Inter-layer Josephson coupling in stripe-ordered superconducting cuprates

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Motivated by experiments on La$_{2-x}$Ba$_x$CuO$_4$ which suggest that stripe order co-exists with two-dimensional pairing without inter-layer phase coherence over an extended range of temperatures, we determine the inter-layer Josephson coupling in the presence of stripe order. We employ a mean-field description of bond-centered stripes, with a zero-momentum superconducting condensate and alternating stripe directions pinned by the low-temperature tetragonal (LTT) lattice structure. We show that the Fermi-surface reconstruction arising from strong stripe order can suppress the Josephson coupling between adjacent layers by more than an order of magnitude.

I. INTRODUCTION

Stripe order is a fascinating phenomenon in cuprate superconductors. Originally detected in neutron-scattering experiments on La$_{2-x}$Nd$_x$Sr$_2$CuO$_4$, this combination of uni-directional spin and charge order was found in other members of the “214” family of cuprates as well. Remarkably, incommensurate low-energy spin fluctuations, often interpreted as precursors to stripe order, are seen not only in La$_{2-x}$Sr$_2$CuO$_4$, but also in YBa$_2$Cu$_3$O$_{6+δ}$ and Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$. Together with STM measurements, which detected signatures of charge stripes (albeit with substantial disorder) on the surface of Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ and Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$, these findings suggest that the tendency toward stripe order is common to underdoped cuprates.

What is less clear is the role of stripes for superconductivity. A large body of experiments appears consistent with the concept of competing superconducting and magnetic order parameters, including e.g. the magnetic-field enhancement of spin-density wave (SDW) order. However, a few observations also point to a cooperative interplay of SDW and pairing. In La$_{15/8}$Ba$_{1/8}$CuO$_4$, the onset of SDW order upon increasing temperature is accompanied by a significant drop in the in-plane resistivity, while bulk Meissner effect sets in at much lower temperatures. This intermediate-temperature regime of La$_{15/8}$Ba$_{1/8}$CuO$_4$ has been interpreted in terms of fluctuating 2d pairing, without inter-layer phase coherence. A related phenomenon is the suppression of the Josephson plasma resonance seen in the optical-plasmon regime of underdoped cuprates.

II. ORDER PARAMETERS AND MEAN-FIELD MODEL

We start by enumerating the relevant order parameters for a superconducting stripe state. Charge and spin density waves, with wavevectors $\vec{Q}_c$ and $\vec{Q}_s$, are related to expectation values of particle-hole bilinears in the singlet and triplet channel, respectively. For instance, a CDW is characterized by non-zero $F_c(k) = \sum_\sigma \langle c^\dagger_{\vec{k}+\vec{Q}_c,\sigma} c_{\vec{k},\sigma} \rangle$ where $c^\dagger_{\vec{k}+\vec{Q}_c,\sigma}$ creates an electron with momentum $\vec{k}$ and spin $\sigma$. The superconducting condensate can have both a uniform component and a modulated (PDW) component with wavevector $\vec{Q}_p$, such that $\langle c_{\vec{k}+\vec{Q}_c,\sigma} c_{\vec{k},\sigma} \rangle \neq 0$. On symmetry grounds, a collinear SDW will induce a CDW with wavevector $\vec{Q}_c = 2\vec{Q}_s$, a PDW will induce a CDW with $\vec{Q}_c = 2\vec{Q}_p$, and in the presence of a uniform condensate a CDW will induce a PDW with $\vec{Q}_p = \vec{Q}_c$.

In our modelling, we start from two CuO$_2$ layers with homogeneous $d$-wave pairing and then add CDW/SDW modulations. Each layer $i = 1, 2$ is described by a quasi-particle model of electrons moving on a square lattice,
with the Hamiltonian
\[
\mathcal{H}^i = \sum_{k \sigma} (\epsilon_k - \mu) c_{k \sigma}^\dagger c_{k \sigma} + \mathcal{H}_{\text{DW}}^i + \mathcal{H}_p^i, \tag{1}
\]
and the in-plane dispersion \( \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) \) with \( t' = -t/4 \) and \( t'' = t/12 \).

