Supraconductivité avec et sans point critique quantique antiferromagnétique

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Institut quantique

Réunion inaugurale, LIA
Jouvence 27 octobre 2016

CIFAR
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VERITATEM IN CHARITATE

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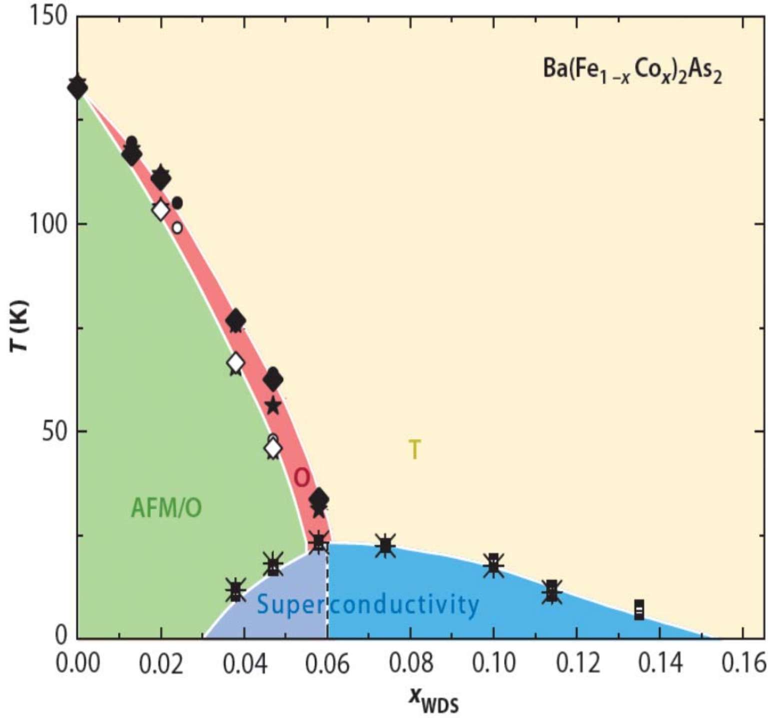
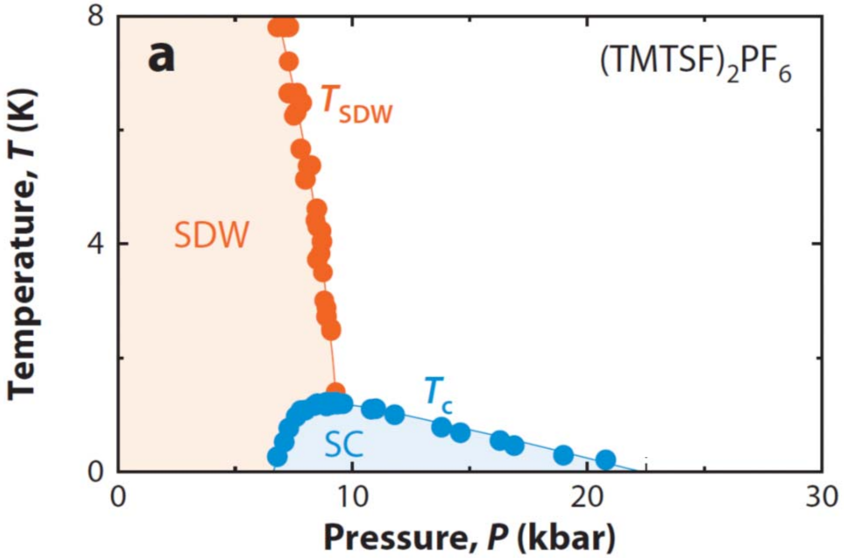
Pnictides and organics

Pnictides



Bechgaard salts



The Archetype

Magnetic superconductivity

Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

Canfield et al. (2010)

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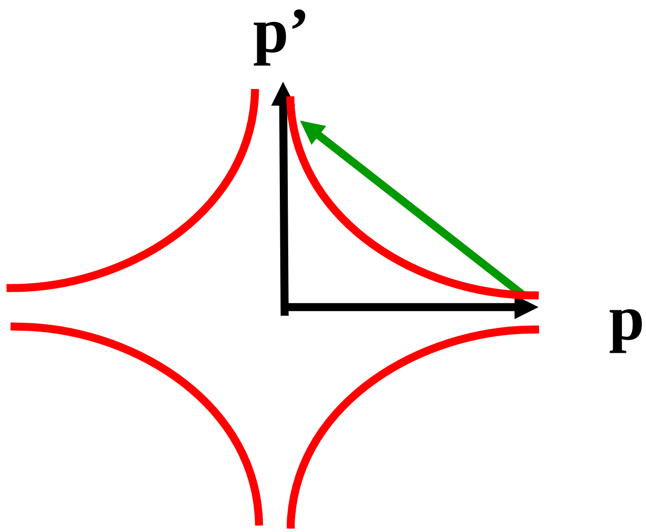
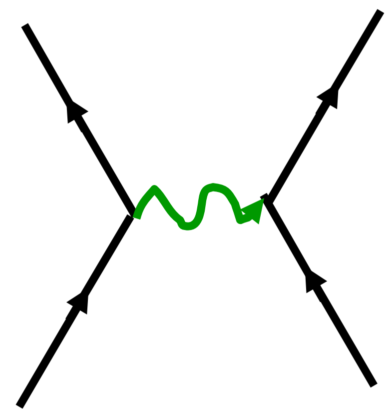
Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





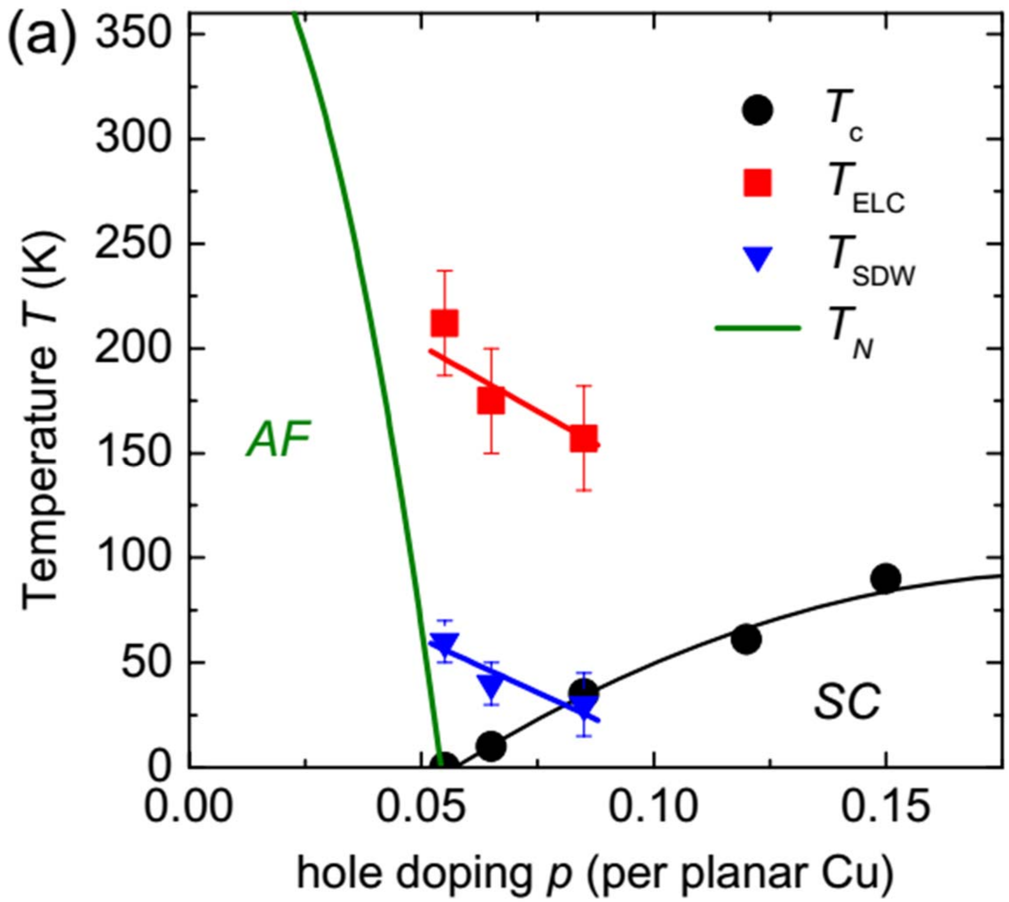
Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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).

P.W. Anderson Science 317, 1705 (2007)

High temperature superconductors



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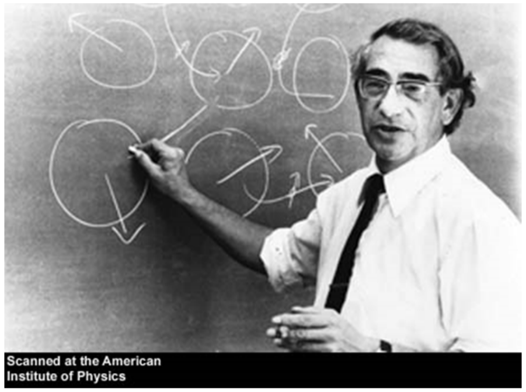
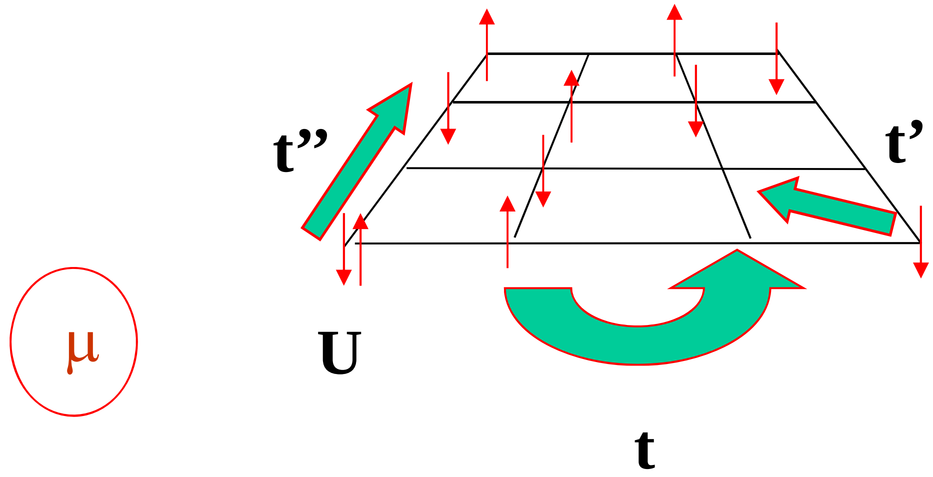
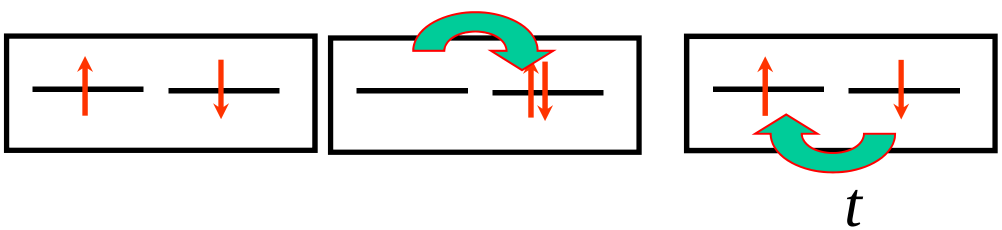
Hubbard model





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

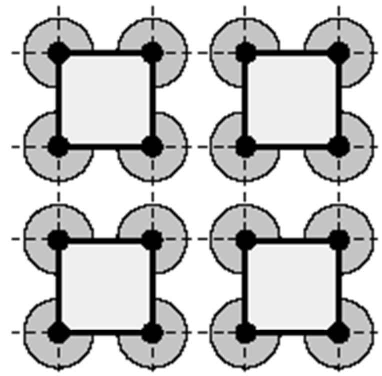
Method for strongly correlated matter

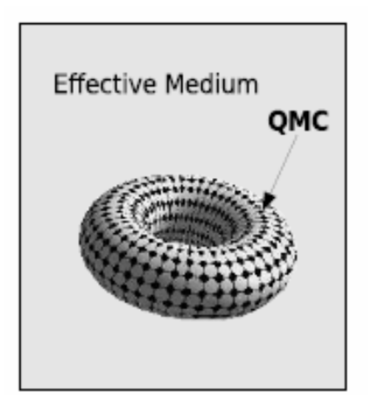
Dynamical Mean Field Theory (+ clusters)

Concept: atomic localized correlations consistent with delocalized aspect

2d Hubbard: Quantum cluster method

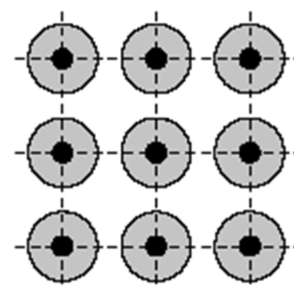
C-DMFT





DCA

DMFT



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

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

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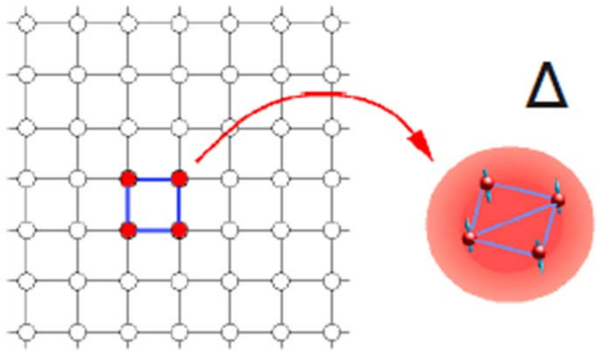
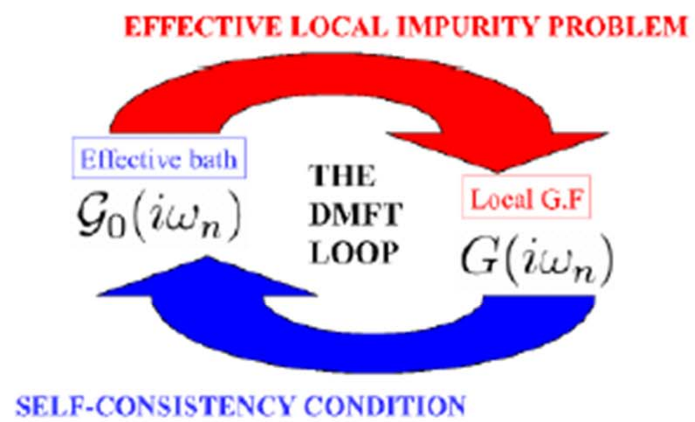
Impurity solver

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





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

$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

+ 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

Wei Wu

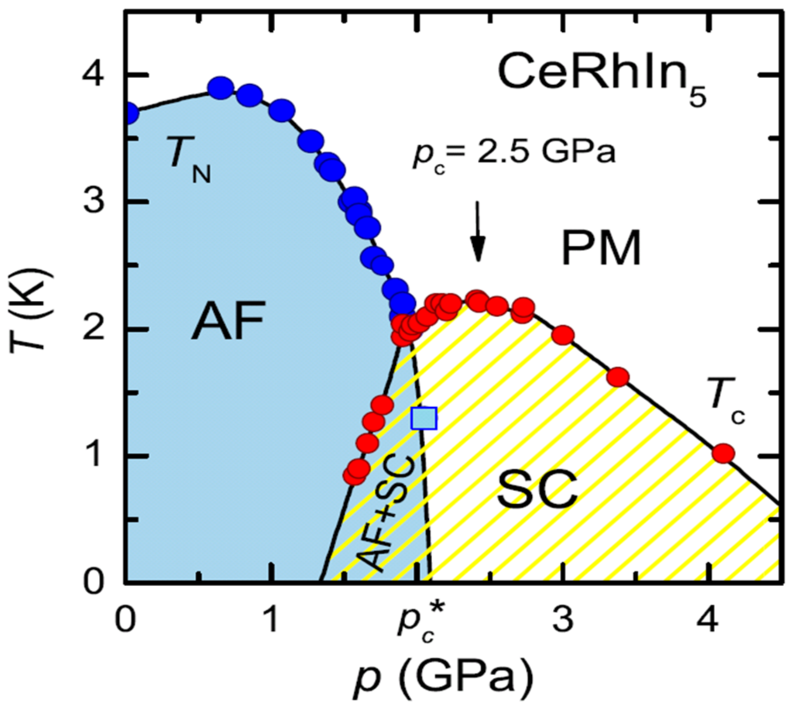
Superconductivity around an AFM quantum critical point

A heavy fermion example

W. Wu A.-M.S.T. Phys. Rev. X, 2015

Heavy fermions

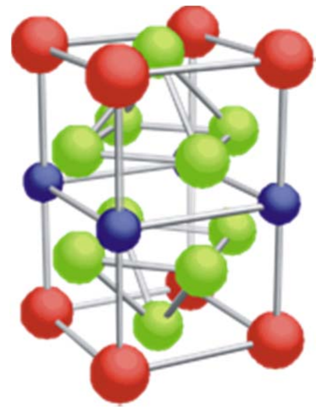
Heavy fermions **3D metals tuned by pressure, field or concentration**



Knebel et al. (2009)

