Spin fluctuations and unconventional superconducting properties

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Introduction to some strongly correlated unconventional superconductors, and general relations between the spin fluctuation and unconventional superconductivity

Theoretical prediction on the pairing symmetry in iron arsenide
Dual effects of the itinerant spin fluctuations and the next-nearest-neighbor localized AFM coupling on the pairing symmetry in newly discovered iron selenide.

Fermi arcs, pseudogap and collective excitations in doped Sr2IrO4 and layered organic SC
Conventional superconductor:
Wavefunction does not change sign around the Fermi surface (s-wave)

What we are knowing:
- s-wave superconductivity can be understood by the phonon-mediated BCS mechanism

Unconventional Superconductor
Unconventional superconductor:
Wavefunction changes sign around the Fermi surface (extended s-wave, d-wave, p-wave, f-wave)

What we are knowing:
unconventional SC is realized due to the formation of Cooper pairs, but the glue to form pair is still under investigation
Copper-based high-Tc (Cuprates)

Structure
La$_{2-x}$Sr$_x$CuO$_4$ $x=0$

- Parent compound: Mott insulator
- SC is a doped Mott insulator
- AF is proximity to SC

Phase diagram

- Strange metal
- Pseudogap
- Antiferromagnet
- Superconductor
- Fermi liquid

hole doping

temperature (K)
**high-Tc cuprates**

**d-wave Superconductivity**

\[ d_{x^2-y^2} \]

Pairing symmetry:

\[
\Delta(k) = \Delta_0 \left( \cos k_x - \cos k_y \right) / 2 \propto \cos(2\phi)
\]

Gap function in BZ

**d-wave**

**s-wave**

**ARPES data**

FIG. 46. Superconducting gap measured at 13 K on Bi2212 \((T_c=87 \text{ K})\) plotted vs the angle along the normal-state Fermi surface (see sketch of the Brillouin zone), together with a \textit{d}-wave fit. From Ding, Norman, et al., 1996.
high-Tc cuprates

Magnetic dispersion of the parent (insulating) compound

La$_2$CuO$_4$

R. Coldea et al., PRL23, 5377 (01)

AF spin wave:

$$\omega_q = \nu q$$

Spin excitation in insulating state can be well described by the spin wave theory
After doping, the AF long-range order disappears rapidly, but the short-range spin correlations or spin fluctuations survives over the whole SC regime.
**high-Tc cuprates**

Universal Dispersion – Hourglass-Type (沙漏)

J.M. Tranquada, cond-mat/0512115

S.M. Hayden, P. Dai et al., Nature 429, 531 (04)
high-Tc cuprates

Frequency dependence of $\chi''(q, \omega)$ --- “Spin resonance”


The “resonance” has not be identified in LaSrCuO
Doping dependence of the spin resonance energy

Temperature dependence of the spin resonance energy

Suggests a close relation of the superconductivity and spin resonance
high-Tc cuprates

Explanation of the Hourglass Dispersion based on the weak-coupling theory

Below Er, Nesting of Fermi surface

Contour plot of the SC quasiparticle energy

\[ E_k = \omega / 2 \]

for \( \omega = 0.1 J , 0.3 J , 0.51 J , 0.7 J \)
high-Tc cuprates

Explanation of the Hourglass Dispersion based on the weak-coupling theory

At Er, Spin resonance—— Spin collective mode (spin exciton)

\[
\text{Im } \chi = \frac{\text{Im } \chi_0}{(1 - |v_q| \text{Re } \chi_0)^2 + (|v_q| \text{Im } \chi_0)^2}
\]

\[1 - |v_q| \text{Re } \chi_0 = 0 \quad \text{Im } \chi_0 \rightarrow 0\]
Conditions for the Formation of the Spin Resonance

1) $\Delta_k = -\Delta_{k+Q}$
   SC coherent factor: $1 - \frac{\varepsilon_k \varepsilon_{k+Q} + \Delta_k \Delta_{k+Q}}{E_k E_{k+Q}}$
   At FS $1 - \frac{\Delta_k \Delta_{k+Q}}{|\Delta_k \parallel \Delta_{k+Q}|}$

2) Enough residual AF exchange interaction $V_q$ to lead the pole to reside in the gap region
   $E_r \approx 2\Delta_Q$

