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Competition between hidden spin and charge orderings in stripe phase

Chitoshi Yasuda,[1,2] Akihiro Tanaka,[1] and Xiao Hu[1]
[1]*Computational Materials Science Center, National Institute for Materials Science, Tsukuba 305-0047, Japan*
[2]*Department of Physics and Mathematics, Aoyama Gakuin University, Sagamihara 229-8558, Japan*
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The correlation between charge and spin orderings in hole-doped antiferromagnets is studied within an effective model of quantum strings fluctuating in an antiferromagnetic background. In particular, we perform the direct estimation of the charge and spin long-range-order parameters by means of the quantum Monte Carlo simulation. A hidden spin long-range order is found to be governed by a competition between the two trends caused by increasing hole mobility: the enhancement of the two-dimensional spin-spin correlation mediated by hole motions and the reformation of a strong stripe order.

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Since the observation of high-temperature superconductivity in a hole-doped antiferromagnetic (AF) insulator, spin dynamics in hole-doped low-dimensional Heisenberg antiferromagnets has turned into a major subject of theoretical and experimental studies. The discovery of an anomalous stripe phase within CuO_2 planes of the Cu-oxide superconductor, $La_{2-x-y}Nd_ySr_xCuO_4$, has stimulated considerable interest in the studies of the correlation between the charge and spin orderings in hole-doped antiferromagnets.[1] The experimental findings suggest that, in the stripe phase, the dopant holes are segregated into one-dimensional (1D) domain walls that separate AF antiphase spin domains.[2,3] The stripe phases have been experimentally observed in a wide range of doped-hole concentrations for the lanthanum cuprate[4,5] and proposed in the two-dimensional (2D) Hubbard-like[6–11] and *t-J* models.[12,13] It is generally accepted that the static stripe order, e.g., observed for $La_{2-x}Sr_xCuO_4$ with $x \simeq 1/8$, is pinned by the lattice modulation in the low-temperature tetragonal phase.

The stripe order with AF antiphase spin domains has also been observed in Ni-oxide $La_{2-x}Sr_xNiO_4$,[14,15] though the material remains insulating except at very high Sr concentrations. There is by now a wide consensus that the formation of stripe is a generic property of hole-doped antiferromagnets.[1] The mean-field theory for the Hubbard-Peierls model proposed by Zaanen and Littlwood[16] suggests a picture in which holes bind to domain walls embedded in an AF background.

Several years ago Zaanen and coworkers reported[17] an appealing model for stripes acting as antiphase boundaries intervening AF spin domains, which captures well the essential features of the interplay between spin and charge degrees of freedom. This effective model, deduced on basis of the Ogata-Shiba principle[18] is described in terms of fluctuating quantum strings. Zaanen's model can be viewed as a variant of the bond-alternated spin model with bond randomness as mentioned below and is interesting in its own rights as a new random quantum spin system. Our main purpose in the present paper is to investigate the correlation between the spin and charge orderings and the tendency of the spontaneous ordering of stripes within the effective model. In particular, we carry out a high precision numerical investigation into the charge and spin orderings by direct calculation of the order parameters at zero temperature in the thermodynamic limit by means of the quantum Monte Carlo (QMC) simulation. We find that a hidden spin long-range order (LRO) is governed by a competition between the two trends caused by increasing hole mobility: the enhancement of the two-dimensional 2D spin-spin correlation and the reformation of a strong stripe order.

The motive of the aforementioned model is to describe the quantum mechanical motion of hard core particles forming extended strings, which fluctuate in an AF background. The strings have an overall orientation that is aligned with the y direction. Each quantum string consists of L_y hardcore particles referred to hereafter as "holes." Each hole moves in the x direction and an effective exchange interaction exists between the two spins neighboring a hole. By regarding the hole as residing on the link between two spins neighboring the hole, we can reduce our system to a spin-only model defined on a squeezed lattice as depicted in Fig. 1. The model thus obtained is described by the Hamiltonian[17]

$$H = \sum_{x,y} [-tP(a^{\dagger}_{(x+1,y)}a_{(x,y)} + \mathrm{h.c.})P + J(1-(1-\alpha)n_{(x,y)})\mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x+1,y)} + J(1 - n_{(x,y)}n_{(x-1,y+1)} - n_{(x-1,y)}n_{(x,y+1)})\mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x,y+1)}], \quad (1)$$

where the summation $\Sigma_{x,y}$ runs over all the lattice sites on the squeezed lattice and $\mathbf{S}_{(x,y)}$ is the $S=1/2$ spin operator at site

