Bond order in two-dimensional metals with antiferromagnetic exchange interactions

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Les Diablerets
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Resistivity \( \sim \rho_0 + AT^\alpha \)

BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\)

The electron spin polarization obeys

\[ \langle \tilde{S}(\mathbf{r}, \tau) \rangle = \varphi(\mathbf{r}, \tau)e^{i \mathbf{K} \cdot \mathbf{r}} \]

where \( \mathbf{K} \) is the ordering wavevector.
Metal with “large” Fermi surface
Fermi surface + antiferromagnetism

“Hot” spots
Fermi surface + antiferromagnetism

Electron and hole pockets in antiferromagnetic phase with antiferromagnetic order parameter $\langle \phi \rangle \neq 0$
Fermi surface + antiferromagnetism

Metal with electron and hole pockets
\[ \langle \tilde{\varphi} \rangle \neq 0 \]

Metal with “large” Fermi surface
\[ \langle \tilde{\varphi} \rangle = 0 \]
\[ \langle c_{k\alpha}^\dagger c_{-k\beta} \rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y) \]

d-wave superconductor: particle-particle pairing at and near hot spots, with sign-changing pairing amplitude
Sign-problem-free Quantum Monte Carlo for antiferromagnetism in metals

\[ \tilde{P}_{\pm}(\tilde{r}_{\text{max}}) \]

\[ L = 10 \]
\[ L = 12 \]
\[ L = 14 \]

\[ s/d \text{ pairing amplitudes } P_+/P_- \]
as a function of the tuning parameter \( r \)

Fluctuating Fermi pockets

Quantum Critical

Large Fermi surface

Underlying SDW ordering quantum critical point in *metal* at $x = x_m$

Spin density wave (SDW)
Fermi surface + antiferromagnetism

Quantum Critical

Large Fermi surface

Fluctuating, paired Fermi pockets

D-wave superconductor

Spin density wave (SDW)

QCP for the onset of SDW order is actually within a superconductor
Resistivity
\sim \rho_0 + AT^\alpha


Magnetic-field-induced charge-stripe order in the high-temperature superconductor YBa$_2$Cu$_3$O$_y$

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8 September 2011 | Vol 477 | Nature | 191
1. Pseudospin symmetry between $d$-wave superconductivity and bond order

*Continuum field theory with exact pseudospin symmetry*

2. Approximate pseudospin symmetry on the lattice $t$-$J$ model

*Pseudogap and bond order in the underdoped cuprates*
1. Pseudospin symmetry between $d$-wave superconductivity and bond order

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*Pseudogap and bond order in the underdoped cuprates*
Pseudospin symmetry of the exchange interaction

\[ H_J = \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

with \( \vec{S}_i = \frac{1}{2} c_{i \alpha}^\dagger \vec{\sigma}_{\alpha \beta} c_{i \beta} \) is the antiferromagnetic exchange interaction. Introduce the Nambu spinor

\[
\Psi_{i \uparrow} = \begin{pmatrix} c_{i \uparrow} \\ c_{i \downarrow} \end{pmatrix}, \quad \Psi_{i \downarrow} = \begin{pmatrix} c_{i \downarrow} \\ -c_{i \uparrow} \end{pmatrix}
\]

Then we can write

\[ H_J = \frac{1}{8} \sum_{i<j} J_{ij} \left( \Psi_{i \alpha}^\dagger \vec{\sigma}_{\alpha \beta} \Psi_{i \beta} \right) \cdot \left( \Psi_{j \gamma}^\dagger \vec{\sigma}_{\gamma \delta} \Psi_{i \delta} \right) \]

which is invariant under independent SU(2) pseudospin transformations on each site

\[ \Psi_{i \alpha} \rightarrow U_i \Psi_{i \alpha} \]

This pseudospin (gauge) symmetry is important in classifying spin liquid ground states of \( H_J \).

