Coexistence of $d_{x^2-y^2}$-wave superconductivity and antiferromagnetism induced by a staggered field

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The two-dimensional t-J model in a staggered field is studied by exact diagonalization of small clusters. For the low-hole-density region and a realistic value of J/t, it is found that the presence of a staggered field strengthens the attraction between two holes. With increasing field, the $d_{x^2-y^2}$-wave superconducting correlations are enhanced while the extended-s-wave ones hardly change. This implies that coexistence of the $d_{x^2-y^2}$-wave superconducting order and the commensurate antiferromagnetic order occurs in a staggered field.

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I. INTRODUCTION

In high-T_c cuprates, the antiferromagnetically ordered phase and the superconducting phase were separately observed in the plane of doping concentration and temperature.[1,2] Thus antiferromagnetism and superconductivity may be thought as competing with each other. However, some of the recent experiments suggest a possibility of their coexistence, although it is still controversial.[3–8]

Elastic neutron-scattering experiments in $YBa_2Cu_3O_y$ with $y=6.5$ and 6.6 show that magnetic intensity emerges near room temperature at the momentum (π,π) in units of the reciprocal-lattice parameter.[3,4,7] The intensity increases continuously with decreasing temperature. Remarkably, an upturn of the intensity is observed at a superconducting transition temperature. This suggests coexistence of superconductivity and the commensurate antiferromagnetic (AF) order. Moreover, nuclear quadrupole resonance measurements have revealed the presence of magnetic moments in the superconducting state on $Hg_{0.8}Cu_{0.2}Ba_2Ca_2Cu_3O_{8+\delta}$.[8] The observed magnetic moments in these materials are often regarded as a consequence of the formation of the d-density wave order.[9] However, this interpretation leaves a difficulty since the d-density wave order suppresses superconductivity.[10] Thus we should also consider an alternative scenario that the magnetic moments are due to the ordered Cu spins.

So far, the possible coexistence of antiferromagnetism and d-wave superconductivity in the two-dimensional (2D) t-J model has been discussed at low hole doping, in a variational approach[11] and quantum Monte Carlo calculations.[12] The possibility of the coexistence[13] poses a fundamental question on interplay between antiferromagnetism and d-wave superconductivity. Before answering whether the coexistence actually takes place in cuprate superconductors, we would like to clarify whether those two orders can coexist in strongly correlated electron systems. To clarify the matter, it would be useful to study the hole pairing and superconductivity in a staggered field, which forces the system to have the AF order. Indeed, for the 1D t-J model in a staggered field, the superconducting correlation was found to be the most dominant for $J/t\sim 0.4$.[14,15]

In this paper, we investigate the 2D t-J model on a square lattice in a staggered field coupled to electron spins. While the staggered field is introduced here as an artificial parameter to induce the AF order, it may arise naturally if three-dimensional interplane interactions are treated in a mean-field theory. We employ exact diagonalization for the 4×4, $\sqrt{18}\times\sqrt{18}$, $\sqrt{20}\times\sqrt{20}$, and $\sqrt{26}\times\sqrt{26}$ clusters with periodic boundary conditions. Our results demonstrate that a staggered field actually enhances the pairing of two holes and the $d_{x^2-y^2}$-wave superconductivity.

II. MODEL

We consider the following Hamiltonian given by

$$\mathcal{H}=-t\sum_{\langle \vec{i},\vec{j}\rangle\sigma}(\tilde{c}^{\dagger}_{\vec{i}\sigma}\tilde{c}_{\vec{j}\sigma}+\mathrm{H.c.})+J\sum_{\langle \vec{i},\vec{j}\rangle}\left(\vec{S}_{\vec{i}}\cdot\vec{S}_{\vec{j}}-\frac{1}{4}n_{\vec{i}}n_{\vec{j}}\right)-h\sum_{\vec{i}\in A}S^z_{\vec{i}}+h\sum_{\vec{j}\in B}S^z_{\vec{j}}, \tag{1}$$

where $\langle \vec{i},\vec{j}\rangle$ is the nearest neighbor. The constrained fermion operator $\tilde{c}_{\vec{i}\sigma}$ is given by $\tilde{c}_{\vec{i}\sigma}=c_{\vec{i}\sigma}(1-n_{\vec{i},-\sigma})$, which means that double occupancy at each site is excluded. The last two terms are due to the presence of a staggered field whose magnitude is denoted by h; A and B represent the two sublattices on a square lattice. We refer to this model as the t-J-h model. In this work we fix $J/t=0.4$ which is considered as a realistic value, and vary h/t as a parameter.