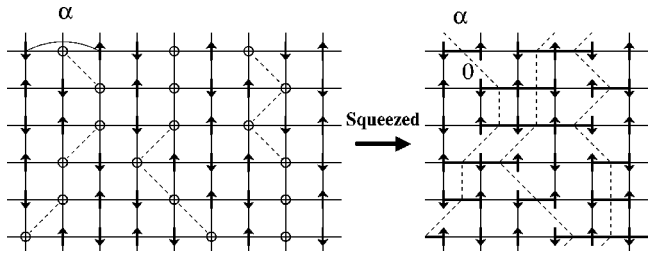

FIG. 1. Transformation from the original lattice to the squeezed lattice. The quantum strings in the original lattice are described by the dashed lines connecting links denoted by bold lines in the squeezed lattice.

(x,y). The first term corresponds to the kinetic energy of holes, where $a^{\dagger}_{(x,y)}$ is the creation operator of the hole sitting on the link between the sites (x,y) and $(x+1,y)$ in the squeezed lattice, and P is the projection operator ensuring that strings are not broken up and are separated by at least one spin site in the original lattice. The second term describes the $S=1/2$ exchange interactions in the x direction. We fix J to unity hereafter. The value of α corresponds to the effective interaction between spins neighboring a hole and $n_{(x,y)}$ is the hole number operator at site (x,y). The third term makes the exchange interaction zero in a link parallel to $\hat{y}$ in the squeezed lattice for bonds connecting to the holes in the original lattice.

In the perfect stripe system with $t=0$, in which case the quantum strings are perfectly straight and line up at regular intervals, the system as described on the squeezed lattice reduces to a spin ladder model with an interladder interaction of strength α.[19] When L_x/N_s is an odd integer, where L_x is the size of the lattice in the x direction and N_s is the number of strings, this system exhibits an even-leg-ladder-like behavior: there is a quantum phase transition between the disordered phase with a finite spin gap for small α and the AF LRO phase for large α.[20] The transition point is located at, e.g., $\alpha_c=0.3138(1)$, 0.0787(2), and 0.0153(1) for the concentrations $x=N_s/L_x=1/3, 1/5$, and $1/7$, respectively. These results are obtained by the finite-size scaling (FSS) analysis of our QMC data of the correlation length with the exponent $\nu=0.71$ fixed to the value of the three-dimensional classical Heisenberg universality class.[21] This disordered phase persists in the presence of the hopping interaction up to a certain value of t_c as mentioned below. On the other hand, when the value of L_x/N_s is even, the system behaves like an odd-leg spin ladder: the system with $\alpha=0$ is in a gapless phase and AF LRO is induced by an infinitesimal value of α.

The strings in the present model, subject to quantum fluctuation viz. the t term, are at the same time in contact with the AF background, and thus induces an imaginary-time dependence of the spin-exchange coupling on the squeezed lattice. To deal with this aspect, the spin configuration is therefore updated by the *discontinuous* imaginary-time loop algorithm[22] with fixed hole configuration. Meanwhile, the hole configuration is described by the Suzuki-Trotter decomposition via the prescription due to Eskes *et al.*[23] and updated by the Metropolis algorithm with a fixed spin configuration. The QMC simulation with the loop algorithm combined with the conventional worldline algorithm is carried out on $L_x \times L_y$ $(L_x=L_y\equiv L\leqslant 36)$ square lattices with the periodic boundary condition. The value of β/N_τ is fixed to be $1/4$, where β is the inverse of temperature T and N_τ is the Trotter number. The error bars are estimated based on about 10^2 samplings. For each sample, 10^4 Monte Carlo steps (MCS) are spent for measurement after 10^4 MCS for thermalization.

