Motivated by the energetic advantage of achieving coherent enhancement of effective spin-dependent interactions through approximate nesting, we propose specific forms of spin ordering, whose form varies over the Fermi surface, for the cuprate superconductors. Competing “spin-orbit” orderings involving order parameters in spatial $d_{xy}$ and $d_{x^-y^+}$ waves at commensurate and incommensurate wavevectors, phase separated in momentum space, support behavior suggestive of observed phenomena. The $d_{xy}$ spin-orbit fluctuation induces an effective interaction that favors $d_{x^-y^+}$-wave pairing, as required for the observed superconductivity. Anisotropic spin susceptibility is a crucial prediction of our mechanism.

High $T_c$ superconductivity in cuprates has been an outstanding problem in condensed matter physics since it was first discovered in 1986. In the meantime, though no consensus theoretical understanding has developed, several striking features of the phenomenology have emerged clearly. These include the strongly 2-dimensional character of the essentially new physics; its proximity to antiferromagnetic spin ordering; the anomalous character of the normal state, especially in the underdoped region, suggestive of emergent energy gaps; the acute sensitivity of the low-temperature state to doping and impurities; the $d$-wave character of the superconductivity; and the apparent uniqueness or near-uniqueness of cuprate layers in supporting this overall phenomenological profile. On the face of it, several of these features suggest that the origin of these phenomena will involve forms of ordering that involve spin and depend sensitively on the precise form of the lattice and the Fermi surface.

There is a simple heuristic that appears to be broadly consistent with these indications. As is familiar from the BCS theory of superconductivity, the effect of weak attractive interactions can be amplified, and can lead to drastic qualitative effects, if there are many low-energy pairs sharing the same quantum numbers. Correlations among these pairs can then be arranged so that their interactions contribute coherently to lowering the energy. The BCS mechanism of superconductivity involves particle-particle and hole-hole correlations. In this context the existence of low-energy pairs with total momentum zero, arising from time-reversed states with momenta $(\mathbf{k}, -\mathbf{k})$ both near the Fermi surface, is generic. By contrast spin-density-wave ordering, at the level of electron creation and destruction operators, involves particle-hole correlations. In this context one finds that many low-energy pairs sharing a common (lattice) momentum only for specially shaped (“nested”) Fermi surfaces. Since the shape of the Fermi surface changes with doping, one might anticipate that at best a nesting condition would be approximately fulfilled at a specific doping level. Our point of departure is to consider that the Fermi surface is not an end in itself, but a step toward constructing the ground state. If changing the pattern of occupied levels — effectively, engineering the Fermi surface — can encourage favorable coherence factors, it might be favorable to make nesting persist. Realizations of this possibility and the properties of the emergent states will, on the face of it, depend sensitively on details of the interactions, lattice structure, and doping level. Two dimensional antiferromagnets on a square (or nearly square) lattice near half filling, as in cuprate layers, provide an especially favorable area for these ideas.

Proposed Ordering At half filling antiferromagnetic (AF) spin ordering is observed. Electrons in the real materials may well be best described as strongly coupled and the spins as localized, but we shall construct our states heuristically by extrapolation from weak or intermediate coupling, anticipating that universal properties, specifically symmetry breaking patterns, might be successfully inferred. (Also, photoemission experiments [1] can be interpreted as revealing a Fermi surface, even at quite small doping.) In that spirit AF ordering can be regarded as follows. On-site Coulomb repulsion induces, in the crossed channel, an attractive interaction between electrons and holes of opposite spin at momentum transfer $\mathbf{q} = (\pi, \pi)$ (modulo reciprocal lattice vectors). This makes it favorable to deform the effective Fermi surface into a diamond shape, which for half filling nests at $\mathbf{q}$ (see Fig. [14]), and allow the electrons to form spin-triplet particle-hole pairs, according to $\langle c_{\mathbf{k},\pi}^\dagger c_{\mathbf{-k},\pi} \rangle \neq 0$. Here, $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are Pauli matrices, and $c_{\mathbf{k}}$ and $c_{\mathbf{k}}^\dagger$ are electron annihilation and creation operators, with two spin components united into a column: $c_{\mathbf{k}}^\dagger = (c_{\mathbf{k},\uparrow}^\dagger, c_{\mathbf{k},\downarrow}^\dagger)$. At finite doping no ansatz seems so uniquely compelling, but the possibility illustrated in Fig. [14] is suggestive. The free Fermi surface has been deformed in two distinct ways, one operating near to and the other far from the zone diagonals. This geometry supports nesting for orderings with wavevector $\mathbf{q}$ in the off-diagonal region and with wavevectors slightly off $\mathbf{q}$, namely, $\pm \Delta \mathbf{q} = (1 \mp \delta)\mathbf{q}$, along the diagonals. This proposal embodies a new phenomenon, phase separation in momentum space, that might find wider...
deed the nearest-neighbor Coulomb interaction
nonzero \( N_r \). These vanish for finite doping.

