Oriental symmetry-breaking correlations in square lattice $t$-$J$ model

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We study a tendency to orientational symmetry breaking of the square lattice $t$-$J$ model by applying the exact diagonalization technique. We introduce a small external anisotropy to $t$ and $J$, and calculate the induced anisotropy of hole-hole correlations as a response. It is found that the response is strongly enhanced for particular band parameters, meaning that the system has a strong tendency to orientational symmetry breaking. The analysis of the momentum distribution function indicates that the correlation develops when the Fermi surface is close to $(\pi, 0)$ and $(0, \pi)$. Some properties of high-$T_c$ cuprates previously attributed to stripes can also be understood from orientational symmetry breaking alone.

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High-$T_c$ cuprate superconductors are realized by a carrier doping into Mott insulators, where strong onsite Coulomb repulsion prohibits double occupation and one electron resides at every sites. Such strong electron-electron correlations are widely recognized to be crucial to the physics of high-$T_c$ cuprates.

Minimal models for high-$T_c$ cuprates are believed to be the two-dimensional (2D) $t$-$J$ and Hubbard models on a square lattice. Cuprate superconductors have $d$-wave gap symmetry, which was successfully reproduced in these models. The models, however, exhibit several ordering tendencies competing with $d$-wave superconductivity: antiferromagnetism, spin-charge stripes, staggered flux, and $d$-density wave. These possible competing orders were recognized as playing crucial roles in high-$T_c$ cuprates and discussed in relation to pseudogap phenomena, vortex structures, and charge ordering.

Recently, through microscopic analyses of the $t$-$J$ and Hubbard models another competing order was proposed, the $d$-wave Fermi surface deformation (dFSD): the Fermi surface (FS) expands along the $k_x$ direction and shrinks along the $k_y$ direction or vice versa. This order is generated by forward scattering of electrons close to the FS near $(\pi, 0)$ and $(0, \pi)$, and hence should be distinguished from all the competing orders mentioned above, which require large momentum transfers.

Some authors termed the spontaneous dFSD as Pomeranchuk instability, referring to a stability criterion for normal Fermi liquids by Pomeranchuk. Note, however, that the dFSD turned out to occur usually through a first order transition at low temperature, namely without breaking Pomeranchuk’s stability condition.

The dFSD competes with other instabilities. In particular, it can be overwhelmed by $d$-wave singlet pairing. However, it was pointed out that even if the spontaneous dFSD was prohibited, the correlations survived and made a system sensitive to an external anisotropy, which led to a noticeable dFSD. This scenario was invoked for high-$T_c$ cuprates through the slave-boson mean-field analysis of the $t$-$J$ model. While the slave-boson theory treats strong correlation effects on average, it still remains a fundamental question whether the dFSD will be relevant to the strongly correlated regime and thus to the physics of high-$T_c$ cuprates. Since the dFSD changes the shape of the FS, possibilities of the dFSD are crucial to the understanding of low energy properties of cuprates.

In this Letter, we study the dFSD by applying the exact diagonalization technique to the 2D $t$-$J$ model at zero temperature and treat strong correlation effects rigorously. We take a $4 \times 4$ cluster with a periodic boundary condition with two holes. Since the dFSD is associated with orientational symmetry breaking of a square lattice, we focus on a tendency to the orientational symmetry breaking. We impose a small $xy$-spatial anisotropy in the original $t$-$J$ model and calculate the induced anisotropy of hole-hole correlations as a response. It is found that the response shows a sharp peak as a function of band parameters, which means that the system has a strong tendency to orientational symmetry breaking for particular band parameters. The analysis of the momentum distribution function indicates that this correlation develops when the FS is close to $(\pi, 0)$ and $(0, \pi)$. The concept of the dFSD, originally proposed in the slave-boson mean-field analysis of the $t$-$J$ model and a renormalization group analysis of the Hubbard model, is thus relevant even to the strongly correlated regime and in this sense is a generic feature of square lattice interacting electron systems. Possibilities of the dFSD are discussed for high-$T_c$ cuprates.

We take the 2D $t$-$J$ model

$$H = - \sum_{i, \tau, \sigma} t^{(l)}_{i, \sigma} \hat{c}^\dagger_{i, \sigma} \hat{c}_{i, \tau, \sigma} + J_x \left( \mathbf{S}_i \cdot \mathbf{S}_{i+\tau} - \frac{1}{4} \hat{n}_i \hat{n}_{i+\tau} \right)$$

(1)

defined in the Fock space with no doubly occupied sites. The $\hat{c}^\dagger_{i, \sigma}$ ($\mathbf{S}_i$) is an electron (a spin) operator, and $\hat{n}_i = \sum_{\sigma} \hat{c}^\dagger_{i, \sigma} \hat{c}_{i, \sigma}$ is the number operator of electrons at site $i$. 