III. NUMERICAL RESULTS

We first discuss the hole correlation function given by $C_{\mathrm{hole}}(\vec{r})=(1/N)\Sigma_{\vec{i}}\langle n_h(\vec{i})n_h(\vec{i}+\vec{r})\rangle$. Here N is the number of lattice sites, $n_h(\vec{i})=1-n_{\vec{i}}$, and $\langle\cdots\rangle$ denotes the expectation value in the zero-momentum ground state. In the left panel of Fig. 1 we show the distance dependence of $C_{\mathrm{hole}}(r)$ with $r\equiv|\vec{r}|$ for the hole densities $N_h/N=2/18\simeq0.111$ and $4/18\simeq0.222$. For two holes and $h=0$, the most dominant correlations are at $r=\sqrt{2}$, namely, when the holes stay at the next-nearest neighbors.[16,17] As h/t increases, correlations at the nearest neighbors ($r=1$) become stronger than those at $r=\sqrt{2}$, and contribution at longer distances is suppressed. For four holes, correlations at $r=1$ are enhanced while ones at the largest distance hardly change. This means that the presence of a staggered field makes the interaction between two holes attractive but the hole pairs are well separated.

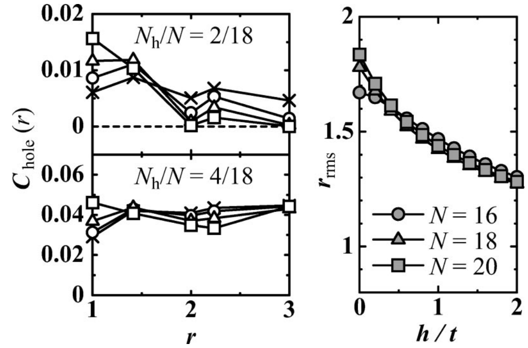

FIG. 1. Left: Equal-time hole correlations as a function of distance in the 2D t-J-h model with $N=18$, $J/t=0.4$, and various values of h/t. Crosses, circles, triangles, and squares are the data for $h/t=0.0,0.4,1.0$, and 2.0, respectively. Right: Root-mean-square separation of the hole pair as a function of h/t. $J/t=0.4$.

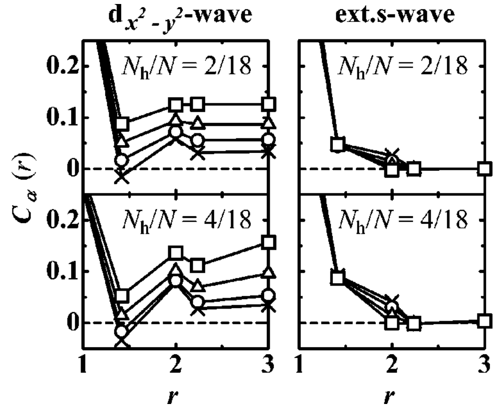

FIG. 3. Equal-time superconducting correlations as a function of distance in the 2D t-J-h model with $N=18$, $J/t=0.4$, and $h/t=0.0,0.4,1.0$, and 2.0. The symbols are the same as in the left panel of Fig. 1.

In order to analyze the obtained data in the two-hole case, we calculate the root-mean-square separation of the hole pair[18,19] defined as $r_{\rm rms}\equiv\sqrt{\langle r^2\rangle}$ where $\langle r^2\rangle=\Sigma_{\vec{r}(\neq\vec{0})}|\vec{r}|^2 C_{\rm hole}(\vec{r})/\Sigma_{\vec{r}(\neq\vec{0})}C_{\rm hole}(\vec{r})$. Here $|\vec{r}|$ takes the shortest distance between two holes on the lattice with periodic boundary conditions. The right panel of Fig. 1 shows the h/t-dependence of $r_{\rm rms}$. It is clear that the separation of the hole pair becomes smaller with increasing staggered field. For larger h/t, the value of $r_{\rm rms}$ is less affected by finite-size effects. The present result suggests that the staggered field does help binding of two holes, and that the hole binding survives in the thermodynamic limit at least for a sufficiently large h/t.

