lanczos alg orithm to calculate the ground-state charge correlation functions for finite-size clusters, we obtai ned a phase diagram of charge stripes shown in Figure 1.

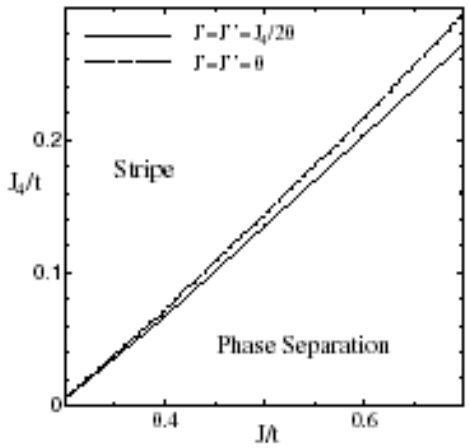

Figure 1. Phase diagram of the charge stripe and the phase separation. J' and J'' are the coup ling constants of the 2nd and 3rd neighbor exchange interactions, respectively.

3. PSEUDOGAP

Using the finite-temperature Lanczos algorithm, we calculated the dynamical spin structure facto r and the spin correlation function of the t-J model at low temperatures. This analysis revealed th at an origin of the pseudogap phenomena observed for the under-doped cuprates can be a crossov er due to a significant enhancement of the short-range antiferromagnetic spin correlation at low t emperatures. The temperature dependences of the Q=(π,π) component of spin correlation functio n S(Q), the dynamical susceptibility Imχ(ω), and the static susceptibility χ calculated by the finit e-temperature Lanczos algorithm for 16-site square lattice t-J model with two holes, are shown in Figures 2 (a), (b), and (c), respectively. These figures suggest that a significant enhancement of t he antiferromagnetic spin correlation corresponds to the pseudogap phenomena, namely broad p eaks of the dynamical and static susceptibilities.

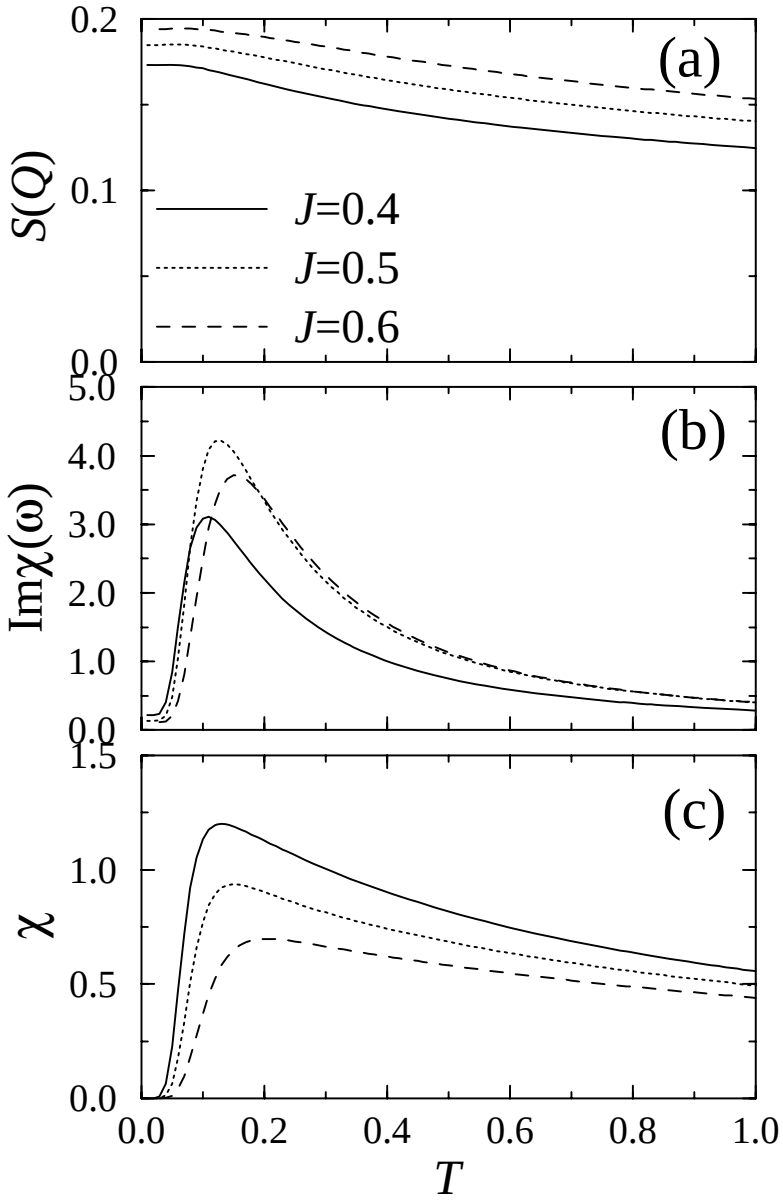

Figure 2. (a) Q=(π,π) component of spin correlation function S(Q), (b)the dynamical susceptibilit y Imχ(ω), and (c) the static susceptibility χ calculated by the finite-temperature Lanczos algorith m for 16-site square lattice t-J model with two holes