Application.

Order parameters with near-uniform s-wave structure do not easily accommodate such phase separation. It is more natural when zeroes of one condensate correspond to maxima of the other. This leads us to propose spin-orbit (SO) orders of the form: 

\[
  d_{2-x^2-y^2} : \langle c_{\mathbf{k}+\pi x}^\dagger \sigma_{\mathbf{k}} \rangle = i\tilde{N}_A \Gamma^A_{\mathbf{k}},
\]

\[
  (k \text{ in off-diagonal})
\]

\[
  d_{xy} : \langle c_{\mathbf{k}+\pm \pi \delta \mathbf{e}_i}^\dagger \sigma_{\mathbf{k}} \rangle = \tilde{N}_B \Gamma^B_{\mathbf{k}} \pm \frac{\pi}{2} \delta \mathbf{e}_j,
\]

(2) \( j = x, y; k \text{ in diagonal} \)

Here \( \tilde{N}_{A,B} \) are constant, real vectors in spin space, and \( \Gamma^A_{\mathbf{k}}, \Gamma^B_{\mathbf{k}} \) are orbital wave basis functions of lattice group \( D_{4h} \), defined by \( \Gamma^A_{\mathbf{k}} \equiv \cos k_x - \cos k_y \) and \( \Gamma^B_{\mathbf{k}} \equiv \sin k_x \sin k_y \). (The lattice constant is set to a unit.) The \( d_{2-x^2-y^2} \) order is purely imaginary, as required by hematicity. Roughly speaking, it describes a state with microscopic spin currents flowing around each plaquette in real space.

The nature of these spin-orbit orderings may be more transparent in real space:

\[
  \langle c_{\mathbf{r}}^\dagger \sigma_{\mathbf{r}'} \rangle = i\tilde{N}_A e^{i\pi \mathbf{r}} \Gamma^A_{\mathbf{r}} + 2\tilde{N}_B e^{i\pi \mathbf{r}} \times [\cos \left( \frac{x+x'}{4} \pi \delta \right) + (x \to y)] \Gamma^B_{\mathbf{r}'}
\]

(3)

where \( \Gamma^A_{\mathbf{r}} = \frac{1}{2} \left[ (\delta_{r',x} + \delta_{r',-x}) - (\hat{x} \to \hat{y}) \right] \) and \( \Gamma^B_{r'} = \frac{1}{2} \left[ \delta_{r',\hat{x}+\hat{y}} - \delta_{r',-\hat{x}+\hat{y}} - \delta_{r',-\hat{x}-\hat{y}} + \delta_{r',\hat{x}-\hat{y}} \right] \). Note that these vanish for \( \mathbf{r} = \mathbf{r}' \).

At mean field level such spin-orbit orderings with nonzero \( N_A \) and \( N_B \) are favored by the nearest and next nearest neighbor Coulomb repulsions, respectively. Indeed the nearest-neighbor Coulomb interaction \( H_V = +V \sum_{(\mathbf{r},\mathbf{r}')} n_{\mathbf{r}} n_{\mathbf{r}'} \) can be transformed to

\[
-\frac{V}{2} \sum_{(\mathbf{r},\mathbf{r}')} \left[ (c_{\mathbf{r}}^\dagger c_{\mathbf{r}}')(c_{\mathbf{r}'}^\dagger c_{\mathbf{r}'}) + (c_{\mathbf{r}}^\dagger \sigma_{\mathbf{r}'} c_{\mathbf{r}})(c_{\mathbf{r}}^\dagger \sigma_{\mathbf{r}'} c_{\mathbf{r}'}) \right]
\]

(4) plus an unimportant term proportional to the density operator. In this form the anticipated electron-hole attraction is manifest. (At this level \( H_V \), with \( V > 0 \), also favors charge-orbit (CO) ordering, known as orbital-antiferromagnetism, staggered flux phase \( \uparrow \), or DDW \( \uparrow \): a non-static version was proposed in \( \uparrow \). We shall not discuss it further here.) Similarly, the next-nearest-neighbor Coulomb interaction favors both \( d_{xy} \) SO and CO orders.