A tendency of hole binding can be obtained also from the binding energy, which is given by[20]

$$E_B=E_0(N_h=2)+E_0(N_h=0)-2E_0(N_h=1). \qquad (2)$$

Here $E_0(N_h)$ denotes the ground-state energy with N_h holes in N sites. A negative value of E_B indicates the presence of hole binding. In Fig. 2(a) we show the dependence of the binding energy on the staggered field h. The binding energy is negative in the whole range of h/t and has a peak at $h/t\sim 0.8,1.2$, 1.2, and 0.8 for $N=16,18$, 20, and 26, respectively. The obtained results apparently imply that hole pairing is suppressed by a small staggered field. However, being an intensive quantity, the binding energy is severely affected by finite-size effects.[18] Figure 2(b) shows the size dependence of the binding energy for various values of h/t. In fact, although at $h=0$ (and $J/t=0.4$) the binding energy for $N\leqslant 26$ takes negative values, an extrapolation from the data rather indicates the absence of hole binding in the thermodynamic limit. This has been already discussed in earlier studies[21,22] for $N\leqslant 32$. On the other hand, for larger h/t, we find the size dependence to be substantially smaller. It seems that the binding energy remains negative with increasing N in the presence of a staggered field. Therefore there is a possibility that the two holes in the bulk limit tend to be bound even by a small field. In particular, for a large h/t ($h/t\gtrsim 1.0$) the weak size dependence of the negative binding energy strongly suggests the hole pairing in the bulk limit.

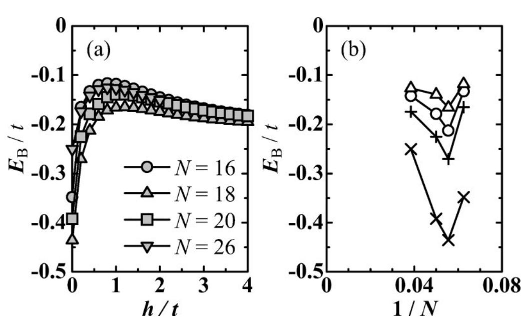

FIG. 2. (a) Binding energy as a function of h/t in the 2D t-J-h model with $J/t=0.4$. (b) Size dependence of the binding energy. Crosses, pluses, circles, and triangles are the data for $h/t=0.0,0.2,0.4$, and 1.0, respectively. $J/t=0.4$.

The pairing of holes is also consistent with the enhanced superconducting correlation discussed below. We calculate the equal-time superconducting correlations given by $C_\alpha(\vec{r})=(1/N)\Sigma_{\vec{i}}\langle\Delta^\dagger_\alpha(\vec{i})\Delta_\alpha(\vec{i}+\vec{r})\rangle$.[23,24] The singlet pairing operator $\Delta_\alpha(\vec{i})$ is defined as $\Delta_\alpha(\vec{i})=(1/\sqrt{2})\Sigma_{\vec{\epsilon}}f_\alpha(\vec{\epsilon})(c_{\vec{i}\uparrow}c_{\vec{i}+\vec{\epsilon},\downarrow}-c_{\vec{i}\downarrow}c_{\vec{i}+\vec{\epsilon},\uparrow})$, where $\vec{\epsilon}$ is $(\pm 1,0)$ and $(0,\pm 1)$. For the extended-s-wave pairing symmetry ($\alpha=s$), we put $f_s(\vec{\epsilon})=+1$ at all $\vec{\epsilon}$. For the $d_{x^2-y^2}$ symmetry ($\alpha=d$), we put $f_d(\vec{\epsilon})=+1$ at $\vec{\epsilon}=(\pm 1,0)$ and $f_d(\vec{\epsilon})=-1$ at $\vec{\epsilon}=(0,\pm 1)$. Figure 3 shows the distance dependence of $C_d(r)$ and $C_s(r)$ for the hole densities 0.111 and 0.222 in 18 sites. For $n_h\lesssim 0.2$, with increasing field, the $d_{x^2-y^2}$-wave superconducting correlations are enhanced at all distances with $r\geqslant 1$. In contrast, the extended-s-wave ones hardly change, especially at long distances. This implies that the presence of a staggered field helps the $d_{x^2-y^2}$-wave superconductivity.

