Supraconductivité avec et sans point critique quantique antiferromagnétique

A.-M. Tremblay

Institut quantique

Réunion inaugurale, LIA
Jouvene 27 octobre 2016
Magnetic superconductivity
Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

Canfield et al. (2010)
\[ \Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta_{p'}}{E_{p'}} (1 - 2n(E_{p'})) \]

Exchange of spin waves?
Kohn-Luttinger
Tc with pressure

Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).

High temperature superconductors
Hubbard model

1931-1980

\[ H = -\sum_{<ij>\sigma} t_{i,j} \left( c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Effective model, Heisenberg: \( J = 4t^2 / U \)

Attn: Charge transfer insulator
Method for strongly correlated matter

Dynamical Mean Field Theory (+ clusters)
Concept: atomic localized correlations consistent with delocalized aspect
2d Hubbard: Quantum cluster method

Hettler …Jarrell…Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar et al. RMP (2006)
AMST et al. LTP (2006)
Impurity solver

\[ Z = \int D[\mathbf{d}^+, \mathbf{d}] \exp \left[ -S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_i [d_i^+(\tau) \Delta_{i'i}(\tau, \tau') d_{i'}(\tau')] \right] \]

Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007
+ and -

• Long range order:
  – Allow symmetry breaking in the bath (mean-field)
• Included:
  – Short-range dynamical and spatial correlations

• Missing:
  – Long wavelength p-h and p-p fluctuations
Groups using these methods for cuprates

• Europe:
  – Georges, Parcollet, Ferrero, Civelli, (Paris)
  – de Medici (Grenoble) Capone (Italy)

• USA:
  – Gull (Michigan) Millis (Columbia)
  – Kotliar, Haule (Rutgers)
  – Jarrell (Louisiana)
  – Maier, Okamoto (Oakridge)

• Japan
  – Imada (Tokyo) Sakai
Superconductivity around an AFM quantum critical point

A heavy fermion example

Heavy fermions 3D metals tuned by pressure, field or concentration

CeRhIn$_5$

Magnetic superconductivity

Knebel et al. (2009)

Quantum criticality

Mathur et al., Nature 1998
Heavy fermions

\[ H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} \epsilon_f f_{k,\sigma}^\dagger f_{k,\sigma} + \sum_{k,\sigma} V_k (f_{k,\sigma}^\dagger c_{k,\sigma} + \text{H.c.}) + \sum_i U \left( n_{\uparrow}^f - \frac{1}{2} \right) \left( n_{\uparrow}^f - \frac{1}{2} \right) \]

Phase diagram

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2: more frustrated case
V'/V = 5: less frustrated case
Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets
Weak vs Strong correlations

\( n = 1 \), unfrustrated \( d = 3 \) cubic lattice

Mott

Slater \( \Rightarrow \)

Heisenberg

AFM

\[ J = \frac{4t^2}{U} \]
Local moment and Mott transition

$n = 1, d = 2$ square lattice

Critical point visible in $V_2O_3$, $BEDT$ organics

Understanding finite temperature phase from a mean-field theory down to $T = 0$
Phase diagram for organics

$\text{Phase diagram (X=Cu[N(CN)\textsubscript{2}]Cl)}$


F. Kagawa, K. Miyagawa, + K. Kanoda

$B_g$ for $C_{2h}$ and $B_{2g}$ for $D_{2h}$

Powell, McKenzie cond-mat/0607078
Influence of Mott transition away from half-filling

$n = 1, \ d = 2$ square lattice
Influence of Mott transition away from half-filling

\( n = 1, \quad d = 2 \) square lattice
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Two crossover lines

P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B 89, 165113/1-6 (2014)
Physics
Plaquette eigenstates

See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges

PRB 80, 064501 (2009)
Finite $T$ phase diagram
Superconductivity

Sordi et al. PRL 108, 216401 (2012)
Fratino et al.
Crossovers inside the AFM phase

\( n = 1, \) unfrustrated \( d = 3 \) cubic lattice
Superconductivity in Doped Mott insulator

\[ n = 1, \ d = 2 \text{ square lattice} \]
An organizing principle
3 bands, charge transfer insulator

Fratino et al. PRB 93, 245147 (2016)

FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pp} = 1.5$, which gives a total occupation $n_{tot}$ equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting total density of states. Color corresponds to the $d$-character of the hybridised bands. The band crossing the Fermi level has mostly oxygen character.
3 bands, charge transfer insulator

Fratino et al. PRB 93, 245147 (2016)
Organics: Phase diagram, finite T

Made possible by algorithmic improvements

P. Sémon et al.
PRB 85, 201101(R) (2012)
PRB 90 075149 (2014);
and PRB 89, 165113 (2014)
Phase diagram for organics

Phase diagram \((X=\text{Cu}[\text{N(CN)}_2]\text{Cl})\)