Quantum criticality

$CeRhIn_5$

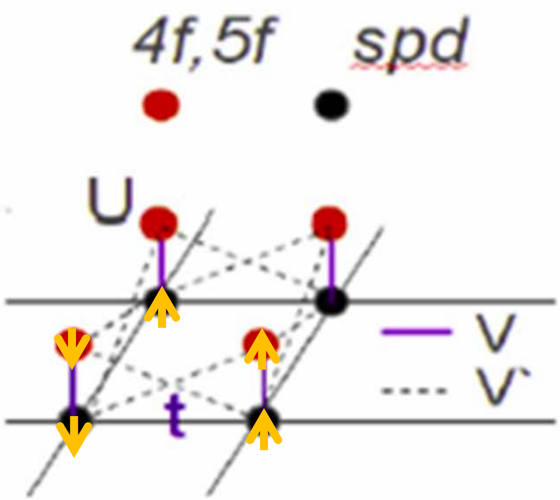


Magnetic superconductivity

Mathur et al., Nature 1998

Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$
$$+ \sum_{k,\sigma} V_k (f^\dagger_{k,\sigma} c_{k,\sigma} + \mathrm{H.c.}) + \sum_i U \left(n_f^\uparrow - \frac{1}{2} \right) \left(n_f^\downarrow - \frac{1}{2} \right)$$



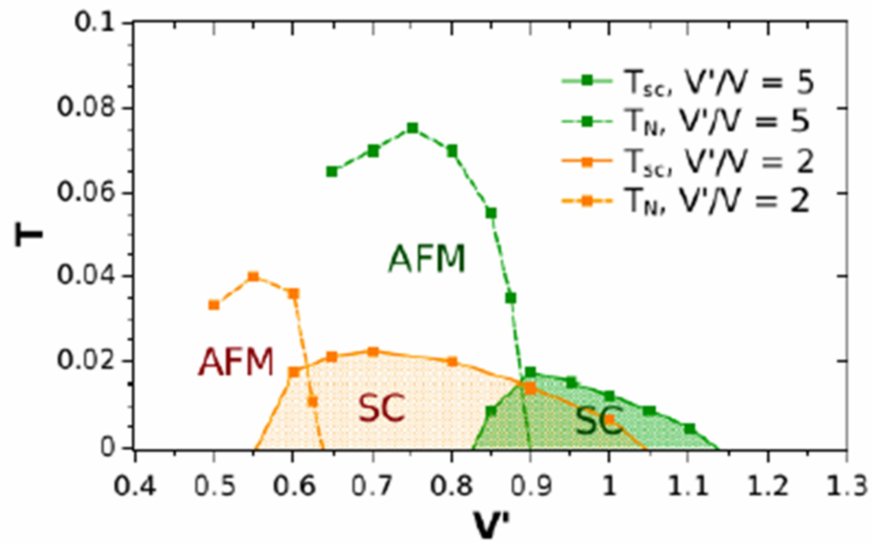
W. Wu A.-M.S.T. Phys. Rev. X, 2015

Phase diagram

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2 : more frustrated case
V'/V = 5 : less frustrated case

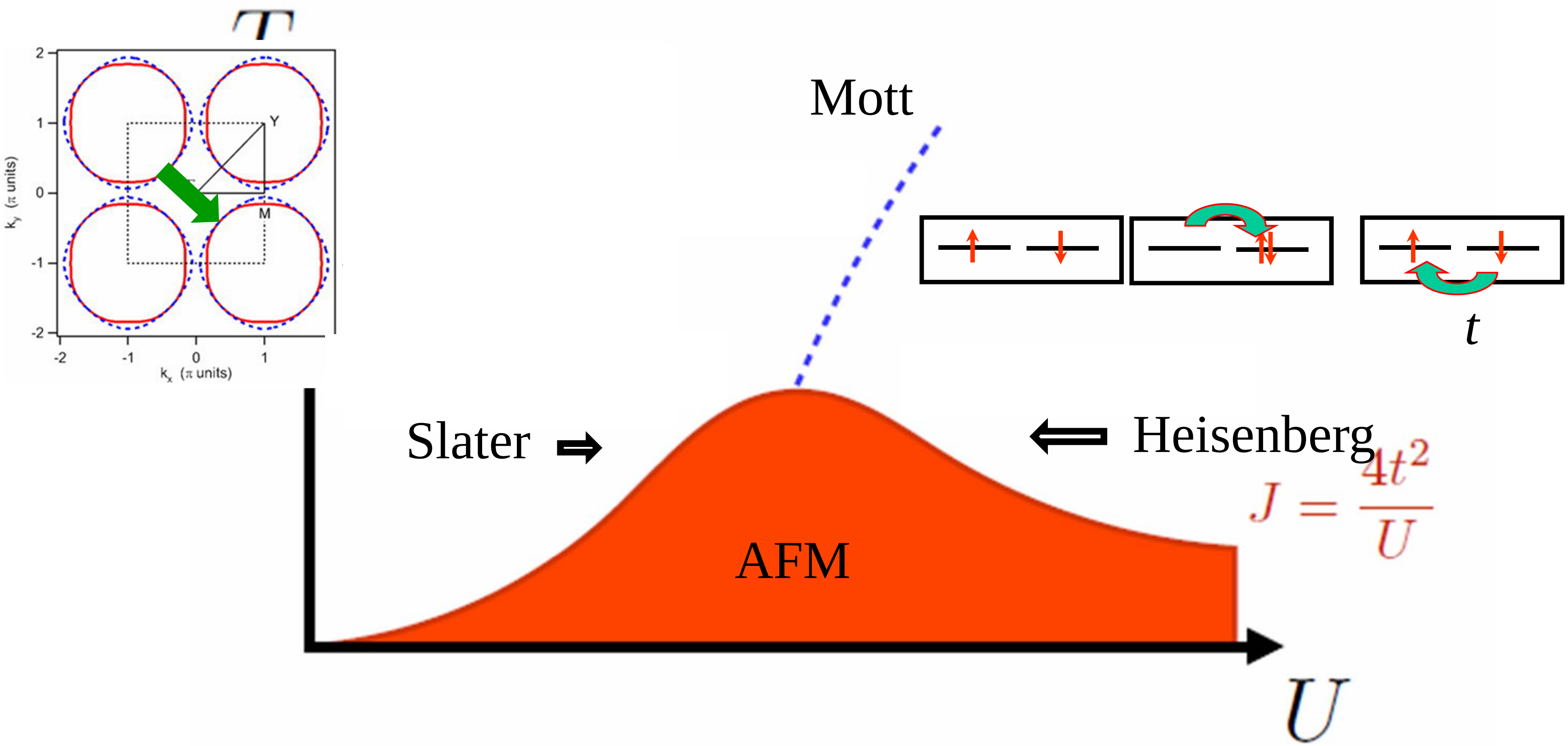


Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

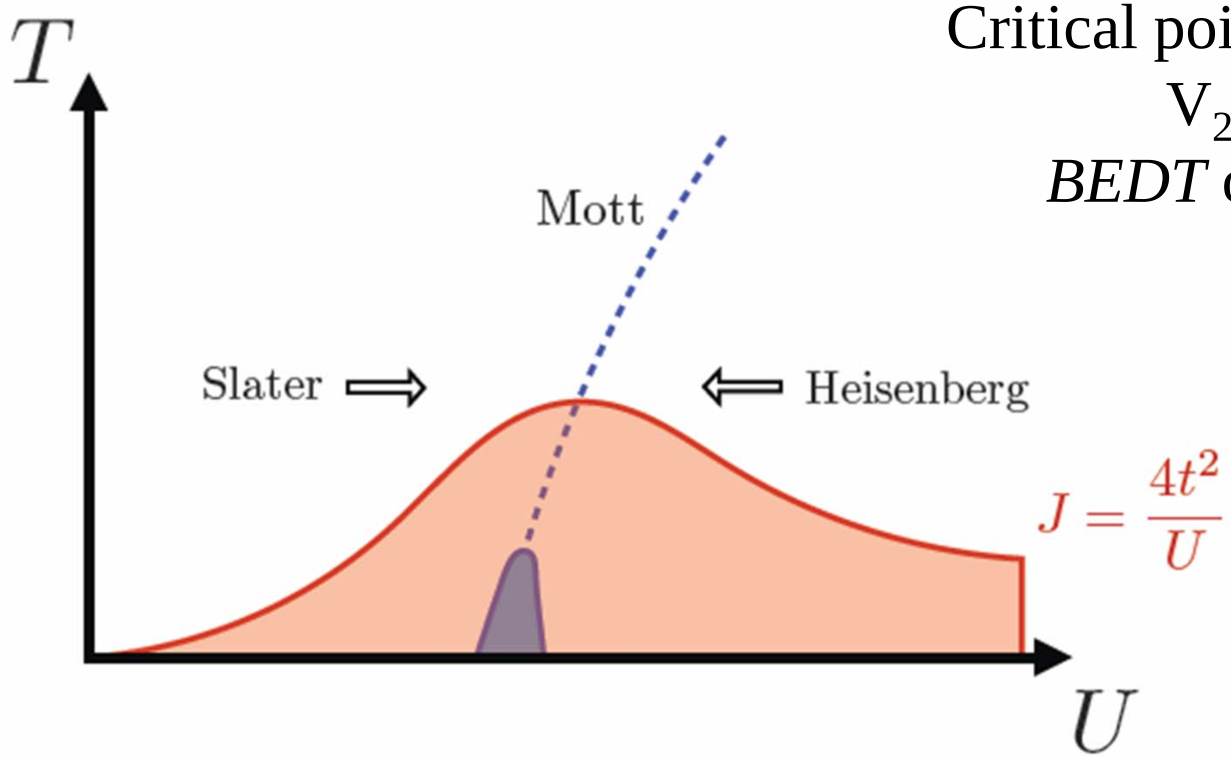
Weak vs Strong correlations

n = 1, unfrustrated *d = 3* cubic lattice



Local moment and Mott transition

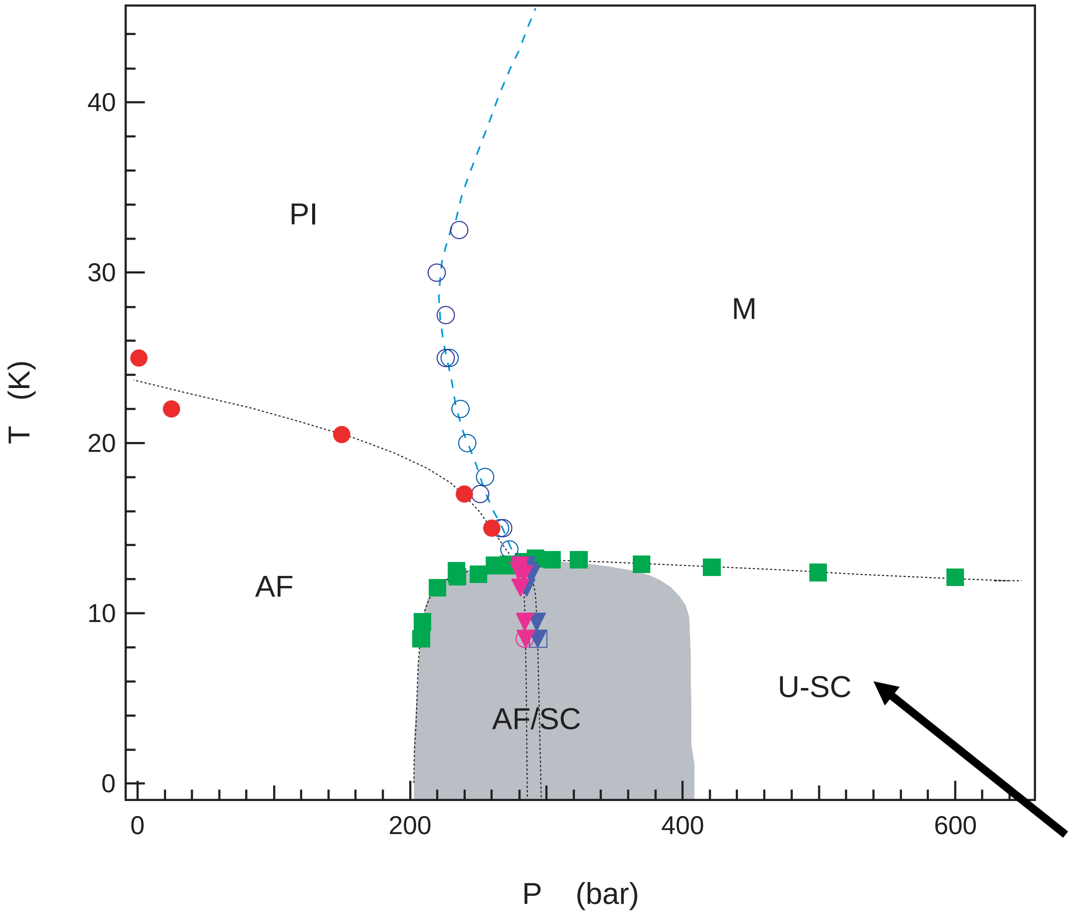
n = *1*, *d* = *2* square lattice



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



F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

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

Powell, McKenzie cond-mat/0607078

Phase diagram (X=$Cu[N(CN)_2]Cl$)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

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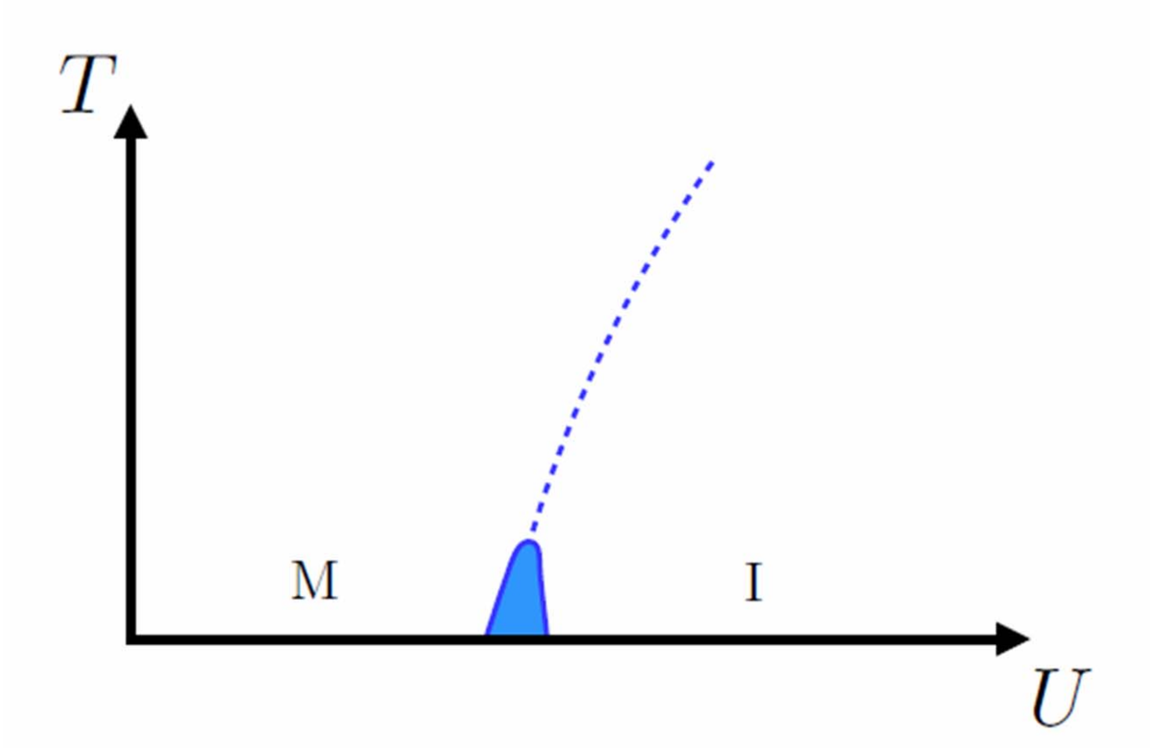
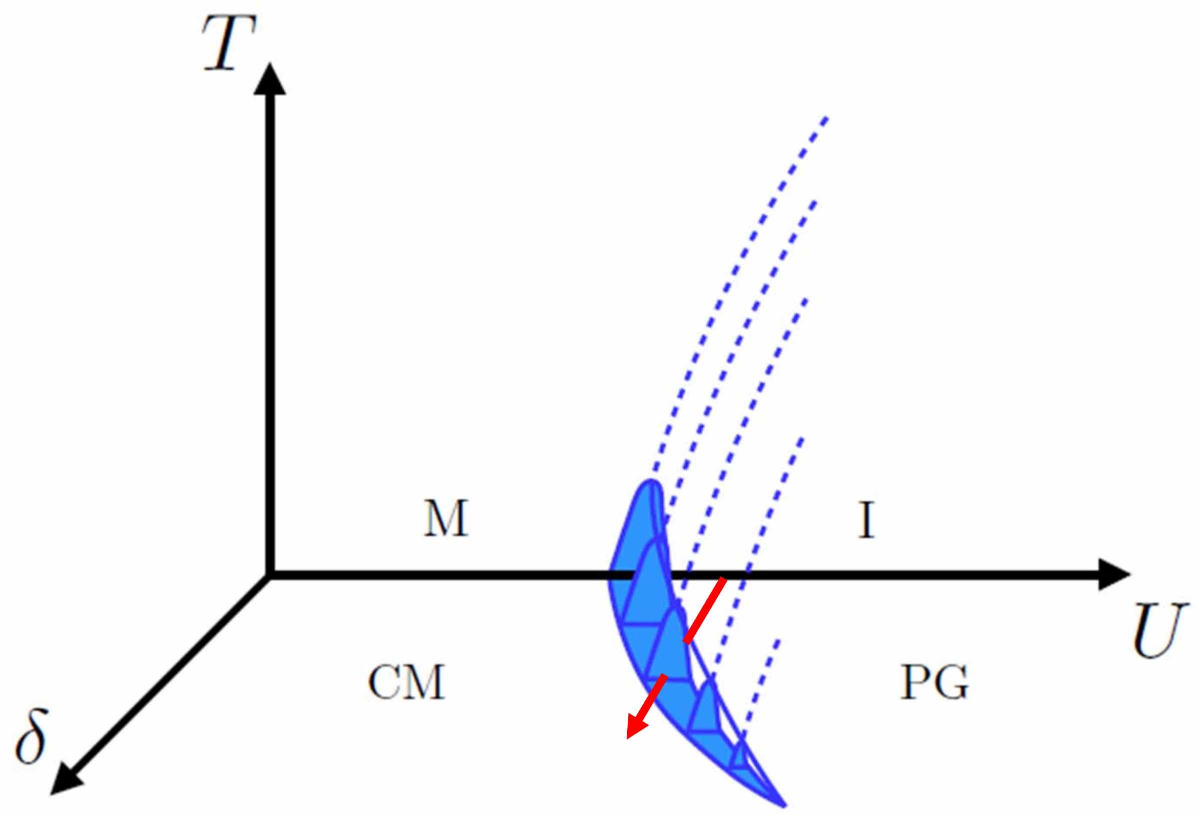
Influence of Mott transition away from half-filling

