Topological states in iridium oxides

$A_2\text{Ir}_2\text{O}_7$

Weak topological insulator:
Protected metallic state at domain wall
Edge state of 1D weak Chern insulator $\Rightarrow$ controllability

$\text{Na}_2\text{IrO}_3$

Ab initio study
Zig-zag order in agreement with experiment
How can we approach Kitaev spin liquid?


Yamaji, Nomura, Kurita, Ryotaro Arita, Imada
Outline

1. Introduction

2. How to identify the mechanism of high-$T_c$?
   Hidden fermion theory for the cuprates
   arXiv:1411.4365

3. Ab initio studies on iron-based superconductors
   arXiv:1409.6536

4. Mechanism of superconductivity for 2D Hubbard

5. Outlook
Introduction
High-$T_c$ superconductors

Superconductivity above 50K

cuprates, iron-based superconductors

2D anisotropy, square lattice close to antiferromagnetic order
1. Introduction
   *Ab initio* Approach

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5. Outlook
How was the mechanism of the conventional BCS electron-phonon superconductivity solved?

**strong-coupling superconductivity**

**Eliashberg eq.**

**anomalous self-energy**

**measured phonon density of states**

**neutron scattering data**

**Bosonic (phonon) glue makes peaks**

McMillan-Rowell 1965, 1969
Similar peak of anomalous self-energy & gap function in cuprate models

\[ \Sigma_{\text{ano}} \]

\[ \Delta(\omega) = z \Sigma_{\text{ano}} \]

\[ \Phi(k, \omega) \]

\[ k = (0, \pi), \quad x = 3\% \]

\[ J/t = 0.3 \]

\[ t-J \] model

Maier, Poilblanc, Scalapino
PRL 100, 237001 (2008)

Kyung et al (08), Civelli (09)

Cluster DMFT
2x2 cluster
exact diagonalization
for \( T > 0 \)

Hubbard model

Origin of peaks is not clear

\[ \text{cf. Spin fluctuation scenario} \]

Le Tacon et al.
Nat. Phys. 7, 725 (2011)
Peak indeed generates high $T_c$

Gap function

$$\text{Re} \Delta(k, \omega = 0) = \frac{2}{\pi} \int_0^\infty \frac{\text{Im} \Delta(k, \omega')}{\omega'} d\omega'$$

$$I(k, \Omega) = \frac{2}{\pi \text{Re} \Delta(k, \omega = 0)} \int_0^\Omega \frac{\text{Im} \Delta(k, \omega')}{\omega'} d\omega'$$

$\Gamma(k_{AN}, \Omega = 0.5) = 0.8$: 80% of the gap is attributed to the peak!

What makes this peak?

cf. Maier, Poiblanc, Scalapino, PRL’08
Poles of $\Sigma^{\text{nor}}$ and $\Sigma^{\text{ano}}$

Peak in $\text{Im} \Sigma^{\text{ano}}$ comes from the pole of $\Sigma^{\text{ano}}$

$\text{Im} \Sigma^{\text{nor}}$ and $\text{Im} \Sigma^{\text{ano}}$ are peaked at the same energy!

arXiv:1411.4365
Pole cancellation between $\Sigma^{\text{nor}}$ and $\Sigma^{\text{ano}}$

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega) \quad G(k, \omega) = \left[ \omega + \mu - \varepsilon_k - \Sigma^{\text{nor}}(k, \omega) - W(k, \omega) \right]^{-1}$$

$$W(k, \omega) = \frac{\Sigma^{\text{ano}}(k, \omega)^2}{\omega - \mu + \varepsilon_k + \Sigma^{\text{nor}}(k, -\omega)^*}$$

$\Sigma^{\text{nor}}$ cancels with $W$!

Poles of $\Sigma^{\text{nor/ano}}$ are invisible in $A(k, \omega)$.