Pseudospin symmetry of the exchange interaction

\[ H_{tJ} = - \sum_{i,j} t_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

with \( \vec{S}_i = \frac{1}{2} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta} \) is the antiferromagnetic exchange interaction. Introduce the Nambu spinor

\[ \Psi_{i\uparrow} = \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}, \quad \Psi_{i\downarrow} = \begin{pmatrix} c_{i\downarrow}^{\dagger} \\ -c_{i\uparrow} \end{pmatrix} \]

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\[ \Psi_{i\alpha} \rightarrow U_i \Psi_{i\alpha} \]

This pseudospin (gauge) symmetry is important in classifying spin liquid ground states of \( H_J \). It is fully broken by the electron hopping \( t_{ij} \) but does have remnant consequences in doped spin liquid states.

Pseudospin symmetry of the exchange interaction

$$H_{tJ} = -\sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

with $\vec{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$ is the antiferromagnetic exchange interaction. Introduce the Nambu spinor

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Then we can write

$$H_J = \frac{1}{8} \sum_{i<j} J_{ij} \left( \Psi_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \Psi_{i\beta} \right) \cdot \left( \Psi_{j\gamma}^\dagger \vec{\sigma}_{\gamma\delta} \Psi_{i\delta} \right)$$

which is invariant under independent SU(2) pseudospin transformations on each site

$$\Psi_{i\alpha} \rightarrow U_i \Psi_{i\alpha}$$

We will start with the Néel state, and find important consequences of the pseudospin symmetry in metals with antiferromagnetic correlations.
Metal with electron and hole pockets

$\langle \varphi \rangle \neq 0$

Metal with “large” Fermi surface

$\langle \varphi \rangle = 0$

Fermi surface + antiferromagnetism
Fermi surface + antiferromagnetism

Metal with "large" Fermi surface

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Rest of the talk

Tuesday, May 14, 13
Fermi surface + antiferromagnetism

“Hot” spots
Fermi surface + antiferromagnetism

Low energy theory for critical point near hot spots
Fermi surface + antiferromagnetism

Low energy theory for critical point near hot spots
\[ S = \int d^2 r d\tau \left[ \psi_{1\alpha}^\dagger (\partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \right. \\
+ \frac{1}{2} (\nabla_r \phi)^2 + \frac{s}{2} \phi^2 + \frac{u}{4} \phi^4 - \lambda \phi \cdot \left( \psi_{1\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \right] \]

This low-energy theory is invariant under independent SU(2) pseudospin rotations on each pair of hot-spots: there is a global $SU(2) \times SU(2) \times SU(2) \times SU(2)$ pseudospin symmetry.
\[ \langle c_{k\alpha}^\dagger c_{-k\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y) \]

d-wave superconductor: particle-particle pairing at and near hot spots, with sign-changing pairing amplitude
Incommensurate d-wave bond order: particle-hole pairing at \textit{and near} hot spots, with sign-changing pairing amplitude.

After pseudospin rotation on \textit{half} the hot-spots.

\[ \left\langle c_{k-\mathbf{Q}/2,\alpha} \hat{c}_{k+\mathbf{Q}/2,\alpha} \right\rangle = \Delta_{\mathbf{Q}} (\cos k_x - \cos k_y) \]

\( \mathbf{Q} \) is ‘2\( k_F \)’ wavevector.

Incommensurate $d$-wave bond order

M. A. Metlitski and S. Sachdev, 

$$\langle c_{k-Q/2,\alpha}^{\dagger} c_{k+Q/2,\alpha} \rangle = \Delta_Q (\cos k_x - \cos k_y)$$
Incommensurate $d$-wave bond order

\[
\left\langle c_{k-Q/2,\alpha}^{\dag} c_{k+Q/2,\alpha} \right\rangle = \Delta_Q (\cos k_x - \cos k_y)
\]
Incommensurate \textit{d}-wave bond order

Consider modulation in an off-site “density” like variable at sites $\mathbf{r}_i$ and $\mathbf{r}_j$

$$\langle c_{i\alpha}^\dagger c_{j\alpha} \rangle \sim \left[ \sum_k \Delta_{\mathbf{Q}}(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2}$$

The wavevector $\mathbf{Q}$ is associated with a modulation in the average coordinate $(\mathbf{r}_i + \mathbf{r}_j)/2$: this determines the wavevector of the neutron/X-ray scattering peak.

