Nematic and Magnetic orders in Fe-based Superconductors

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Discussion with B. Halperin
Nematic and Magnetic orders in Fe-based Superconductors

Outline:

1. Ising nematic and magnetic transitions at finite temperature

2. Quantum nematic and magnetic transitions at finite doping and pressure

3. Special system, FeTe, FeSe

4. Quantum nematic order with SC, experimental observables
Common phenomena:

1, SDW and structure distortion in almost all samples: neutron scattering...

2, Lattice distortion and SDW do not always occur at the same temperature: $T_{c1,ld} \sim 150\text{K}$, $T_{c2,sdw} \sim 137\text{K}$, $T_{c1} \geq T_{c2}$

3, both lattice distortion and SDW suppressed by doping and pressure

First goal: unified picture of lattice distortion and SDW
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Simplest toy model for SDW: Abrahams, Si, 2008

\[ H = \sum_{\langle i, j \rangle} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\langle\langle i, j \rangle\rangle} J_2 \vec{S}_i \cdot \vec{S}_j. \]

Critical point: \( J_1 = 2J_2 \). If \( J_1 < 2J_2 \), Classical ground state is \( S^2 \otimes S^2 \). Fluctuations will lead to GSM (moduli space) \( S^2 \otimes \mathbb{Z}_2 \).
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Natural Ising quantity: \( \sigma = \vec{\phi}_1 \cdot \vec{\phi}_2 \)

Has the same symmetry as the lattice distortion!
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\[ \sigma = \vec{\phi}_1 \cdot \vec{\phi}_2 \]

Can deform fermi surface
\textit{i.e. nematic order}

Energy scales:

In pure 2d system, Ising order transition at \( T_{Ising} \sim J_{in} \), and there is no SDW O(3) transition.

In weakly coupled 2d layers, \( T_{sdw} \sim J_{in} / \ln(J_{in}/J_{\perp}) \)
The Ising order parameter breaks reflection symmetry along

\[ x = \pm y \]

Lattice distortion may be driven by magnetism

Straightforward conclusion:

Nature of transitions: two separate transitions, one 3D Ising, one 3D O(3); if one single transition, first order.

PRB, 78, 020501, 2008, Cenke Xu et.al.
Similar story, Chen Fang et.al.

P. Dai et.al.
Mazin et.al.
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LaFeAsO

0806.3878 McGuire et.al.

MFe$_2$As$_2$

0807.1077 Zhao et.al.

0806.1043 Krellner et.al.
SDW and lattice distortion are intimately related.

Question: Why are 1111 and 122 samples different?

\[ F_{GL} = (\nabla \mu \sigma)^2 + r_\sigma \sigma^2 + \sum_{a=1}^{2} (\nabla \mu \Phi_a)^2 + r_\phi |\Phi_a|^2 + \hat{u} \sigma \Phi_1 \cdot \Phi_2 + \cdots \]

\[ r = r_\sigma + r_\phi \]
\[ \Delta r = r_\phi - r_\sigma \]
$r$ is tuned by temperature, how about $\Delta r$?

Recall equations:

\[ r = r_\sigma + r_\phi \quad \Delta r = r_\phi - r_\sigma \]

\[ T_{ising} \sim J_{in} \]

\[ T_{sdw} \sim J_{in}/ \ln(J_{in}/J_\perp) \]

$\Delta r$ is tuned by the anisotropy of the system.
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122 materials are much more isotropic than 1111 materials

Evidence 1: Strong $z$ direction electron dispersion for 122 samples from LDA calculation, APRES;

![122 vs 1111](image)

0806.3526 Ma et.al. 0806.1869 Mazin et.al.

Evidence 2: almost isotropic $H_{c2}$ for 122s. 0807.3137 Yuan et.al.

$$H_{c2,z}/H_{c2,xy} \sim 1.5 - 2 \text{ for 122s, } \sim 7 - 8 \text{ for 1111s.}$$

Evidence 3: Strong $z$ direction spin wave dispersion for 122s, from inelastic neutron, $J_z/J_{in} \sim 1/20 - 1/10$. 0808.2455 Zhao et.al.
Electron doped 122s:

After electron doping, the transition splits into two second order transitions. It turns out, electron doping rapidly suppresses z direction spin coupling. \[0904.3775\] Harriger, et.al.

