Innovations in Strongly Correlated Electronic Systems: School and Workshop

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Interplay between superconductivity, magnetism and nematic order in the iron pnictides - Part II

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Interplay between superconductivity, magnetism, and nematic order in the iron pnictides

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Iron pnictides: typical phase diagram

- How these different ordered states interact with each other?
- Is there a primary degree of freedom?
Outline

1. **The superconducting state (Lecture I)**
   - unconventional superconductivity

2. **The magnetic state (Lectures I & II)**
   - itinerant or localized?

3. **The nematic state (Lecture II)**
   - a new electronic phase that emerges from magnetism and triggers structural and orbital order

4. **Competing orders (Lecture II)**
   - competition between SC, magnetism, and nematics
Iron pnictides: magnetic order

• How to describe the magnetically ordered state?

➢ *itinerant or localized picture?*

\[ Q_1 = (\pi, 0) \quad Q_2 = (0, \pi) \]
Digression: localized and itinerant magnetism

- **Localized limit**: strong Coulomb repulsion
  - Hubbard model at half-filling
    \[ H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i \sigma}^+ c_{j \sigma} + c_{j \sigma}^+ c_{i \sigma} \right) + U \sum_i n_{i \uparrow} n_{i \downarrow} \quad t \ll U \]
  - perturbation theory: energy gain due to virtual hopping

![Diagram showing virtual hopping between sites in a lattice configuration.](image-url)
Digression: localized and itinerant magnetism

- **Localized limit**: strong Coulomb repulsion

- Effective Heisenberg Hamiltonian

\[ H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \]

\[ J = \frac{t^2}{U} \]

Energy gain comes from the kinetic term.
Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

  the ground state of non-interacting electrons is non-polarized
Digression: localized and itinerant magnetism

- *Itinerant limit:* to simplify, first consider the case of a ferromagnet (Stoner model)

  forcing a polarized state costs kinetic energy

\[ \Delta E_{\text{kin}} \approx \rho_F^{-1} \]
**Digression: localized and itinerant magnetism**

- **Itinerant limit**: to simplify, first consider the case of a ferromagnet (Stoner model)

  however, when the electrons are polarized, they pay less local Coulomb energy due to Pauli principle

\[
\Delta E_{\text{kin}} \approx \rho_F^{-1}
\]

\[
\Delta E_{\text{Coul}} \approx -U
\]
Digression: localized and itinerant magnetism

- *Itinerant limit*: to simplify, first consider the case of a ferromagnet (Stoner model)

**Stoner criterion for ferromagnetism:**

\[ \Delta E_{\text{kin}} + \Delta E_{\text{Coul}} = 0 \implies U \rho_F = 1 \]

[Diagram showing energy levels and spin polarization]

energy gain comes from the Coulomb repulsion term
Digression: localized and itinerant magnetism

- **Itinerant limit**: to simplify, first consider the case of a ferromagnet (Stoner model)

  - Hubbard model in the limit of small $U \ll t$

  $$H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i \sigma}^+ c_{j \sigma} + c_{j \sigma}^+ c_{i \sigma} \right) + U \sum_i n_{i \uparrow} n_{i \downarrow}$$

  - Coulomb repulsion enhances uniform susceptibility (RPA)

  $$\chi = \frac{\chi_{\text{Pauli}}}{1 - U \rho_F}$$

  favored near van-Hove singularity
Digression: localized and itinerant magnetism

- **Itinerant limit**: Stoner condition can be generalized for the case of a magnetically ordered state with ordering vector $\mathbf{Q}$

  \[
  \chi(Q) = \frac{\chi_0(Q)}{1 - U_Q \chi_0(Q)}
  \]

- Instability usually assisted by nesting: $\varepsilon(k + Q) = -\varepsilon(k)$

  \[
  \chi_0(Q) = -T \sum_{k, \omega_n} G(k, \omega_n) G(k + Q, \omega_n)
  \]

  \[
  \chi_0(Q) = \sum_k \frac{\text{tanh}(\varepsilon_k / 2T) - \text{tanh}(\varepsilon_{k+Q} / 2T)}{2(\varepsilon_k - \varepsilon_{k+Q})}
  \]
Digression: localized and itinerant magnetism