The usual charge-density-wave has only $c_s \neq 0$, and so the density wave is non-zero only if $\mathbf{r}_i = \mathbf{r}_j$. The bond-ordered state has only $c_d$: in this case the density wave is non-zero only if $\mathbf{r}_i$ and $\mathbf{r}_j$ are nearest neighbors.

Incommensurate \textit{d}-wave bond order relative co-ord.

average co-ord.
Incommensurate $d$-wave bond order

Consider modulation in an off-site “density” like variable at sites $r_i$ and $r_j$

$$
\langle c_i^{\dagger} c_{j\alpha} \rangle \sim \left[ \sum_k \Delta_Q(k) e^{ik \cdot (r_i - r_j)} \right] e^{iQ \cdot (r_i + r_j)/2}
$$

The wavevector $Q$ is associated with a modulation in the average co-ordinate $(r_i + r_j)/2$: this determines the wavevector of the neutron/X-ray scattering peak.

The interesting part is the dependence on the relative co-ordinate $r_i - r_j$. Assuming time-reversal, the order parameter $\Delta_Q(k)$ can always be expanded as

$$
\Delta_Q(k) = c_s + c_s'(\cos k_x + \cos k_y) + c_d(\cos k_x - \cos k_y) + \ldots
$$

Tuesday, May 14, 13
Incommensurate $d$-wave bond order

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$$\langle c_{i\alpha}^\dagger c_{j\alpha} \rangle \sim \left[ \sum_k \Delta_Q(k) e^{i k \cdot (r_i - r_j)} \right] e^{i Q \cdot (r_i + r_j) / 2}$$

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The usual charge-density-wave has only $c_s \neq 0$, and so the density wave is non-zero only if $r_i = r_j$. 

Tuesday, May 14, 13
Incommensurate $d$-wave bond order

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\Delta_Q(k) = c_s + c_s'(\cos k_x + \cos k_y) + c_d(\cos k_x - \cos k_y) + \ldots
$$

The usual charge-density-wave has only $c_s \neq 0$, and so the density wave is non-zero only if $\mathbf{r}_i = \mathbf{r}_j$.

The bond-ordered state has only $c_d$ non-zero: in this case the density wave is non-zero only if $\mathbf{r}_i$ and $\mathbf{r}_j$ are nearest neighbors.
Incommensurate \(d\)-wave bond order

\[
\langle c_{r\alpha}^\dagger c_{s\alpha} \rangle = \sum_{Q} \sum_{k} e^{iQ \cdot (r+s)/2} e^{-i k \cdot (r-s)} \langle c_{k-Q/2,\alpha}^\dagger c_{k+Q/2,\alpha} \rangle
\]

where \(Q\) extends over \(Q = (\pm Q_0, \pm Q_0)\) with \(Q_0 = 2\pi/(7.3)\) and

\[
\langle c_{k-Q/2,\alpha}^\dagger c_{k+Q/2,\alpha} \rangle = \Delta_Q \left( \cos k_x - \cos k_y \right)
\]

Note \(\langle c_{r\alpha}^\dagger c_{s\alpha} \rangle\) is non-zero only when \(r, s\) are nearest neighbors.
1. Pseudospin symmetry between $d$-wave superconductivity and bond order

*Continuum field theory with exact pseudospin symmetry*

2. Approximate pseudospin symmetry on the lattice $t$-$J$ model

*Pseudogap and bond order in the underdoped cuprates*
1. Pseudospin symmetry between $d$-wave superconductivity and bond order