**Phase diagram**

We shall focus on the following competing orders, that we believe play major roles: AF, \( d_{x^2-y^2}-\text{SO} \) and \( d_{xy}-\text{SO} \), and \( d_{x^2-y^2} \)-wave superconducting state (dSC). The two SO orders compete for particle-hole pairing states, plausibly with different outcomes in different domains, whose size depends on overall doping level. This can be understood by reference to Fig. 1b. With increasing density \( x \) of doped holes, the total area of the four triangles along the zone diagonals increases at first while the size of off-diagonal regions shrinks. For sufficient large doping, e.g., \( x = 3 \), the triangles are no long sustainable. This explains the trends of phase transition lines of \( T_{\text{SO}}^{x^2-y^2} \) (for \( d_{x^2-y^2} \)-SO) and \( T_{\text{SO}}^{xy} \) (for \( d_{xy} \)-SO) as functions of doping.

For low doping up to \( x_2 \), there are several competing spin orders (including AF) that are connected by first-order phase transitions. On general grounds, one expects that phase separation (in real space) may occur, plausibly in the form of stripes \( \uparrow \).
Effective Theory

We now propose an effective Lagrangian for the unconventional normal state, based on
the hypothesis of $d_{x^2-y^2}$-SO ordering:

$$L = \sum_r \epsilon_r^\dagger (i\partial_t + \mu)\psi_r - H_0 + V_A \sum_r \phi_r^\dagger \phi_r$$

(5)

where $\phi_r = \frac{1}{\sqrt{N}} \sum_r \Gamma_r A_r \psi_r$, $\hbar c$ is a composite operator, $V_A > 0$ is assumed, and $H_0$ collects the hopping
next-nearest-neighbor Coulomb interaction.

A $d_{x^2-y^2}$-SO ordered state is characterized by a non-vanishing order parameter field $\phi$, corresponding to
the imaginary part of $c_r^\dagger \sigma c_{r'}$, pointing to (say) the 3-direction in spin space,

$$\langle \phi_r^\dagger \rangle = 0, \quad \langle \phi_r^3 \rangle = e^{i\pi \cdot r} |N_A| \neq 0.$$  

(6)

This correlation spontaneously breaks SU(2) spin symmetry down to a U(1) corresponding to spin rotation
about the 3-axis. Two Nambu-Goldstone bosons appear as gapless collective spin excitations, corresponding to
transverse fluctuations of the order parameter field $\phi_r$. We will call them orbital magnons.

We can describe the low energy interactions of these collective modes using an effective Lagrangian. Following
the standard technique, we isolate the Nambu-Goldstone part (two transverse spin fluctuations) in the
electron field. Expressing the electron field as a local SU(2) spin rotation acting on a new fermion $\psi$:

$$c_r = \frac{1 + i \epsilon_{\alpha\beta} \sigma_\alpha \zeta_r \phi_r}{\sqrt{1 + \zeta_r^2}} \psi_r \equiv U_r \psi_r, \quad (\alpha, \beta = 1, 2; \text{ no } 3).$$

(7)

This defines a new fermion $\psi_{r\sigma}$ that carries the full charge and the spin $\sigma$ quantum numbers but does not carry transverse spin. $\zeta_r^{1,2}$ parameterize the slowly-varying orbital magnons. They are given by the 3-component $\phi$ via: $U_r^\dagger \phi \sigma U_r = R^a_\sigma \phi^a$ and $\phi^a = R^a_\sigma (\phi_{x}\mathbf{a} + \phi_{y}\mathbf{b})$ with $a, b = 1, 2, 3$, where $\mathbf{a}$ represents the (gapped) longitudinal spin-orbit fluctuation. With the above transformations, we now have a prescription of deriving an effective Lagrangian for the orbital magnons and new fermions: $L[\psi, \psi^\dagger, \zeta^a, \phi]$ from the Lagrangian [10].