$n = 1, d = 2$ square lattice

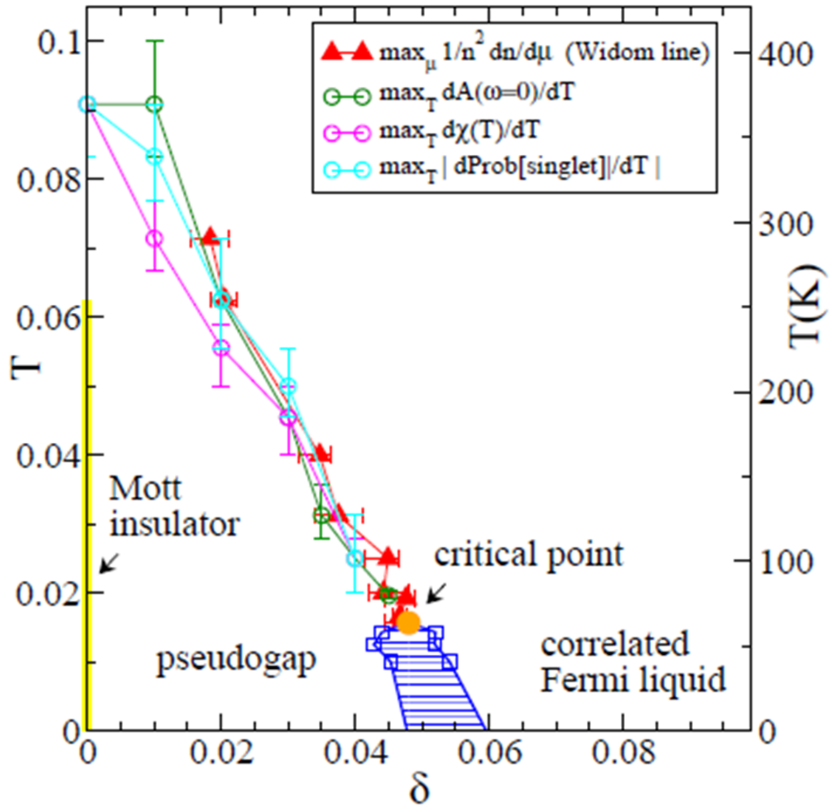


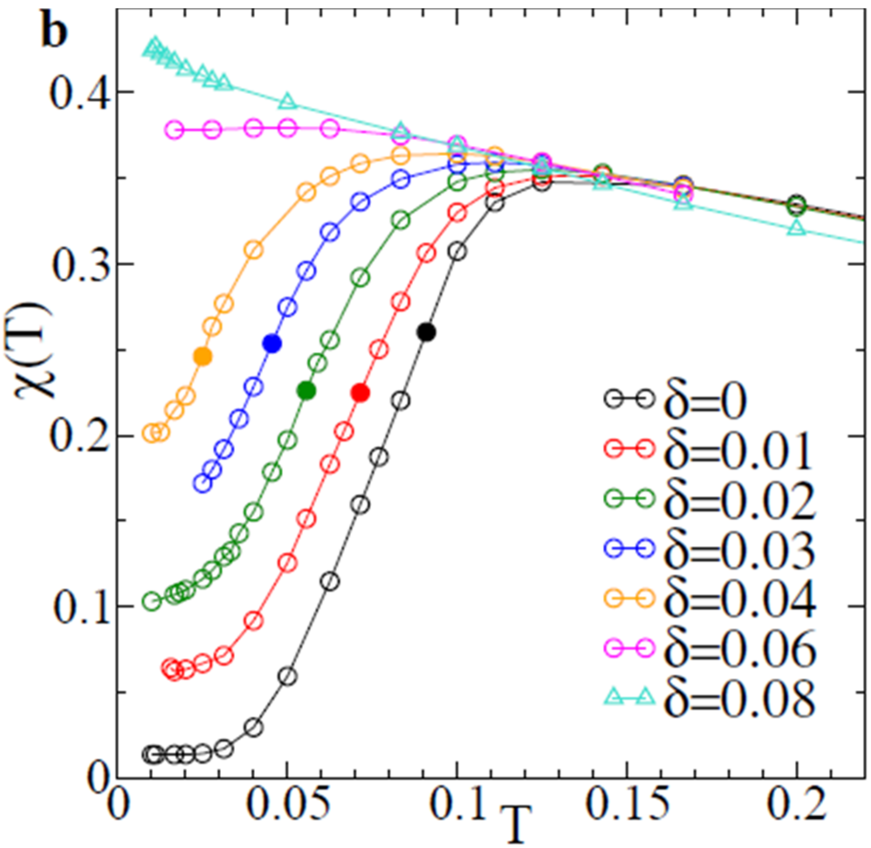
Influence of Mott transition away from half-filling

n = 1, *d = 2* square lattice



Spin susceptibility





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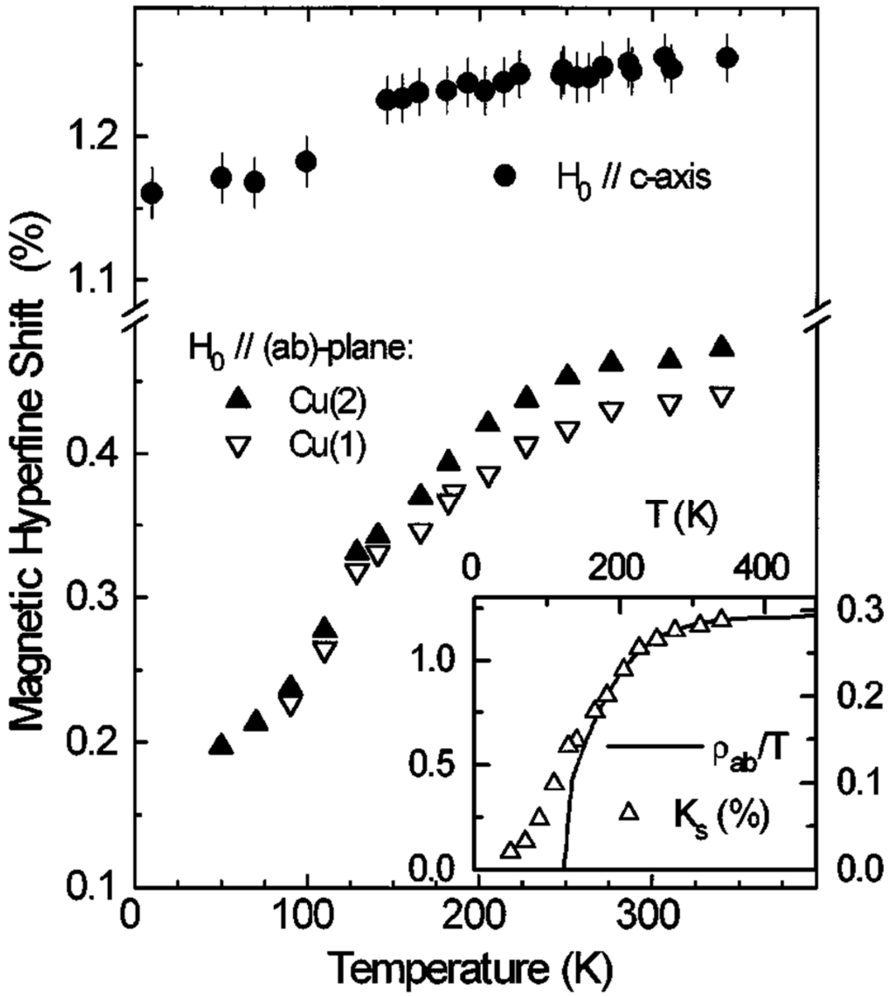
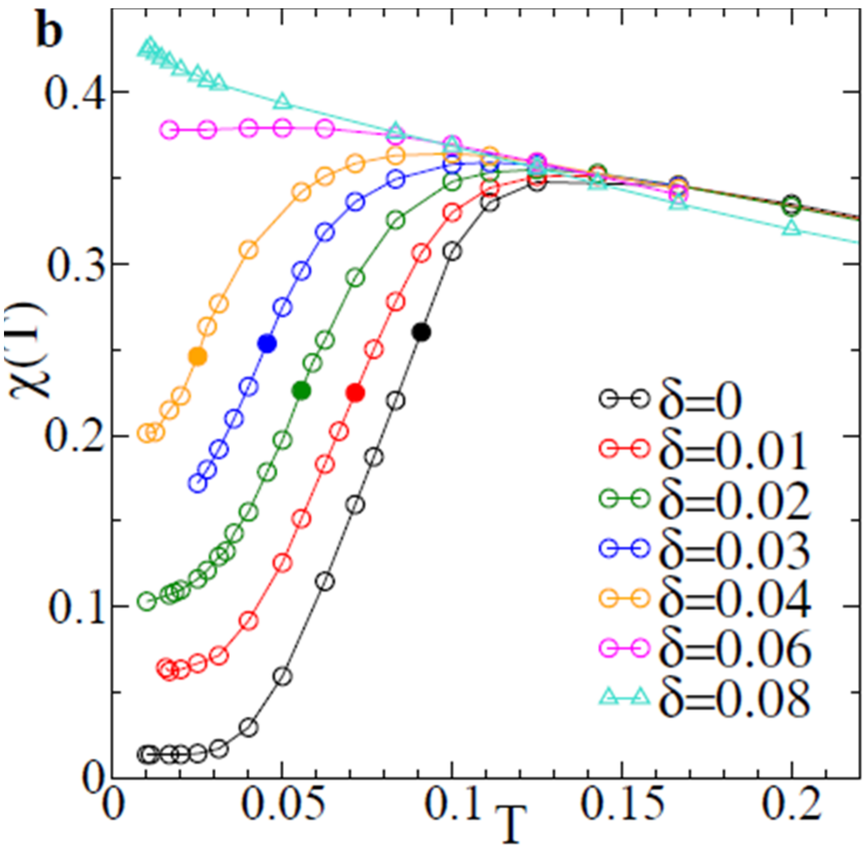
Spin susceptibility





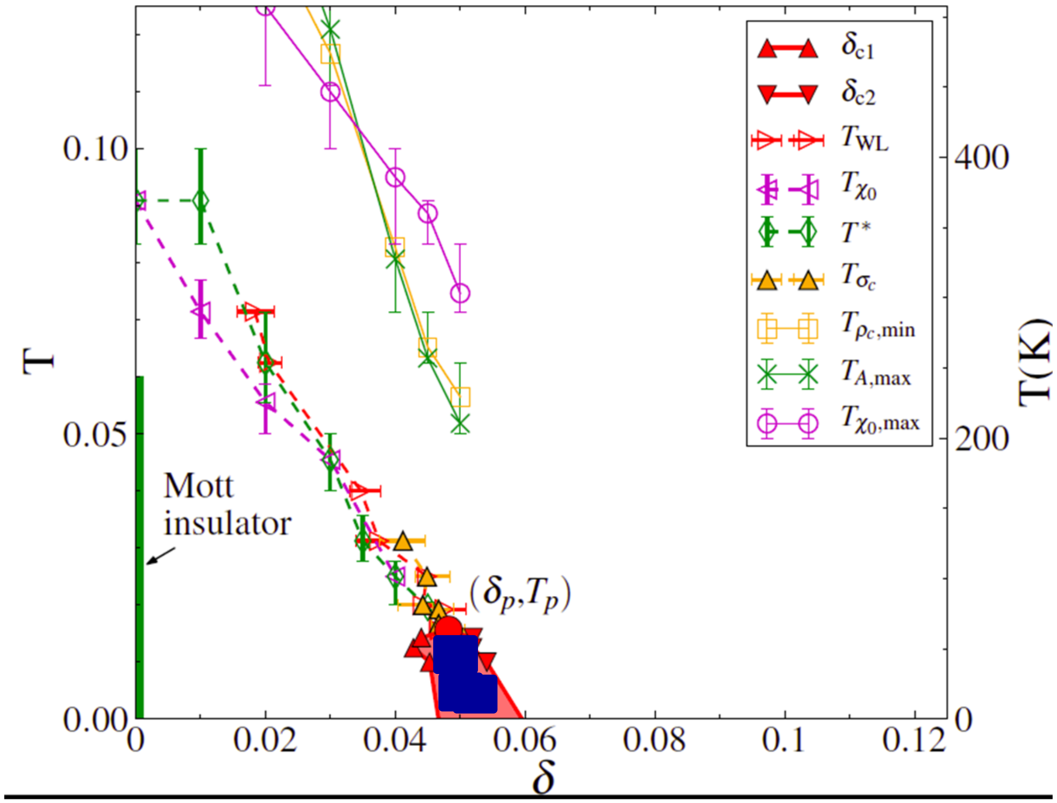
Underdoped Hg1223

Julien et al. PRL **76,** 4238 (1996)

Two crossover lines

Giovanni Sordi

Patrick Sémon



G. Sordi et al. Phys. Rev. Lett. 108, 216401/1-6 (2012)
P. Sémon, G. Sordi, A.-M.S.T., Phys. Rev. B **89**, 165113/1-6 (2014)

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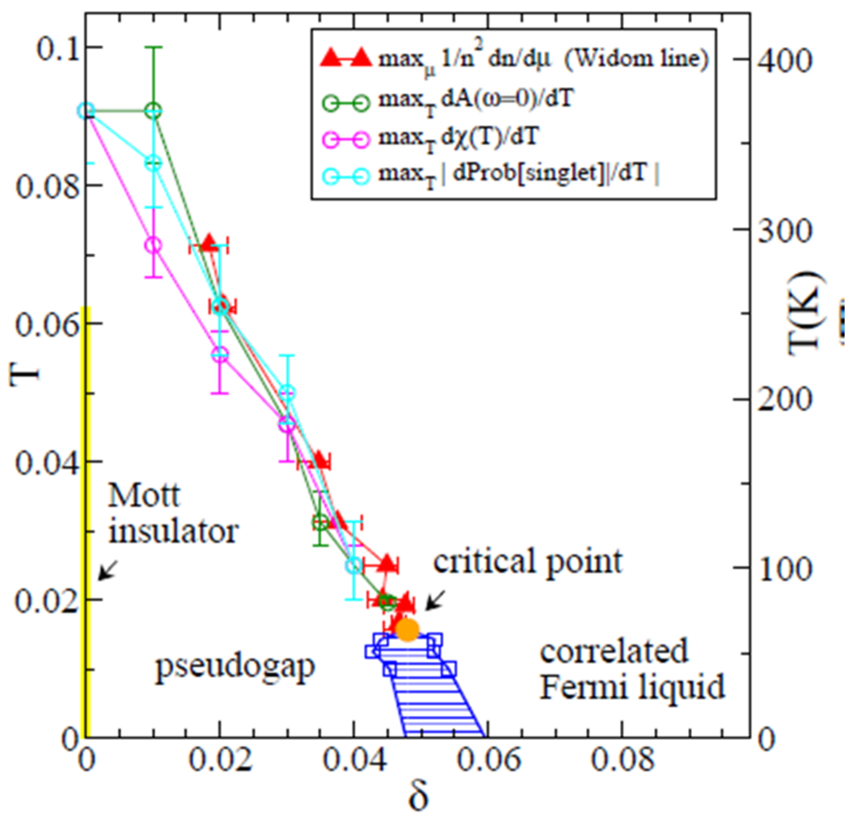
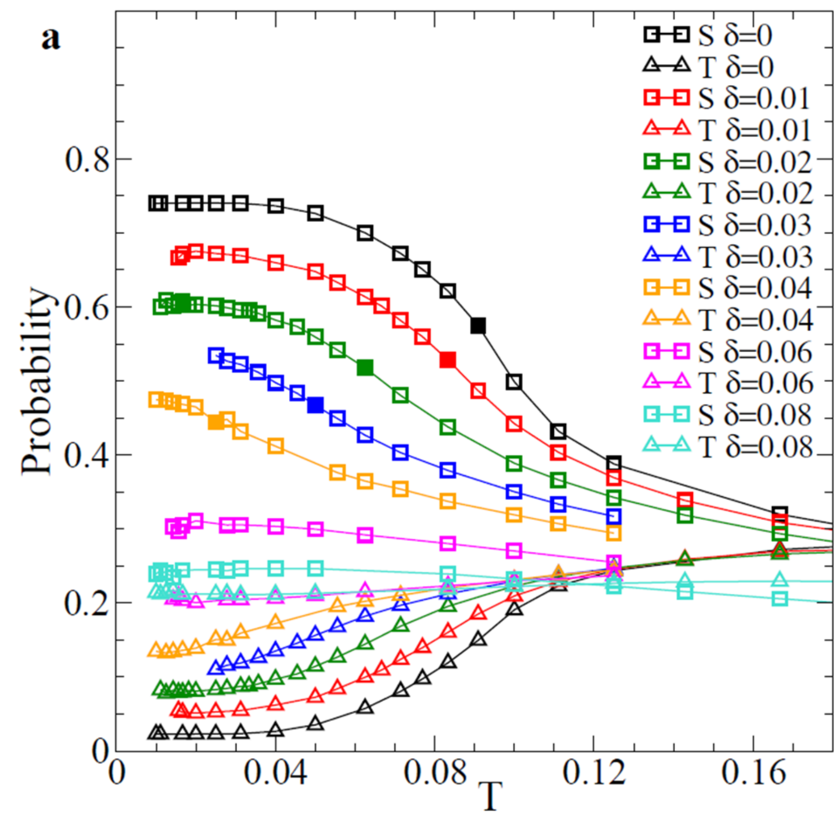
Physics