Whether the spin resonance is the driving force or the consequence of the SC is still under debate.
Discovery of New Non-cuprate High-Tc Superconductors

Iron-based superconductors

Materials
Iron-based superconductors

Spin-Density-Wave (SDW) V.S. Superconductivity

Phase Diagram

- AF is proximity to SC

S. Nandi et al., PRL 104, 057006 (2010)
Difference in the Magnetic Ground States of the Parent Compounds

J. Dong, et al., arXiv: 0803.3426

Indicates that Fe-arsenide SC may be in the intermediate correlated regime
Multi-band Structure in the Energy Band

D.J. Singh and M.H. Du, PRL 100, 237003 (2008)

Multi-band crosses
Fermi surface

High-Tc cuprate superconductor

Single-band crosses
Fermi surface
Layered organic SC

It shares some similarities with high-Tc cuprates

\( T_c \approx 10 \text{k} \)

\( \kappa - (\text{BEDT-TTF})_2 X \)

Similarities: 1) Quasi 2D
2) AF is proximity to SC
3) Relatively strong correlation

Maybe a d-wave SC
Chiral $p$-wave superconductivity

-- Sr$_2$RuO$_4$

Maeno et al., in 1994  $T_c \sim 1k$

$$d(k) = \Delta_0 \hat{z}(k_x \pm ik_y)$$

- Triplet pairing
- topological order & Majorana fermions
- spontaneous supercurrents
This is a half-filling system. Why is not a metal?

$3d^9$

$T_N \sim 500K$

Mott Insulator

Strongly correlated electron system
Simplest model to describe the strongly correlated system

**Hubbard model:**

Since the short-range interaction is important, Coulomb interaction between electrons is taken to be point-like in real space and hence constant in momentum space—On-site interaction U

\[ H = -t \sum_{\langle i,j \rangle, \alpha} (c_{i\alpha}^{\dagger} c_{j\alpha} + c_{j\alpha}^{\dagger} c_{i\alpha}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

The case of \( U > W \) (bandwidth) is called strongly correlated system!!

The difficulty to treat Hubbard model is that there is no small parameter

→ The usual perturbation theory fails
Heisenberg model for the interaction between spins in a crystal:

\[ H = \sum_{ij} J_{ij} S_i \cdot S_j \]

The interaction is generally short ranged

\[ J_{ij} = \begin{cases} J, & \text{If i and j are neighbors} \\ 0, & \text{otherwise} \end{cases} \]

\( J > 0 \) antiferromagnetic correlations \( J < 0 \) Ferromagnetic correlations

In materials where electrons both generate magnetic moments and form conduction bands, only the Heisenberg model can’t account for the magnetism. Because the spins are not localized.
**t-J model**

low-energy effective model at larger $U$

t-J model is an effective model governing the low energy excitations in a larger $U/t$ regime

$$H = -t \sum_{<ij>,\sigma} (\hat{C}^+_i \hat{C}^-_j + h.c.) + J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)$$

$$J = 4t^2 / U > 0$$

$$\hat{C}_i^+ = (1 - n_{i\uparrow}) C_i^+$$

Electron can move only through the single occupied sites

At half-filling, the t-J model is reduced to the Heisenberg model

An illustration of the derivation of the J term from the Hubbard model

Due to $U>>t$, treat $t$-term as a perturbation

$$\mathcal{H}^t \rightarrow \frac{1}{u} \mathcal{H}^t \rightarrow |\uparrow, \downarrow\rangle \rightarrow |\uparrow\downarrow, 0\rangle \rightarrow |\downarrow, \uparrow\rangle \rightarrow |0, \uparrow\downarrow\rangle \rightarrow |\downarrow, \uparrow\rangle.$$ 

The operators that connect these initial and final states can be written as a product of $\frac{1}{2}$ spin operators

$$H_2 = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j$$
Spin Fluctuations and Superconductivity

➢ Berk-Schrieffer weak coupling theory

EFFECT OF FERROMAGNETIC SPIN CORRELATIONS ON SUPERCONDUCTIVITY*

N. F. Berk and J. R. Schrieffer
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania
(Received 24 June 1966)

In this note we show from first principles that ferromagnetic spin correlations which arise from strong Coulomb interactions between the valence electrons lead to an enhanced singlet-state repulsion. For realistic values of system parameters, this spin-induced repulsion can be many times larger than the conventional Coulomb pseudopotential. For example, in systems like Pd, whose static spin susceptibility is strongly exchange enhanced, this repulsion is sufficient to suppress superconductivity totally.