Calculation of the pair spectral function[25,26] should provide another evidence for the $d_{x^2-y^2}$-wave pairing enhanced by a staggered field. The pair spectral function is given by

$$P_\alpha(\omega)=\sum_n |\langle\Psi_n(N_h=2)|\Delta^{\rm tot}_\alpha|\Psi_0(N_h=0)\rangle|^2 \times\delta[\omega-E_n(N_h=2)+E_0(N_h=0)+\mu], \qquad (3)$$

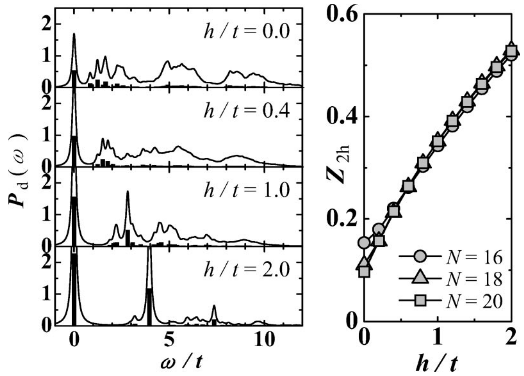

FIG. 4. Left: Pair spectral function with $d_{x^2-y^2}$-wave symmetry in the 2D t-J-h model with 18 sites, $J/t=0.4$, and various values of h/t. The delta functions (vertical bars) are broadened by a Lorentzian with a width of $0.1t$ (solid curves). Right: Spectral weight Z_{2h} as a function of h/t in the 2D t-J-h model with $J/t=0.4$.

where $\Delta_\alpha^{\rm tot}=\Sigma_{\vec{i}}\Delta_\alpha(\vec{i})/\sqrt{N}$, $\mu=E_0(N_h=2)-E_0(N_h=0)$, and $|\Psi_n(N_h)\rangle$ denotes an eigenstate with energy $E_n(N_h)$ in the N_h-hole system. The left panel of Fig. 4 shows the ω-dependence of $P_d(\omega)$ for various values of h/t. The overall feature approximated by a Lorentzian is insensitive to the system size at each h/t. The peak at $\omega=0$ (i.e., the coherent peak) grows with increasing h/t, which means that the pairing becomes strong. The contribution for $\omega>0$, which seems to be a continuum spectrum, is relatively suppressed, but a peak with secondary dominant intensity appears. Concerning this peak for $h/t=2.0$, the values of energy ω and residue z are $(\omega/t,z)=(3.95,0.268),(3.96,0.273)$, and $(3.95,0.265)$ for $N=16,18$, and 20, respectively. The weak size dependence of both values of ω and z indicates that the secondary peak may be a delta-function contribution rather than a part of continuum spectrum in the bulk limit.

We estimate the spectral weight defined as[26,27]

$$Z_{2h}=\frac{|\langle\Psi_0(N_h=2)|\Delta_d^{\rm tot}|\Psi_0(N_h=0)\rangle|^2}{\langle\Psi_0(N_h=0)|(\Delta_d^{\rm tot})^\dagger\Delta_d^{\rm tot}|\Psi_0(N_h=0)\rangle}, \qquad (4)$$

which corresponds to the coherent peak of $P_d(\omega)$ at $\omega=0$. Note that Z_{2h} is between 0 and 1 because the denominator of Eq. (4) is equal to the integration of $P_d(\omega)$ over ω. The right panel of Fig. 4 shows Z_{2h} as a function of h/t. The weight is monotonically increasing function of h/t. Again, the size dependence of Z_{2h} is weak for a large h/t. Therefore we expect that the coherent peak survives in the thermodynamic limit for a sufficiently large h/t.