Can we measure anisotropic spin correlation in the window?
Nature of the transitions:

The lattice distortion transition is mean field like, while the SDW transition is a nontrivial WF universality class in 3D

Mean field is only applicable to dimensions higher than 4, where is the extra dimension? Why SDW unaffected?
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Soft lattice coupled with 3D Ising transition:

\[ g\sigma(\partial_x u_y + \partial_y u_x) + K (\vec{\nabla} \cdot \vec{u})^2 + \cdots \]

Integrating out displacement vector, obtaining angle dependent quadratic term:

\[ F_{\theta,\phi} \sim f(\theta, \phi)|\sigma_{k,\theta,\phi}|^2 \sim 10K \]

Expanded at the minima:

\[ F = \int q^2 dq d\theta d\phi (q^2 + \chi \theta^2 + r)|\sigma_{q,\theta}|^2 + O(\sigma^4) \]

\[ F = \int dq_x dq_y dq_z (q_x^2 + q_y^2 + q_z^2 + \frac{q_x^2 + q_y^2}{q_z^2})|\sigma_q|^2 + O(\sigma^4) \]

Equivalent to 5 dimension! → mean field transition!
Soft lattice coupled with 3D O(3) transition (SDW):

\[ |\vec{\phi}|^2 (\partial_x u_x + \partial_y u_y + \lambda' \partial_z u_z) \]

Only generates irrelevant terms at the 3D O(3) transition, because \( \alpha < 0 \) for 3D O(3) or XY transition.

The lattice elasticity will leave the SDW transition unaffected, but drive the Ising transition more mean field like.

Yang Qi, Cenke Xu, arXiv:0812.0016
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2. Quantum phase transitions at zero temperature:
Without the charge sectors, the transitions in the spin sector will have dynamical exponent $z=1$. By coupling to the Fermi pockets, the exponent $z$ may be modified.
The exponent $z$ depends on the overlapping between hole and electron pockets, after translation by the SDW wave-vector:

Phase diagram tuned by pressure and doping:
Transitions at large doping, low pressure

\[
L = \sum_{i=1}^{2} \sum_{\mu=\tau,x,y} \partial_{\mu} \vec{\phi}_i \cdot \partial_{\mu} \vec{\phi}_i - r \vec{\phi}_i^2 + u|\vec{\phi}_i|^4 + L', \\
L' = \gamma \vec{\phi}_1 \partial_x \partial_y \cdot \vec{\phi}_2 + \gamma_1 |\vec{\phi}_1|^2 |\vec{\phi}_2|^2 - \alpha (\vec{\phi}_1 \cdot \vec{\phi}_2)^2,
\]

Estimate the scaling dimensions at the 3D O(3) transition

\[
\Delta[\gamma] = D - (2 + D - 2 + \eta) = -\eta. \\
\Delta[\gamma_1] = D - 2\Delta[|\vec{\phi}|^2] = D - 2(D - \frac{1}{\nu}) = \frac{2}{\nu} - D,
\]

\[
\Delta[\alpha] \approx 0.581
\]

One obvious relevant perturbation, can split the transition to one SDW transition and one Ising nematic transition
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Ising nematic transition without SC

Ordered at (0, 0), ferromagnetic type, decay with \( ph \)-pair

\[
\text{Im}[\chi(\omega, q)] \sim \int \frac{d^2 k}{(2\pi)^2} [f(\epsilon_{k+q}) - f(\epsilon_k)] \delta(\omega - \epsilon_{k+q} + \epsilon_k) \\
\times |\langle k|\Phi_q|k+q\rangle|^2 \sim c_0 \frac{\omega}{q}.
\]

\[
L = \Phi_{-q}(\frac{|\omega|}{c_0 q} + c_1 q^2 + r)\Phi_q + \cdots
\]

\[
C_u \sim T^d/z = T^{2/3},
\]

\[
T_{c1} \sim \delta x^{z/(d-2+z)} = \delta x,
\]

\[
\rho \sim T^{(d+2)/z} = T^{4/3}.
\]