➢ AF spin flu. leads to d-wave pairing
Scalapino-Loh,Jr.-Hirsch, PRB34, 8190 (1986)
What causes Cooper pairings in the repulsive Hubbard model?

Let us first review two approaches to the Cooper instability

Hamiltonian:

\[ H = \sum_{k\sigma} \varepsilon_k c_k^\sigma c_k - V_0 \sum_{k,k'>k_F} c_{k'}^\uparrow c_{-k'}^\downarrow c_{-k}^\downarrow c_k^\uparrow \]

➤ Wave function method:

Assuming:

\[ \psi = \sum_{|k|>k_F} \alpha_k c_k^\uparrow c_{-k}^\downarrow |FS> \]

Solving the eigen equation:

\[ H\psi = E\psi \]

\[ E = -2\hbar \omega_D \exp\left[-\frac{2}{V_0 N(E_F)}\right] \quad \Rightarrow \text{A pair of electrons forms a bound state} \]

Cooper pair
Perturbation method

Underlying physics: starting from the normal state, we can do perturbation calculations. If the perturbation is broken down, it means that the system will undergo an instability.

It has been known that the Cooper instability arises in the particle-particle scattering channel with zero total momentum

\[
V(k-p, \varepsilon_k - \varepsilon_p) \approx \begin{cases} 
-V_0, & |\varepsilon_k - \varepsilon_p| < \omega_D \\
0, & |\varepsilon_k - \varepsilon_p| > \omega_D 
\end{cases}
\]

Scattering T-matrix

\[
T = \frac{V_0}{1 - V_0 T_0}
\]

When T-matrix divergent, then Cooper forms:

\[
1 - V_0 T_0 = 0 \implies k_B T_C = \hbar \omega_D \exp\left[-\frac{2}{V_0 N(E_F)}\right]
\]
What causes Cooper pairings in the Hubbard model?


For a bare interaction, the electron-electron interaction is just the Hubbard $U$ which is repulsive.

\[ \Gamma_i = U + \ldots \]

If we include the interaction perturbatively, i.e., in the form of RPA then, the effective interaction will gain a q-dependence $\Gamma_i(q)$ via the exchange of spin excitations

\[ \chi_{\pi\pi} = \ldots \]

\[ \chi_{+-} = \ldots \]
What causes Cooper pairings in the Hubbard model?

However, the effective particle-particle interaction is still positive

Can such an interaction cause pairing?
The answer is yes!

It is useful to look at the interaction at real space

\[ \Gamma_l(r) = \frac{1}{N} \sum_q e^{iqr} \Gamma_l(q) \]

If the two electrons can spatially arrange themselves to take advantage of the attractive regions of the interactions, then it is possible that they can pair.
Pairing symmetry mediated by spin fluctuations

The pairing function is given by the eigenvector $\Delta(k)$ corresponding to the largest eigenvalue $\lambda$ of the linear “Eliashberg equation”

$$\lambda \Delta(k) = -\frac{T}{N} \sum_{k'} \Gamma(k - k') |G(k')|^2 \Delta(k')$$

It describes a pair of electrons $k$ and $-k$ is scattered into the pair of $k'$ and $-k'$ via the exchange of spin fluctuations.

If $\lambda$ is equal to 1, then a bound state forms -- Cooper pair

For the spin-singlet pairing, $\Gamma(q) > 0$

so, the favorable gap function $\Delta(k)$ satisfies:

**Condition:** $\Delta_i(k)\Delta_i(k + Q) < 0$

$Q$ the wavevector at which $\chi_s$ peaks
For spin triplet: \[ \hat{\Gamma}'(q) < 0 \quad \Delta_l(k)\Delta_l'(k + Q) > 0 \]

For the phonon mediated pairing
\[
\Gamma(q) < 0 \approx -V(\text{const.}) \quad \Delta_k = \Delta \text{ is isotropic}
\]

Eliashberg equation is reduced to the usual BCS gap:

\[
1 = \frac{V}{2} \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta_k^2}}
\]
Theoretical prediction on the pairing symmetry in iron arsenide