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The $t'^{(l)}_r$ is the $l$th ($l \leq 3$) neighbor hopping integral to the direction $\tau = r_j - r_i$, and we denote $t'^{(1)}_r = t$, $t'^{(2)}_r = t'$, and $t'^{(3)}_r = t''$; the latter two are assumed isotropic. The $J_{r'}(> 0)$ is the superexchange coupling between nearest-neighbor sites. We introduce an external anisotropy to $t_r$ and $J_r$,

$$t_x = (1 + \alpha)t, \ t_y = (1 - \alpha)t,$$  \hspace{1cm} (2) \\
$$J_x = (1 + \gamma)J, \ J_y = (1 - \gamma)J,$$  \hspace{1cm} (3)

where we assume $\gamma = \frac{t}{t_J}$ so that the anisotropy between $J_x$ and $J_y$ is twice as large as that between $t_x$ and $t_y$. As a response to this anisotropy, we consider an anisotropy of hole-hole correlation

$$\Delta C(r) = C(r) - C(\bar{r}),$$  \hspace{1cm} (4)

where $r = (x, y)$ and $\bar{r} = (y, x)$, and

$$C(r) = \frac{1}{(Nm)^2} \sum_{n} \langle (1 - \tilde{n}_i)(1 - \tilde{n}_{i+r}) \rangle$$  \hspace{1cm} (5)

is a hole-hole correlation function; $N$ is the total number of lattice sites; $\delta(> 0)$ is hole density; the factor $\frac{1}{(Nm)^2}$ is taken to normalize $\sum_r C(r)$ to be unity. Note that $\Delta C(r)$ vanishes as long as the system has orientational symmetry of the lattice.

To treat strong correlation effects rigorously, we take a $4 \times 4$ cluster with a periodic boundary condition and diagonalize the Hamiltonian using the Lanczos algorithm at zero temperature; the coordinates of the cluster are defined in Fig. 1(a). Although the cluster size is rather small for usual exact diagonalization studies, the $4 \times 4$ cluster has square lattice symmetry and enables us to treat $k = (\pi, 0)$ and $(0, \pi)$. These aspects are crucial in the present study. We introduce two holes ($\delta = 1/8$) and assume that the total momentum of the wave function is zero. For $\alpha = 0$, the system has orientational symmetry and hence $\Delta C(r) = 0$. When a small $\alpha$ is introduced, $\Delta C(r)$ can become finite. It has four inequivalent points: (i) $r = (2, 0)$, (ii) $r = (1, 0)$, (3, 0), (iii) $r = (2, 1), (2, 3)$, and (iv) $r = (1, 1), (2, 2), (3, 3), (3, 1)$. In the latter case $\Delta C(r) = 0$. We refer to the former three cases as $\Delta C_m$ with $m = 1, 2$, and 3, respectively. Setting $\alpha = 0.01$, we calculate $\Delta C_m$ as a function of $t''/t$ for $t/J = 4$ and $t''/t = -0.17$.

In Fig. 1(b), we see that $\Delta C_m$ is nearly zero for $|t''| \geq 0.15t$, that is the hole-hole correlation is almost isotropic even in the presence of the external anisotropy ($\alpha \neq 0$). For $|t''| \leq 0.1t$, $\Delta C_m$ becomes noticeable and is strongly enhanced near $t''/t = 0.05$ to form a sharp peak. This peak is seen in all $\Delta C_m$, indicating that the system has a strong tendency to the orientational symmetry breaking for particular band parameters.

In the inset of Fig. 1(b), we show the following quantity as a function of $t''$: $C_x$ to see a degree of the orientational symmetry breaking: $C_x = \sum_y C(r)$, where the summation is over $r = (1, 0), (2, 0), (3, 0)$, similarly $C_y = \sum_y C(r)$ over $r = (0, 1), (0, 2), (0, 3)$, and $C_{xy} = \sum_{x'y'} C(r)$ over $r = (1, 1), (2, 2), (3, 3)$. The $C_x$ ($C_y$) and $C_{xy}$ describe hole-hole correlation along the horizontal (vertical) direction and a diagonal direction, respectively. Around $t''/t = 0.05$ the value of $C_x$ is about twice as large as that of $C_y$. The breaking of orientational symmetry at $t''/t \approx 0.05$ is thus very large. The hole-hole correlation, however, does not become one-dimensional like. The sum rule, $\sum_r C(r) = 1$, suggests that the value of $C_{xy}$ is appreciably smaller than the mean value of $C(r)$ is $\frac{t}{t_J}$ and that of $C_{xy}$ becomes $\frac{\overline{t'}}{t_J}$. Furthermore we found that $C_{xy}$ was almost the same as that for $\alpha = 0$, that is the correlation along the diagonal direction still remained. Moving away from $t''/t \approx 0.05$ the difference between $C_x$ and $C_y$ gets smaller as expected.