• *Itinerant limit*: Stoner condition can be generalized for the case of a magnetically ordered state with ordering vector \( Q \)

\[
\chi(Q) = \frac{\chi_0(Q)}{1 - U_Q \chi_0(Q)}
\]

• Instability usually assisted by nesting: \( \varepsilon(k + Q) = -\varepsilon(k) \)

\[
\chi_0(Q) = \rho_F \int_0^\Lambda \frac{d\varepsilon}{\varepsilon} \tanh\left(\frac{\varepsilon}{2T}\right)
\]

same equation as BCS!

\[
\chi_0(Q) \propto \rho_F \log\left(\frac{\Lambda}{T}\right)
\]

\[
T_{\text{mag}} \propto \Lambda \exp\left(-\frac{1}{U_Q \rho_F}\right)
\]
Iron pnictides: magnetic order

- from itinerant to localized magnetism
  - several known systems are in the intermediate coupling regime (such as elemental Ni and Fe)

- since the ground state of the iron pnictides is a metal, we choose here the itinerant limit as our starting point
Iron pnictides: magnetic order

- from itinerant to localized magnetism
  - several known systems are in the intermediate coupling regime (such as elemental Ni and Fe)
  - optical conductivity: transfer of spectral weight from the Drude peak to the mid-infrared region

Nakajima et al, PRB (2010)
Iron pnictides: itinerant approach to SDW

- Fermi surface of the iron pnictides:
Iron pnictides: itinerant approach to SDW

- Bands have good nesting features (but not perfect)

\[ \chi_0(Q) \propto \log \frac{E_F}{\max(T, \delta_{\text{nesting}})} \]
Iron pnictides: itinerant approach to SDW

- Bands have good nesting features (but not perfect)

\[ \chi_0(Q) \propto \log \frac{E_F}{\max(T, \delta_{\text{nesting}})} \]

Electronic interaction above threshold leads to a magnetically ordered state (SDW) with ordering vector \( Q_i \)

\[ \chi(Q) = \frac{\chi_0(Q)}{1 - U \chi_0(Q)} \]
Theory of the itinerant magnetic state

Two simultaneous spin-density wave instabilities:

\[ S = M_1 e^{iQ_1 \cdot r} + M_2 e^{iQ_2 \cdot r} \]

Microscopic calculation of the magnetic free energy by integrating out the electrons (Hertz-Millis approach)
derivation of the magnetic free energy

step 1: start with purely multi-band electronic interactions

\[ H_0 = \sum_{k} \varepsilon_{0,k} \quad d_{k \alpha}^{+} d_{k \alpha} + \sum_{i,k} \varepsilon_{i,k} \quad c_{i,k \alpha}^{+} c_{i,k \alpha} \]

electrons in the hole pocket  
electrons in the electron pockets

\[ H_{\text{int}} = \sum_{i,k} u_1 d_{k_1 \alpha}^{+} d_{k_3 \alpha} c_{i,k_2 \beta}^{+} c_{i,k_4 \beta} + \sum_{i,k} u_2 d_{k_1 \alpha}^{+} c_{i,k_2 \beta}^{+} d_{k_4 \beta} c_{i,k_3 \alpha} \]

\[ + \sum_{i,k} \frac{u_3}{2} d_{k_1 \alpha}^{+} d_{k_2 \beta}^{+} c_{i,k_4 \beta} c_{i,k_3 \alpha} + (\cdots) \]

equivalent to multi-orbital Hubbard model
derivation of the magnetic free energy

step 2: project the interactions in charge channel and spin channel

use the identity between Kronecker deltas and Pauli matrices:

$$\delta_{\alpha\beta}\delta_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\gamma\beta} - \vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta}$$

$$H_{\text{int}} = -u_s \sum_{q,i} \left( d_{k+q\alpha}^+ \vec{\sigma}_{\alpha\beta} c_{i,k\beta} \right) \cdot \left( c_{i,p-q\gamma}^+ \vec{\sigma}_{\gamma\delta} d_{i,p\delta} \right)$$