**Suggestion:** Superconducting pairing is mediated by spin fluctuations

**Effective two-band Hubbard model**

**Tight binding energy bands**

![Energy bands diagram](image)

**The on-site Coulomb Interactions:** $U, U', J, J'$

Intra-band, inter-band, Hund’s coupling, Pair hopping
Brief introduction to the FLEX Calculation

Set of Equations for the renormalization Green’s Function $G$

1. \( \hat{G} = \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G} \)

2. \( \hat{\Sigma}_{mn}(k, i\omega_n) = \)

3. \( \hat{V} \) is a function of $G$’s
   (a) Hartree-Fock term
   (b) Longitudinal Spin and charge Flu.
   (c) Transverse Spin Flu.
   (d) Particle-particle Flu.

Eqs.(1)-(3) form a closed set of Eqs. and be solved self-consistently using $32 \times 32$ k-space lattice and 1024 Matsubara frequency to get $G$. 
Our FLEX Calculation on the two-band Model

For $U=5.5$, $U'=4.0$, $J=J'=1.0$

Spin susceptibility

It has no nodes around each Fermi pockets, but changes sign between the electronic and hole Fermi pockets $\rightarrow$ extended s-wave ($S_{\pm}$-wave)

The interband SF near $(0, \pi)$ comes from the FS nesting between the electron-hole pockets

$\Delta_{ee}$

$\Delta_{hh}$
Theoretical prediction on the pairing symmetry in iron arsenide

\[ \Delta_p = -\Delta_{p+Q} \]

\[ Q = (0, \pm \pi), \]

\[ (\pm \pi, 0) \]
Exp. Data on the Spin-density-wave Order


Real Space Structure

order wave-vector \((0, \pi)\)

So, the spin fluctuation peaks most likely at \((0, \pi)\)
As a result, the pairing symmetry is likely the extended s-wave.

As shown before, this suggests that the superconductivity is mediated by the interband spin fluctuations
Exp. Data on the Unconventional Superconductivity

**ARPES** on Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$  H. Ding, et al., arXiv:0807.0419

nodeless and nearly isotropic SC gap
Exp. Data on the Unconventional Superconductivity

Unconventional superconductivity in Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ from inelastic neutron scattering

A. D. Christianson$^1$, E. A. Goremychkin$^{2,5}$, R. Osborn$^3$, S. Rosenkranz$^2$, M. D. Lumsden$^1$, C. D. Malliakas$^{2,4}$, I. S. Todorov$^5$, H. Claus$^5$, D. Y. Chung$^2$, M. G. Kanatzidis$^{2,4}$, R. I. Bewley$^6$ & T. Guiji$^7$

Spin resonance

\[ \frac{\pi}{2.77(\text{Å}^{-1})} \approx 1.15(\text{Å}^{-1}) \]

Coherent factor:

\[ 1 - \frac{E_k E_{k+Q}}{\Delta_k \Delta_{k+Q}} \approx 1 - \frac{\Delta_k \Delta_{k+Q}}{\left| \Delta_k \right| \left| \Delta_{k+Q} \right|} \]

\[ \Rightarrow \Delta_{k+Q} = -\Delta_k \]

Suggestion: s+/- pairing gap
One of the most essential ingredient of the weak-coupling scenario based on spin fluctuations is:

Approximately equal sizes of the hole and electron pockets
Iron selenide $A_xFe_{2-y}Se_2$ (A=K,Rb,Cs) with only electron pockets


Absence of hole pockets at $\Gamma$ point

KFe$_2$Se$_2$

I.R. Shein, et al, PLA 375, 1208 (11)

ARPES experiments

Y. Zhang et al., Nature Mater., 10, 273 (11)
T. Qian et al., PRL106,187001 (11)
D. Mou et al., PRL106,107001 (11)
Consequences of the absence of the hole Fermi pocket in $A_xFe_{2-y}Se_2$


$KFe_{2-x}As_2$

Itinerant spin fluctuation (five-orbital model) by FLEX

Spin susceptibility

SC gap function

Two sets of peaks around $Q = (\pi, \pi)$ $Q = (\pi, 0.6\pi)$

$\Delta_{k+Q} = -\Delta_k$

F. Wang et al., EPL93, 57003 (01)
T. Maier et al., PRB 83, 100515 (01)
ARPES measurements of the pairing symmetry


Nodeless gap in the large electron Fermi pockets around M

M. Xu et al., arXiv:1205.0787 (2012)

Rule out the d-wave

Neutron scattering results in superconducting $A_xFe_{2-y}Se_2$

G. Friemel et al., PRB85, 140511(12); J.T.Park et al., PRL107, 177005(11)

- Spin resonance at $(\pi, 0.5\pi)$
- No peak is observed around $(\pi, \pi)$
- New peaks are observed around $(\pi, 0)$

It can’t be explained by the nesting effect.