To understand the origin of the sharp peaks in Fig. 1(b), we calculate the momentum distribution function $n_k = \frac{1}{\sqrt{V}} \langle \sum_{\sigma} \epsilon_{k, \sigma} \sigma_{k, \sigma} \rangle$ for $\alpha = 0$ [Fig. 2(a)]. The maximal value of $n_k$ is about 0.56. This comes from strong correlation effects, namely the constraint that double occupation is forbidden at every site, which leads to $n_k \leq \frac{1}{4}(1 + \delta)$. The distribution of $n_k$ is shown in Figs. 2(b)-(d) for several choices of $t''$; the FS is inferred under the assumption of the Luttinger theorem, and may represent a typical FS in $-0.2 \leq t''/t \leq -0.05 (b)$, $-0.05 \leq t''/t < 0.05 (c)$, and $0.05 < t''/t < 0.2$ (d), respectively. This change of FS as a function of $t''$ agrees with one expected for interacting electrons with $t, t'$, and $t''$ as emphasized before. Around $t''/t \approx -0.15$ the FS is expected to cross the point $k = (\pi/2, \pi/2)$. But an appreciable change of $n_k$ is
not seen in Fig. 2(a). This is probably due to a finite size effect since the total number of electron has to be distributed over a small number of k points constrained by the geometry of the cluster. A jump of $n_{\mathbf{k}}$ is seen at $t''/t = 0.05$ in Fig. 2(a). This jump itself is probably a finite size effect, which we interpret as a level crossing between a state with an electron like FS [Fig. 2(c)] and a state with a hole like FS [Fig. 2(d)]. The free energy shows a cusp there as a function of $t''$. Moreover, the jump disappears for $\alpha \neq 0$ and $n_{\mathbf{k}}$ changes smoothly, which will be due to realization of an “intermediate” state in the sense that the FS will close along the $k_x$ direction (electron like) and open along the $k_y$ direction (hole like). To confirm that an electron like FS actually changes into a hole like FS near $t''/t = 0.05$ as inferred from Figs 2(a)- (d), we look at the change of $n_{\mathbf{k}}$ at $(\pi, 0)$ and $(0, \pi)$ by small $\alpha$, which we define as $\Delta n_{\mathbf{k}} = n_{\mathbf{k}, \alpha=0.01} - n_{\mathbf{k}, \alpha=0}$. In Fig. 2(c), we see an appreciable change of $\Delta n_{\mathbf{k}}$ around $t''/t = 0.05$ and a positive (negative) sign of $\Delta n_{\mathbf{k}}$ at $(0, \pi)$ ($(\pi, 0)$). This is expected when a FS is close to $(\pi, 0)$ and $(0, \pi)$ at $t''/t = 0.05$, where the small $\alpha$ moves the $(0, \pi)$ $(\pi, 0)$ point inside (outside) the FS. Therefore, considering that $\Delta C_m$ shows a sharp peak at $t''/t = 0.05$ [Fig. 2(b)], we conclude that an electronic state with a FS being near $(\pi, 0)$ and $(0, \pi)$ has strong correlations toward orientational symmetry breaking.

Since our anisotropy ($\alpha = 0.01$) is a weak perturbation to the original t-J model, $\Delta C_m$ can be a linear response quantity. This actually holds for most of $t''$. When $t''$ approaches $0.05t$, however, the linear susceptibility grows rapidly and the value of $\alpha = 0.01$ is no longer in the linear response regime; $\Delta C_m$ begins to show saturation as a function of $\alpha$.

So far we have investigated the anisotropy of hole-hole correlation as a function of $t''$. A similar enhancement of the anisotropy would be expected as a function of $t'$ (with $t'' = 0$), since an electron like FS may cross $(\pi, 0)$ and $(0, \pi)$, and evolve to a hole like FS with decreasing $t'(< 0)$. However, $n_{\mathbf{k}}$ did not indicate a hole like FS, but an electron like FS [Fig. 2(c)] in a wide range $-0.1 \gtrsim t'/t \gtrsim -0.43$. This is probably due to larger finite size effects at smaller $t'$, since $n_{\mathbf{k} = (0, 0)}$ decreases drastically at $t'/t \approx -0.44$ and becomes smaller than $n_{\mathbf{k}}$ at $k = (\pi/2, 0), (\pi, 0), (\pi/2, \pi/2)$, indicating realization of a hole pocket around $k = (0, 0)$. This is not expected in infinite systems for such parameters and in fact does not occur in the slave-boson mean-field analysis. Regardless of this possible finite size effect, $\Delta C_m$ shows a pronounced enhancement near $t'/t = -0.43$, where we expect a FS to be closest to $(\pi, 0)$ and $(0, \pi)$ from the same observation as in Fig. 2(c).