If the peak directly comes from bosonic excitations such as spin fluctuations, the cancellation cannot happen.
Two-component fermion

mutually hybridizing $c$ and $d$ fermions

$$H = \sum_k [\varepsilon(k)c_k^\dagger c_k + \Lambda(k)(c_k^\dagger d_k + h.c) + \varepsilon'(k)d_k^\dagger d_k]$$

$$G = (\omega - H)^{-1} = \begin{pmatrix} c & d \\ \omega - \varepsilon & -\Lambda \end{pmatrix}^{-1} = \frac{1}{(\omega - \varepsilon)(\omega - \varepsilon') - \Lambda^2} \begin{pmatrix} \omega - \varepsilon' & \Lambda \\ \Lambda & \omega - \varepsilon \end{pmatrix}$$

$$G_{cc^\dagger} = \frac{\omega - \varepsilon'}{(\omega - \varepsilon)(\omega - \varepsilon') - \Lambda^2} = \frac{1}{(\omega - \varepsilon) - \frac{\Lambda^2}{\omega - \varepsilon'}}$$

$$G = \frac{1}{\omega - \varepsilon - \Sigma} \quad \Sigma = \frac{\Lambda^2}{\omega - \varepsilon'}$$

zero of $G_c = \text{pole of } \Sigma_c = \text{pole of } G_d$

hybridization gap = origin of mean field gap of CDW, SDW(AF), ....
Two-component fermion II

\[
H = \sum_k \left[ \varepsilon_c(k) c_{k\sigma}^\dagger c_{k\sigma} + \Lambda(k) (c_{k\sigma}^\dagger d_{k\sigma} + h.c) + \varepsilon_d(k) d_{k\sigma}^\dagger d_{k\sigma} \right]
\]
\[
+ \Delta_c c_{k\sigma}^\dagger c_{k\sigma}^\dagger + \Delta_d d_{k\sigma}^\dagger d_{k\sigma}^\dagger + \text{H.c.}
\]

\[
\Sigma_{c}^{\text{nor}}(k, \omega) = \Lambda_k^2 \left[ \omega - \varepsilon_d - \frac{\Delta_d^2}{\omega + \varepsilon_d} \right]^{-1}
\]

\[
G_{dd^\dagger}(k, \omega)
\]

becomes complicated, but

\[
G_{dd^\dagger}^{(0)}(k, \omega) = \left[ \omega - \varepsilon_d - \frac{\Delta_d^2}{\omega + \varepsilon_d} \right]^{-1}
\]
for \( \Lambda = 0 \)
Zeros of Green’s function

\[ G_{c^\dagger c}(k, \omega) = \frac{1}{\omega - \epsilon_c(k) - \Sigma_c^{\text{nor}}(k, \omega) - V_c(k, \omega)} \]

Poles of \( \Sigma_c^{\text{nor}} \) and \( V_c \) completely cancel
\( \Rightarrow \) \( G \) does not have zeros at the poles of the self-energy!

This cancellation disappears in the pseudogap phase
\( \Rightarrow \) Zeros of the quasiparticle Green’s function emerge at the poles of \( d \)-fermion Green’s function
\( = \) pseudogap
Origin of pseudogap

pole of hidden fermion

→ pole of $\Sigma^{\text{nor}}$

Below $T_c$ it disappears because of the cancellation by $\Sigma^{\text{ano}}$. 
Excellent agreement between CDMFT and TCFT

\[ \text{Im}\Sigma^{\text{nor}}(k,\omega) \]

\[ \text{Im}\Sigma^{\text{ano}}(k,\omega) \]

\( U=8 \)

\( t'=0.2 \)

\( n=0.96 \)

\( T=0.01 \)

\[ \epsilon_f(k) \sim \epsilon_c(k+Q), \quad Q=(\pi,\pi). \]
What is the hidden fermion $d$?
Candidate: Quasiparticle vs. Composite fermion

**Quasiparticle:**

- kinetic energy gain

**Composite fermion:**

- interaction energy gain
- hybridization

natural extension of exciton

\[
d^\dagger_{i\sigma} \equiv \sqrt{\frac{m}{1-m}} c^\dagger_{i\sigma} \left(1 - \frac{1}{m} n_{i\bar{\sigma}}\right), \quad m \equiv \langle n_{i\bar{\sigma}} \rangle \quad \text{incoherent part of fermion}
\]

\[
U n^\uparrow_n^\downarrow = -U (1 - \gamma) \frac{\sqrt{m(1-m)}}{4} \sum_{\sigma} \left(c^\dagger_{\sigma} d_{\sigma} + d^\dagger_{\sigma} c_{\sigma}\right) + U \gamma \frac{m(1-m)}{2(1-2m)} \sum_{\sigma} d^\dagger_{\sigma} d_{\sigma} + U \frac{m}{2} \left(1 - \gamma \frac{1-m}{1-2m}\right) \sum_{\sigma} n_{\sigma}
\]

hybridization


\[d \text{ and } f \text{ satisfy fermion anticommutation approximately}\]
Peak of \( \text{Im} \Delta = \) pole of hidden fermion (composite fermion)