*PRB, 64, 195109, 2001, V. Oganesyan et.al.*

*PRB, 78, 020501, 2008, C. Xu et.al.*
The exponent $z$ depends on the overlapping between hole and electron pockets, after translation by the SDW wave-vector:

Phase diagram tuned by pressure and doping:
The exponent $z$ depends on the overlapping between hole and electron pockets, after translation by the SDW wave-vector:

Phase diagram tuned by pressure and doping:
Transitions at low doping, large pressure

\[ L = \sum_{i=a,b} \left| \omega \right| \left| \Phi_i \right|^2 + c^2(k_x^2 + r k_y^2)\left| \Phi_a \right|^2 + c^2(k_y^2 + r k_x^2)\left| \Phi_b \right|^2 \]

\[ + A \left| \Phi_i \right|^4 + B(\Phi_a \cdot \Phi_b) + C\left| \Phi_a \right|^2\left| \Phi_b \right|^2 \]

\[ \Phi_{a,b} = \Phi_1 \pm \Phi_2 \]

Perturbative RG equation around a \( z = d = 2 \) fixed point:

\[ \frac{dA}{d\ln l} = -22A^2 - \frac{1}{2}B^2 - \frac{3}{2}C^2 - BC, \]

\[ \frac{dB}{d\ln l} = -5\alpha B^2 - 8AB - 8\alpha BC, \]

\[ \frac{dC}{d\ln l} = -\alpha B^2 - 4AB - 20AC - 4\alpha C^2. \]

Extremely weak run-away flow, relevant only very close to critical point

Cut-off: \(~50K\)
Special multicritical point

\[ Q = 2k_f \text{ decay rate} \]

\[ \frac{|\omega|}{\sqrt{|q_x|}} + \frac{|\omega|}{\sqrt{|q_y|}} \]

Naively, \( z = 5/2 \), but singular term generated:

\[ |\phi|^{5/2} \]

No longer a mean field solution

Similar: nematic-smectic transition, K. Sun et.al. 2008

Phase diagram tuned by pressure and doping:

\( x_c = 7.6\% \)
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Global Phase diagram of 1111

For 122, more 3d, more mean field like, less splitting

Yang Qi, Cenke Xu, arXiv:0812.0016
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The 11 family: FeTe

4-sublattice Neel order

Shiliang Li, et.al. 2008

Lattice distortion:
Tetragonal to monoclinic
(in contrast to orthorhombic)
The 11 family: FeTe

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Shiliang Li, et.al. 2008

Lattice distortion:

Tetragonal to monoclinic (in contrast to orthorhombic)
Lattice symmetry guarantees that reversing the direction of the spins on any two sublattices simultaneously will not change the energy.

There are in total two independent Ising quantities defined.

Richer phase diagrams!

$S^2 \times Z_2 \times Z_2$

In contrast to $S^2 \times Z_2$

Commensurate v.s. incommensurate order, both observed.

Cenke Xu, Jiangping Hu, arXiv:0903.4477

Wei Bao, et.al. 2008
Commensurate v.s. incommensurate order, both observed.

Wei Bao, *et al.* 2008
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Quantum transition inside the superconductor:

![Graph showing temperature vs. x for SDW and SC phases](image)

![Graph showing Tc onset vs. nominal composition of F](image)

![Graph showing Tc onset at different T](image)

![Graph showing Tc onset at different temperature](image)
Why s±-wave ??

1, Approach 1: starting with Hubbard model, numerical RG, Fa Wang et.al.