Plaquette eigenstates





See also:

Michel Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges
PRB **80**, 064501 (2009)

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Giovanni Sordi

Patrick Sémon

Lorenzo Fratino

Finite *T* phase diagram
Superconductivity

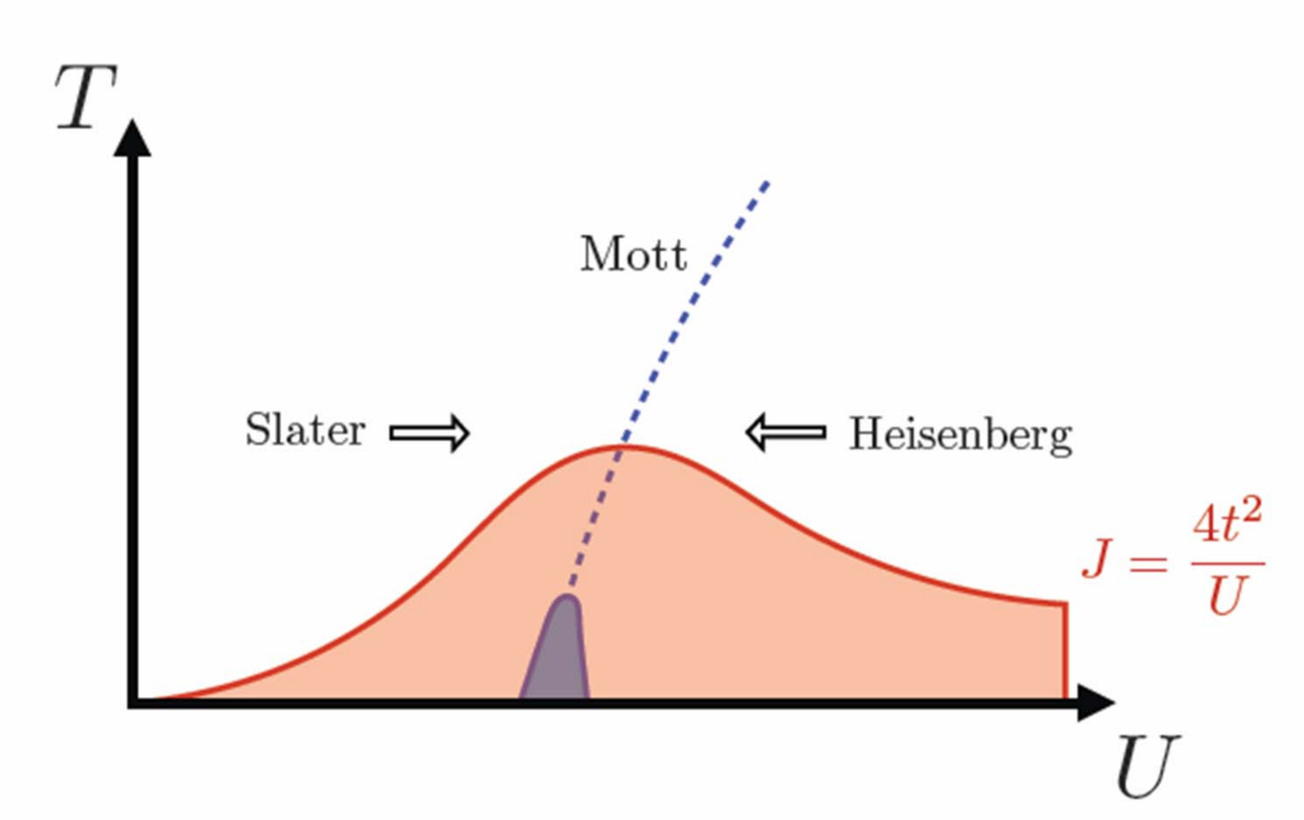
Sordi et al. PRL **108**, 216401 (2012)

Fratino et al.

Sci. Rep. **6**, 22715 (2016)

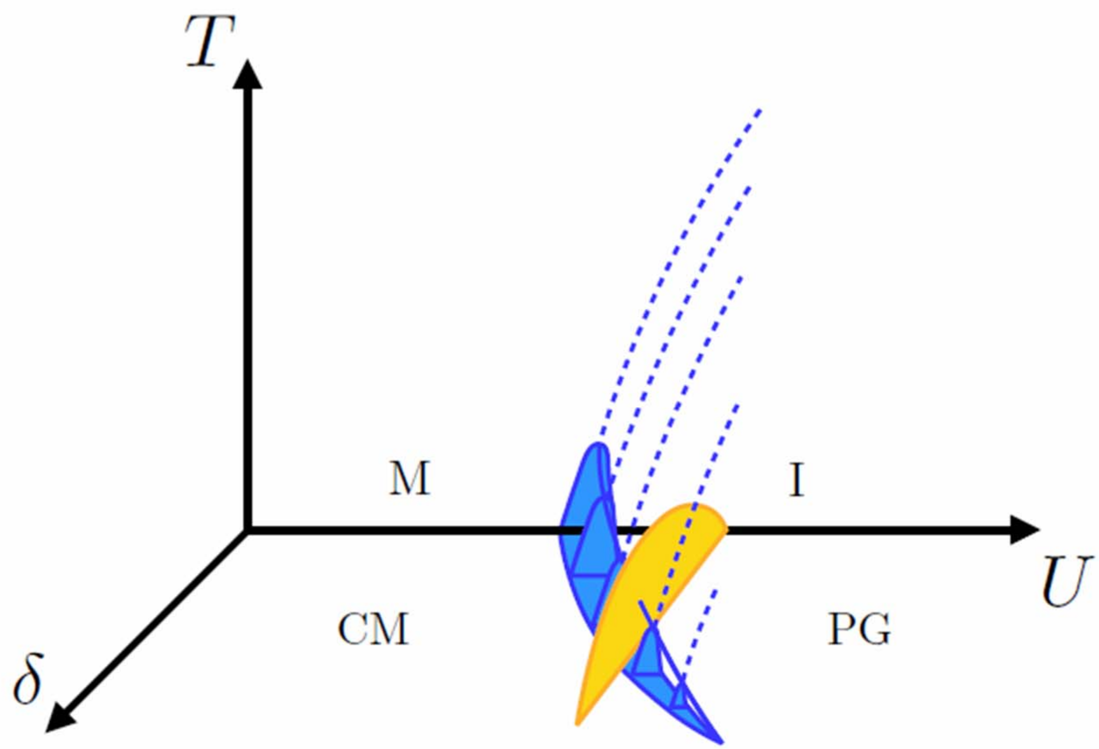
Crossovers inside the AFM phase

$n = 1$, unfrustrated $d = 3$ cubic lattice

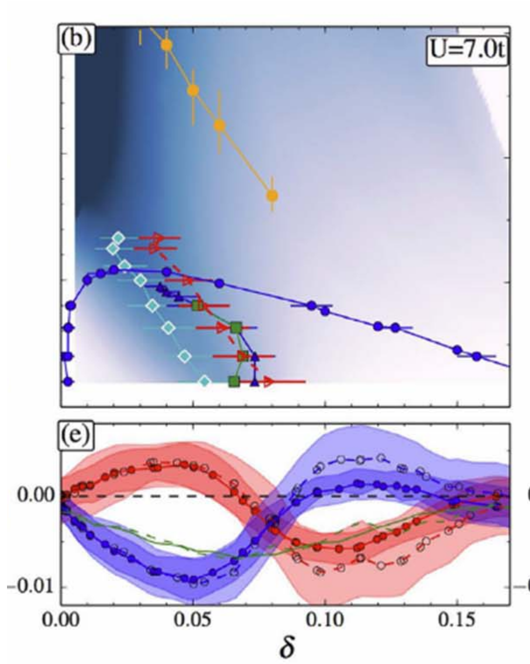


Superconductiviy in Doped Mott insulator

$n = 1, d = 2$ square lattice



An organizing principle



Fratino et al.
Sci. Rep. **6**, 22715

3 bands, charge transfer insulator

Fratino et al. PRB **93**, 245147 (2016)

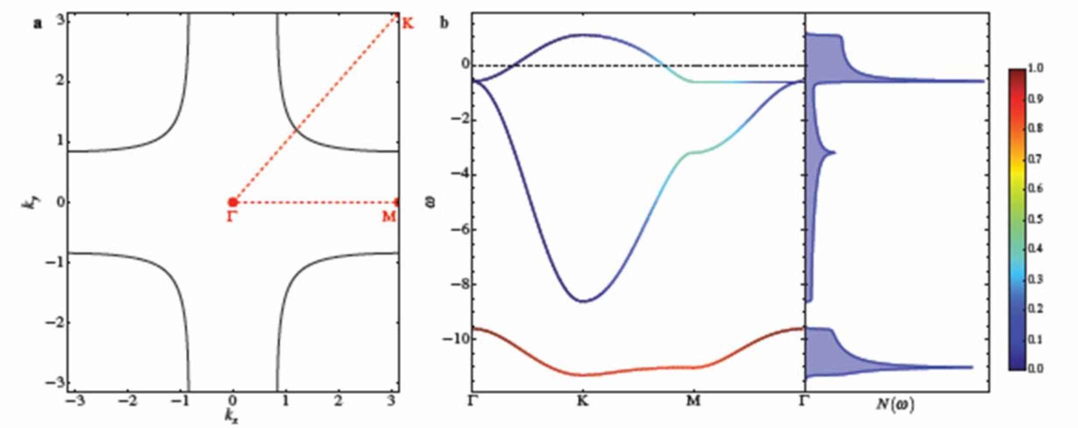
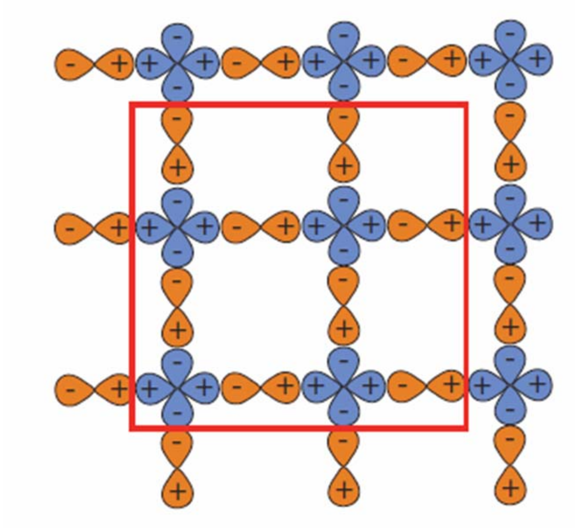


FIG. 2. (a) Noninteracting Fermi surface for the model parameter investigated in Fig. 1a of main text, namely $\epsilon_p = 9$, $t_{pp} = 1$, $t_{pd} = 1.5$, which gives a total occupation n_{tot} equal to five. (b) Non-interacting band structure for the same model parameter along with the resulting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

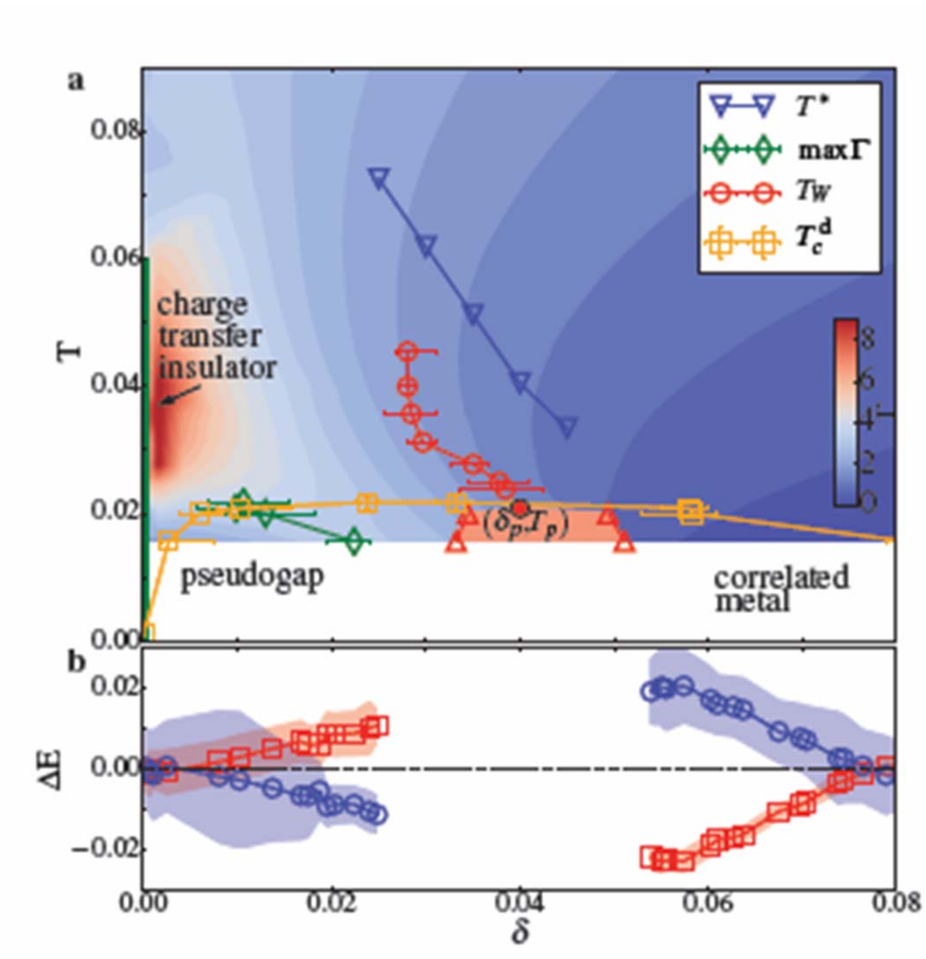


Giovanni Sordi

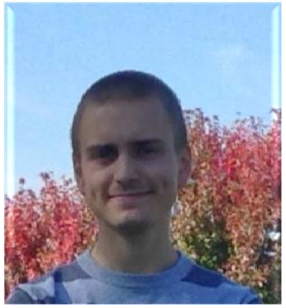
Lorenzo Fratino

Université de Sherbrooke

3 bands, charge transfer insulator



Fratino et al. PRB **93**, 245147 (2016)



Charles-David Hébert

Patrick Sémon

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)

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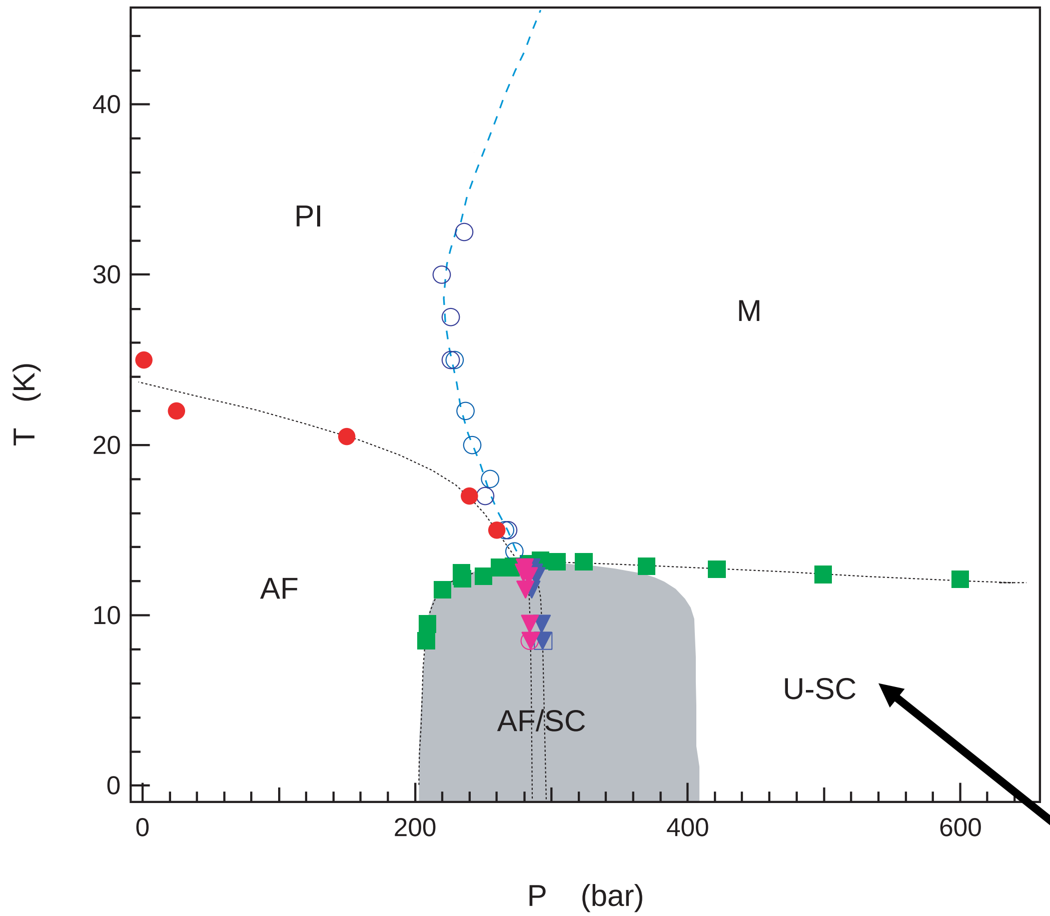
Phase diagram for organics