$$u_s = u_1 + u_3$$
derivation of the magnetic free energy

**step 3: introduce collective variables for the two SDW instabilities**

\[ Z \propto \int dc_k df_k \exp(-H/T) \]

\[ \mathbf{M}_i \propto \sum_k \langle d^+_k \bar{\sigma}_{\alpha\beta} c_{i,k\beta} \rangle \]

use the Hubbard-Stratonovich transformation:

\[
\exp\left[u_s \left( d^+_{k+q\alpha} \bar{\sigma}_{\alpha\beta} c_{i,k\beta} \right) \cdot \left( c^+_{i,p-q\gamma} \bar{\sigma}_{\gamma\delta} d_{p\delta} \right) \right] =
\]

\[
\int d\mathbf{M}_i \exp\left[ -\frac{u_s}{2} \mathbf{M}_{i,q} \cdot \mathbf{M}_{i,-q} + \mathbf{M}_{i,q} \cdot \left( c^+_{i,k-q\alpha} \bar{\sigma}_{\alpha\beta} d_{k\beta} \right) + \mathbf{M}_{i,-q} \cdot \left( d^+_{k+q\alpha} \bar{\sigma}_{\alpha\beta} c_{i,k\beta} \right) \right]
\]
derivation of the magnetic free energy

step 4: introduce “Nambu operators” (simplify the notation)

\[ \hat{\Psi}_k^+ = \left( d_{k\uparrow}^+ \quad d_{k\downarrow}^+ \quad c_{1,k\uparrow}^+ \quad c_{1,k\downarrow}^+ \quad c_{2,k\uparrow}^+ \quad c_{2,k\downarrow}^+ \right) \]

\[ Z \propto \int d\hat{\Psi}_k \, dM_i \, \exp(-F[\hat{\Psi}_k, M_i]) \]

\[ F = -\int \hat{\Psi}_k^+ \hat{G}^{-1}_k \hat{\Psi}_k + \frac{2}{u_s} \int M_i^2 \]

\[ \hat{G}_k^{-1} = \begin{pmatrix} G_{0,k}^{-1} & M_1 \cdot \sigma & M_2 \cdot \sigma \\ M_1 \cdot \sigma & G_{1,k}^{-1} & 0 \\ M_2 \cdot \sigma & 0 & G_{2,k}^{-1} \end{pmatrix} \]

with: \[ G_{j,k}^{-1} = i\omega_n - \varepsilon_{j,k} \quad k = (\omega_n, \mathbf{k}) \]
derivation of the magnetic free energy

step 5: “integrate out” the electrons (Gaussian integration)

\[
\hat{G}_k^{-1} = \left(\hat{G}_k^0\right)^{-1} - \hat{V}
\]

\[
\left(\hat{G}_k^0\right)^{-1} = \begin{pmatrix}
G_{0,k}^{-1} & 0 & 0 \\
0 & G_{1,k}^{-1} & 0 \\
0 & 0 & G_{2,k}^{-1}
\end{pmatrix}
\]

\[
\hat{V} = \begin{pmatrix}
0 & M_1 \cdot \sigma & M_2 \cdot \sigma \\
M_1 \cdot \sigma & 0 & 0 \\
M_2 \cdot \sigma & 0 & 0
\end{pmatrix}
\]

\[
Z \propto \int dM_i \exp \left( - F_{\text{mag}} [M_i] \right)
\]

with the effective action:

\[
F_{\text{mag}} = - \text{Tr} \log \left( 1 - \hat{G}_k^0 \hat{V} \right) + \frac{2}{u_s} \int M_i^2
\]
derivation of the magnetic free energy

step 6: do perturbation theory

\[
\left(\hat{G}_k^0\right)^{-1} = \begin{pmatrix}
G_{0,k}^{-1} & 0 & 0 \\
0 & G_{1,k}^{-1} & 0 \\
0 & 0 & G_{2,k}^{-1}
\end{pmatrix}
\]