The ground-state phase diagram parametrized by α and t for $x=1/3$ was previously presented by Zaanen *et al.*.[17] Our result is qualitatively consistent with theirs: the system is in the charge-ordered and spin-disordered phase for small t and small α and the phase transition to the charge-ordered and hidden AF LRO phase occurs as the value of t or α is increased. Hereafter, the AF LRO in the squeezed lattice will also be referred to as the hidden AF LRO in terms of the original lattice. The spin-disordered state is effectively the same as the state realized in the spin-1/2 even-leg-ladder system with the interladder interaction α as mentioned above. When $\alpha=0.1$ and $x=1/3$, our FSS analysis of the Binder parameter[24] shows that the phase transition occurs at $t_c=0.21(1)$. The charge-ordered and hidden AF LRO phase for $t>t_c$ is characterized by peaks of the charge-charge structure factor $S_c(k_x,k_y)\equiv 1/L^2\langle[\Sigma_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} n_{\mathbf{r}}]^2\rangle$ at $(k_x,k_y)=\left(\pm\frac{2}{3}\pi,0\right)$, where $n_{\mathbf{r}}$ is the hole number operator at site $\mathbf{r}$, and those of the spin-structure factor $S_s(k_x,k_y)\equiv 1/L(L-N_s)\langle[\Sigma_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} S^z_{\mathbf{r}}]^2\rangle$ at $(k_x,k_y)=\left(\pm\frac{2}{3}\pi,\pm\pi\right)$ as shown in Figs. 2(a) and 2(b). The results show that the hidden AF correlations with antiphase boundaries are present, consistent with the stripe structure, namely, the peaks of $S_c(k_x,k_y)$ and $S_s(k_x,k_y)$ are at $(k_x,k_y)=(\pm 2\pi x,0)$ and $[\pm(1-x)\pi,\pm\pi]$, respectively. Note that there are no additional peaks corresponding to other modes, except for the one at $(k_x,k_y)=(0,0)$ for $S_c(k_x,k_y)$ in the thermodynamic limit. While the $x=\frac{1}{3}$ system exhibits an even-leg-ladder–like behavior, the system at $x=\frac{1}{4}$ is odd-leg ladderlike. This is evident from the peaks that are observed at the positions $(k_x,k_y)=\left(\pm\frac{1}{2}\pi,0\right)$ and $\left(\pm\frac{3}{4}\pi,\pm\pi\right)$ as shown in Figs. 3(a) and 3(b), respectively. It shows that at least in the parameter range we calculated, the stripe configuration consisting of only three-leg ladders is realized rather than an alternating series of two- and four-leg ladders, which was suggested in Ref. 17, where interactions from holes were neglected. The peaks of $S_c(k_x,k_y)$ at $k_y=0$ shows that each string selects a overall direction in space, though it can locally fluctuate. This is associated with the "directedness" observed in a quantum string model.[23] On the other hand, the peaks at $k_x=\pm 2\pi x$ corresponding to strings lined up at regular intervals might have their primary origin in the effective repulsion coming from the constraint that the stripes be separated by at least one spin site.

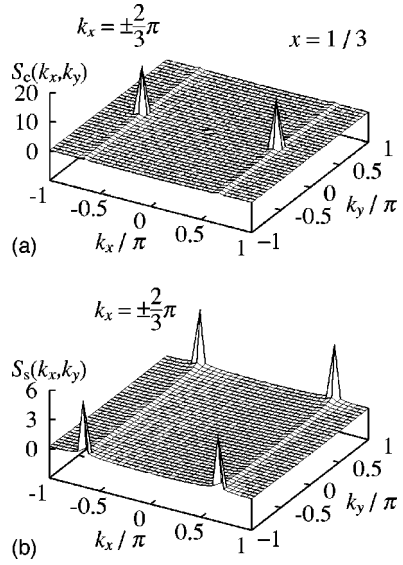

FIG. 2. Plots of (a) the charge-charge structure factor and (b) the spin structure factor in the original lattice for $x=1/3$ at $T=0.01$ in the charge-ordered and hidden AF long-range ordered phase with $\alpha=0.1$ and $t=1$. Note that the peak at (0,0) of the charge-charge structure factor is subtracted.