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

PRB **69** (2004) +Nature **436** (2005)

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

Powell, McKenzie cond-mat/0607078

Phase diagram (X=$Cu[N(CN)_2]Cl$)

S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

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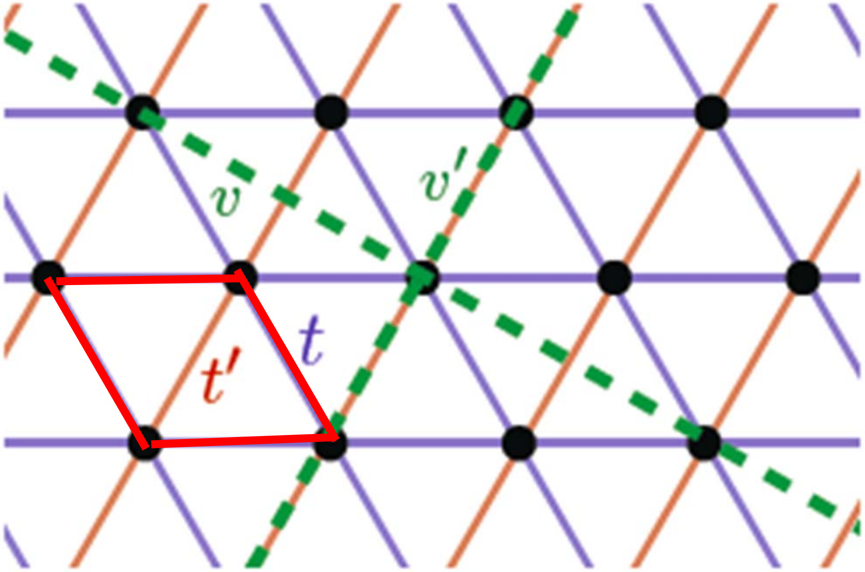
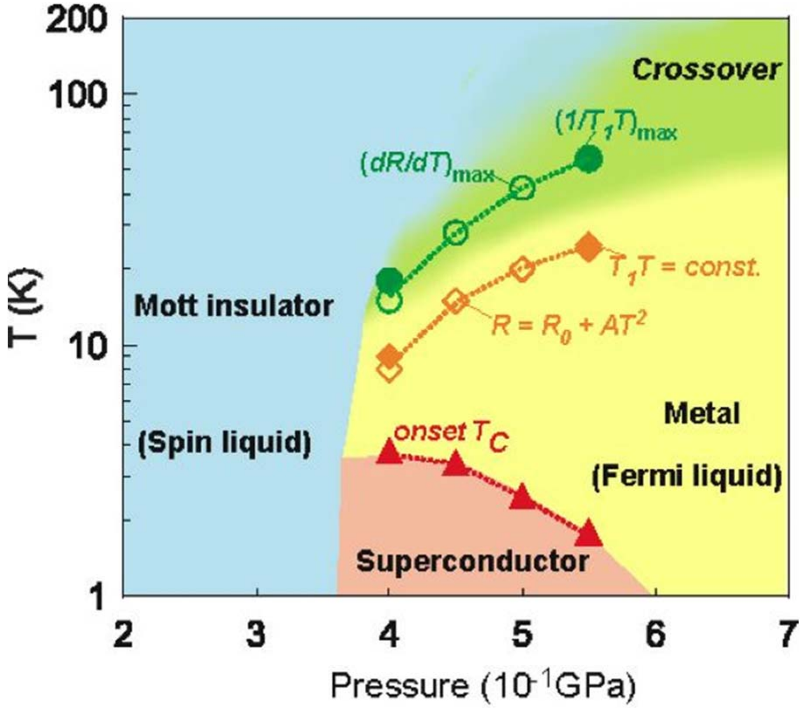
Anisotropic triangular lattice



See: Poster Shaheen Acheche

Phase diagram at $n = 1$

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

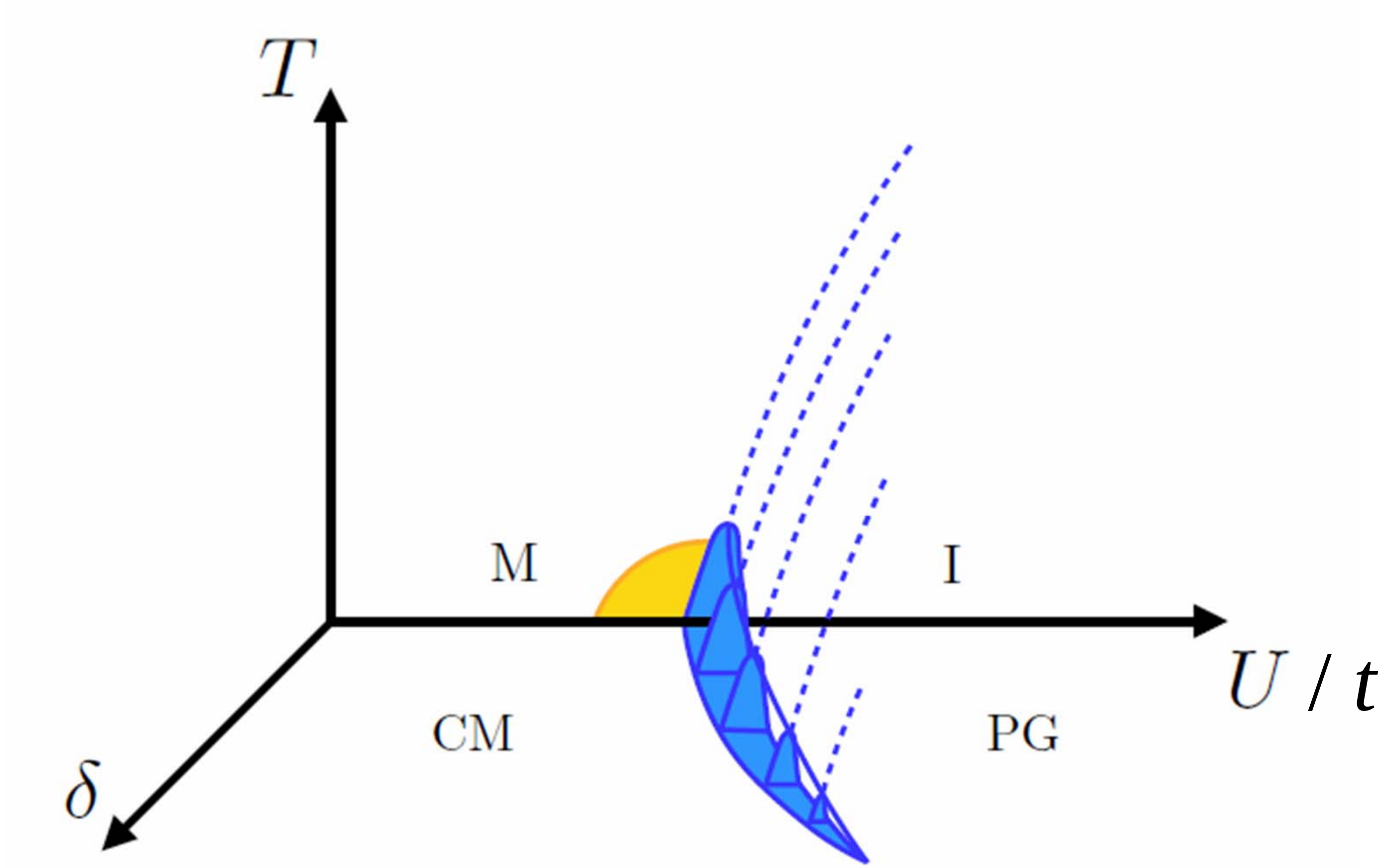


Y. Kurisaki, et al.
Phys. Rev. Lett. **95**, 177001(2005)

Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

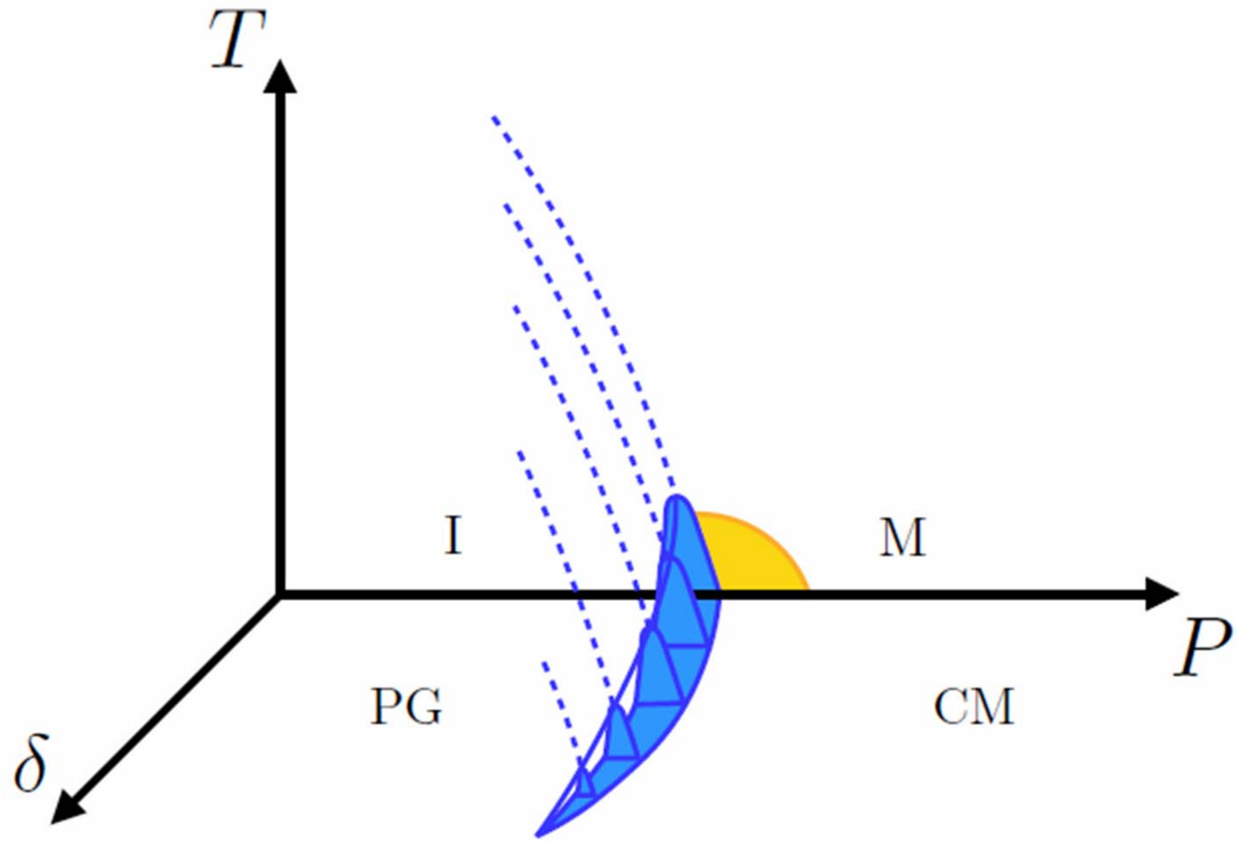
Superconductivity near the Mott transition

n = 1, d = 2 square lattice



Superconductivity near the Mott transition

n = 1, d = 2 square lattice



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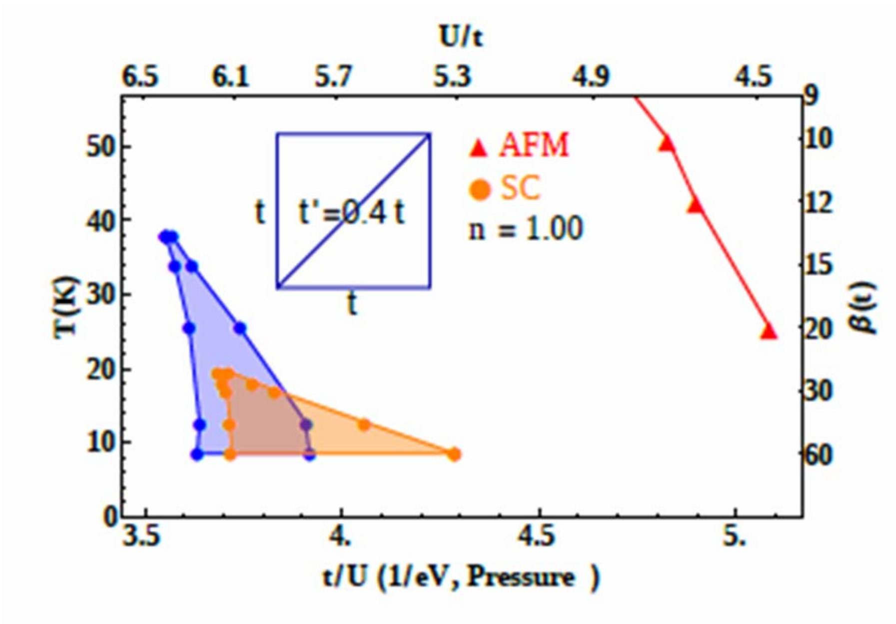
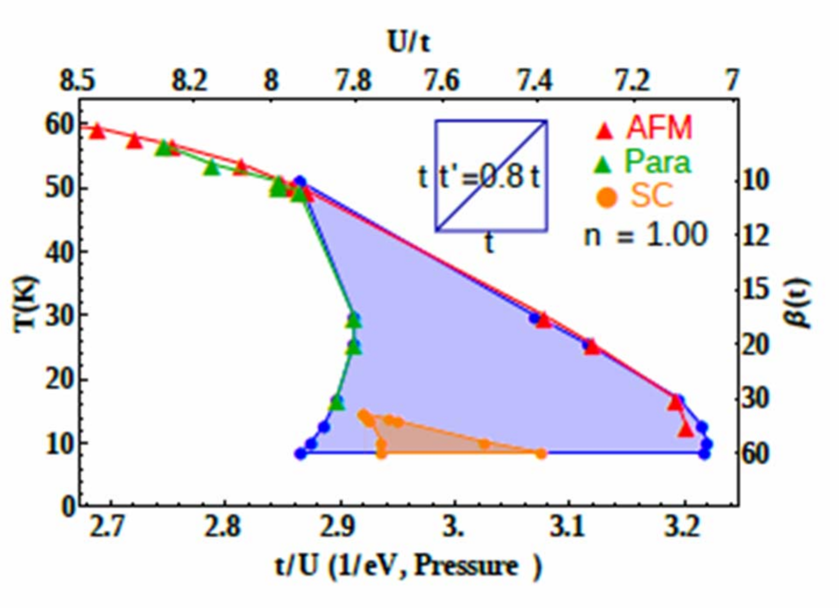
Superconductivity near Mott transition (*n = 1*)





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

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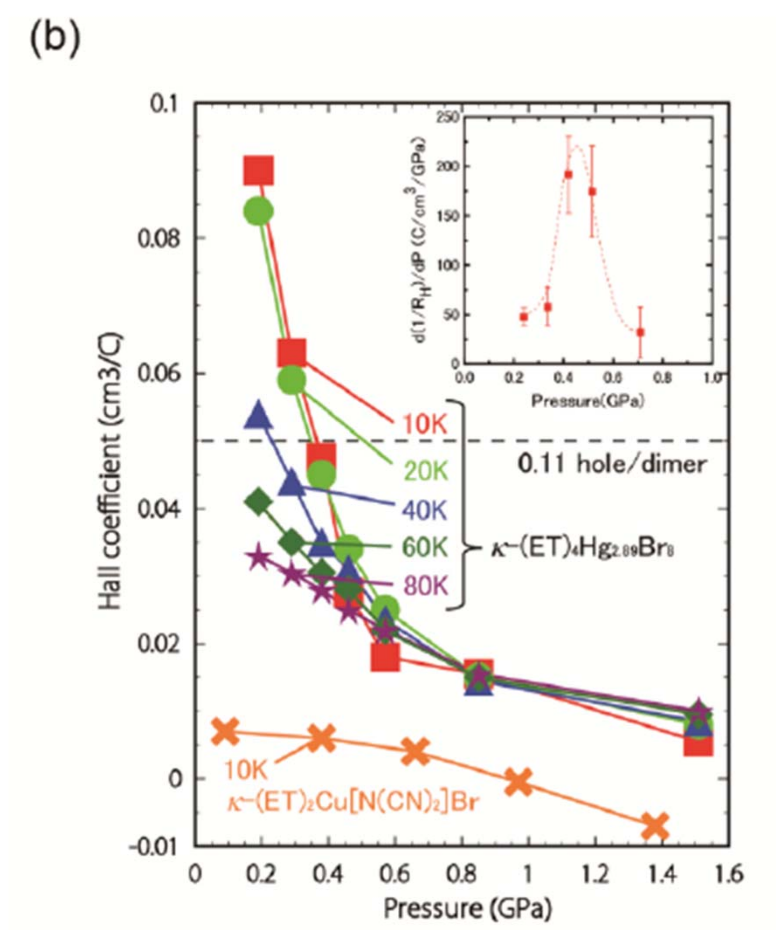
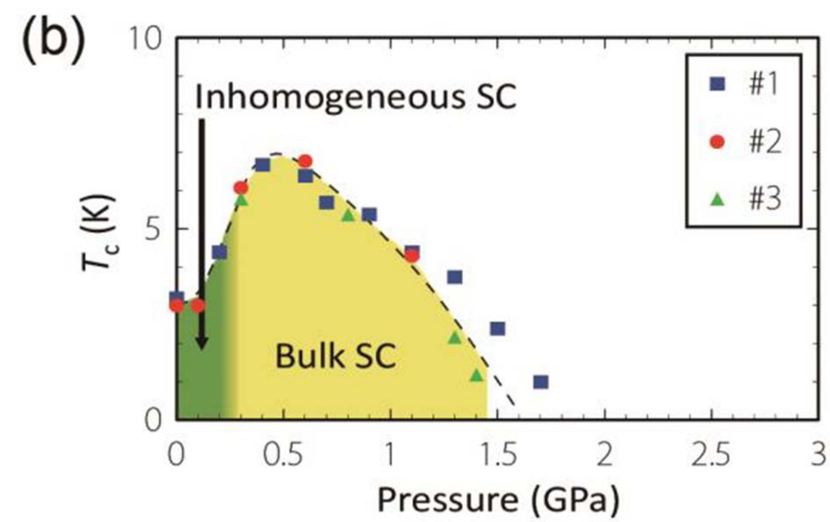
Doped Organics