M. Wang et al., arXiv:1201.3348 (12)
The usual itinerant picture does not work

The parent compound is an AFM insulator => Local correlation

Dual effect of both the itinerant and localized magnetism

**The on-site Coulomb Interactions:** \( U, U', J, J' \)
Intra-band, inter-band, Hund’s coupling, Pair hopping

**The NNN AF Interactions:**

\[
H_{J_2} = J_2 \sum_{\langle\langle ij\rangle\rangle, l \neq l'} \vec{S}_{il} \cdot \vec{S}_{jl'}
\]

Five-orbital energy band:

Calculations are carried out by the FLEX approximation

Results for the superconducting gap

When \( J_2 > 0.045 \text{eV} \), \( s \)-wave pairing is the dominant pairing symmetry.

A small \( J_2 \) can help \( s \)-wave to be dominant over \( d \)-wave.

\[
U = 1.2 \text{ eV}, \quad U' = 0.35 \text{ eV}, \quad J_H = 0.2 \text{ eV}
\]

Gap function on the FS

\( J_2 = 0 \)

\( d \)-wave

\( J_2 = 0.05 \text{eV} \)

\( s \)-wave

Gap magnitude on the FS for the \( s \)-wave state
Results for the spin susceptibility

\[ J_2 = 0 \]

\[ J_2 = 0.01 \text{eV} \]

\[ J_2 = 0.04 \text{eV} \]

\[ J_2 = 0.05 \text{eV} \]

Turning on the \( J_2 \) term:

- The broad peak around \((\pi, \pi)\) decreases rapidly.
- The four satellite peaks move to \((\pm \pi, 0)\). For \(0.03 \text{eV} < J_2 < 0.05 \text{eV}\), they are at \((\pm 0.5 \pi, 0)\)
- The \((\pm \pi, 0)\) spin fluctuations also emerges for \(J_2 > 0.04 \text{eV}\)

Neutron exp.

M. Wang et al., arXiv:1201.3348 (12)

\((\pi, 0)\) : contribution from the \( J_2 \) term

\( \Rightarrow \) localized magnetism

\((\pi, 0.5 \pi)\) : contribution from the FS nesting

\( \Rightarrow \) itinerant magnetism
Analysis of the origin of the pairing

Results for $J_2=0.05$

Extended s-wave

$xz : \Delta(k) = \Delta_1 \cos(ky) + \Delta_2 \cos(kx) \cos(ky)$
$yz : \Delta(k) = \Delta_1 \cos(kx) + \Delta_2 \cos(kx) \cos(ky)$
$xy : \Delta(k) = \Delta_3 \cos(kx) \cos(ky)$  $S_\pm$-wave

Spatial Fourier transform of the gap

<table>
<thead>
<tr>
<th>xz</th>
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<tr>
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Strongly enhance the next-nearest-neighbor pairing in all three orbits

Results for $J_2=0$

d-wave

$xz : \Delta(k) = \Delta_1 \cos(ky) - \Delta_2 \cos(kx)$
$yz : \Delta(k) = -\Delta_2 \cos(kx) + \Delta_1 \cos(ky)$
$xy : \Delta(k) = \Delta_3 (\cos(kx) - \cos(ky))$

$\Delta_3 = 2.0 \Delta_1$

Pairing in the xy orbital is dominant
Spin fluctuations and unconventional phenomena in doped Mott insulator

Fermi arcs, pseudogap and collective excitations in doped Sr2IrO4
Ref: H. Wang, S.L. Yu and J.X. Li, PRB 91, 165138 (2015)