\[
\hat{V} = -\begin{pmatrix}
0 & M_1 \cdot \sigma & M_2 \cdot \sigma \\
M_1 \cdot \sigma & 0 & 0 \\
M_2 \cdot \sigma & 0 & 0
\end{pmatrix}
\]

\[
F_{\text{mag}} \approx \frac{1}{2} \text{Tr}\left(\hat{G}_k^0 \hat{V}\right)^2 + \frac{1}{4} \text{Tr}\left(\hat{G}_k^0 \hat{V}\right)^4 + \frac{2}{u_{s,x,i}} \int M_i^2 + O(M_i^6)
\]

we obtain the Ginzburg-Landau derived from the microscopic model!

\[
F_{\text{mag}} = \frac{a}{2} \left(M_1^2 + M_2^2\right) + \frac{u_{11}}{4} M_1^4 + \frac{u_{22}}{4} M_2^4 + \frac{u_{12}}{4} M_1^2 M_2^2 + (\cdots)
\]
Theory of the itinerant magnetic state

For perfect nesting:

\[ F_{\text{mag}} = \frac{a}{2} \left( M_1^2 + M_2^2 \right) + \frac{u}{4} \left( M_1^2 + M_2^2 \right)^2 \]

\[
\begin{align*}
a &= \frac{2}{u_s} + 2 \int_k G_{\Gamma,k} G_{X,k} \\
u &= \frac{1}{2} \int_k G_{\Gamma,k}^2 \left( G_{X,k} + G_{Y,k} \right)^2
\end{align*}
\]

\[ G_{j,k}^{-1} = i \omega_n - \varepsilon_{j,k} \]
Theory of the itinerant magnetic state

For perfect nesting:

\[ F_{\text{mag}} = \frac{a}{2} \left( M_1^2 + M_2^2 \right) + \frac{u}{4} \left( M_1^2 + M_2^2 \right)^2 \]

mean-field solution:

\[ \frac{\partial F_{\text{mag}}}{\partial M_i} = 0 \]

\[ M_1^2 + M_2^2 = \text{constant} \]
Theory of the itinerant magnetic state

For perfect nesting:

\[ Q_1 = (\pi, 0) \]
\[ Q_2 = (0, \pi) \]

\[ M_1 = 0 \land M_2 \neq 0 \]
\[ M_1 \neq 0 \land M_2 = 0 \]

\[ M_1 \perp M_2 \]
\[ M_1 \parallel M_2 \]
Theory of the itinerant magnetic state

Away from perfect nesting:

\[ F_{\text{mag}} = -\frac{a}{2} (M_1^2 + M_2^2) + \frac{u}{4} (M_1^2 + M_2^2)^2 - \frac{g}{4} (M_1^2 - M_2^2)^2 \]

\[ g = -\frac{1}{2} \sum_k G_{\Gamma,k}^2 \left( G_{X,k} - G_{Y,k} \right)^2 > 0 \]
Theory of the itinerant magnetic state

mean-field solution: \[ \frac{\partial F_{\text{mag}}}{\partial M_i} = 0 \]

\[ F_{\text{mag}} = \frac{a}{2} (M_1^2 + M_2^2) + \frac{u}{4} (M_1^2 + M_2^2)^2 - \frac{g}{4} (M_1^2 - M_2^2)^2 \]

\begin{align*}
M_1 &\neq 0 \\
M_2 &= 0
\end{align*}

\begin{align*}
M_1 &= 0 \\
M_2 &\neq 0
\end{align*}

OR
Iron pnictides: itinerant magnetism

- Solving the mean-field microscopic gap equations, we can also obtain the doping-dependence of the magnetization and transition temperature.

**good agreement with experimental measurements**

RMF et al, PRB (2010)
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   • competition between SC, magnetism, and nematics
Why nematics???
Iron pnictides: normal state properties

magnetic and structural transition lines follow closely each other

SDW

Ort.