Doped BEDT





H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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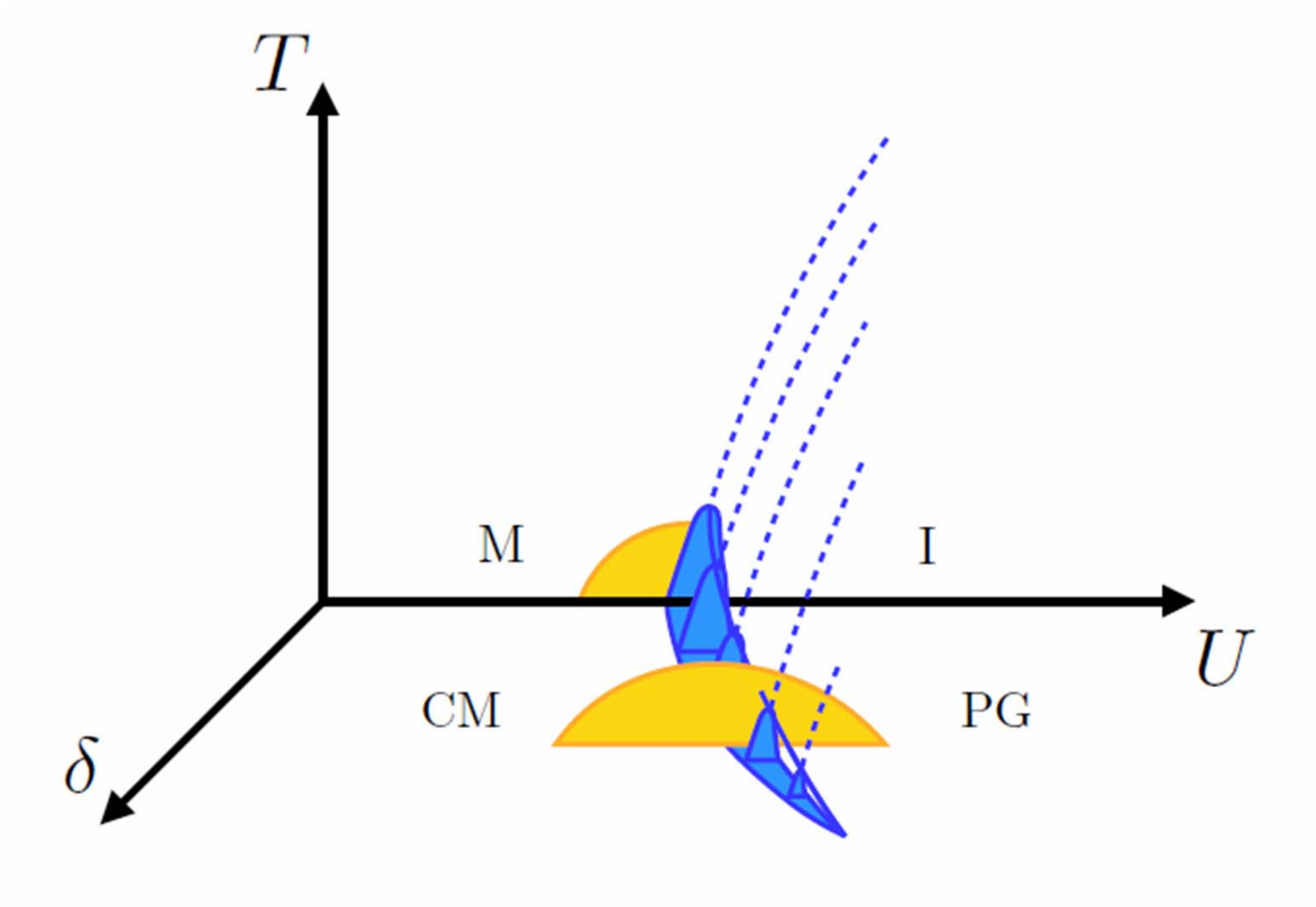
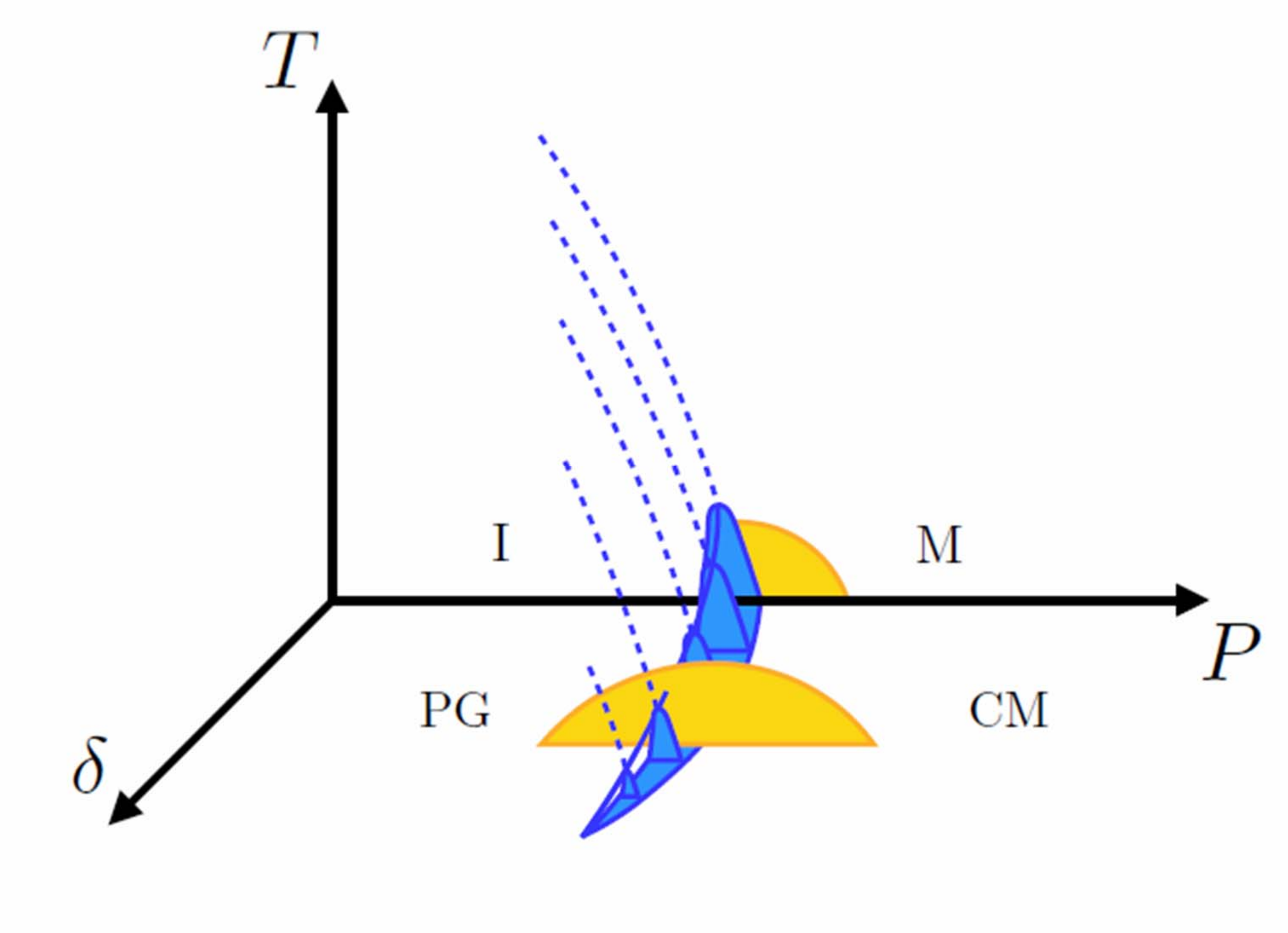
Doped organics

$n = 1$, $d = 2$ square lattice



Doped organics

n = 1, d = 2 square lattice



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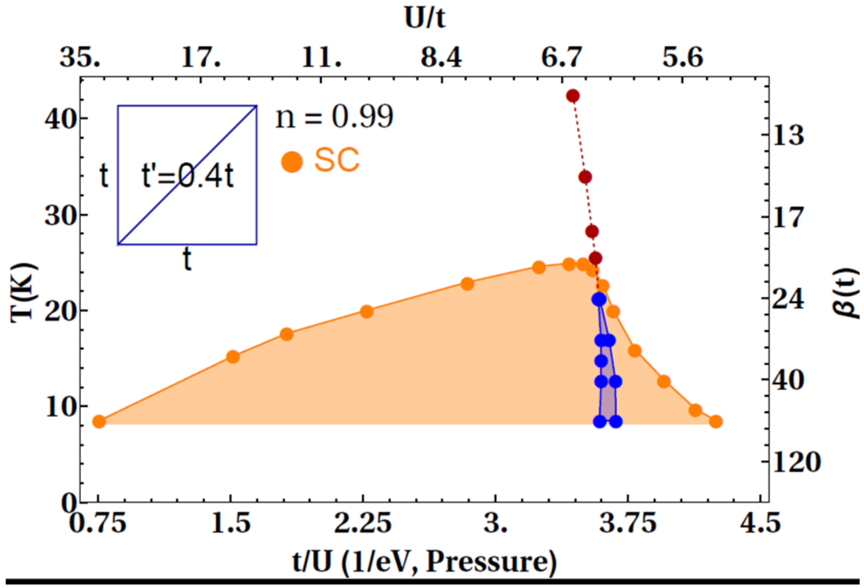
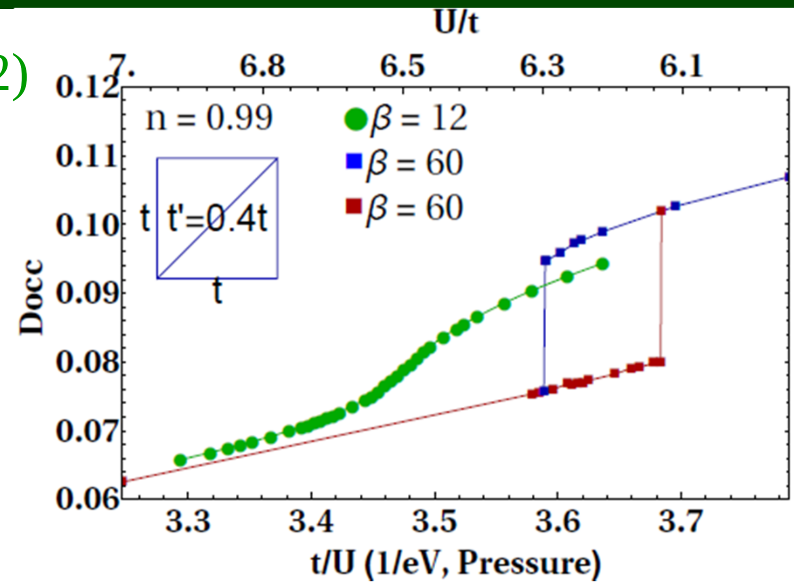
First order and Widom line in organics

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

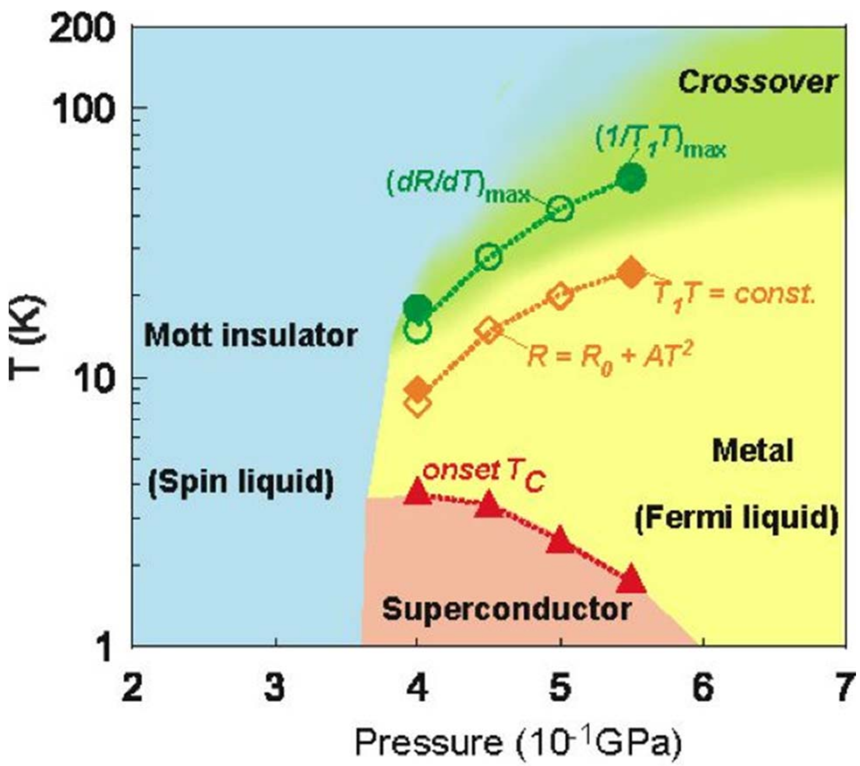


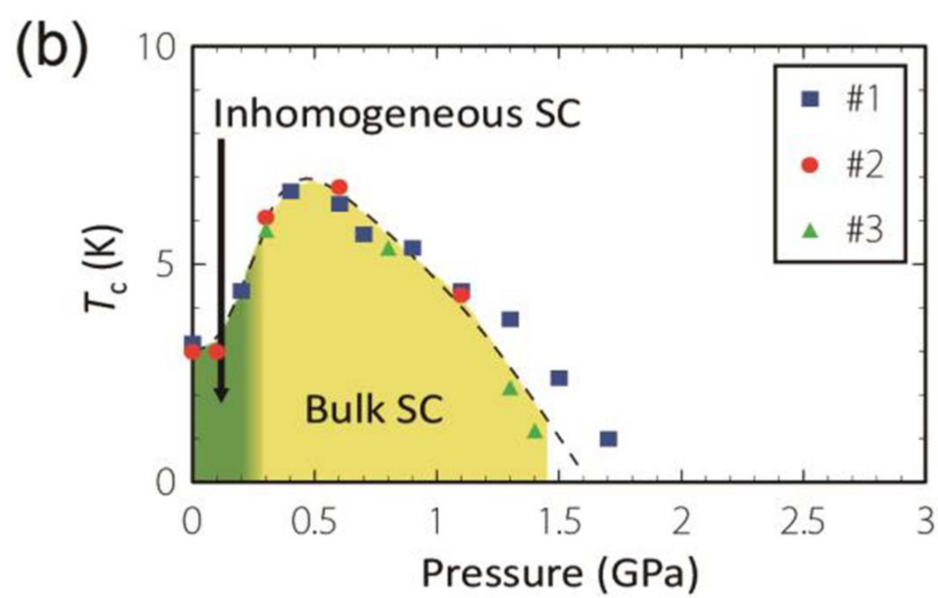


Compare: T. Watanabe, H. Yokoyama and M. Ogata JPS Conf. Proc. **3**, 013004 (2014)