The free part of the effective theory for the $\psi$-fermion is

$$L_\psi = \sum_k \left\{ \psi_k^\dagger \left[ i \partial_t - \epsilon(k) + \mu \right] \psi_k^\dagger + i \Delta_k |\psi_k^\dagger \sigma^3 \psi_k - \text{h.c.} | \right\}$$

(8)

where $\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ and $\Delta_k = \Delta_A(\cos k_x - \cos k_y)$ with $\Delta_A = \frac{1}{2} V_A N_A$. Due to unit cell doubling, the fermion energy spectrum is split into two bands

$$E^\pm_k = \frac{1}{2} (\epsilon_k + \epsilon_{k+\pi}) \pm \sqrt{\epsilon_k^2 + \Delta_k^2},$$

(9)

each being spin up and down degenerate. For weak $d_{x^2-y^2}$-SO order, the Fermi surface of the $E^-$ band is near the diagonals of the Brillouin zone while the Fermi surface of the $E^+$ band is near the off-diagonal region (see Fig. 4). Note that the fermion field $\psi$, appropriate to describing the low-energy excitations, does not carry the full spin quantum numbers of the electron. This is a form of partial spin-charge separation.

**FIG. 3:** The Fermi surface in $d_{x^2-y^2}$-SO state. $E^- = 0$ is shown as the dotted ellipses, inside which all states are empty. $E^+_k = 0$ is shown as the boundaries of the four patches (in dark) which are completely occupied.

The effective theory for $d_{xy}$-SO can be constructed in the same manner from a model Lagrangian similar to [10], with $V_A \rightarrow V_B$ and $\phi_r \rightarrow \phi_r \equiv 2 \sum_r \Gamma_{r-r'} \psi_r^\dagger \sigma c_{r'} + \text{h.c.}$ ($d_{xy}$-SO order parameter). The ordering wavevector is changed from $\pi$ to $Q_{h,v}$.

Origin of $d$-wave Superconductivity

In the effective theory of $d_{xy}$-SO, fermions are coupled to the longitudinal spin-orbit fluctuation $\phi$,

$$H_{\text{int}} = -2V_B \sum_{kq} [\Gamma_{k}^B + \Gamma_{k+q}^B] (\psi_{k}^\dagger \sigma \psi_{k-q}) \phi_q.$$ (10)

Broken spin symmetry implies that the $\phi$ propagator has the form $(\omega^2 - \epsilon_q^2)(\omega^2 + i\gamma_q(\omega, \omega')^{-1})$ with $\gamma_q(\omega)$ having minima at $q = \pm Q_{h,v}$ and the damping rate $\gamma_q(\omega) \rightarrow 0$ as $\omega \rightarrow 0$. Given the coupling [10], we have calculated the effective interaction between fermions induced by the longitudinal SO fluctuation (Fig. 4). In the low energy (static) limit, the spin-singlet component of the Cooper channel interaction is described by the Hamiltonian

$$H_{\text{int}}^{S=0} = \sum_{kp} v_{kp} [\psi_{k}^\dagger \sigma \psi_{k-q}] \phi_q.$$ (11)

where $v_{kp} = 2g_{\phi} V_B^2 \Gamma_{k}^B + \Gamma_{k}^B |\Gamma_{q}^B|^{-1/2} (k-p) > 0$ and the spin indices $\rho, \sigma = \uparrow, \downarrow$. Here $g_{\phi}$ is a positive normalization constant of the SO field. The interaction is repulsive in both s-wave and $d_{xy}$-wave pairing. Note that $v_{kp}$, as function of $k-p$, peaks at the incommensurate wavevectors $\pm Q_{h,v}$ (Fig. 4). By examining a typical superconducting gap equation, $\Delta_{k}^c = -\sum_{q} v_{kp} \Delta_{k-q}^c[(\epsilon_p - \mu)^2 + \Delta_{k-q}^{sc} - 1/2]$, one finds nontrivial solution if $\Delta_{k}^c$ and $\Delta_{k-q}^{sc}$ have opposite sign. By the arguments similar to Ref. [11],
we conclude that the favored superconducting pairing is $d_{x^2-y^2}$-wave. Fermions near $(\pm \pi, 0)$ and $(0, \pm \pi)$ will pair as: $\langle \psi_{k_0} \psi_{-k_0} \rangle \sim \epsilon_{\sigma} \Gamma_{k_0}^{\pm} \neq 0$. The $\psi$-fermion pair condensate is equivalent to an electron pair condensate

$$
\epsilon_{\rho\sigma} \langle \psi_{k\rho} \psi_{\sigma^c} \rangle = \langle \epsilon_{ \rho^c} \Gamma_{k_{\rho}}^{\pm} \psi_{\sigma} \rangle = \epsilon_{\rho\sigma} \langle \epsilon_{\rho^c} \Gamma_{k_{\rho}}^{\pm} \psi_{\sigma} \rangle
$$

for uniform $q$. Thus an exotic normal state can be associated with conventional electron pairing.