The symmetry-breaking orders are implemented non-selfconsistently at the mean-field level by \( \mathcal{H}_{\text{DW}} \) and \( \mathcal{H}_p \). We restrict our attention to bond-centered stripes of period 4 (8) in the charge (spin) sector which appear most compatible with experiments at doping 1/8,\(^{12} \) The density-wave part \( \mathcal{H}_{\text{DW}} \) is given by
\[
\mathcal{H}_{\text{DW}}^i = \sum_{k \sigma} \Phi_c(k \sigma) = -e^{i \frac{\pi}{2}} \left( \cos(k_x + \frac{\pi}{4}) - \cos(k_y) \right) \delta t,
\]
\[
\Phi_s(k \sigma) = -\sigma \frac{1 + e^{i \frac{\pi}{2}}}{\sqrt{2}} \delta \mu \sigma \tag{2}
\]
where \( \Phi_c^1 = (\pi/2,0), \Phi_c^1 = (3\pi/4,\pi) \), and the \( \Phi_s^2 \) are obtained from \( \Phi_c^1 \) by \( x \leftrightarrow y \). \( \Phi_c \) implements a hopping modulation on the bonds of strength \( \delta t \), resulting in so-called valence-bond stripes.\(^{13,14} \) Such bond-charge modulation, Fig. 1, is compatible with the STM data of Ref. \(^7 \) and implies a strong d-wave component in the form factor \( F \), of the CDW order parameter. The associated collinear spin order, Fig. 1b, is implemented via a spin-dependent chemical potential \( \delta \mu \) in \( \Phi_c \).\(^{15} \)

The pairing part \( \mathcal{H}_p \) is dominated by a uniform \( d_{x^2-y^2} \)-wave pairing mean field \( \Delta_0 \). In addition, a pairing modulation of amplitude \( \delta \Delta \) is assumed along with the CDW, resulting in a pattern of bond pairing amplitudes qualitatively similar to Fig. 1, but with d-wave sign structure.

\[
\mathcal{H}_p^i = \sum_{\vec{k}} \Delta_c(k_{\vec{k} \vec{l} \sigma}) c_{k \vec{k} \vec{l} \sigma}^\dagger c_{-k \vec{l} \vec{k} \sigma} + \Phi_p^1(k_{\vec{k} \vec{l} \sigma}) c_{k \vec{l} \vec{k} \sigma}^\dagger c_{-k \vec{l} \vec{k} \sigma}^\dagger c_{-k \vec{k} \vec{l} \sigma} + \Phi_p^2(k_{\vec{k} \vec{l} \sigma}) c_{k \vec{l} \vec{k} \sigma}^\dagger c_{-k \vec{l} \vec{k} \sigma} + \text{h.c.},
\]
\[
\Delta(k) = \Delta_0 (\cos k_x - \cos k_y),
\]
\[
\Phi_p^1(k) = -e^{i \frac{\pi}{2}} \left( \cos(k_x + \frac{\pi}{4}) + \cos(k_y) \right) \delta \Delta, \tag{3}
\]
and \( \Phi_p^2 \) is obtained from \( \Phi_p^1 \) by \( x \leftrightarrow y \).

### III. INTER-LAYER JOSEPHSON COUPLING

#### A. Inter-layer tunneling

The Hamiltonian of the full system of two adjacent CuO\(_2\) layers is given by
\[
\mathcal{H} = \mathcal{H}^1 + \mathcal{H}^2 + \sum_{k \sigma} \left[ t_{\perp}(\vec{k}) c_{k \sigma}^\dagger c_{-k \sigma} + \text{h.c.} \right] \tag{4}
\]
with \( \mathcal{H}^i \) given in Eq. (1), and the inter-layer hopping matrix element\(^{17} \)
\[
t_{\perp}(\vec{k}) = \frac{t_1}{4} (\cos k_x - \cos k_y)^2. \tag{5}
\]

To calculate the Josephson coupling it is convenient to multiply global phase factors \( \theta \) to the superconducting mean fields \( \Delta_0 \) and \( \delta \Delta \) in layer \( i \). Then, the Josephson coupling measures the inter-plane phase stiffness:
\[
J_J = \frac{1}{2} [ F(\delta \theta = \pi) - F(\delta \theta = 0) ] \tag{6}
\]
where \( F = F^1 + F^2 + \delta F(\delta \theta) \). \( F^i \) is the free energy of the isolated layer \( i \), \( \delta F \) is the inter-layer tunneling contribution to the free energy, and \( \delta \theta \) is the inter-plane phase difference.