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

Doped BEDT

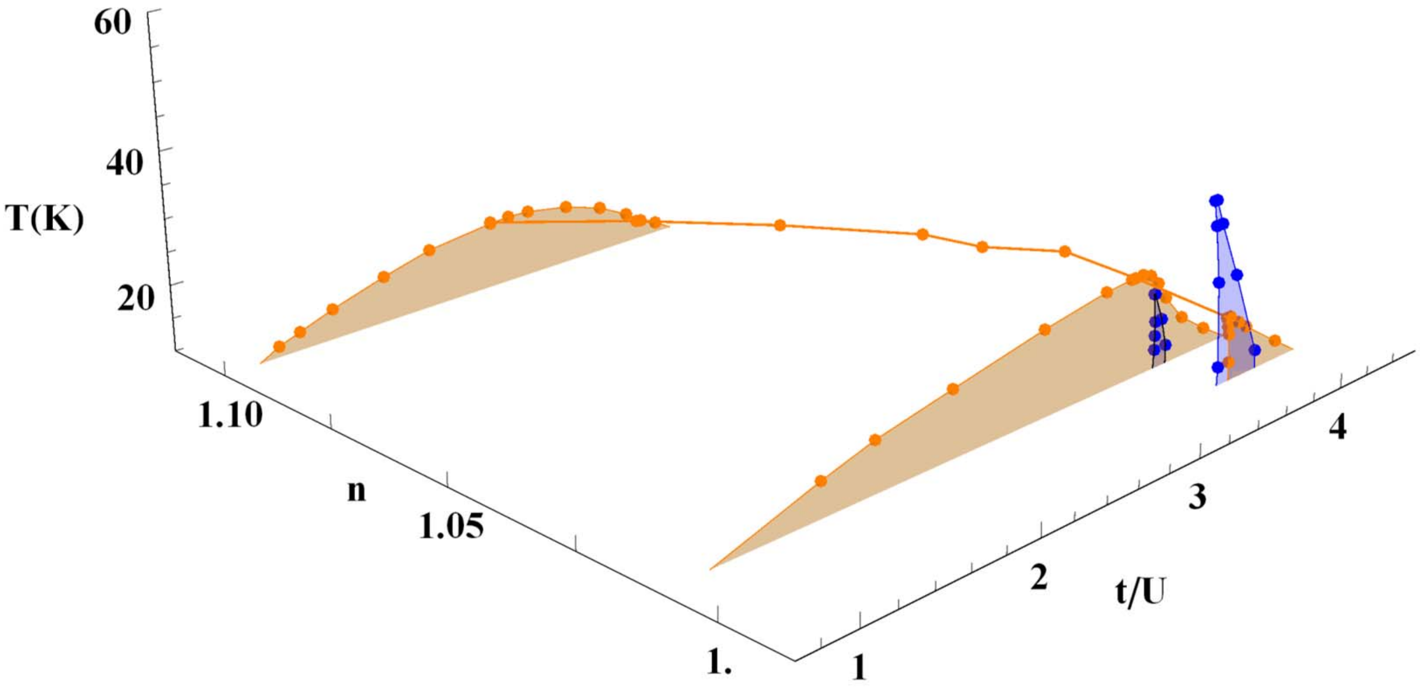




$n = 1$

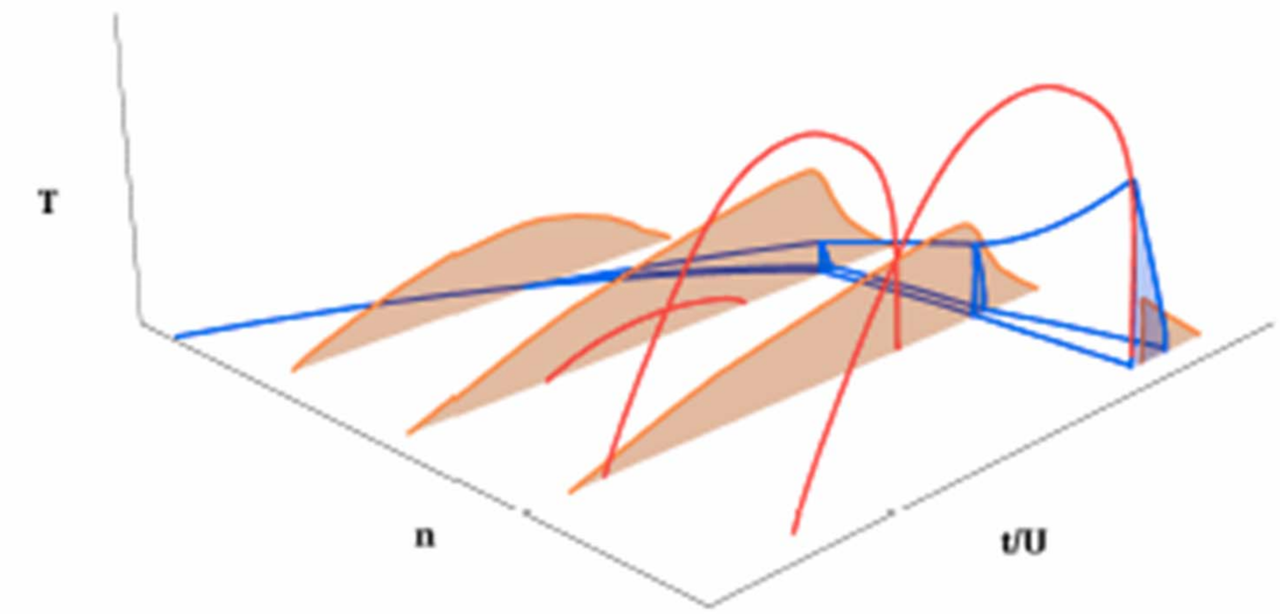
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

t' = 0.4t overview



Compare: T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

Generic case highly frustrated case



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Summary : organics

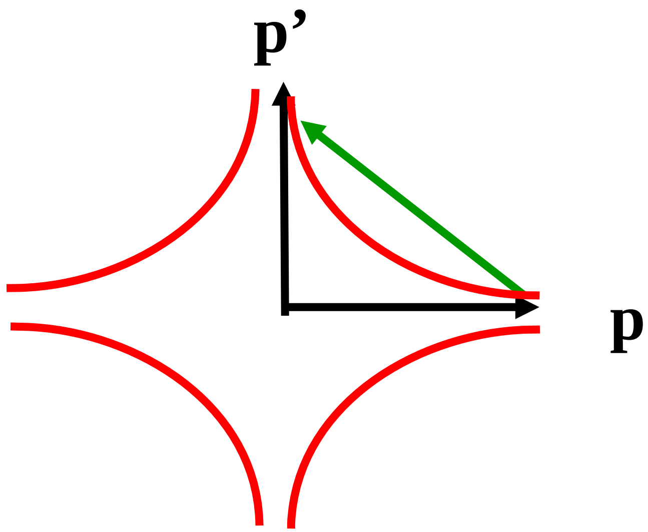
- Agreement with experiment
  - SC: larger T_c and broader P range if doped
  - Larger frustration: Decrease T_N *much more* than T_c
  - Normal state metal to pseudogap crossover
- Predictions
  - First order transition at low T in normal state (B induced)
  - Crossovers in SC state associated with 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

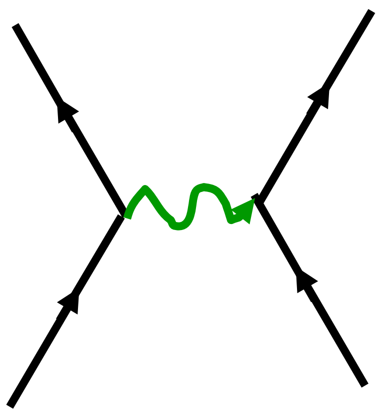
Pairing mechanism

Back to high T_c

Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





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).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

P.W. Anderson Science 317, 1705 (2007)

A cartoon strong coupling picture

$$J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j = J\sum_{\langle i,j\rangle}\left(\frac{1}{2}c_i^{\dagger}\vec{\sigma}c_i\right)\cdot\left(\frac{1}{2}c_j^{\dagger}\vec{\sigma}c_j\right)$$

$$d = \langle\hat{d}\rangle = 1/N\sum_{\vec{k}}(\cos k_x - \cos k_y)\langle c_{\vec{k},\uparrow}c_{-\vec{k},\downarrow}\rangle$$

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

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

P.W. Anderson Science 317, 1705 (2007)

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

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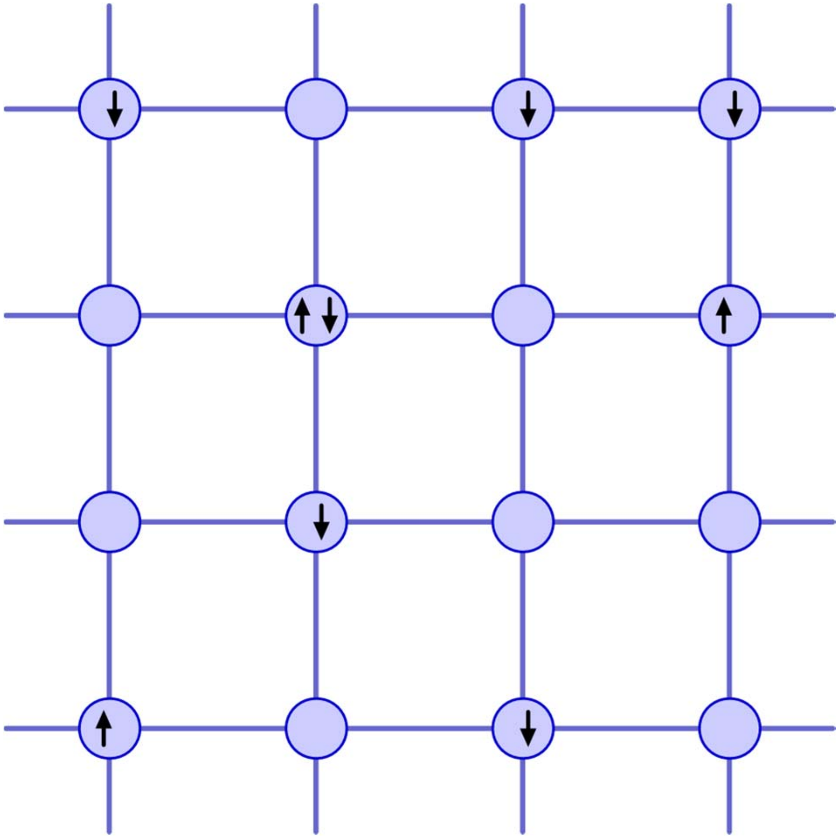
Extended Hubbard model



$$\hat{\mathcal{H}} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + c.h \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j - \mu \sum_{i} \hat{n}_i$$

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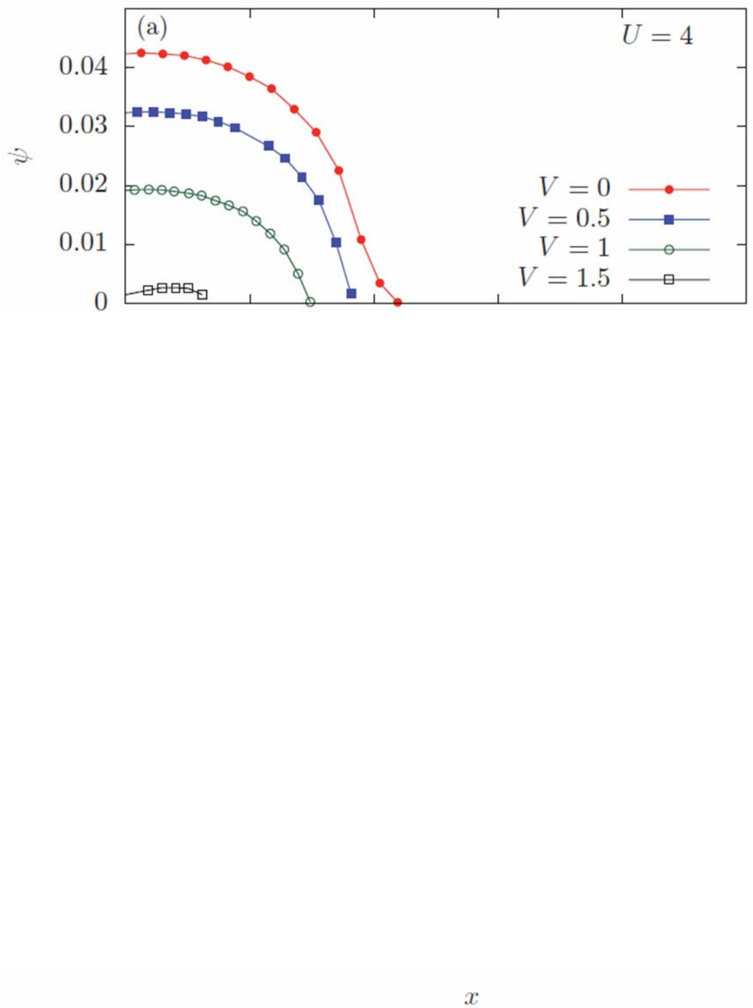
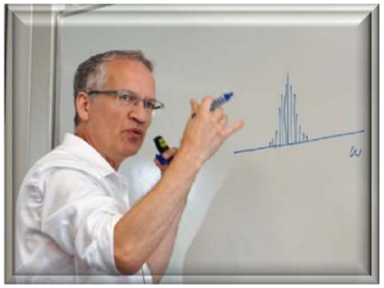
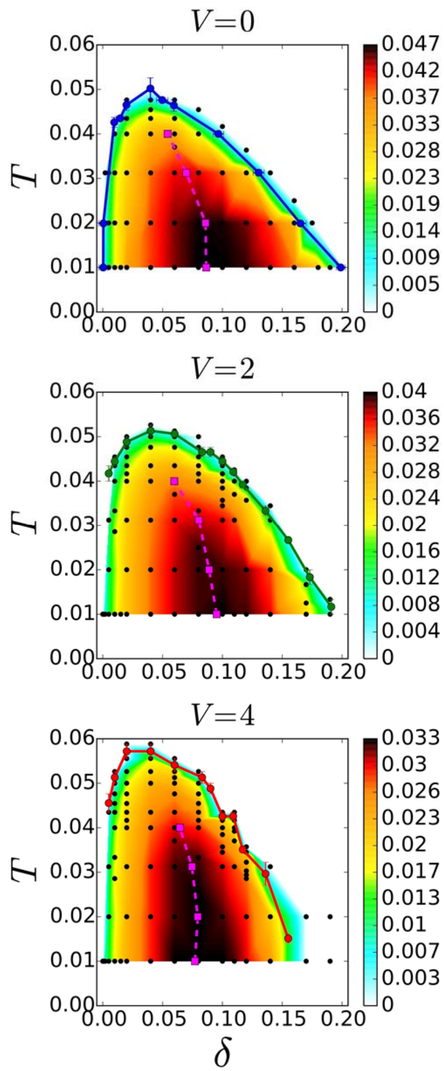
Strongly correlated: From *J*, yet retarded



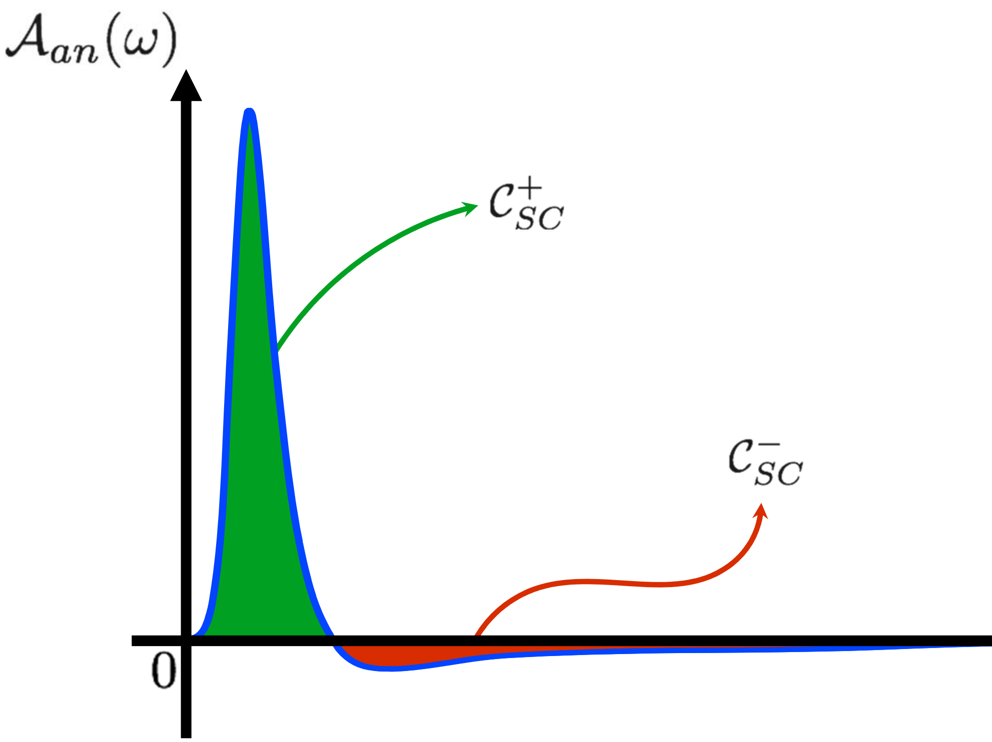


Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013)

Antagonistic effects of *V* at finite T



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



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

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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

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BÂTIR L'ÉCONOMIE NUMÉRIQUE

Calcul Québec

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Review: A.-M.S.T. arXiv: 1310.1481

Merci

Thank you

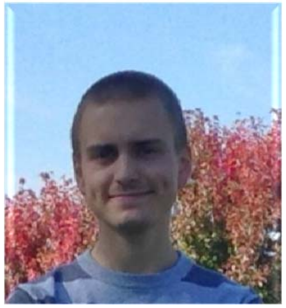
A.-M.S. Tremblay

"Strongly correlated superconductivity"

Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation, Vol. 3*, E. Pavarini, E. Koch, and U. Schollwöck (eds.)