- Not boson but fermion boosts up \( T_c \)
- Nearly localized incoherent electron acquire local large binding energy of pair

Hybridization

Proximity to quasiparticle
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   - arXiv:1409.6536,

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Experimental Discovery

$\text{LnFeAs(O}_{1-x}\text{F}_x\text{)}$

$\text{Ln} = \text{La, Pr, Sm, ...}$

$T_c \approx 26K-55K$

Kamihara et al, JACS 130, 3296 (2008)

Mukuda et al. PRB 89 (2013) 064511

Zhao et al. Nat. Mat. 7, 963 (2008)

Antiferromagnetic metal
First Principles Approach

downfolding; Fe 3d 5 band models (d model)
dimensional downfolding → 2 D effective model

\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}, \]
\[ \mathcal{H}_0 = \sum_{\sigma} \sum_{i,j} \sum_{\nu,\mu} t_{i,j,\nu,\mu} c_{i,\nu,\sigma}^\dagger c_{j,\mu,\sigma}, \]
\[ \mathcal{H}_{\text{int}} = \mathcal{H}_{\text{on-site}} + \mathcal{H}_{\text{off-site}}. \]

1. Global electronic structure by DFT far from Fermi level tens eV
2. downfolding constrained RPA
   (1) Screened Coulomb interaction
   (2) Self-energy
3. Low-energy solver
   Low-energy effective Hamiltonian 1/10-1/100 eV
   variational Monte Carlo (VMC), path-integral renormalization group (PIRG), (cluster) dynamical mean-field theory (DMFT),

**Ab initio derivation of $U$ by constrained RPA**

<table>
<thead>
<tr>
<th>Material</th>
<th>$d$ model</th>
<th>$dp/dpp$ model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\bar{U}$ (eV)</td>
<td>$\bar{\nu}$ (eV)</td>
</tr>
<tr>
<td>LaFePO</td>
<td>2.47</td>
<td>14.15</td>
</tr>
<tr>
<td>LaFeAsO</td>
<td>2.53</td>
<td>14.85</td>
</tr>
<tr>
<td>BaFe$_2$As$_2$</td>
<td>2.80</td>
<td>15.59</td>
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<tr>
<td>LiFeAs</td>
<td>3.15</td>
<td>15.82</td>
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<tr>
<td>FeSe</td>
<td>4.24</td>
<td>17.53</td>
</tr>
<tr>
<td>FeTe</td>
<td>3.41</td>
<td>16.89</td>
</tr>
</tbody>
</table>

$U / t : d$ model

<table>
<thead>
<tr>
<th>Material</th>
<th>$U / t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaFePO</td>
<td>8</td>
</tr>
<tr>
<td>LaFeAsO</td>
<td>9</td>
</tr>
<tr>
<td>FeTe</td>
<td>11</td>
</tr>
<tr>
<td>FeSe</td>
<td>14</td>
</tr>
</tbody>
</table>

smaller size of Wannier $\Rightarrow$ larger bare Coulomb
smaller covalency $\Rightarrow$ poor screening

Miyake, Nakamura, Arita, Imada
JPSJ 79 (2010) 044705
\[ |\psi\rangle = \mathcal{P}_J \mathcal{P}^{\text{ex.}}_d \mathcal{P}_G \mathcal{L}^{S=0} |\phi_{\text{pair}}\rangle \]

\[ |\phi_{\text{pair}}\rangle = \left[ \sum_{i,j} f_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right]^{N/2} |0\rangle \]

\( f_{ij} \): pair-dependent variational parameter

Optimization of 1000-10000 variables to overcome bias

\[ \mathcal{P}_G = \exp \left[ -g \sum_i n_{i\uparrow} n_{i\downarrow} \right] \]

Gutzwiller factor

\[ \mathcal{L}^S = \frac{2S + 1}{8\pi^2} \int d\Omega P_S(\cos \beta) \hat{R}(\Omega) \]