1, Approach 2: starting with $t$-$J_1$-$J_2$ model, K. Seo et.al.

\[
J_1 \vec{S} \cdot \vec{S} + J_2 \vec{S} \cdot \vec{S} \sim \sum_{k,k'} V_{k,k'} c_{\alpha,k,\uparrow}^\dagger c_{\alpha,-k,\downarrow}^\dagger c_{\alpha,-k',\downarrow} c_{\alpha,k',\uparrow}
\]

\[
V_{k,k'} = -\frac{2J_1}{N} \sum_\pm (\cos k_x \pm \cos k_y)(\cos k'_x \pm \cos k'_y)
\]

\[
-\frac{8J_2}{N} (\cos k_x \cos k_y \cos k'_x \cos k'_y + \sin k_x \sin k_y \sin k'_x \sin k'_y)
\]
**Nematic and Magnetic orders in Fe-based Superconductors**

**Do SDW and SC compete with each other?**

Direct calculations: \[ \kappa |\Delta|^2 |\phi|^2 \]

SDW competes with d-wave pairing, but not s±-wave; nematic order always competes with SC.
Superconductor (partially) gaps out the fermi surface, if the SC is $s$-wave, the low energy, long wavelength nature of the spin sector transition is unaffected, $z = 1$.

$d$-wave SC, the nematic order parameter couple with the nodal particle, and deform the location of the nodes

\[\sigma = 1\]

\[\sigma = -1\]
Effective low energy theory for nodal particles: Dirac fermions E. Kim et.al.

\[
L = L_\Psi + L_\phi + L_{\Psi\phi},
\]

\[
L_\Psi = \sum_{a=1}^{N_f} \Psi_1^\dagger_a (\partial_\tau - iv_f \partial_x \tau^z - iv_\Delta \partial_y \tau^x) \Psi_1^a + \Psi_2^\dagger_a (\partial_\tau - iv_f \partial_y \tau^z - iv_\Delta \partial_x \tau^x) \Psi_2^a,
\]

\[
L_\phi = \frac{1}{2} (\partial_\tau \phi)^2 + \frac{c^2}{2} (\nabla \phi)^2 + \frac{r}{2} \phi^2 + \frac{u_0}{4!} \phi^4,
\]

\[
L_{\Psi\phi} = \lambda_0 \phi \sum_{a=1}^{N_f} (\Psi_1^\dagger_a \tau^x \Psi_1^a + \Psi_2^\dagger_a \tau^x \Psi_2^a).
\]

Quantum fluctuation makes the velocity energy dependent, fixed point: \( \nu_\Delta = 0 \), Y. Huh et.al.
$1/N_f$ RG equations:

\[
\frac{d\Sigma_1}{d \ln \Lambda} = C_1(-i\omega) + C_2 v_f k_x \tau^z + C_3 v_\Delta k_y \tau^x,
\]

\[
\frac{dv_f}{d \ln \Lambda} = (C_1 - C_2)v_f,
\]

\[
\frac{dv_\Delta}{d \ln \Lambda} = (C_1 - C_3)v_\Delta,
\]

\[
\frac{d(v_\Delta/v_f)}{d \ln \Lambda} = (C_2 - C_3)(v_\Delta/v_f).
\]

$C_i$ are functions of $1/N_f$ and $v_\Delta/v_f$

\[
C_1 = -0.4627 \frac{(v_\Delta/v_F)}{N_f} + \mathcal{O} \left( (v_\Delta/v_F)^3 \right)
\]

\[
C_2 = -0.3479 \frac{(v_\Delta/v_F)}{N_f} + \mathcal{O} \left( (v_\Delta/v_F)^3 \right)
\]

\[
C_3 = \left( \frac{8}{\pi^2} \ln(v_F/v_\Delta) - 0.9601 \right) \frac{(v_\Delta/v_F)}{N_f} + \mathcal{O} \left( (v_\Delta/v_F)^3 \right).
\]

Fixed Point: $v_\Delta = 0$. Y. Huh et.al. 2008
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How does the nematic quantum critical point change the physical quantities?