Continuum field theory with exact pseudospin symmetry

2. Approximate pseudospin symmetry on the lattice $t$-$J$ model

Pseudogap and bond order in the underdoped cuprates
\[ H_{tJ} = - \sum_{i,j} t_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet charge order \( (\Delta_Q(k)) \):

\[ H_{MF} = - \sum_{i,j} t_{ij} c_{i\alpha}^{\dagger} c_{j\alpha} + \sum_{k,Q} \Delta_Q(k) c_{k+Q/2,\alpha}^{\dagger} c_{k-Q/2,\alpha} \]
\[ H_{tJ} = - \sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet charge order \( \Delta_Q(k) \):

\[ H_{MF} = - \sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{k,Q} \Delta_Q(k) c_{k+Q/2,\alpha}^\dagger c_{k-Q/2,\alpha} \]

Expanding the free energy in powers of the order parameters we obtain

\[ F = F_0 + \sum_{k,Q} \Delta_Q^*(k) \mathcal{M}_Q(k, k') \Delta_Q(k') \]

We compute the eigenvalues, \( 1 + \lambda_Q \), and eigenfunctions, \( \Delta_Q(k) \) of the kernel \( \mathcal{M}_Q(k, k') \)
Charge-ordering eigenvalue $\lambda_Q/J_0$. 

S. Sachdev and R. La Placa, arXiv:1303.2114
Minimum at $Q = (Q_m, Q_m)$ with

$$
\Delta_Q(k) = 0.993(\cos k_x - \cos k_y) \\
-0.069(\cos(2k_x) - \cos(2k_y)) \\
-0.009(\cos k_x - \cos k_y) \\
\times \sqrt{8} \sin k_x \sin k_y
$$

**Incommensurate $d$-wave bond order**

Charge-ordering eigenvalue $\lambda_Q / J_0$. 

S. Sachdev and R. La Placa, arXiv:1303.2114
Remarkable agreement between the value of $Q_m$ from Hartree-Fock in a metal with short-range *incommensurate* spin correlations, and the value of $Q_0$ from hot spots of *commensurate* antiferromagnetism.
Minimum at $Q = (Q_m, Q_m)$ with

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Incommensurate $d$-wave bond order

Charge-ordering eigenvalue $\lambda_Q/J_0$. 

S. Sachdev and R. La Placa, arXiv:1303.2114
Charge-ordering eigenvalue $\lambda_Q / J_0$. 
\[ Q = (Q_m, 0) \] with

\[ \Delta Q(k) = 0.963(\cos k_x - \cos k_y) \\
-0.231 \\
-0.067(\cos(2k_x) - \cos(2k_y)) \\
-0.044(\cos k_x + \cos k_y) \\
-0.046(\cos(2k_x) + \cos(2k_y)) \]

**Incommensurate**

\( d^+_s \) -wave bond order

Charge-ordering eigenvalue \( \lambda_Q / J_0 \).

S. Sachdev and R. La Placa, arXiv:1303.2114
Remarkable agreement between the value of $Q_m$ from Hartree-Fock in a metal with short-range *incommensurate* spin correlations, and the value of $Q_0$ from hot spots of *commensurate* antiferromagnetism.
\[ \mathbf{Q} = (Q_m, 0) \text{ with} \]

\[
\Delta_{Q}(k) = \begin{align*}
0.963(\cos k_x - \cos k_y) \\
-0.231 \\
-0.067(\cos(2k_x) - \cos(2k_y)) \\
-0.044(\cos k_x + \cos k_y) \\
-0.046(\cos(2k_x) + \cos(2k_y))
\end{align*}
\]

Incommensurate \( d_{+s} \)-wave bond order

Charge-ordering eigenvalue \( \lambda_{\mathbf{Q}} / J_0 \).
Charge-ordering eigenvalue $\lambda_Q / J_0$. 

