Unconventional superconductivity with and without an antiferromagnetic quantum critical point

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Quantum criticality and topology in itinerant electron systems
15 to 19 August 2016
Magnetic superconductivity
Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

Canfield et al. (2010)
Heavy fermions

3D metals tuned by pressure, field or concentration

Heavy fermions

$\text{CeRhIn}_5$

Magnetic superconductivity

Quantum criticality

$\text{CeRhIn}_5$

$T_N$, $p_c = 2.5 \text{ GPa}$

$T_c$

$\rho_0^*$

Knebel et al. (2009)

Mathur et al., Nature 1998
Method for strongly correlated matter

Dynamical Mean Field Theory (+ clusters)

Concept: atomic localized correlations consistent with delocalized aspect
Dynamical “variational” principle

\[ \Omega_t[G] = \Phi[G] - Tr[(G_{0t}^{-1} - G^{-1})G] + Tr \ln(-G) \]

\[ \Phi[G] = \text{\includegraphics[width=0.5\textwidth]{variational_principle.png}} \]

\[ \frac{\delta \Phi[G]}{\delta G} = \Sigma[G] \]

\[ \frac{\delta \Omega_t[G]}{\delta G} = \Sigma[G] - G_{0t}^{-1} + G^{-1} = 0 \]

DMFT

\[ \Phi[G] = \sum_{i} \Phi[G_{ii}(i\omega_n)] \]

Luttinger and Ward 1960, Baym and Kadanoff (1961)
Impurity solver

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

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
Some not Feynman diagrams
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)
+ 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

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

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

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

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

Mott

Heisenberg

AFM

U/t
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
One-band Hubbard model of BEDT organics


$t \approx 50$ meV

$\Rightarrow U \approx 400$ meV

$t'/t \sim 0.6 - 1.1$
Phase diagram at $n = 1$

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


Influence of Mott transition away from half-filling

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

3D plot with axes labeled \( \delta \), \( T \), and \( U \), showing the transition region labeled as M and I.
Influence of Mott transition away from half-filling

$n = 1, d = 2$ square lattice
\[ U = 6.2 \, t \] Normal state. Density of states
Density of states

Khosaka et al. *Science* **315**, 1380 (2007);
Spin susceptibility

![Graph showing the relationship between temperature (T) and susceptibility (χ(T)) for different values of δ. The graph includes markers for max_{σ} dn/dμ (Widom line), max_{σ} dA(ω=0)/dT, max_{σ} dχ(T)/dT, and max_{σ} |dProb[singlet]/dT|. The graph also highlights the transition from a Mott insulator to a pseudogap and a correlated Fermi liquid.]
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)
Plaquette eigenstates

See also:

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

PRB 80, 064501 (2009)
Crossovers inside the AFM phase

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

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

[Diagram showing phase transitions between Slater, AFM, Mott, and Heisenberg phases.]
Finite $T$ phase diagram
Superconductivity

Sordi et al. PRL 108, 216401 (2012)
Fratino et al.
n = 1, d = 2 square lattice
An organizing principle

Fratino et al.
Sci. Rep. 6, 22715
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 $t_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, 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)
Anisotropic triangular lattice
Superconductivity near the Mott transition

\[ n = 1, \ d = 2 \] square lattice
Phase diagram at $n = 1$

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

Y. Kurisaki, et al.

Effect of frustration on Mott transition \((n = 1)\)
Doped Organics
Doped organics

$n = 1, \, d = 2$ square lattice
Doped BEDT

Doped BEDT

\[ t' = 0.4t \]

Compare: T. Watanabe, H. Yokoyama and M. Ogata
\( t' = 0.4t \) overview

Compare: T. Watanabe, H. Yokoyama and M. Ogata
\[ t' = 0.8 \, t \]
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
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 (not shown)
André-Marie Tremblay

Sponsors:
C'est fini…
A.-M.S.T. Tremblay

“Strongly correlated superconductivity”
Verlag des Forschungszentrum Jülich, 2013


Merci
Thank you

A.-M.S. Tremblay