Self-masking of spontaneous symmetry breaking in layer materials

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We study d-wave Fermi surface deformations (dFSD), the so-called Pomeranchuk instability, on bilayer and infinite-layer square lattices. Since the order parameter of the dFSD has Ising symmetry, there are two stacking patterns along the c axis: (+, +) and (+, −). We find that, as long as the c axis dispersion is finite at the saddle points of the in-plane band dispersion, the (+, −) stacking is usually favored independently on the details of interlayer coupling, yielding no macroscopic anisotropy. The dFSD provides unique spontaneous symmetry breaking that is self-masked in layer materials.

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Spontaneous symmetry breaking is a key concept in physics. Typical examples in condensed matter are crystallization, ferromagnetism, antiferromagnetism, ferroelectricity, and superconductivity. Recently a new type of symmetry breaking was found in the shape of the Fermi surface (FS) [1, 2]. The FS usually fulfills the point-group symmetry of the underlying lattice structure. However, it was shown that such symmetry of the FS can be broken by electron correlation effects in the two-dimensional (2D) t-J [1, 3, 4] and Hubbard [2, 5, 6, 7] models on a square lattice: The FS expands along the k_x direction and shrinks along the k_y direction, or vice versa. This instability is characterized by a d-wave order parameter and we refer to it as d-wave Fermi surface deformations (dFSD) or d-wave Pomeranchuk instability.

The dFSD state has the same symmetry as the electronic nematic state [8]. Implications of such reduced symmetry were widely discussed for high-T_c cuprates [9]. In particular, the strong ab-anisotropy of magnetic excitation spectrum observed for untwinned YBa_2Cu_3O_y [10] was well explained in terms of the dFSD and its competition with singlet pairing [11]. Moreover many peculiar features observed for the bilayer ruthenate Sr_3Ru_2O_7 [12, 13] also turned out to be well captured in terms of the dFSD instability [14, 15, 16, 17].

The dFSD is expected in layer materials, which are characterized by weak interlayer coupling. Since the order parameter of the dFSD has Ising symmetry, the interlayer coupling drives two possible stacking patterns between the layers: (+, +) and (+, −); we call the former ferro-type (F) stacking and the latter antiferro-type (AF). In the latter case, macroscopic anisotropy does not appear, leading to self-masking of the underlying dFSD instability.

In this Letter, we propose a microscopic theory for the dFSD phenomenon in realistic layer materials. We find that AF dFSD state is usually favored independently on the details of interlayer coupling. Thus the dFSD instability provides unique spontaneous symmetry breaking that is self-masked macroscopically. This generic conclusion is applicable to a wide range of layer materials, including recently discovered iron-based superconductors [18, 19].

We consider both bilayer and infinite-layer models. We first focus on a bilayer square lattice and analyze the following pure forward scattering model

\[ H = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2N} \sum_{\mathbf{k}, \mathbf{k}', i=A, B} f_{\mathbf{k}k'} n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma} \]

\[ + \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}}^A c_{\mathbf{k}\sigma}^A c_{\mathbf{k}\sigma} + \epsilon_{\mathbf{k}}^B c_{\mathbf{k}\sigma}^B c_{\mathbf{k}\sigma} \]

where \( c_{\mathbf{k}\sigma}^A (\epsilon_{\mathbf{k}}) \) creates (annihilates) an electron with momentum \( \mathbf{k} \) and spin \( \sigma \) on the i = A and B planes; \( n_{\mathbf{k}\sigma} = \sum_\sigma c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \), is the number operator; \( N \) is the total number of sites on the i plane and \( \mu \) is the chemical potential. For hopping amplitudes \( t \) and \( t' \) between nearest and next-nearest neighbors on the square lattice, \( \epsilon_{\mathbf{k}} \) is given by \( \epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \). The forward scattering interaction, \( f_{\mathbf{k}k'} = -g d_{\mathbf{k}} d_{\mathbf{k}'} \), drives the dFSD instability, where \( d_{\mathbf{k}} = \cos k_x - \cos k_y \) and \( g > 0 \) [20, 21]. The last term in Hamiltonian (1) is the hybridization between A and B planes. We consider three types of c axis dispersions, \( \epsilon_{\mathbf{k}}^F = -t z + 2t' (\cos k_x + \cos k_y) \), and \( -4t_z \cos \frac{k_x}{2} \cos \frac{k_y}{2} \); the latter two dispersions vanish at \( k = (\pi, 0) \) and \( (0, \pi) \) while the former does not. This difference is crucial to the stacking of the dFSD.