4. PHONON EFFECTS

The recursion method combined with the Lanczos algorithm proposed by Gagliano and Balseiro [5] can be applied to derive the ground-state dynamical charge structure factor of quantum syste ms.We investigated the phonon effect of the in-plane oxygen atoms in high-Tc cuprates, applying this method for the t-J Hamiltonian including the phonon degrees of freedom, so-called t-J-Holst ein model. This analysis indicated that a shift of the chemical potential and a broadening of the q uasi-particle spectrum observed in the recent ARPES measurement can be explained by the phon on effect. The dynamical spectral weight of a single quasiparticle excitation calculated by the pre

sent method for the Cu_8O_{16} cluster with the electron-phonon coupling constant λ_0=0, 0.2, 0.4, an d 0.6 is shown in Figures 3 (a), (b), (c), and (d), respectively. These figures reveal that with incre asing electron-phonon interaction the quasiparticle peak becomes broader and the position shifts. These behaviors are consistent with the experimental ARPES spectrum.

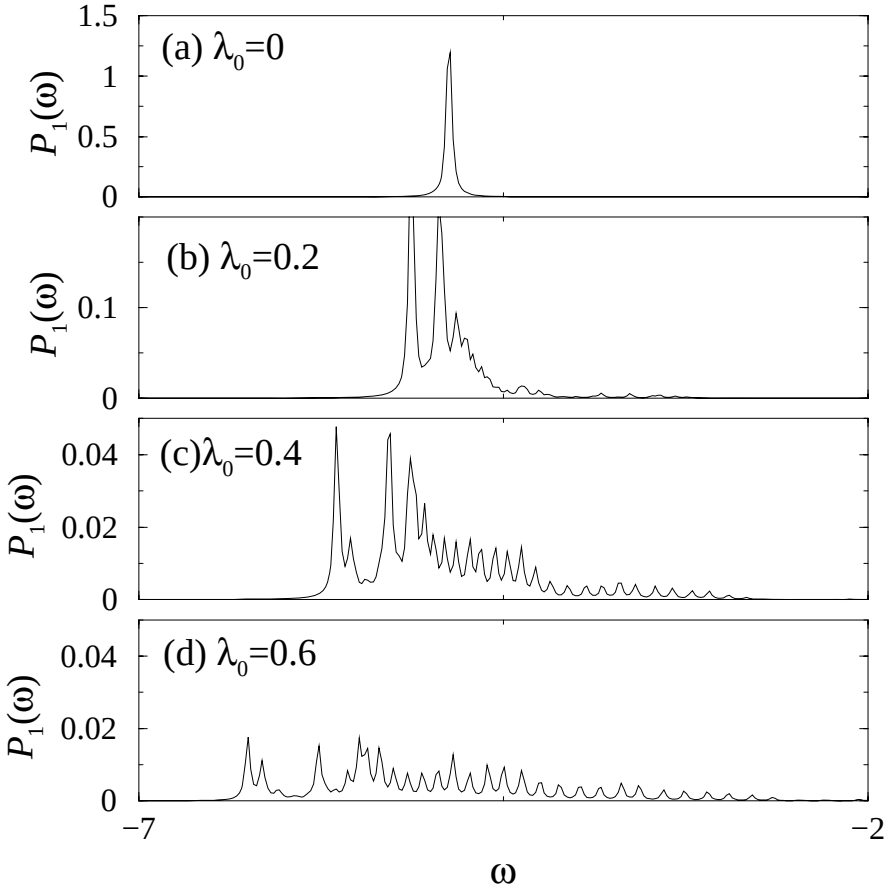

Figure 3. Dynamical spectral weights calculated by the Gagliano and Balseiro method for t-J-Hol stein model to describe the Cu_8O_{16} cluster with the electron-phonon coupling constant λ_0=0, 0.2, 0.4, and 0.6 is shown in Figures 3 (a), (b), (c), and (d), respectively.

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