Superconductivity and spin excitations in orbitally ordered FeSe

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Motivation: FeSe

- FeSe
  - simplest compound
  - superconducting without doping
- interesting properties
  - non-magnetic
  - nematic phase
    possibility to study origin of nematicity without presence of magnetic order
Motivation: FeSe

- **pressure experiments**
  
  [Graph showing pressure experiments]

  Medvedev et al. (2010) enhancement of Tc up to 37K


- **intercalation**
  
  Burrard-Lucas et al. 2012
  Tc → 43K molecular intercalation

- **thin films**
  
  [Graph showing thin films]


  ARPES gap Tc → 65K


  Transport on monolayer: Tc ~ 100K

FeSe

- ARPES: unusual band renormalization, no agreement to DFT

- pragmatic approach TB engineering
  - shifts of tight binding parameters
  - orbital order
    - site centered orbital order
    - bond centered orbital order

\[
H = H_{\text{TB}} + H_{\text{OO}},
\]

\[
H_{\text{TB}} = \sum_{k,\mu,\nu,\sigma} t_{\mu\nu}(k)c_{\mu\sigma}^\dagger(k)c_{\nu\sigma}(k),
\]

\[
H_{\text{OO}} = \Delta_s(T) \sum_{k,\sigma} [n_{x\sigma}(k) - n_{y\sigma}(k)].
\]

Maletz, et al. PRB 89, 220506(R) (2014)
FeSe: tight binding model

- ARPES

Watson et al., PRB 91, 155106 (2015); no color code

orbital order: 50 meV

$T_s$=87K

Shimojima, et al. PRB 90, 121111(R) (2014)

Model

Eschrig et al., Phys Rev B, 80, 104503 (2009)

+shift of hoppings
+inclusion of orbital order

10-orbital model based on:

$H_{OO} = \Delta_b g(t) \sum_{k\sigma} (\cos k_x - \cos k_y)[n_{xz\sigma}(k) + n_{yz\sigma}(k)]$

$+ \Delta_s g(t) \sum_{k\sigma} [n_{xz\sigma}(k) - n_{yz\sigma}(k)]$. 
FeSe: tight binding model

- orbital order
  - bond centered OO
  - site centered OO

- sign changing orbital splitting

\[ H_{OO} = \Delta_b g(t) \sum_{\mathbf{k}\sigma} (\cos k_x - \cos k_y) [n_{x\sigma}(\mathbf{k}) + n_{y\sigma}(\mathbf{k})] \]
\[ + \Delta_s g(t) \sum_{\mathbf{k}\sigma} [n_{x\sigma}(\mathbf{k}) - n_{y\sigma}(\mathbf{k})]. \]

ARPES on detwinned samples

Unidirectional bond order:
Watson et al., arXiv:1603.04545 (2016)
FeSe: tight binding model

- Quantum oscillations

   ![Quantum oscillation image](image1)

   **Watson et al., PRB 91, 155106 (2015)**

   ![Quantum oscillation image](image2)

   **Terashima, et al. PRB 90, 144517 (2014)**

   ![Quantum oscillation image](image3)

   **Daniel Guterding: https://github.com/danielguterding/dhva**

- **Question:** Can model electronic structure account for various other experimental results?
  - NMR: no spin-fluctuations until very low T
  - Neutron diffraction: Stripe fluctuations at intermediate energies, Neutron resonance in SC state
  - Scanning tunnelling microscopy: V-shaped DOS
  - ...
NMR: Knight shift, $1/T_1T$

orbital order visible in Knight shift

no enhanced low-energy spin fluctuations visible in NMR


\[
\frac{1}{T_1 T} = \lim_{\omega_0 \to 0} \frac{\gamma_0^2}{2 N k_B} \sum_{q \alpha \beta} |A^{q\beta}_{hf}(q)|^2 \frac{\text{Im}\{\chi^{\alpha\beta}_{RPA}(q, \omega_0)\}}{\hbar \omega_0}
\]
Spin fluctuations at higher energies

- FeSe: close to magnetic instability (tune interactions accordingly)
- transfer from Néel fluctuations to Stripe fluctuations on lowering temperature
- spin resonance at low energies from transfer of spectral weight in the superconducting state
Inelastic neutron scattering

Inelastic neutron scattering

Superconducting order parameter

• spin-fluctuation driven superconductivity

$$\frac{1}{V_G} \sum_j \int_{FS_j} dS' \Gamma(k, k') \frac{g_{\alpha}(k')}{|v_{Fj}(k')|} = \lambda_{\alpha} g_{\alpha}(k)$$

STM on FeSe: Kasahara et al. (2014)

Song et al., Science 332, 1410 (2011)
Magnetic field penetration depth

Fermi velocity (sensitive to nodes)

\[
\frac{1}{\lambda_{\nu,i}^2} = \frac{4\pi e^2}{c^2 \hbar^2} \sum_k \frac{d\xi_{\nu}(k)}{dk_i} \left( \frac{d\xi_{\nu}(k)}{dk_i} |\Delta_k|^2 - \frac{d|\Delta_k|}{dk_i} |\Delta_k| \xi_{\nu}(k) \right) \\
\times \frac{1}{E_{\nu,k}} \left( \frac{1}{E_{\nu,k}} \tanh\left( \frac{E_{\nu,k}}{2k_B T} \right) - \frac{1}{2k_B T} \text{sech}\left( \frac{E_{\nu,k}}{2k_B T} \right)^2 \right). 
\]

superfluid density tensor

Linear behavior nodal in y-direction

“full gap” in x-direction \(\sim T^3\)
Summary

- model electronic structure for FeSe consistent with ARPES and quantum oscillations
- further experimental findings consistent with
  - spin-fluctuation driven superconductivity
  - absence of magnetic order, but nematic order (orbital order, origin not explained yet)
- Predictions:
  - linear $T$-dependence in magnetic penetration depth
  - impurity bound states: possible to model with given electronic structure

Acknowledgements:


Spin fluctuations under pressure

- Close to magnetic instability: pressure experiments

Medvedev et al. (2010)

Bendele et al. 2012: magnetic state at low pressure

enhanced spin fluctuations
Imai, Cava PRL (2009)

INS: stripe orbital order

Superconducting order parameter: stripe OO

- spin-fluctuation driven superconductivity

\[- \frac{1}{V_G} \sum_j \int_{\text{FS}_j} dS' \Gamma(k, k') \frac{g_\alpha(k')}{|v_{Fj}(k')|} = \lambda_\alpha g_\alpha(k)\]

STM on FeSe: Kasahara et al. (2014)

Song et al., Science 332, 1410 (2011)