SC

correlated phases!
Iron pnictides: normal state properties

orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

Tanatar et al, PRB (2010)
resistivity anisotropy cannot be attributed only to the orthorhombic distortion

\[
\frac{a - b}{a + b} \approx 0.01
\]  

maximum orthorhombic distortion

\[
\frac{\rho_b}{\rho_a} \approx 2
\]  

maximum resistivity anisotropy

resistivity anisotropy cannot be attributed only to the orthorhombic distortion

Iron pnictides: normal state properties

- resistivity
- optical spectrum
- orbital polarization
- density of states...

orthorhombic state displays strong anisotropies that cannot be attributed to the lattice distortion only

underlying electronic order that spontaneously breaks tetragonal symmetry: nematic phase
Nematic order: qualitative argument

- Symmetry breaking in a regular antiferromagnet:

$$O(3)$$ (spin-rotational) symmetry breaking

disordered state

magnetic state
Symmetry breaking in the striped magnetic state of the iron pnictides:

- **Nematic order:** qualitative argument

\[ O(3) \times \mathbb{Z}_2 \]

Doubly-degenerate ground states

Symmetry breaking

\[ (0, \pi) \]

\[ (\pi, 0) \]
Nematic order: qualitative argument

- A state that breaks $Z_2$ symmetry but remains paramagnetic

$\langle S_i \cdot S_{i+x} \rangle = -\langle S_i \cdot S_{i+y} \rangle$

$\langle S_i \rangle \neq 0$
Itinerant approach to the nematic state

To consider the possibility of a nematic state, we need to include fluctuations

\[ F_{\text{mag}} = \chi_{\text{mag}}^{-1}(q)(M_1^2 + M_2^2) + \frac{u}{2}(M_1^2 + M_2^2)^2 - \frac{g}{2}(M_1^2 - M_2^2)^2 \]

\[ Z = \int dM_i \exp(-F_{\text{mag}}[M_i]) \]

Hubbard-Stratonovich transformation: auxiliary fields

\[ \exp\left[-\frac{u}{2}(M_1^2 + M_2^2)^2\right] = \int d\psi \exp\left[-\psi(M_1^2 + M_2^2) + \frac{\psi^2}{2u}\right] \]

\[ \psi \propto M_1^2 + M_2^2 \quad \text{Gaussian fluctuations} \]
Itinerant approach to the nematic state

To consider the possibility of a nematic state, we need to include fluctuations

\[ F_{\text{mag}} = \chi_{\text{mag}}^{-1}(q)(M_1^2 + M_2^2) + \frac{u}{2}(M_1^2 + M_2^2)^2 - \frac{g}{2}(M_1^2 - M_2^2)^2 \]

\[ Z = \int dM_i \exp(-F_{\text{mag}}[M_i]) \]

Hubbard-Stratonovich transformation: auxiliary fields

\[ \exp\left[\frac{g}{2}(M_1^2 - M_2^2)^2\right] = \int d\phi \exp\left[\phi(M_1^2 - M_2^2) - \frac{\phi^2}{2g}\right] \]

\[ \phi \propto M_1^2 - M_2^2 \quad \text{nematic order parameter} \]
Itinerant approach to the nematic state

To consider the possibility of a nematic state, we need to include fluctuations

\[ Z = \int dM_i \, d\psi \, d\varphi \exp\left(-F_{\text{mag}}[M_i, \psi, \varphi]\right) \]

Now the partition function is quadratic in the magnetic degrees of freedom, which can be integrated out analytically

\[ F_{\text{mag}} = \chi^{-1}_{\text{mag}}(q) \left( M_1^2 + M_2^2 \right) + \psi \left( M_1^2 + M_2^2 \right) - \varphi \left( M_1^2 - M_2^2 \right) - \frac{\psi^2}{2u} + \frac{\varphi^2}{2g} \]
Itinerant approach to the nematic state

To consider the possibility of a nematic state, we need to include fluctuations

\[ Z = \int d\psi \ d\phi \exp(-F_{\text{eff}}[\psi, \phi]) \]

Now the partition function is quadratic in the magnetic degrees of freedom, which can be integrated out analytically

\[ F_{\text{eff}}[\psi, \phi] = \int_q \left( \frac{\phi^2}{2g} - \frac{\psi^2}{2u} \right) + \frac{3}{2} \text{tr} \log \left[ (\chi_{\text{mag}}^{-1} + \psi)^2 - \phi^2 \right] \]
Itinerant approach to the nematic state