Quantum number projection
Tomonaga Luttinger liquid

\[ S(0)S(r) \propto (\log r)^{1/2} 1/r^{1+K_\rho} \]

algebraic decay

Capello et al. PRB 72(2005) 085121

R. Kaneko, S. Morita, MI
Solution of low-energy solver

ordered magnetic moment

VMC result for ab initio models of mother compounds

near magnetic quantum critical point

Misawa et al.
JPSJ 80 (2011) 023704
PRL 108 (2012) 177007

see also Yin Haule Kotliar Nat. Mat. (2011)
Detailed Study on Doping Effect

Orbital Selective Mottness and Charge Inhomogeneity

Mottness and Stripe Order

$d_{x^2-y^2}$ stays at half filling for $\delta < 0.05$

Ishida, Liebsch
Misawa, Imada

Orbital selective Mott insulator

two first-order transitions of stripe order *cf.* nematic

Stripe order driven by $d_{X^2-Y^2}$ order

high-spin to low-spin transition by $J_H$

$\Rightarrow$ strong first order transition
Phase separation necessarily appears around the first-order transitions 

\[ 0.1 < \delta < 0.16 \]

Maxwell construction

NQR

- Takeshita, Kadono
- Charnukha et al. PRL 109, 017003 (2012)
- Lang et al. PRL 104, 097001 (2010)
- Park et al. PRL 102 (2009) 117006
- Inosov et al. PRB 79, 224503 (2009)
Superconducting Mechanism
Superconductivity

\( s_{\pm} \) symmetry (3s)

\( d_{X^2-Y^2} \) orbital gives dominant contribution

\( d_{X^2-Y^2} \) governs magnetism & superconductivity

⇒ similarity to cuprates

\[ 0.08 < \delta < 0.32; \]

SC, N

two local minima

\[ 0.2 < \delta < 0.32 \]

SC ground state

\[ \left\langle \Delta_{3s, X^2-Y^2} \right\rangle = \sqrt{\lim_{r \to \infty} P_{3s, X^2-Y^2}(r)} \]

Superconducting order has domes near first-order jumps
Role of Electron Correlation

\[ \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}, \]

\[ \mathcal{H}_0 = \sum_{\sigma} \sum_{i,j} \sum_{\nu,\mu} t_{i,j,\nu,\mu} c^\dagger_{i,\nu,\sigma} c_{j,\mu,\sigma}, \]

\[ \mathcal{H}_{\text{int}} = \mathcal{H}_{\text{on-site}} + \mathcal{H}_{\text{off-site}}. \]

\[ \mathcal{H} = \mathcal{H}_0 + \lambda \mathcal{H}_{\text{int}} \]

Sensitive dependence on \( \lambda \)

\( \lambda = 0.95 \)
Phase Diagram

λ \sim 0.96 \Leftrightarrow \text{experiment}

Possible small role of electron phonon int.

Nomura et al. (2013)

0.4 eV attraction within 0.02 eV

LaFePO

LaFeAsO_{1-x}H_x

Yamaura et al.
Smoking Gun of Superconducting Mechanism

\[ \left\langle \Delta_{3s, X^2 - Y^2} \right\rangle \] and \(-d^2E/d\delta^2\) show same peak structure:
One-to-one correspondence

Superconductivity around 1st order trans. and PS
Summary

1. *Ab initio* electronic model shows $s\pm$ superconducting phase by electron doping into stripe AF phase of LaFeAsO. Agreement with experiment.

2. Orbital selective Mottness of $d_{x^2-y^2}$ orbital holds an underlying key for the emergence of the high-$T_c$ superconductivity. Major role for both magnetism and superconductivity.

3. Superconductivity emerges because of the charge instability accompanied by the PS caused by the strong 1st order AF/nematic transition. Smoking gun is found in one-to-one correspondence between charge compressibility and superconductivity in various cases.
Single band Hubbard model

Misawa & Imada
Single band Hubbard model

Charge fluctuation has one-to-one correspondence to SC
Conclusion

1. “Hidden fermion” boosts up $\Delta$ and hence $T_c$

2. Cancellation of $\Sigma^{\text{nor}}$ and $\Sigma^{\text{ano}}$ in $A(k,\omega)$

3. Hidden fermion may represent incoherent and excitonic electron $\Leftrightarrow$ large gap proximity to QP

4. Iron-based SC emerges from density fluct.

5. Hubbard model has a similar origin of SC
Thank you