Hamiltonian (1) is analyzed in the Hartree approximation, which becomes exact in the thermodynamic limit in our model. We obtain the mean field

\[ \eta^{A(B)} = -\frac{g}{N} \sum_{\mathbf{k}} d_{\mathbf{k}} \langle n_{\mathbf{k}}^{A(B)} \rangle \]

which is nonzero only if the electronic state loses the four-fold symmetry of the square lattice and is thus the order parameter of the dFSD in the A(B) plane. The FS is elongated along the k_x and k_y directions for \( \eta^{A(B)} > 0 \) and \( \eta^{A(B)} < 0 \), respectively, i.e., the order parameter has Ising symmetry. AF (F) stacking is defined by \( \eta^{A(B)} > 0 \). We determine the mean fields self-consistently under the constraint that each plane has the same electron density. We choose \( t'/t = 0.35 \) and \( t_z/t = 0.1 \), which is appropriate for the bilayer ruthenate. \( \epsilon_{\mathbf{k}} \) has saddle points in \( \mathbf{k} = (\pi, 0) \) and \( (0, \pi) \), and thus the van Hove energy of \( \epsilon_{\mathbf{k}} \) is given by \( \mu_{\text{vH}} = 4t' = 1.4t \). In the following we set \( t = 1 \) and shift the energy such that \( \mu_{\text{vH}} = 0 \).
We first consider the $c$ axis dispersion, $\varepsilon_k^z = -t_z$, from which we can extract a generic conclusion about the stacking of the dFSD. Figure 1(a) shows the phase diagram obtained for $g = 1$. The dFSD instability occurs around the van Hove energy of the in-plane dispersion, i.e. $\mu = 0$ as in the case of the single-layer model (Ref. 21). $T_c$ is almost unchanged by the presence of $\varepsilon_k^z$. The AF dFSD state, namely $\eta^A = -\eta^B \neq 0$, is stable in most of the region of the phase diagram. The F stacking appears in a very small region, as shown in the inset of Fig. 1(a). When the coupling constant $g$ is reduced, the $F$ regions increase, close to the edges of the transition line. Yet the AF region is still much larger than the $F$ ones, as it is shown in Fig. 1(b). Upon further reducing $g$, the $F$ and AF regions split from one another [Fig. 1(c)]. After this “intermediate” phase, the property of the phase diagram drastically changes below $g = 0.5$, as shown in Fig. 1(d): No dFSD instability appears around $\mu = 0$, but the transition occurs around the van Hove energy of the bonding and antibonding bands, namely around $\mu_{dH} = \pm t_z = \pm 0.1$. The phase diagram eventually contains only $F$ regions. This property does not change down to an infinitesimally small $g$.

To gain an understanding of the dFSD stacking, we consider the Landau expansion of the grand canonical potential (per lattice site) with respect to $\eta^A$ and $\eta^B$,

$$\omega(\eta^A, \eta^B) = \frac{T}{2} \left( (\eta^A)^2 + (\eta^B)^2 \right) + J \eta^A \eta^B + \cdots. \quad (3)$$

The condition, $\mathcal{I}^2 - \mathcal{J}^2 = 0$, determines a second order transition. $\mathcal{J}$ drives AF and F stacking for $\mathcal{J} > 0$ and $\mathcal{J} < 0$, respectively, and is given by

$$\mathcal{J} = \frac{1}{2N} \sum_k d_k^2 \left( f'(\lambda^+_k) + f'(\lambda^-_k) - \frac{f(\lambda^+_k) - f(\lambda^-_k)}{\epsilon_k} \right). \quad (4)$$

where $\lambda^\pm_k = \epsilon_k - \mu \pm \varepsilon_k^z$ is the dispersion of the bonding and antibonding bands; $f(\lambda) = (e^{\lambda/T} + 1)^{-1}$ is the Fermi function at temperature $T$ and $f'$ is its derivative.

As long as a second order transition occurs around $\mu = 0$ [Figs. 1(a) and (b)], we can analyze Eq. 3 by expanding it with respect to $\varepsilon_k^z$ and obtain

$$\mathcal{J} = \frac{1}{3} \frac{\partial^2}{\partial \mu^2} \int d\epsilon N_d^z(\epsilon) f'(\epsilon - \mu) \quad (5)$$

where

$$N_d^z(\epsilon) = \frac{1}{N} \sum_k d_k^2 (\epsilon_k^z)^2 \delta(\epsilon_k - \epsilon). \quad (6)$$

Since the $k$ summation in Eq. 6 is dominated by the contribution from the saddle points of $\epsilon_k$, we expand $\epsilon_k$ and $\varepsilon_k^z$ around the saddle points. $\epsilon_k$ is then written as $\epsilon_k = \frac{k_z}{2m}$ after choosing a suitable choice of momentum variables $k_\perp$ and $k_z$ with a cutoff momentum $\Lambda$, namely $|k_z| < \Lambda$; $m$ is related to $t$ and $t'$; $d_k$ is replaced by a constant, which just rescales $\varepsilon_k^z$, and we set $d_k = 1$.