Assuming \( t_{\perp} \ll t, \delta F \) can be determined in second-order perturbation theory in \( t_{\perp} \):
\[
\delta F = \frac{1}{\beta} tr \left( \hat{G}^1 \hat{T} \hat{G}^2 \hat{T} \right) = \frac{1}{N} \sum_{\vec{k}} \delta F_{\vec{k}},
\]
\[
\delta F_{\vec{k}} = \frac{1}{\beta} \sum_{\omega_n} t_{\perp}^{\vec{k}} \frac{1}{2} \sum_{\alpha,\beta=0}^{1,2} (-)^{\alpha+\beta} g_{\vec{k} \alpha \beta} g_{\vec{k} \alpha \beta} \tag{7}
\]
where \( \hat{G} \) is the full Green’s operator on layer \( i \). \( \hat{T} \) is the inter-layer tunneling operator from \( t_{\perp} \), \( \beta \) is the inverse temperature, and \( N \) the number of unit cells. The indices \( \alpha, \beta \) denote particle-hole space. Since the stripe directions are orthogonal, we have to consider the full (non-reduced) Brillouin zone (BZ). For a period-4 CDW (period-8 CDW+SDW) in each superconducting layer, the calculation of \( \delta F \) involves the diagonalization of a \( 8 \times 8 \) (16 \times 16) Hamiltonian matrix to construct the Green’s functions required in Eq. (7).

#### B. Results

The numerical calculations have been performed at zero temperature, with parameters \( t = 0.15 \text{ eV}, \Delta_0 = 0.024 \text{ eV}, \) and fixed doping \( x = 1/8 \). For the homogeneous case, this corresponds to \( \mu = -0.126 \text{ eV} \).

Results for \( J_J \) for charge-only stripes as function of the hopping modulation \( \delta t (\delta \Delta = \delta \mu \sigma = 0) \) are shown in Fig. 3a. For large modulation amplitude, the Josephson coupling is seen to be strongly suppressed, e.g. by roughly a factor 10 for \( \delta t = 0.07 \text{ eV} \). A simultaneous

![FIG. 1: Schematic real-space structure of valence-bond stripes at doping 1/8. a) Paramagnetic state with dominant d-wave modulation. b) Additional spin modulation with anti-phase domain walls on hole-rich stripes.](image-url)
modulation in the condensate mean field by $\delta \Delta$ (here chosen to produce similar relative modulation strengths in the resulting bond kinetic energies and pairings) suppresses the Josephson coupling even further, Fig. 2.

Figs. 2c and d show the corresponding evolution of the homogeneous and modulated condensate amplitudes, $\psi_0$ and $\psi_{Q_c}$, calculated from the solution of the mean-field Hamiltonian $H^t$. Here, we define $\psi$ as the sum of the magnitudes of the $s$-wave (on-site), $s_{x^2+y^2}$-wave and $d_{x^2-y^2}$-wave condensates calculated from the real-space pairing amplitudes extracted from the solution of $H^t$ (note that the $s$ and $d_{x^2-y^2}$ representations of the point group mix in the presence of stripe order). A modulated condensate $\psi_{Q_c}$ is always present for $\delta t \neq 0$, but remains small if $\delta \Delta = 0$. In contrast, for $\delta \Delta \propto \delta t$ as in Fig. 2d, $\psi_{Q_c}$ increases and eventually dominates over $\psi_0$. A comparison between the evolution of $J_J$ and $\psi_0$ reveals that in the range of $\delta t$ where $J_J$ drops dramatically, the uniform condensate $\psi_0$ displays a much weaker depletion. This is also true for panels b and d where, at $\delta t \approx 0.08 \text{ eV}$, $J_J$ is reduced by a factor 200 while $\psi_0$ still has half of its original value. From this we conclude that the primary source of the suppression of the Josephson coupling in our calculation is different from that of the PDW proposal by Berg et al., where the layer decoupling is due to the absence of a homogeneous condensate.