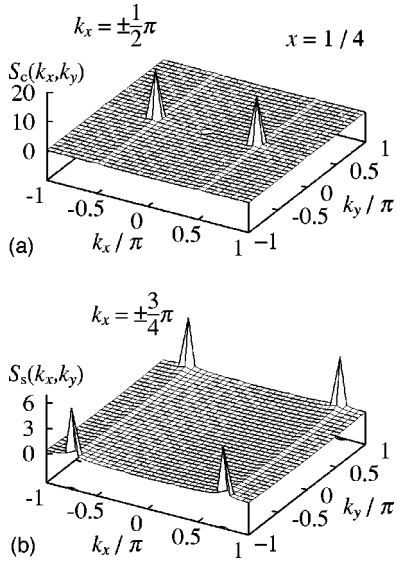

FIG. 3. Plots of (a) the charge-charge structure factor and (b) the spin-structure factor in the original lattice for $x=1/4$ at $T=0.01$ in the $\alpha=0.1$ and $t=1$ system.

We make direct estimations of the t-dependent stripe LRO parameter defined by

$$\langle O_{\text{stripe}}\rangle \equiv \lim_{L\to\infty}\lim_{T\to 0}\sqrt{\frac{S_c(2\pi x,0)}{L^2}}. \tag{2}$$

The value of $S_c(2\pi x,0)$ converges to its zero-temperature value at T lower than an energy scale related to the finiteness of the system size. Thus, $S_c(2\pi x,0)$ at low temperatures, where its T dependence becomes indiscernible within the error bars is taken as the values in the $T\to 0$ limit. Furthermore, the value in the limit of $L\to\infty$ is obtained by fitting the QMC data to $\sqrt{S_c(2\pi x,0)/L^2}\simeq\langle O_{\text{stripe}}\rangle + a/L$. The results of the extrapolation are shown in Fig. 4. When the system is in the perfect stripe phase with $t=0$, the value of $\langle O_{\text{stripe}}\rangle$ equals x, because the strings are perfectly straight and align at regular intervals, from which follows that $S_c(2\pi x,0)=N_s^2$. For $t<3$ the value of $\langle O_{\text{stripe}}\rangle$ reduces as t is increased. This is consistent with the picture that hole fluctuation competes with the stripe order. For $t>3$, however, the strong stripe order is reformed and the ground state approaches the perfect stripe. This reformation of the strong stripe will be discussed later.

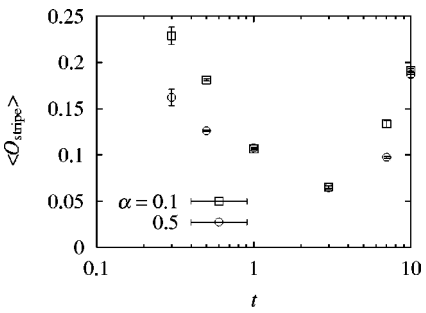

FIG. 4. The t dependence of the stripe LRO parameter at $T=0$ for $x=\frac{1}{3}$. The square and circle denote the QMC results of the stripe LRO parameter for $\alpha=0.1$ and 0.5, respectively.

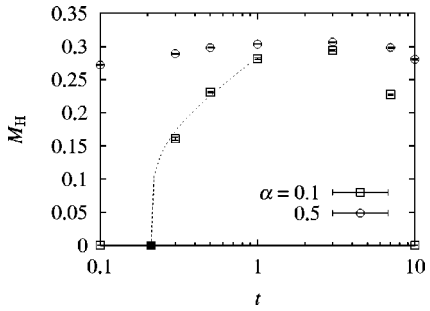

FIG. 5. The t dependence of the hidden AF LRO parameter at $T=0$ for $x=\frac{1}{3}$. The open square and circle denote the QMC results of the hidden AF LRO parameter for $\alpha=0.1$ and 0.5, respectively. The filled square denotes the critical point $t_c\simeq 0.21$ for $\alpha=0.1$. The dashed line is obtained by the least-squares fitting with the fitting function $M_H=c(x-0.21)^b$ in the range of $0.3\leqslant t\leqslant 1$. The values of c and b are estimated to be 0.30(1) and 0.23(4), respectively.