To consider the possibility of a nematic state, we need to include fluctuations

\[
F_{\text{eff}}[\psi, \varphi] = \int_q \left( \frac{\varphi^2}{2g} - \frac{\psi^2}{2u} \right) + \frac{3}{2} \text{tr} \log \left[ \left( \chi_{\text{mag}}^{-1} + \psi \right)^2 - \varphi^2 \right]
\]

Saddle-point approximation gives two non-linear coupled equations:

\[
\begin{align*}
\frac{\partial F_{\text{eff}}}{\partial \psi} &= 0 \\
\frac{\partial F_{\text{eff}}}{\partial \varphi} &= 0
\end{align*}
\]

\[
\Rightarrow \begin{align*}
\psi &= \frac{u}{2} \int_q \left[ \frac{1}{\chi_{\text{mag}}^{-1}(q) + \psi - \varphi} + \frac{1}{\chi_{\text{mag}}^{-1}(q) + \psi + \varphi} \right] \\
\varphi &= \frac{g}{2} \int_q \left[ \frac{1}{\chi_{\text{mag}}^{-1}(q) + \psi - \varphi} - \frac{1}{\chi_{\text{mag}}^{-1}(q) + \psi + \varphi} \right]
\end{align*}
\]
Itinerant approach to the nematic state

Equation of state for the nematic order parameter:

\[ \varphi^3 = \varphi \left[ g \int \chi_{\text{mag}}^2(q) - 1 \right] \]

\( \varphi \neq 0 \) solution already in the paramagnetic phase, when the magnetic susceptibility is large enough

\[ \langle M_1^2 \rangle \neq \langle M_2^2 \rangle \]

magnetic fluctuations \( \rightarrow \) nematic order
Itinerant approach to the nematic state

- Magnetic fluctuations become stronger around one of the ordering vectors in the paramagnetic phase

\[ Q_2 = (0, \pi) \]
\[ Q_1 = (\pi, 0) \]

\( x \) and \( y \) directions become inequivalent:

**tetragonal symmetry breaking**

*(structural transition driven by magnetic fluctuations)*
Enhanced magnetic fluctuations due to nematic order

- Strong increase of the magnetic correlation length at the nematic transition

\[ \xi^{-2} \rightarrow \xi^{-2} - \varphi \]
Enhanced magnetic fluctuations due to nematic order

- NMR reveals the enhancement of magnetic fluctuations at the nematic transition

$RMF, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)$

$RMF & Schmalian, SUST (2012)$
Phase diagrams for the magnetic and structural transitions

magnetic fluctuations give rise to nematic order

enhances transitions naturally follow each other
magneto-structural phase diagram: itinerant approach

Temperature

BaFe$_2$As$_2$
(under pressure)

BaFe$_2$As$_2$
(electron-doped)

nematic

magnetic

(nematic coupling)$^{-1}$
Nematic transition triggers orbital order

- Distinct Fermi pockets have different orbital content

DFT calculation

simplified 2-orbital model
Nematic transition triggers orbital order

- Nematic order leads to different onsite energies for the $d_{xz}$ and $d_{yz}$ orbitals: *ferro-orbital order*

$$H_{\text{orb}} = - \sum_{\mathbf{k}} \Delta_{\text{orb}} \left( c_{X,\mathbf{k} \alpha}^+ c_{X,\mathbf{k} \alpha} - c_{Y,\mathbf{k} \alpha}^+ c_{Y,\mathbf{k} \alpha} \right) \Rightarrow \langle \Delta_{\text{orb}} \rangle \propto \langle \varphi \rangle$$

RMF, Chubukov, Eremin, Knolle, Schmalian, PRB (2012)
Nematic transition triggers orbital order

- polarized ARPES observes orbital splitting in BaFe$_2$As$_2$

Yi et al, PNAS (2011)