**Due to coupling with nematic order, velocities are functions of frequency:**

Physical Quantity 1: LDOS, measured by STM

Naive equation:

\[ \rho(\omega/\Lambda) \sim \frac{\omega}{v_\Delta v_f} \]

- \( v_{\Delta_0}/v_{f0} = 1/5, \quad \rho \sim \omega^{0.91}, \)
- \( v_{\Delta_0}/v_{f0} = 1/10, \quad \rho \sim \omega^{0.935}, \)
- \( v_{\Delta_0}/v_{f0} = 1/20, \quad \rho \sim \omega^{0.955}. \)
Physical Quantity 2: Specific heat

Naive equation:

\[ C \sim \frac{1}{v_{\Delta} v_f} T^2 \]

\[ \frac{v_{\Delta 0}}{v_{f 0}} = \frac{1}{5}, \quad C \sim T^{1.86} \]

\[ \frac{v_{\Delta 0}}{v_{f 0}} = \frac{1}{10}, \quad C \sim T^{1.91} \]

\[ \frac{v_{\Delta 0}}{v_{f 0}} = \frac{1}{20}, \quad C \sim T^{1.95} \]
Physical Quantity 3: NMR spin lattice relaxation rate

\[ F(\omega) \sim \int dq_x dq_y \frac{1}{\omega} \chi''(q_x, q_y, \omega), \]

Local probe, momentum integrated susceptibility, contribution from all the “slow” spin density wave should be considered.

Wave-function + vertex corrections

\[ \vec{q} = (0, 0), \quad \Psi_1^\dagger \sigma^a \Psi_1 + \Psi_2^\dagger \sigma^a \Psi_2; \]
\[ \vec{q}_{1A} = (2Q, 0), \quad \Psi_2^\dagger \sigma^a \Psi_1; \]
\[ -\vec{q}_{1A} = (-2Q, 0), \quad \Psi_1^\dagger \sigma^a \Psi_2; \]
\[ \vec{q}_{1B} = (0, 2Q), \quad \Psi_1^\dagger \tau^y \sigma^a \sigma^a \Psi_2; \]
\[ -\vec{q}_{1B} = (0, -2Q), \quad \Psi_2^\dagger \tau^y \sigma^a \sigma^a \Psi_1^*, \]
\[ \vec{q}_{11} = (2Q, 2Q), \quad \Psi_1^\dagger \tau^y \sigma^a \sigma^a \Psi_1; \]
\[ -\vec{q}_{11} = (-2Q, -2Q), \quad \Psi_1^\dagger \tau^y \sigma^a \sigma^a \Psi_1^*; \]
\[ \vec{q}_{22} = (-2Q, 2Q), \quad \Psi_2^\dagger \tau^y \sigma^a \sigma^a \Psi_2; \]
\[ -\vec{q}_{22} = (2Q, -2Q), \quad \Psi_2^\dagger \tau^y \sigma^a \sigma^a \Psi_2^*. \]
Physical Quantity 3: NMR spin lattice relaxation rate

\[ F(\omega) \sim \int dq_x dq_y \frac{1}{\omega} \chi''(q_x, q_y, \omega), \]

Naive equation:

\[
\frac{1}{T_1 T} \sim T^2
\]

\[
v_{\Delta 0}/v_f \quad = \quad 1/5, \quad \frac{1}{T_1 T} \sim T^{1.74},
\]

\[
v_{\Delta 0}/v_f \quad = \quad 1/10, \quad \frac{1}{T_1 T} \sim T^{1.83},
\]

\[
v_{\Delta 0}/v_f \quad = \quad 1/20, \quad \frac{1}{T_1 T} \sim T^{1.89}.
\]

PRB, 78, 134508 (2008), C. Xu, Y. Qi, S. Sachdev
Summary of Fe-SC:

1. Global phase diagram:

2. Unified theory of lattice distortion and SDW.

3. Nature of the transitions when coupled to a soft lattice.

4. Physical observables at the nematic transition in SC.