Fermi arcs and pseudogap in layered organic superconductors
Ref: J. Kang, S.L. Yu, T. Xiang and J.X. Li, PRB 84, 064520 (2011)
5d transition-metal oxides Sr2IrO4

Sr2IrO4 vs La2CuO4:

F. Ye et al., PRB 87, 140406 (13)
H. Das et al., PRB 79, 134522 (09)

Magnetic dispersion

Coldea et al, PRL 86, 5377 (01)
Kim et al. PRL 108, 177003 (12)

waterfall features

Liu et al, Arxiv: 1501.04687v1
Inosov PRL 99, 237002 (2007)
5d transition-metal oxides Sr\textsubscript{2}IrO\textsubscript{4}

Sr\textsubscript{2}IrO\textsubscript{4}: 5d\textsuperscript{5}, t\textsubscript{2g} Configuration, weak correlation


- **Insulator**

- **LDA+U**

- **LDA+U+SO**

Strong SOC entangle the spin and orbital spaces → isospin \(1/2\) state
Pseudogap and Fermi arc in Sr$_2$IrO$_4$

Electron doping via in situ surface doping technique


Issues

- The validity of the Jeff=1/2 Mott physics and its robustness to doping
  time-resolved optical conductivity; Hard X-ray spectroscopy, STM, LDA numerical calculations
  PRB 86, 035128 (2012); PRL 108, 086403 (2012); PRB 89, 165115 (2014);

- The possible origin of the pseudogap and Fermi arc
Model and method

- t2g three-orbital model (xz, yz, xy) including the spin-orbital coupling and interactions U, U', J, J'

  Parameters: $\xi_{SOC} = 1.03$
  
  $(U, U', J, J') = (5, 3.5, 0.75, 0.75)$

- Generalized FLEX method—SU(2) broken
Results for susceptibility

Orbital susceptibility > Spin susceptibility

T=0.01, 3% electron doping

Define $J_{\text{eff}} = \frac{1}{2}$ isospin susceptibility

$$a_{k,\uparrow/\downarrow} = (d_{k,xz,\downarrow/\uparrow}^+ \pm id_{k,yz,\downarrow/\uparrow}^+ + d_{k,xy,\uparrow/\downarrow}^+) / \sqrt{3}$$

$$S_{q}^{\alpha} = \sum_{k} (a_{k+q,\uparrow}^+ a_{k+q,\downarrow}^+ a_{k,\uparrow} a_{k,\downarrow}) \sigma^{\alpha}(a_{k,\uparrow}, a_{k,\downarrow})^T$$
Stability of the $\text{Jeff}=1/2$ isospin picture

As a function of dopings

The validity of the $\text{Jeff}=1/2$ picture in an extended doping and SOC regime
Weak pseudogap and Fermi arc

Single-particle spectral function $A(k, \omega) = -\text{Im}G(k, \omega) / \pi$


Suppressions of the spectral weights near $(\pi,0)$
Weak pseudogap and Fermi arc

Temperature dependence

T=0.02

T=0.01

EDC

Possible origin

The weak pseudogap is most likely to result from the scattering of quasiparticles by isospin fluctuations.

3% e-doiping

17% hole doping

Experiments:
15% hole doping

Y. Cao et al., arXiv:1406.4978
Pseudogap in $\kappa$-(BEDT-TTF)$_2$X

Geometrical arrangement of the $\kappa$-(BEDT-TTF)$_2$X

BEDT-TTF

- NMR
- The experimental indications merely come from the transport measurements, there are no direct probes of the single-particle spectrum, such as the ARPES etc.

Pseudogap

Takigawa et al., PRB(1991)
- PRL 89, 017003(2002)
- PRL 75, 4122(1995)
- PRB 52, 10364(1995)
- PRL 74, 3455(1995)

Nernst effect

Nam et al., Nature 449, 584(2007)
Hubbard Model on Square and Triangle lattice

\[ H^0_m = -t \sum_{\langle i,j \rangle, \sigma} c^+_i,\sigma c_{j,\sigma} - t' \sum_{\langle i,j \rangle', \sigma} c^+_i,\sigma c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \]

High-Tc cuprates
\[ t'/t = -0.45 \]

K-(BEDT-TTF)\_2X
\[ t'/t = 0.7 \sim 1.1 \]