For $\varepsilon_k^z = -t_z$, Eq. 6 becomes

$$N_d^z(\epsilon) = \frac{2m t_z^2}{\pi^2} \log \frac{\epsilon_k}{|\epsilon|}. \quad (7)$$

FIG. 1: $\mu$-$T$ phase diagrams in the bilayer model with $\epsilon_k^z = -t_z$ for several choices of $g$ at $t_z = 0.1$. Solid lines, $T_{c2}$, denote second order transitions, while first order transitions are denoted by open circles, $T_{c1}$, and dotted lines, $T_{d1}$; the latter, present in panels (a) and (b), corresponds to a transition between $F$ and $AF$; solid circles represent tricritical points. The insets magnify the regions around $\mu \approx -0.33$ and $T \approx 0.15$ in (a), and around $\mu \approx 0.08$ and $T \approx 0.02$ in (b).
In the present case and thus \( \Lambda \) originates from the singular contribution of \( f \) to AF stacking of the\( J \) and antibonding bands, i.e. at\( \mu = 0 \). Therefore \( \mathcal{J} \) becomes positive for \( |\mu| \lesssim T_c \), as shown in Fig. 2(a). Because of the universal property of the dFSD instability obtained for a single layer model \( [21] \), the dFSD phase is stabilized in the region \( |\mu| \lesssim T_c \). Therefore the sign of \( \mathcal{J} \) is expected to be positive, leading to AF stacking of the dFSD in a major region of the phase diagram, as seen in Figs. 1(a) and (b).

If the coupling constant \( g \) is reduced, the temperature scale of the dFSD becomes small and the energy scale of \( \epsilon_k^0 \) must be taken into account. We consider Eq. (1) instead of its lowest order expansion of Eq. (5). The scale of \( \epsilon_k^0 \) is defined as the bilayer splitting at the saddle points of the in-plane dispersion, namely

\[
\Lambda_z = |\epsilon_k^0| \quad \text{at} \quad k = (\pi, 0) \quad \text{and} \quad (0, \pi) \tag{8}
\]

in the present case and thus \( \Lambda_z = t_z \). The positive \( \mathcal{J} \) region is bounded by the scale \( \Lambda_z \), rather than \( T \), as seen in Fig. 2(b). Then \( \mathcal{J} \) becomes negative for \( |\mu| \gtrsim \Lambda_z \) and shows steep dips at the van Hove energy of the bonding and antibonding bands, i.e. at \( \mu_{\text{H}} = \pm t_z \). This structure originates from the singular contribution of \( f' \) in Eq. (1). When the temperature scale becomes much smaller than \( \Lambda_z \), we have seen that the dFSD instability occurs around \( \mu = \mu_{\text{H}} \). Therefore we obtain F stacking, as seen in Fig. 1(d).

So far we have considered a simple c axis dispersion. However, the above analysis holds also for other choices of a c axis dispersion, e.g. \( \epsilon_k^0 = -t_z \sqrt{\cos k_x + \cos k_y} \), as long as \( \Lambda_z \neq 0 \). Hence we obtain a generic conclusion for bilayer systems: F stacking prevails when the temperature scale of the dFSD is much smaller than \( \Lambda_z \), otherwise the major stacking is AF \([22]\).

What happens for \( \Lambda_z = 0 \)? This can be seen from the analysis of Eq. (5). When \( \epsilon_k^0 \) is expanded as \( \epsilon_k^0 = (a_1 k_x + b_1 k_y) t_z \) around the saddle points of the in-plane band dispersion, the logarithmic singularity in Eq. (7) is weakened to \( \epsilon \log |\epsilon| \), leading to \( \mathcal{J} \approx \frac{2m^2 \epsilon^2 \alpha_{\text{H}}}{\mu} \). The dispersion in this case may be taken as \( \epsilon_k^0 = -4t_z \sqrt{\cos k_x \cos k_y} \), for which we obtain \( a_1 b_1 < 0 \). The phase diagram indeed showed AF and F stacking for \( \mu < 0 \) and \( \mu > 0 \).