While our results suggest the enhancement of hole pairing by a staggered field, it is possible that the attraction between holes leads to phase separation. We calculate the clustering energy given by[20]

$$E_C=E_0(N_h=4)+E_0(N_h=0)-2E_0(N_h=2). \qquad (5)$$

If this quantity is negative, the phase separation is expected to occur. The results for $N=18$ and 20 are shown in Fig. 5, which suggests that the region $0\leqslant h/t\lesssim 2$ is not interrupted by the phase separation.[28]

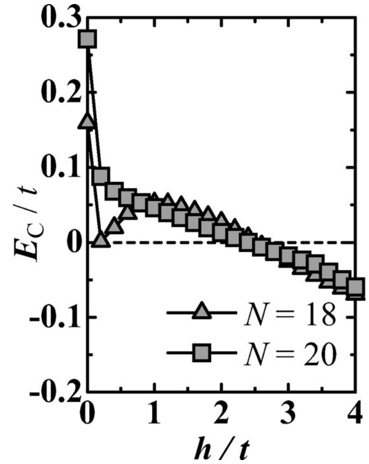

FIG. 5. Clustering energy as a function of h/t in the 2D t-J-h model with $J/t=0.4$.

The staggered field should induce a finite magnetic moment on each site, and consequently the commensurate AF long-range order. In Fig. 6 we show the result on the staggered-spin correlations given by $C_{\rm spin}(\vec{r})=(1/N)\Sigma_{\vec{i}}(-1)^{r_x+r_y}\langle S_{\vec{i}}^z S_{\vec{i}+\vec{r}}^z\rangle$ with $\vec{r}=(r_x,r_y)$. Indeed, the correlations seem to remain finite in the long-distance limit for $h/t>0$, as expected. An important point is that *both* the $d_{x^2-y^2}$-wave superconducting correlations and the staggered-spin ones are enhanced by a staggered field. Therefore we expect the simultaneous presence of the $d_{x^2-y^2}$-wave superconducting order and the commensurate AF order in a certain range of h/t.

IV. PERTURBATION FROM LARGE-h/t LIMIT

Why does the presence of a staggered field help the pairing formation? This may be understood from the large-h/t limit. In order to treat analytically, we consider the t-J_z-h model where the isotropic Heisenberg term (J) in Eq. (1) is replaced by the Ising term (J_z), following Refs. 14 and 15. For $h/t\gg 1$, we can regard the single-particle hopping term (t) as a perturbative one. In the Hilbert space with all spins along the direction of the staggered field, the second-order perturbation leads to the effective Hamiltonian given by $\mathcal{H}_{\rm eff}=P\tilde{\mathcal{H}}_{\rm eff}P$ where

$$\tilde{\mathcal{H}}_{\rm eff}=J_z\sum_{\langle\vec{i},\vec{j}\rangle}\left(S_{\vec{i}}^zS_{\vec{j}}^z-\frac{1}{4}n_{\vec{i}}n_{\vec{j}}\right)-\tilde{t}\sum_{\langle\vec{i},\vec{j},\vec{\ell}\rangle\sigma}[\tilde{c}_{\vec{i}\sigma}^\dagger(1-n_{\vec{j}})\tilde{c}_{\vec{\ell}\sigma}$$
$$+(1-n_{\vec{i}})(1-n_{\vec{j}})n_{\vec{\ell}\sigma}+\text{H.c.}]+(\text{other terms}). \qquad (6)$$

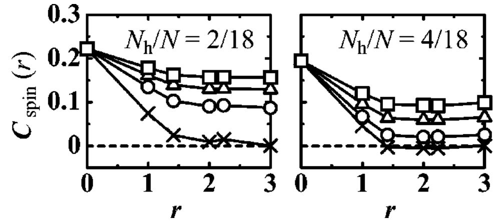

FIG. 6. Equal-time staggered-spin correlations as a function of distance in the 2D t-J-h model with $N=18$, $J/t=0.4$, and $h/t=0.0,0.4,1.0$, and 2.0. The symbols are the same as in the left panel of Fig. 1.