- so far, this is the only mechanism that, starting from an itinerant microscopic model, gives orbital order in the absence of long-range magnetic order
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   • competition between SC, magnetism, and nematics
Competing phases: experimental observations

- Neutron diffraction: suppression of the magnetic order parameter below $T_c$
Competing phases: experimental observations

- X-ray diffraction: suppression of the **orthorhombic order parameter** below $T_c$

_Nandi,..., RMF et al, PRL (2010)
Competition between SDW and SC: coexistence or phase separation?

second-order transition
(microscopic coexistence)

first-order transition
(phase separation)
• In some conventional superconductors, magnetism can only coexist with superconductivity when the two phenomena involve different electrons.
In some conventional superconductors, magnetism can only coexist with superconductivity when the two phenomena involve different electrons. Here, the electrons that cause magnetism are the same that cause superconductivity.
Competition between SDW and SC: phenomenological model

\[ F[M, \Delta] = \frac{a_m}{2} M^2 + \frac{u_m}{4} M^4 + \frac{a_s}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2 \]

Minimization with respect to \( M \) leads to

\[ a_m + u_m M^2 = -\gamma |\Delta|^2 \]

and we obtain the effective free energy

\[ F[\Delta] = -\frac{a_m^2}{4u_m} + \frac{a_s}{2} \left( 1 - \frac{a_m \gamma}{a_s u_m} \right) |\Delta|^2 + \frac{u_s}{4} \left( 1 - \frac{\gamma^2}{u_s u_m} \right) |\Delta|^4 \]

<0 : first-order

>0 : second-order
Competitive between SDW and SC: phenomenological model

\[
F[M, \Delta] = \frac{a_m}{2} M^2 + \frac{u_m}{4} M^4 + \frac{a_s}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2
\]

\[
g = \frac{\gamma}{\sqrt{u_m u_s}} - 1
\]

Kosterlitz et al, PRB (1976)

coexistence phase separation
Competition between SDW and SC: phenomenological model

\[ F[M, \Delta] = \frac{a_m}{2} M^2 + \frac{u_m}{4} M^4 + \frac{a_s}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2 \]

\[ g < 0 \]

\[ g > 0 \]

Graphs showing the phase diagram of \( \text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_2\text{As}_2 \) and \( \text{LaFeAsO}_{1-x}\text{F}_x \) with respect to temperature and nominal F content.
Competition between SDW and SC: phenomenological model

How to describe this competition from a microscopic model?

\[ g < 0 \quad g > 0 \]
Competition between SDW and SC: microscopic model

- Hertz-Millis approach to the two-band model

\[
H = H_0 + H_{\text{SDW}} + H_{\text{SC}}
\]

\[
\begin{align*}
H_0 &= \sum_{\mathbf{k},\sigma} \left( \varepsilon_{1,\mathbf{k}+\mathbf{Q}} - \mu \right) c_{\mathbf{k}+\mathbf{Q}\sigma}^+ c_{\mathbf{k}+\mathbf{Q}\sigma}^- + \sum_{\mathbf{k},\sigma} \left( \varepsilon_{2,\mathbf{k}} - \mu \right) d_{\mathbf{k}\sigma}^+ d_{\mathbf{k}\sigma}^- \\
H_{\text{SDW}} &= -\sum_{\mathbf{k},\sigma} \sigma M \left( c_{\mathbf{k}+\mathbf{q}\sigma}^+ d_{\mathbf{k}\sigma}^- + d_{\mathbf{k}\sigma}^+ c_{\mathbf{k}+\mathbf{q}\sigma}^- \right) \\
H_{\text{SC}} &= -\sum_{\mathbf{k}+\mathbf{Q}} \Delta_1 \left( c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ + c_{-\mathbf{k}\downarrow}^+ c_{\mathbf{k}\uparrow}^- \right) - \sum_{\mathbf{k}} \Delta_2 \left( d_{\mathbf{k}\uparrow}^+ d_{-\mathbf{k}\downarrow}^+ + d_{-\mathbf{k}\downarrow}^+ d_{\mathbf{k}\uparrow}^- \right)
\end{align*}
\]
We can then **derive** the Ginzburg-Landau coefficients