S. Sachdev and R. La Placa, arXiv:1303.2114
Charge-ordering eigenvalue $\lambda_Q / J_0$. 

$Q = (\pi, \pi)$ with 

$$\Delta_Q(k) = i(\sin k_x - \sin k_y)$$

Orbital currents
Charge-ordering eigenvalue $\lambda_Q / J_0$. 
Charge-ordering eigenvalue $\lambda_Q/J_0$. 

$Q = (0, 0)$ with

$$\Delta_Q(k) = \cos k_x - \cos k_y$$

Ising-nematic order
Incommensurate $d$-wave bond order

High $T$ pseudogap: Fluctuating composite order parameter of nearly degenerate $d$-wave pairing and incommensurate $d$-wave bond order. (Approximate) SU(2) symmetry of composite order prevents long-range order $T > 0$.

Incommensurate \textit{d}-wave bond order

Our computations show that the charge order is predominantly \textit{d}-wave also at this $\mathbf{Q}$. This $\mathbf{Q}$ is preferred in computations of bond order within the superconducting phase.

S. Sachdev and R. La Placa, arXiv:1303.2114
Evidence bond order is along (1,0), (0,1) directions in low $T$ superconducting phase

We point out that unidirectional bond-centered charge-density-wave states in cuprates involve electronic order in both $s$- and $d$-wave channels, with nonlocal Coulomb repulsion suppressing the $s$-wave component.
Incommensurate $d$-wave bond order

Our computations show that the charge order is predominantly $d$-wave also at this $Q$.

This $Q$ is preferred in computations of bond order within the superconducting phase.

S. Sachdev and R. La Placa, arXiv:1303.2114
An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates

Y. Kohsaka,1 C. Taylor,1 K. Fujita,1,2 A. Schmidt,1 C. Lupien,3 T. Hanaguri,4 M. Azuma,5 M. Takano,5 H. Eisaki,6 H. Takagi,2,4 S. Uchida,2,7 J. C. Davis1,8*

9 MARCH 2007 VOL 315 SCIENCE
Distinct Charge Orders in the Planes and Chains of Ortho-III-Ordered YBa$_2$Cu$_3$O$_{6+\delta}$ Superconductors Identified by Resonant Elastic X-ray Scattering


PRL 109, 167001 (2012)

Moreover, the energy dependence of the CDW order in the planes is shown to result from a spatial modulation of energies of the Cu 2p to 3d$_{x^2-y^2}$ transition, similar to stripe-ordered 214 cuprates.

These energy shifts are interpreted as a spatial modulation of the electronic structure and may point to a valence-bond-solid interpretation of the stripe phase.
Electron spectral function

\[ \text{Im} G(k, \omega + i\eta) \quad \text{log Im} G(k, \omega + i\eta) \]

\[
\left\langle c_{k-Q/2,\alpha}^\dagger c_{k+Q/2,\alpha} \right\rangle \propto \Delta_Q(k) = \begin{cases} 
\Delta_s + \Delta_d(\cos k_x - \cos k_y) & , \quad Q = (\pm Q_0, 0) \\
\Delta_s - \Delta_d(\cos k_x - \cos k_y) & , \quad Q = (0, \pm Q_0) 
\end{cases}
\]

with \( \Delta_s/\Delta_d = -0.234 \).

S. Sachdev and R. La Placa, arXiv:1303.2114
Antiferromagnetism in metals and the high temperature superconductors

Antiferromagnetic quantum criticality leads to d-wave superconductivity (supported by sign-problem-free Monte Carlo simulations)
Antiferromagnetic quantum criticality leads to d-wave superconductivity (supported by sign-problem-free Monte Carlo simulations)

Metals with antiferromagnetic spin correlations have nearly degenerate instabilities: to d-wave superconductivity, and to a charge density wave with a d-wave form factor. This is a promising explanation of the pseudogap regime.