Verlag des Forschungszentrum Jülich, 2013

Collaborators for this work



Charles-David Hébert

Patrick Sémon

Wei Wu

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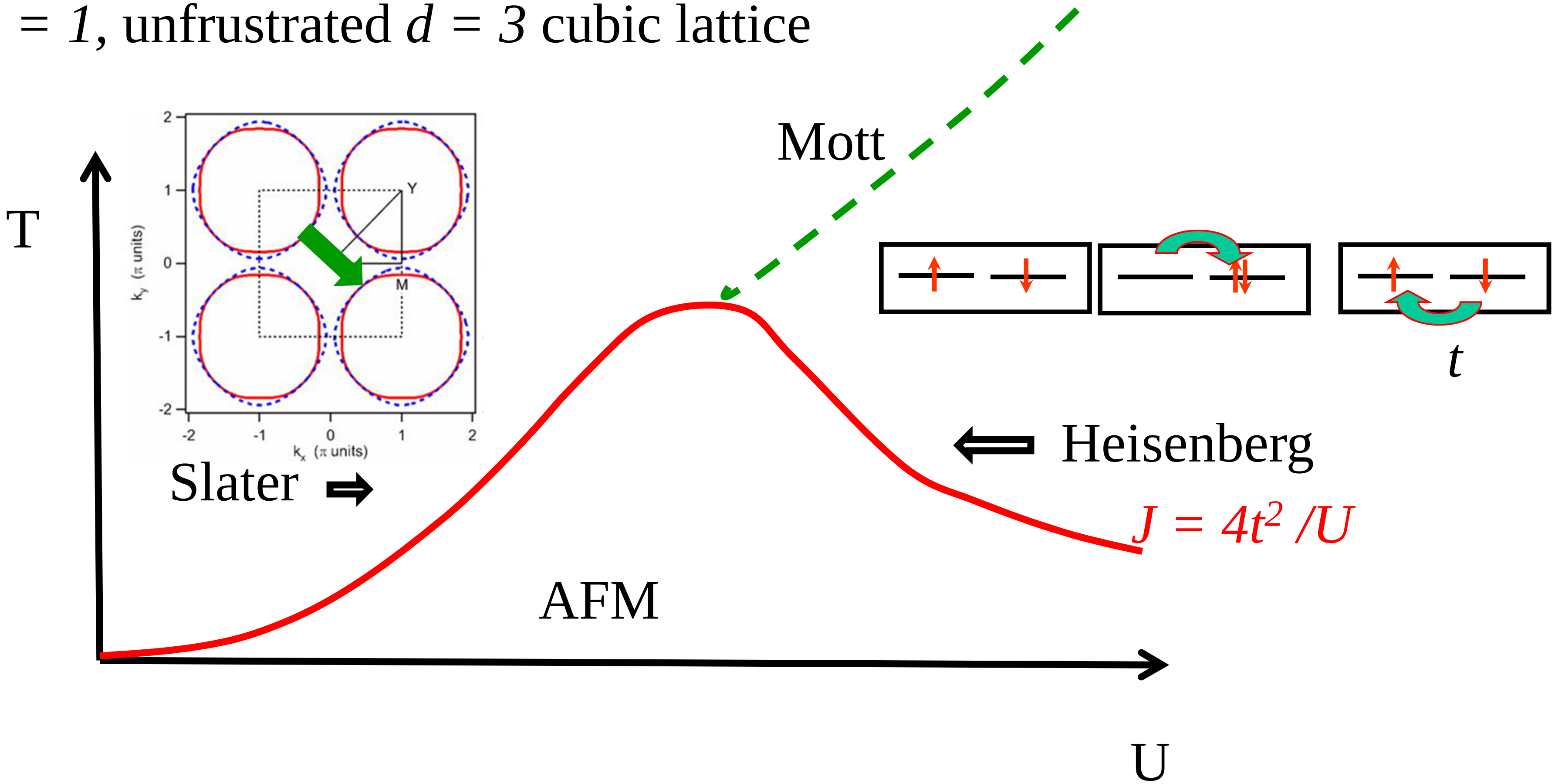
Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

Weak vs Strong correlations

$n = 1$, unfrustrated $d = 3$ cubic lattice



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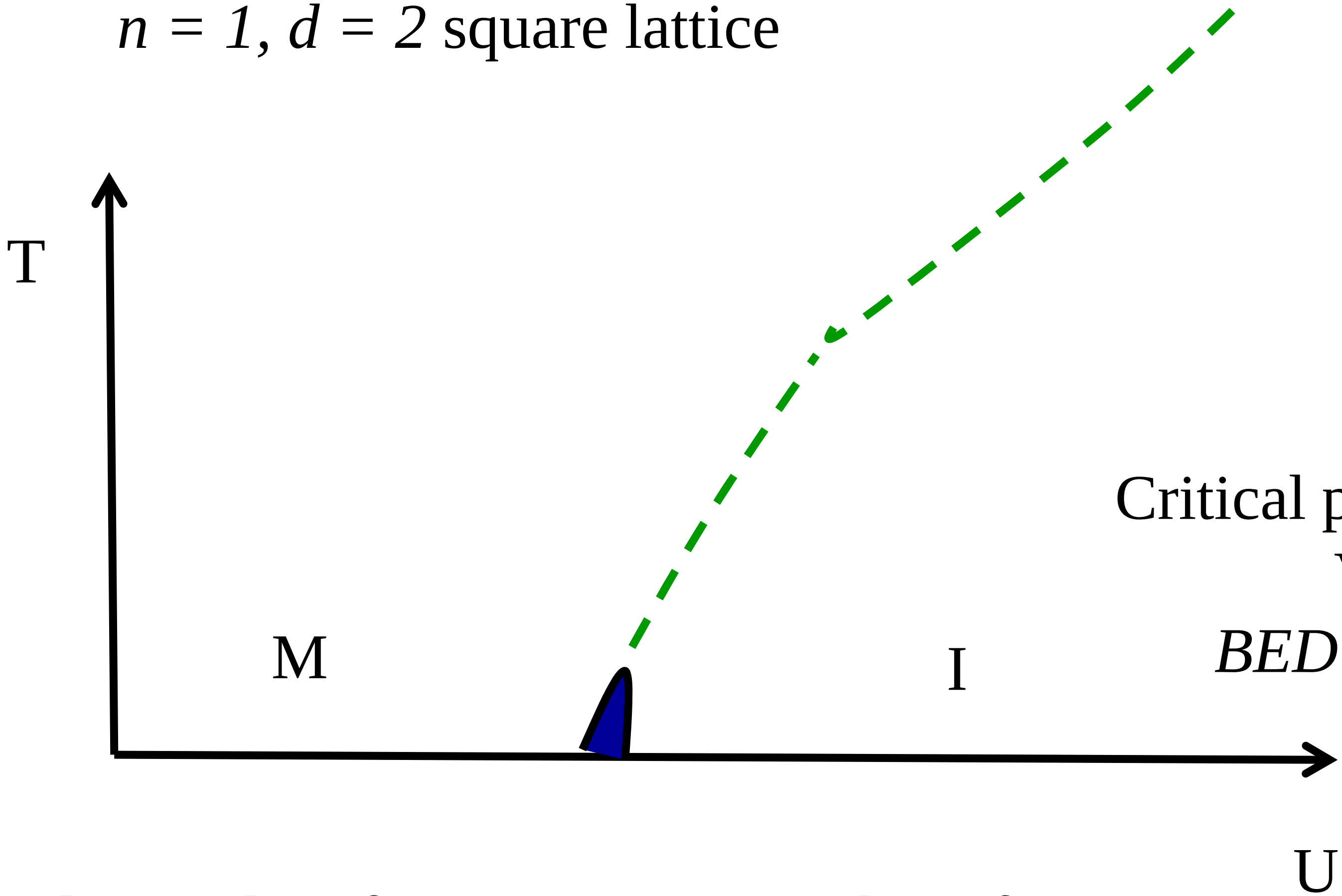
Local moment and Mott transition

n = 1, d = 2 square lattice

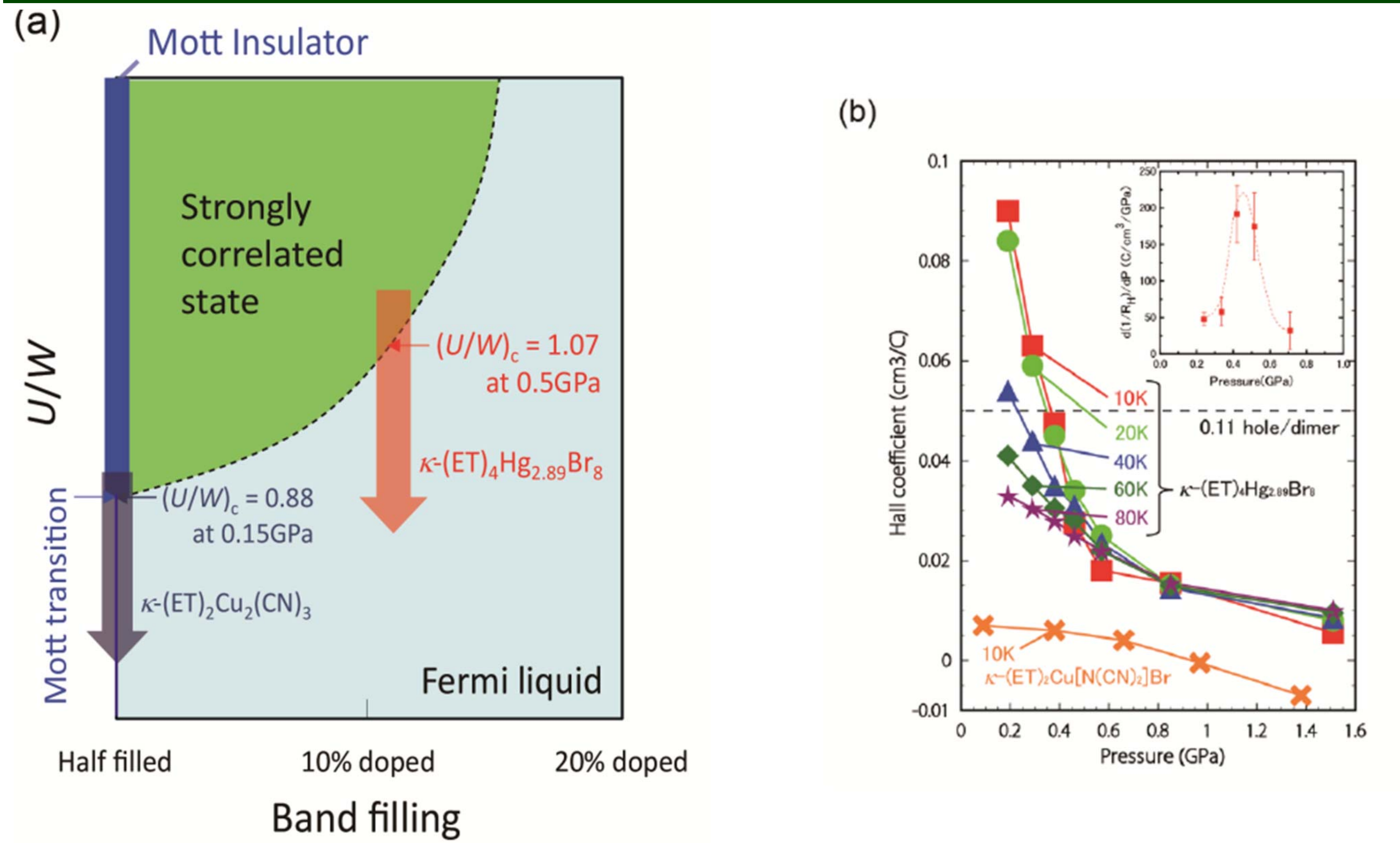


Critical point visible in
V_2O_3,
BEDT organics

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

Doped organic: experiment

Doped BEDT



H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

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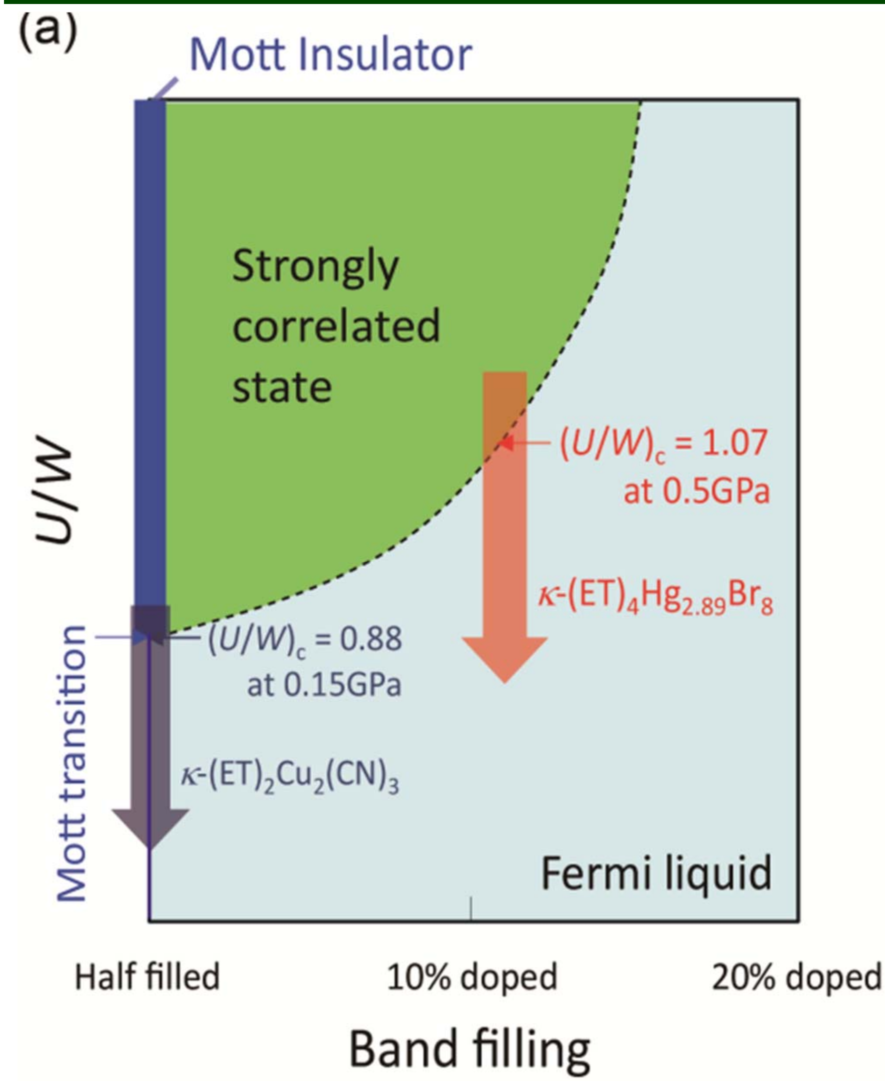
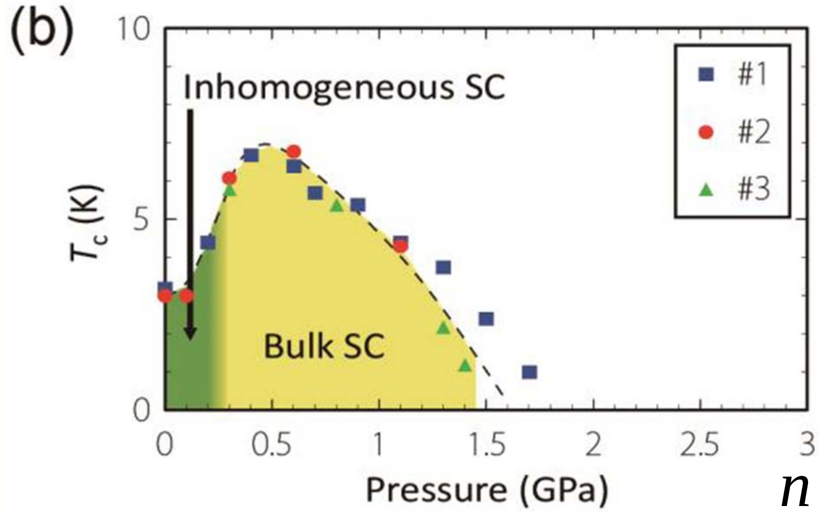
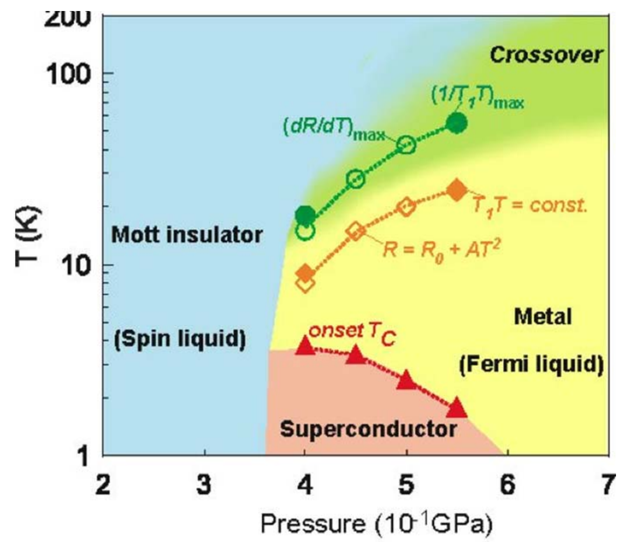
Doped BEDT





n = 0.90



n= 1

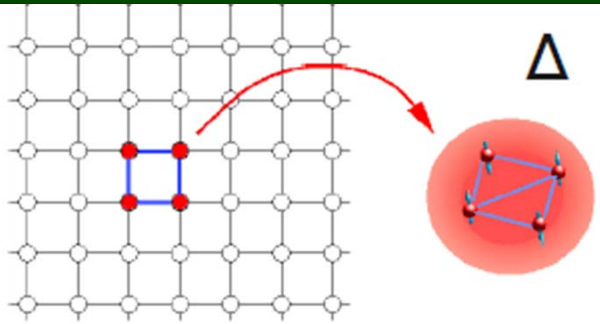
H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

Method

Concept: Cluster - DMFT

Tools: Impurity solver

CTQMC impurity solver (tool) (*T* finite)

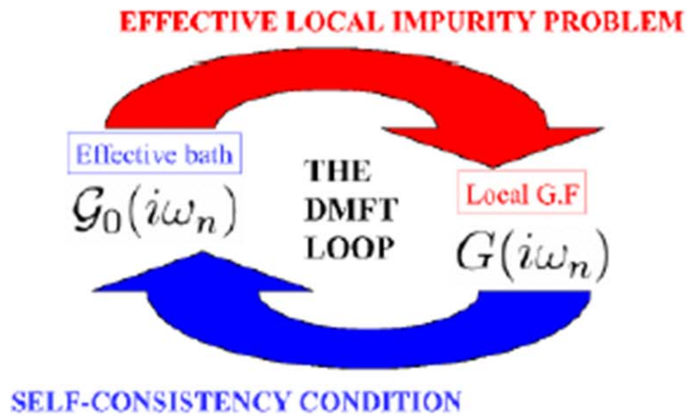


$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau) \Delta_{\mathbf{K}}(\tau,\tau') \psi_{\mathbf{K}}(\tau')}$$

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



$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

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