\[
F[M, \Delta] = \frac{a_m}{2} M^2 + \frac{u_m}{4} M^4 + \frac{a_s}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2
\]

\[
g = \frac{\gamma}{\sqrt{u_m u_s}} - 1
\]
• We can then derive the Ginzburg-Landau coefficients

\[ G_i(k, \omega_n) = \frac{1}{i\omega_n - \xi_{i,k}} \]
We can then derive the Ginzburg-Landau coefficients

\[ G_i(k, \omega_n) = \frac{1}{i \omega_n - \xi_{i,k}} \]
Competition between SDW and SC: microscopic model

- Strength of the competition term depends on the symmetry of the superconducting state

\[ \gamma_{12} \propto M^2 |\Delta|^2 \cos \theta \]

\[ \begin{align*}
\theta &= 0 \\
& \text{s}^{++} \text{ state} \\
\theta &= \pi \\
& \text{s}^{+-} \text{ state}
\end{align*} \]

RMF and Schmalian, PRB (2010)
Vorontsov, Vavilov, and Chubukov, PRB (2010)
Coexistence between AFM and SC: perfect nesting

- For perfect nesting:

\[ F = \frac{a}{2} \left( |\Delta|^2 + M^2 \right) + \frac{u}{4} \left( |\Delta|^2 + M^2 \right)^2 + g \frac{u}{2} |\Delta|^2 M^2 \]

\[ g = \frac{1 + \cos \theta}{2} \]

- \( s^{-+} \) state: \( g = 0 \) (borderline)

- \( s^{++} \) state: \( g = 1 \) (phase separation)
Coexistence between AFM and SC: perfect nesting

- For perfect nesting:

\[ F = \frac{a}{2} \left( |\Delta|^2 + M^2 \right) + \frac{u}{4} \left( |\Delta|^2 + M^2 \right)^2 + g u |\Delta|^2 M^2 \]

\[ s^{+-} \text{ state: } g = 0 \]
\[ s^{++} \text{ state: } g = 1 \]

Borderline

Phase separation

Note that \( g = 0 \implies \text{emergent SO(5) symmetry} \)

\[ \tilde{N} = (\text{Re} \Delta, \text{Im} \Delta, M) \]

Podolsky et al, EPL (2009)
Competition between SDW and SC: coexistence

Perfect nesting: \[ g = \frac{1 + \cos \theta}{2} \]
Competition between SDW and SC: coexistence

- $s^{++}$ cannot coexist with magnetism
- $s^{+-}$ may or may not coexist
Observation of microscopic coexistence in some iron arsenides rules out the possibility of an $S^{++}$ state

Phase sensitive STM measurements confirm that the SC state is $s^{+-}$

Competition between superconductivity and nematicity

• Due to its magnetic origin, nematicity also competes (indirectly) with superconductivity

$$\varphi^3 = \varphi \left[ g \int \chi_{\text{mag}}^2 (\mathbf{q}) - 1 \right]$$

- magnetic fluctuations suppressed by superconductivity

$$F[M, \Delta] = \frac{a_m}{2} M^2 + \frac{a_s}{4} M^4 + \frac{u_m}{2} |\Delta|^2 + \frac{u_s}{4} |\Delta|^4 + \frac{\gamma}{2} |\Delta|^2 M^2$$

$$\tilde{\chi}_{\text{mag}}^{-1} = \chi_{\text{mag}}^{-1} + \gamma \Delta^2$$
Due to its magnetic origin, nematicity also competes (indirectly) with superconductivity.

\[ \varphi^3 = \varphi \left[ g \int \chi_{\text{mag}}^2 (q) - 1 \right] \]

*even in the absence of long-range magnetic order*
Competition between superconductivity and nematicity

- X-ray diffraction: experimental observation of the suppression of the orthorhombic distortion below $T_c$

*Nandi,..., RMF et al, PRL (2010)*
magnetic phase

superconducting phase

nematic phase

• structural order
• orbital order

competing order

emergent order

fluctuations

indirect competition