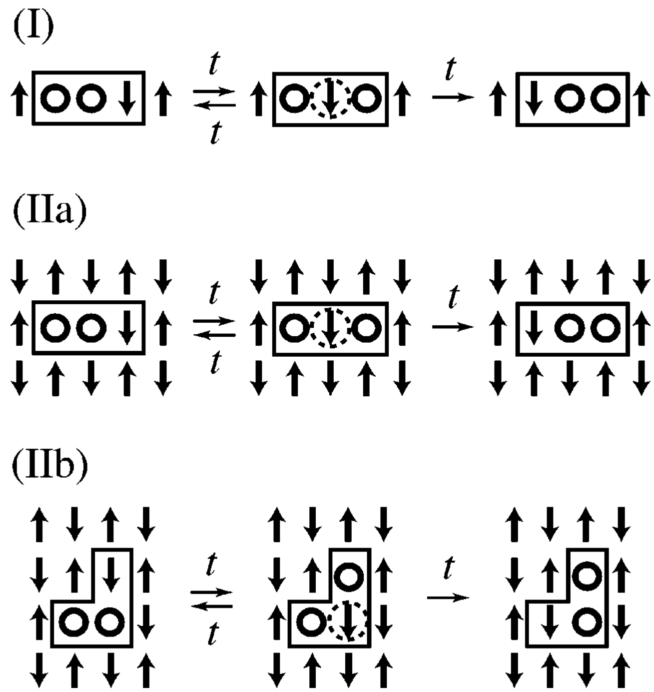

FIG. 7. Typical processes of the second-order perturbation in the t-J_z-h model for $h/t \gg 1$. (I) is the 1D case, while (IIa) and (IIb) are the 2D case. The spin surrounded by a broken circle is against the direction of the staggered field. The three sites surrounded by a box correspond to $\langle \vec{i},\vec{j},\vec{\ell} \rangle$ in the second term of Eq. (6).

Here $\langle \vec{i},\vec{j} \rangle$ and $\langle \vec{i},\vec{j},\vec{\ell} \rangle$ are the nearest neighbors, and $P = \prod_{\vec{i} \in A}(1-n_{\vec{i}\downarrow})\prod_{\vec{j} \in B}(1-n_{\vec{j}\uparrow})$. The second term in the right-hand side of Eq. (6) includes hopping of a hole which occurs only if there is another hole in the neighboring site. Namely, it gives hopping of a hole pair. This is generated in the second-order processes shown in Fig. 7. In the 2D case the pair-hopping integral $\tilde{t}$ is given by $t^2/(h+3J_z/2)$ where the denominator indicates the energy difference between the initial state and the intermediate one [see Fig. 7(IIa) and 7(IIb)]. We note that $\tilde{t}$ is replaced by $t^2/(h+J_z/2)$ in the 1D case [see Fig. 7(I)].[14,15]

The fact that the effective Hamiltonian includes the hole-pair hopping implies that hole binding and superconductivity may be naturally realized in the antiferromagnetic background forced by the staggered field. The effective pair-hopping integral $\tilde{t}$ decreases as h/t increases. This suggests that a too large staggered field makes the hole pairs less mobile, which may be related to the phase separation at large h/t discussed above. On the other hand, it does not mean that a smaller h/t is better for superconductivity, because the calculation is based on the perturbation theory in t/h.

V. SUMMARY

We have investigated the binding energy and various correlation functions for the 2D t-J model in a staggered field. For the low-hole-density region at $J/t=0.4$, the presence of a staggered field strengthens the attraction between two holes and helps the $d_{x^2-y^2}$-wave superconductivity. This implies that the commensurate antiferromagnetic order and the $d_{x^2-y^2}$-wave superconductivity can coexist in a strongly correlated electron system in two dimensions.

One may ask whether calculation of small clusters with $N\sim20$ provides some conclusive statements in a model. In fact, for the 2D t-J model without a staggered field, binding effects for $N\sim20$ can be different from those with much larger size.[22,29,30] However, the presence of a staggered field makes the coherence length (i.e., the size of a Cooper pair) small, and therefore the data for $N\sim20$ is likely to reach the bulk limit for a sufficiently large staggered field, as evidenced by the weak size dependence. Thus our conclusion regarding the coexistence of superconductivity and antiferromagnetism should hold at least near the boundary of the phase separation $(h/t\sim2)$.[31] This would be of a conceptual interest, although such a large staggered field seems unrealistic. An open question is whether the picture for such a large field connect continuously to that for smaller field. For a realistic application of the present model, perhaps we need to know the effect of a small staggered field, as the effective staggered field produced by the interlayer coupling would be tiny. Unfortunately, for a small staggered field, the size dependence is still large and we cannot draw a definite conclusion from our present study based on small clusters. We hope future studies to clarify this question and its relation to the experiments.

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