The state of $d_{x^2-y^2}$-SO is different. A similar coupling involving the longitudinal SO fluctuation in the $d_{x^2-y^2}$ leads to an effective interaction that disfavors the $d_{x^2-y^2}$-SC pairing.

$d_{xy}$-SO order does not forbid the existence of Fermi nodal points in the dSC state. It splits the quasiparticle energy band around the four triangles along the zone diagonals (Fig. 1), with Fermi surfaces being carved out from the lowest possible band.

**Incommensurate spin excitations** The translational symmetry broken by the SO orderings leads to multibands of orbital magnons in a reduced zone scheme, each having the degeneracy of two transverse spin modes. The orbital magnons associated with the $d_{xy}$-SO are gapless at the four incommensurate momenta $\pm \mathbf{Q}_h$ and $\pm \mathbf{Q}_o$. With coexisting $d_{xy}$ and $d_{x^2-y^2}$ SO orders, there will be another band that is gapless at $\pi$. Dynamical spin-spin correlation functions are affected by particle-hole pair mixing with two orbital magnon channels. Combining magnons from $d_{xy}$ and $d_{x^2-y^2}$ can yield two branches of spin excitation resonance at finite energies, one dispersing upward and another downward from momentum $\pi$. The two branches cross at $\pi$, with zero gap energy. This structure seems qualitatively consistent with the inelastic neutron scattering experiments in YBCO (e.g. as in D. Reznik, et al. [12] and references therein; see also [13]). A full investigation is in progress.

**Anisotropic spin susceptibility** The state of SO ordering has $\langle \mathbf{S}_r \rangle = 0$, so the static correlation of local spins does not exhibit conventional long range order. A straightforward exercise confirms $\langle \mathbf{S}_r \cdot \mathbf{S}_{r'} \rangle = -\frac{\mu_B^2}{\hbar^2} (c_{\sigma}^d c_{\sigma'}^d)^2 + \frac{1}{2} (c_{\sigma}^d \sigma c_{\sigma'}^d)^2 \to 0$ as $|\mathbf{r} - \mathbf{r}'| \to \infty$.

We have calculated the uniform, static spin susceptibility for the $d_{x^2-y^2}$-SO state, using the effective Lagrangian $\mathcal{L}_\text{SO}$. We find that the susceptibility is anisotropic,

$$
\chi^{ab} = -\mu_B^2 \int \frac{d^3k}{(2\pi)^3} f'(E^+_k) + f'(E^-_k)
\times \left[ 1 + 2\left( \Delta^a_{\parallel} \Delta^b_{\parallel} - \delta^{ab} \Delta^2_k \right)/(E^+_k - E^-_k) \right]
$$

where $f(E) = \frac{1}{e^{\beta E} + 1}$, $f'(E) = \partial f/\partial E$, and the ordering direction is assumed arbitrary (cf. Eq. (3)). Fig. 5 shows the anisotropy of susceptibility predicted by the mean field theory (without corrections due to orbital magnon scatterings). Measurement of $\chi^{||}$ and $\chi^\perp$ could therefore provide important tests of our proposals. The result is quite different from the AF state, for which $\chi^{||} < \chi^\perp$.

**FIG. 4** Effective attraction between spin-broken electrons induced by longitudinal spin-orbit fluctuation $g$. The arrows indicate spin. The free electron fermi surface is plotted for simplicity. The off-diagonal regions for dSC or $d_{x^2-y^2}$-SO need to not change qualitatively from the state of $d_{xy}$-SO.

**FIG. 5** Anisotropic spin susceptibility in the $d_{x^2-y^2}$-SO state at different temperatures. Energy units are chosen such that $t = 1$. Other parameters: $t' = -0.45$ and $\mu = -1.2$ (chemical potential). Integration was performed numerically using a mesh of 500 × 500 in each quarter of the Brillouin zone. $\chi^{||}$ and $\chi^\perp$ denote the susceptibilities parallel or perpendicular to the direction of the $d_{x^2-y^2}$ SO.

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