Analyzing our results further, we identify the momentum-space mismatch of the Fermi surfaces of the two layers, arising from the orthogonal stripe modulation, as the main source of the suppression of $J_J$. This mismatch is also accompanied by a mismatch of the nodal lines of the superconducting order parameter in the two layers, due to broken rotational symmetry in each layer. These effects can be nicely seen in the momentum-resolved contributions $J_J(\vec{k}) = \delta F^t(\delta \theta = \pi) - \delta F^t(\delta \theta = 0)$ to the Josephson coupling, shown in Fig. 3. In the homogeneous case, the largest contributions to $J_J$ arise near the antinodal points of the (bare) Fermi surface. These contributions are drastically reduced (note the logarithmic intensity scale) with increasing stripe modulation, as a result of the Fermi-surface distortions accompanying the stripe order. For sizeable $\delta \Delta$, the combination of Fermi-surface and order-parameter reconstruction even generates regions in momentum space with $J_J(\vec{k}) < 0$, Fig. 3b. (For $\delta \Delta = 0$, this effect occurs only near the BZ diagonals due to the shift of nodal lines from stripe order, but this has little influence on $J_J$ due to the specific momentum dependence of the inter-layer tunneling.) The imposed pairing modulation $\delta \Delta$ is seen to contribute to the reduction of $J_J$, Fig. 3d.

We now turn to the influence of magnetic SDW order as in Fig. 1b. As shown in Fig. 4a, SDW order alone (with CDW being parasitic only) leads to a moderate suppression of $J_J$. Similarly, SDW order in combination with a CDW suppresses $J_J$ further compared to the non-magnetic case, mainly because of the additional Fermi-surface reconstruction arising from the SDW wavevector. Note that the relative spin orientation between the two layers does not enter the result.

Finally, we link our findings to the experimental situation. Unfortunately, the magnitude of the charge modulation in cuprate stripes is not well known: From re-

FIG. 2: Inter-layer Josephson coupling $J_J$ (a,b) and superconducting condensate amplitudes $\psi_0$ (solid) and $\psi_{Q_c}$ (dashed) (c,d) as functions of the hopping modulation strength $\delta t$, at fixed doping $x = 1/8$ and in the absence of magnetic order. The modulation in the pairing field is $\delta \Delta/\delta t = 0$ (a,c) and 1.3 (b,d). The couplings and condensates are normalized w.r.t. the values of $J_J$ and $\psi_0$ at $\delta t = \delta \Delta = 0$.

FIG. 3: Positive (top) and negative (bottom) momentum-resolved contributions to $J_J$. Each panel shows $|J_J(\vec{k})/t^2_0|$ (see text) as a function of $\vec{k}$ on a logarithmic intensity scale. The modulation strength $\delta t$ is zero in a) and increases from b) to c). The other parameters are as in Fig. 2d. From a) to c) the positive contributions near the antinodal points are reduced, moreover negative contributions appear. Note that the momentum dependence of the inter-layer tunneling [5] suppresses the contributions near the diagonals.
and gives an additional factor 2 suppression of compound.

J 20% reduction of calculation, a modulation of ±δt energies is obtained from ± amplitude in the charge sector of ±dent. From the STM data factor 4, but the quantitative analysis is model dependent. Modulation on the oxygens was concluded to be of order δt ... maximum moment size is 50 factor 90 reduction of J δt with magnetic modulation set by 0.5 (dashed), 1.3 (dotted), and b) antiferromagnetic stripes in cuprates is known reasonably well, at x special).

quasiparticle theory does not account for half filling being Mott physics makes this number less meaningful, as the calculation of ±25% in the bond kinetic energies is obtained from δt = 0.023 eV, which gives a 20% reduction of J (Fig. 2b), while δt = 0.07 eV with a factor 90 reduction of J corresponds to a kinetic-energy modulation of about a factor 10 (here, the neglect of Mott physics makes this number less meaningful, as the quasiparticle theory does not account for half filling being special).