On the other hand, when \( \epsilon_k^0 \) is expanded as \( \epsilon_k^0 = (a_2 k_x^2 + b_2 k_x^2 + c_2 k_y k_y) t_z \), we obtain \( \mathcal{J} \approx \frac{16m^3 \epsilon^2}{\pi} (2a_2 b_2 + c_2^2) \log |\epsilon| \). Thus F (AF) stacking is stabilized for \( 2a_2 b_2 + c_2^2 > 0 \) (\( < 0 \)). However, the above analysis holds also for other choices of \( \epsilon_k^0 \) in Eq. (5) and just yields a factor of \( \frac{1}{2} \) after the \( k_z \) summation. AF stacking is thus stabilized in a major region of the phase diagram for \( \Lambda_z \neq 0 \).

Unlike the situation in the bilayer model, bonding and antibonding bands now depend on \( \mu \). In (a), the forward scattering interaction \( \sum_{i,j} V_{ij} n_i^A n_j^B \) and spin-spin interaction \( \sum_{i,j} J_{ij} S_i^A \cdot S_j^B \). However, these interactions do not yield a direct coupling between \( \eta^A \) and \( \eta^B \). They may just shift the chemical potential and renormalize the c axis dispersion, which is indeed the case in the Hartree-Fock approximation, as long as the in-plane interaction \( f_{kk} \) is dominant.

While our Hamiltonian (1) is simple, it is known that a forward scattering model works very well for \( \text{Sr}_3\text{Ru}_2\text{O}_7 \) \([14, 13, 16, 17]\) and that such a forward scattering interaction turns out to be inherent in the t-J \([1, 3, 4]\) and Hubbard \([2, 5, 6, 7]\) models, minimal models for cuprate superconductors. In addition, although the symmetry is different from the dFSD, a forward scattering model is also known to work for \( \text{URu}_2\text{Si}_2 \) \([22]\).

The bilayer ruthenate \( \text{Sr}_3\text{Ru}_2\text{O}_7 \) is a promising material for the dFSD instability \([12, 13]\). LDA calculations \([22]\) show that the intrabilayer dispersion does not van-
ish at the saddle points $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, that is $\Lambda_z \neq 0$. Since the temperature scale of the dFSD is about 1 K and is much smaller than $\Lambda_z$, we expect F dFSD stacking within each bilayer. On the other hand, there is a very weak interbilayer dispersion, which is expected to have the form factor $t_z' \cos \frac{k_y}{2} \cos \frac{k_y}{2}$ because the Ru sites shift by $(\frac{1}{2}, \frac{1}{2})$ between adjacent bilayers. The interbilayer dispersion thus vanishes at $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, i.e. $\Lambda_z = 0$. In this case, $J \sim -1/\mu$ as calculated above. This suggests AF and F stacking between adjacent bilayers, namely the stacking $(\cdots + + + +, \cdots)$ and $(\cdots + + + +, \cdots)$ for $\mu \lesssim 0$ and $\mu \gtrsim 0$ respectively.

High-temperature cuprate superconductors are also promising materials for the dFSD instability \[1\]. While competition with singlet pairing may suppress the instability, the dFSD is still important, yielding strong correlations \[1, 4\], which may lead to a giant anisotropic response to a small external anisotropy, e.g. lattice anisotropy. Hence the stacking is determined by the external anisotropy and we expect F stacking for Y-based cuprates \[11\] and AF stacking in La-based cuprates in the low temperature tetragonal structure \[4\].

We have studied a generic tendency for the dFSD stacking in bilayer and infinite-layer models. We have found that the stacking does not depend on the details of interlayer coupling as long as the $c$ axis dispersion is finite at the saddle points of the in-plane band dispersion, namely as long as $\Lambda_z \neq 0$. For bilayer systems we have found F stacking only when the temperature scale of the dFSD is much smaller than $\Lambda_z$ \[Fig. 1(d)\], and AF stacking otherwise \[Figs. 1(a)-(c)\]. For infinite-layer systems instead the major stacking pattern is always AF \[Fig. 3\].

The dFSD instability is a generic tendency in correlated electron systems as found in different theoretical models \[1, 2, 5, 27\]. The dFSD is thus expected for various materials except if other instabilities prevail over the dFSD instability. Since the condition $\Lambda_z \neq 0$ is fulfilled for most materials unless there is a special symmetry reason, typical materials with a high critical temperature for the dFSD instability may have AF stacking. While spontaneous symmetry breaking is by definition recognized by symmetry breaking of the system, the dFSD provides a conceptually interesting property that spontaneous symmetry breaking can be self-masked in realistic materials.

Given the fact that antiferromagnetism was recognized about twenty centuries later than ferromagnetism \[28, 29\], it is not difficult to believe that the dFSD instability is hidden in various layer materials. Because of a coupling to the lattice, the easiest step to find AF dFSD materials is to test a twofold lattice modulation along the $c$ axis.

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