F. Kagawa, K. Miyagawa, + K. Kanoda

B_g for \(C_{2h}\) and \(B_{2g}\) for \(D_{2h}\)
Powell, McKenzie cond-mat/0607078

Anisotropic triangular lattice

See: Poster Shaheen Acheche
Phase diagram at $n = 1$

$X = Cu_2(CN)_3 \ (t' \sim t)$


Superconductivity near the Mott transition

\[ n = 1, \, d = 2 \text{ square lattice} \]
Superconductivity near the Mott transition

\[ n = 1, \ d = 2 \] square lattice
Superconductivity near Mott transition ($n = 1$)

C.-D. Hébert, P. Sémon, A.-M.S. T PRB 92, 195112 (2015)
Doped Organics
Doped BEDT

Doped organics

\[ n = 1, \ d = 2 \] square lattice
Doped organics

\[ n = 1, \ d = 2 \] square lattice
First order and Widom line in organics

G. Sordi et al. Scientific Reports, 2, 547 (2012)

Compare: T. Watanabe, H. Yokoyama and M. Ogata

C.-D. Hébert, P. Sémon, A.-M.S. T PRB 92, 195112 (2015)
Doped BEDT

$t' = 0.4t$ overview

Compare: T. Watanabe, H. Yokoyama and M. Ogata
Generic case highly frustrated case
Summary: organics

• Agreement with experiment
  • SC: larger $T_c$ and broader $P$ range if doped
  • Larger frustration: Decrease $T_N$ much more than $T_c$
  • Normal state metal to pseudogap crossover

• Predictions
  • First order transition at low $T$ in normal state (B induced)
  • Crossovers in SC state associated with normal state.

• Physics
  • SC dome without an AFM QCP. Extension of Mott
  • SC from short range $J$.
  • $T_c$ dome maximum near normal state 1st order
Pairing mechanism

Back to high $T_c$
$\Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta p'}{E_{p'}} \left( 1 - 2n\left(E_{p'}\right) \right)$

Exchange of spin waves?
Kohn-Luttinger
$T_c$ with pressure

Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).

A cartoon strong coupling picture

\[ J \sum_{\langle i,j \rangle} S_i \cdot S_j = J \sum_{\langle i,j \rangle} \left( \frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left( \frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right) \]

\[ d = \langle \hat{d} \rangle = \frac{1}{N} \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} ^\dagger c_{-\vec{k},\downarrow} \rangle \]

\[ H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0 \]

Pitaevskii Brückner:
Pair state orthogonal to repulsive core of Coulomb interaction

Miyake, Schmitt–Rink, and Varma  P.R. B 34, 6554-6556 (1986)
More sophisticated Slave Boson: Kotliar Liu PRB 1988
Extended Hubbard model

\[ \hat{H} = -t \sum_{\langle i,j \rangle \sigma} \left( \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + c.h. \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_i \hat{n}_i \]
Strongly correlated: From $J$, yet retarded

Antagonistic effects of $V$ at finite $T$

$$J = \frac{4t^2}{U - V}$$

$\mathcal{A}_n(\omega)$

$\mathcal{C}^+_{SC}$

$\mathcal{C}^-_{SC}$

A. Reymbaut et al. PRB 94 155146 (2016)
Summary

• AFM QCP for a heavy-fermion model
• No QCP: First order transition that extends Mott physics away from half-filling
• Is an organizing principle for
  – The normal and superconducting states
  – Cuprates and organics are examples
  – Predictions for organics
• Mechanism: $J$ short-range
Mammouth

 Merci

Thank you

A.-M.S. Tremblay

“Strongly correlated superconductivity”


Verlag des Forschungszentrum Jülich, 2013
Collaborators for this work

Charles-David Hébert

Patrick Sémon

Wei Wu
Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets
Weak vs Strong correlations

\[ n = 1, \text{ unfrustrated } d = 3 \text{ cubic lattice} \]

\[ J = \frac{4t^2}{U} \]

Mott

Heisenberg

Slater

AFM

T

U
Local moment and Mott transition

$n = 1, d = 2$ square lattice

Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

Critical point visible in $V_2O_3$, $BEDT$ organics
Doped organic: experiment
Doped BEDT

Doped BEDT

Method

Concept: Cluster - DMFT
Tools: Impurity solver
CTQMC impurity solver (tool) \((T \text{ finite})\)

Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

\[ Z = \int D[\psi^\dagger, \psi] e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_K \psi_k^\dagger(\tau) \Delta(\tau, \tau') \psi_K(\tau')} \]

\[ \Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) \]

\[ - \left[ \sum_k \frac{1}{i\omega_n + \mu - t_c(\vec{k}) - \Sigma_c(i\omega_n)} \right]^{-1} \]

P. Sémon \textit{et al.}
PRB 85, 201101(R) (2012)
PRB 90 075149 (2014);
and PRB 89, 165113 (2014)