The correlation of orientational symmetry breaking found in Fig. 4(b) is identical to the dFSD correlation that was discussed in the slave-boson mean-field analysis of the t-J model [11] and in various other models. [12] A crucial point of the present study is that the dFSD correlation is found in the exact diagonalization where strong correlation effects are treated exactly. Hence the dFSD is relevant even to a strongly correlated regime and in this sense is a generic feature when a FS is close to $(\pi, 0)$ and $(0, \pi)$.

While the present calculation has been done at a fixed hole density, the dFSD correlation may be prominent in a certain hole doping region. The slave-boson analysis of the t-J model showed that the dFSD correlation was noticeable in $0 \leq \delta \lesssim 0.20$ for $t'/J = 4, t'/t = -1/6, t''/t = 0$ and became stronger with decreasing $\delta$. [11]

The strong correlation effects are treated exactly in this study. But the system size is finite. Does a spontaneous dFSD take place when the system size becomes infinite? This is an open question. Since the dFSD competes with other instabilities such as d-wave superconductivity, there is a possibility that a spontaneous dFSD is hindered by a more dominant instability. [11] [19]

Even if a spontaneous dFSD does not occur, appreciable correlations of the dFSD make a system sensitive to a small external anisotropy, which leads to a noticeable dFSD — the FS is softened. [11] [21] This scenario was proposed for La-based cuprates from strong band parameter dependence of the dFSD correlation [see Fig. 4(b)]. [11] The shape of the FS was interpreted in terms of the dFSD under the assumption of a coupling to the low-temperature tetragonal lattice distortion that gave a small external anisotropy to the electron system. [11] Magnetic excitations were investigated on the basis of the dFSD scenario and turned out to catch essential features of neutron scattering data. [25] Recently anisotropic neutron scattering signals were observed for untwinned yttrium barium copper oxides. [25] and effects of the dFSD will be interesting for this material also.
The dFSD correlation is the same as electronic "nematic" correlations\[^{34}\] from the view of symmetry — orientational symmetry breaking of a square lattice. The possibility of nematic order has been discussed for high-$T_c$ cuprates.\[^{10}\] It is, however, currently envisaged as melting of spin-charge stripe order; the underlying physics is different from the dFSD. In the stripe scenario, some interaction with large momentum transfer near $q = (\pi, \pi)$ is requisite to realize spin-charge stripe formation. On the other hand, the dFSD comes from forward scattering of electrons close to the FS near $(\pi, 0)$ and $(0, \pi)$; stripes are not necessary to get the nematic order. It should be noted that the dFSD scenario does not preclude realization of stripes, which could be driven by interactions with large momentum transfers in the dFSD state. In the $t$-$J$ model, however, this is unlikely. The hole-hole correlation is not one-dimensional even in the presence of the anisotropy [set of Fig. 11(b)]. In addition, various numerical studies of the $t$-$J$ model reported that stripe formation was not favored, especially in the presence of $t'$ and $t''$,\[^{31, 32}\] that is for realistic band parameters of cuprates.

In summary, we have investigated a tendency to orientational symmetry breaking of the square lattice $t$-$J$ model. To treat strong correlation effects rigorously, we have applied the exact diagonalization technique to a $4 \times 4$ cluster with a periodic boundary condition with two holes at zero temperature. Introducing a small anisotropy to $t$ and $J$, we have calculated the induced anisotropy of hole-hole correlations as a response. We have found that the response is strongly enhanced for particular band parameters, meaning that the system has a strong tendency to orientational symmetry breaking of the square lattice.

The analysis of momentum distribution function indicates that this correlation develops when the FS is close to $(\pi, 0)$ and $(0, \pi)$. The present study shows that the idea of a dFSD, originally proposed in the slave-boson mean-field analysis of the $t$-$J$ model\[^{11}\] and a renormalization group analysis of the Hubbard model,\[^{12}\] is relevant even to a strongly correlated regime and is thus a generic feature of square lattice interacting electron systems. Possibilities of the dFSD are interesting for high-$T_c$ cuprates as well as other materials.\[^{32}\]

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