The magnitude of the magnetic order in striped 214 cuprates is known reasonably well, at x = 1/8 the maximum moment size is 50 . . . 60% of that of the undoped compound. In our mean-field calculation, δµ = ±0.07 eV corresponds to a maximum moment of 0.36µB and gives an additional factor 2 suppression of J I, as is the case in 214 cuprates with LTT lattice structure. For realistic stripe modulation strengths, we find that the inter-layer coupling can be easily reduced by an order of magnitude. The primary cause of this reduction is the momentum-space mismatch between the reconstructed Fermi surfaces of adjacent layers, while the depletion of the zero-momentum superconducting condensate (in favor of a modulated one) is secondary. Whether this effect is sufficient to explain the unusual properties of La15/8Ba1/8CuO4 is not yet clear.

IV. CONCLUSIONS

Using a mean-field quasiparticle framework, we have calculated the inter-layer Josephson coupling in superconducting stripe states. We have assumed that the in-plane stripe orientations alternate from layer to layer, as is the case in 214 cuprates with LTT lattice structure. For realistic stripe modulation strengths, we find that the inter-layer coupling can be easily reduced by an order of magnitude. The primary cause of this reduction is the momentum-space mismatch between the reconstructed Fermi surfaces of adjacent layers, while the depletion of the zero-momentum superconducting condensate (in favor of a modulated one) is secondary. Whether this effect is sufficient to explain the unusual properties of La15/8Ba1/8CuO4 is not yet clear.

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1 S. A. Kivelson, I. P. Bindloss, E. Fradkin, V. Oganesyan, J. M. Tranquada, A. Kapitulnik, and C. Howald, Rev. Mod. Phys. 75, 1201 (2003).
2 M. Vojta, Adv. Phys. (in press), preprint arXiv:0901.3145
3 J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature 375, 561 (1995).
4 S. M. Hayden, H. A. Mook, P. Dai, T. G. Perring, and F. Doğan, Nature 429, 531 (2004).
5 V. Hinkov, D. Haug, B. Fauqué, P. Bourges, Y. Sidis, A. Ivanov, C. Bernhard, C. T. Lin, and B. Keimer, Science 319, 597 (2008).
6 G. Xu, G. D. Gu, M. Hücke, B. Fauqué, T. G. Perring, L. P. Regnault, and J. M. Tranquada, Nature Phys. (in press), preprint arXiv:0902.2802.
7 Y. Kohsaka et al., Science 315, 1380 (2007).
8 Q. Li, M. Hücke, G. D. Gu, A. M. Tsvelik, and J. M. Tranquada, Phys. Rev. Lett. 99, 067001 (2007).
9 J. M. Tranquada et al., Phys. Rev. B 78, 174529 (2008).
10 A. A. Schafgans et al., to be published.
11 E. Berg, E. Fradkin, E.-A. Kim, S. A. Kivelson, V. Oganesyan, J. M. Tranquada, and S. C. Zhang, Phys. Rev. Lett. 99, 127003 (2007).
12 E. Berg, E. Fradkin, and S. A. Kivelson, Phys. Rev. B 79, 064515 (2009).
13 M. Vojta and S. Sachdev, Phys. Rev. Lett. 83, 3916 (1999).
14 M. Vojta and O. Rösch, Phys. Rev. B 77, 094504 (2008).
15 A. J. Millis and M. R. Norman, Phys. Rev. B 76, 220503(R) (2007).
16 A. Wollny and M. Vojta, preprint arXiv:0808.1163.
17 O. K. Andersen, A. I. Lichtenstein, O. Jepsen and F. Paulsen, J. Phys. Chem. Solids 56, 1573 (1995).
18 S. Smadici, G. D. Gu, G. A. Sawatzky, D. L. Feng, P. Ab cabamonte, and A. Rusydi, Nat. Phys. 1, 155 (2005).
19 B. Nachumi et al., Phys. Rev. B 58, 8760 (1998).