We also make direct estimations of the t-dependent hidden AF LRO parameter defined by

$$M_H \equiv \lim_{L\to\infty}\lim_{T\to 0}\sqrt{\frac{3S(\pi,\pi)}{L(L-N_s)}}, \tag{3}$$

where $S(\pi,\pi)$ is the size-dependent staggered structure factor in the squeezed lattice. The extrapolation is performed by a procedure similar to that for $\langle O_{\text{stripe}}\rangle$. A finite M_H is induced at $t>t_c=0.21(1)$ for $\alpha=0.1$, with the value increasing with t in the region $t_c<t\leqslant 3$ as shown in Fig. 5. This result suggests that the hole motion enhances the effective spin-spin interactions, which, in turn, obscures the ladderlike structure, and yields instead the 2D magnetic LRO. To paraphrase, the magnetization, which had been suppressed in the underlying bond-alternating spin system due to quantum fluctuations, is recovered by the randomness of the spin interaction brought on by turning on a finite t. Randomness-induced LRO is expected to occur also in 2D quantum spin systems with bond randomness.[25] The present case differs in that the randomness is present also in the imaginary-time direction, i.e., one may view it as a "2+1D random quantum spin system." A further increase in the hole motions, however, eventually leads to the reduction of the spin LRO due to the reformation of the strong stripe order, leading to the spin system with alternating structure, which was seen for $0<t<t_c$. The properties mentioned above are also seen for $\alpha=0.5$, where the system with $t\to 0$ does not belong to the spin-disordered phase.

The values of $\langle O_{\text{stripe}}\rangle$ for $\alpha=0.1$ are larger than those for $\alpha=0.5$ as shown in Fig. 4. This result is in conflict with the following naive energetics: a kink, arising when one hole in the straight string moves to a neighboring site, yields an energy loss proportional to a nearest spin-spin correlation. In the hidden AF LRO phase, a naive mean-field-like argument gives the correlation proportional to M_H^2. This implies then that in order to gain energy the value of the stripe LRO parameter for $\alpha=0.5$ should become larger than that for α

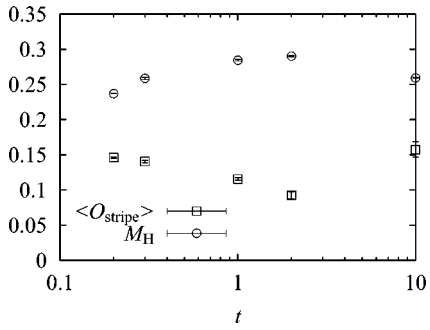

FIG. 6. The t dependence of the LRO parameters at $T=0$ for $x=\frac{1}{4}$. The square and circle denote the values of the stripe LRO and the hidden AF LRO parameters for $\alpha=0.1$.

$=0.1$ because of the α dependence of M_{H}. Our results indicate that the speculation is too naive to explain quantitatively the magnitude of the order parameters.

The t dependences of $\langle O_{\mathrm{stripe}}\rangle$ and M_{H} for $\alpha=0.1$ and $x=\frac{1}{4}$ are also shown in Fig. 6, where the system in the limit of $t\rightarrow 0$ becomes odd-leg-ladderlike. Though a similar upturn behavior of the order parameters to that for $x=1/3$ is observed, the t dependence is indiscernible due to the weak effective repulsion between quantum strings. We thus expect, in general, that it becomes harder in practice to see the correlation between spin and charge orderings as one goes to lower hole densities, in particular for the odd-leg-ladder-like system.

To conclude, we have demonstrated that the magnitude of the hidden AF LRO is governed by the competition between the enhancement of the 2D spin-spin correlation and the reformation of the strong stripe order. The question as to why the stripe tends to reorder at large t remains to be resolved. Although we have not yet found a rigorous description of the reformation of the strong stripe order, it may be due to the effective Coulomb repulsion coming from the constraint that the stripes are separated by at least one spin site. The present model with the constraint is not realistic at large t. There are two further issues along the line of the present study left for future work. One is the effect of adding a next-nearest-neighbor interaction on the squeezed lattice. In that case, the diagonal stripe, observed in Cu oxides and Ni oxides, would be expected to emerge in a certain parameter region. The other is to incorporate the dislocation of the strings. In the present paper, we have restricted the string mobility so as to ensure that the strings are not broken up. In order to access a superconducting regime, however, it would be crucial to study the situation where the stripes start to get destroyed.[17] The numerical simulation for this situation is a major challenge and new ideas are in need.

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