Fermi surface
Cluster perturbation theory

Senechal et al., PRL84,522 (2000); PRB66, 075129 (2002)

i) Dividing the lattice into clusters

ii) Exact diagonalization of clusters

Cluster Green function

\[ G_{a,b}(z) = \langle \Omega | c_a \frac{1}{z - H_0} c_b^+ | \Omega \rangle + \langle \Omega | c_b^+ \frac{1}{z + H_m} c_a | \Omega \rangle \]

iii) Treating intercluster hopping with a perturbation theory

Approx. Green function for the whole lattice has a RPA-like form

\[ G_{a,b}(Q, z) \approx \left( \frac{\hat{G}(z)}{1 - \hat{V}(Q)\hat{G}(z)} \right)_{a,b} \]

\[ G_{\text{CPT}}(k, z) = \frac{1}{N} \sum_{a,b} e^{-i(k(a-b))} G_{a,b}(Q, z) \]
Test of the cluster perturbation theory

Kane-Mele Hubbard model

\[ H = H_{KM} + U \sum_i n_{i\uparrow}n_{i\downarrow} \]


Cellular dynamical mean-field theory

W. Wu et al., arXiv: 1106.0943 (2011)


PRL (2011)
In square lattice, it coexists with the Mott gap, so that it persists to the $\mathbf{U} \to \infty$ limit.
Pseudogap

It evolves into the Mott gap with the further increase of Hubbard U.

- The pseudogap here is the precursor state of the Mott gap
- To differentiate the bandwidth-controlled systems (κ-type organic salts) and the band-filling-controlled systems (cuprates).
Pseudogap and spin fluctuations

The pseudogap (not include the Mott gap partially opened in k-space) is likely due to the short-range antiferromagnetic spin fluctuations.

\[ Q = (\pi, \pi) \]
Superconducting pairing mediated by spin fluctuations in $\kappa-(\text{BEDT-TTF})_2 X$

J. Schmalian, Phys. Rev. Lett. 81, 4232 (1998);

FIG. 2. Effective pairing interaction for intra and inter-band excitations along the high symmetry lines of the Brillouin zone. Note the pronounced peak at $\mathbf{q} = (\pi, 0)$ for inter-band excitations.
Preliminary experimental data of the d-wave like symmetry

T. Arai et al., Phys.Rev.B63, 104518 (01)
We have tried to summarize the results on the spin fluctuation and superconducting pairing symmetry in unconventional (iron-based) superconductors based on the weak-coupling scenario.

Spin fluctuations preserve at most unconventional superconductors.

Superconductivity mediated by spin fluctuations gives rise to the pairing symmetry which is consistent with many experimental results.

Spin fluctuations may also be taken to explain some exotic phenomena in these strongly correlated superconductors.

There are also some experimental results which are not consistent with the pairing symmetry mediated by spin fluctuations. In fact, the iron-based superconductors are complicated because of the multi-orbital nature of the energy band and the sensitivity of some physical properties to the compositions of materials.

Therefore, further extensive studies are needed.
“...We used to think that if we knew one, we knew two, because one and one are two. We are finding that we must learn a great deal more about ‘and’. ”

Sir Arthur Eddington.

- New exotic quantum phases(orders) have emerged in 2D quantum materials => emergent materials
...at each new level of complexity, entirely new properties appear, and the understanding of this behavior requires research which I think is as fundamental in its nature as any other.

P. W. Anderson, More is different, 1972

“Continuous Revolution” ----- P.W. Anderson

继续革命
You have as many chances of success as the number of materials which is infinite.
Thank you
Experiments Probing Magnetic Properties

Physical quantity characters the magnetic properties:

- **Spin susceptibility:** \( M = \chi H \)
- **In the textbook:** \( \chi = \text{const.} \)
- **Real materials:** \( \chi(q, \omega) = \text{Re} \chi(q, \omega) + i \text{Im} \chi(q, \omega) \)

**Neutron Scattering – Spin susceptibility (full freq. and momentum)**

\[
I \propto \frac{d^2\sigma}{d\Omega dE_f} \propto \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) S^{\alpha\beta}(q, \omega)
\]

\[
S^{\alpha\beta}(q, \omega) = \frac{1}{\pi} [1 + n(\omega)] \text{Im} \chi^{\alpha\beta}(q, \omega)
\]
dynamical spin susceptibility