Et pourtant ils s'attirent: les supraconducteurs organiques et la supraconductivité fortement corrélée

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CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

UNIVERSITÉ DE SHERBROOKE

Sherbrooke, 22 juillet 2015

VERITATEM IN CHARITATE

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Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

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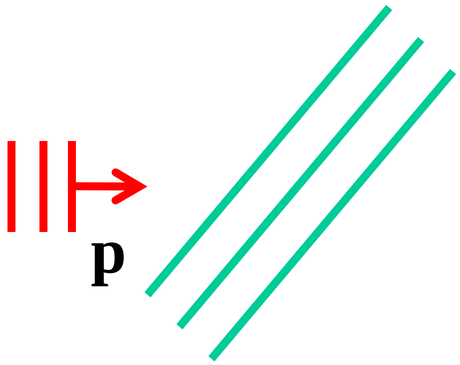
BCS Superconductivity

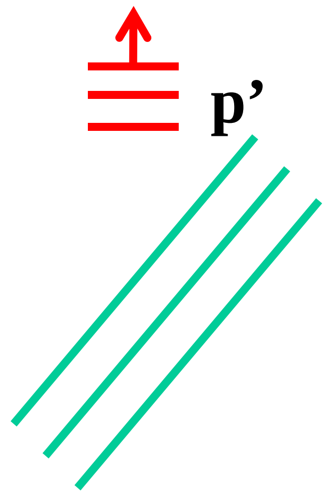
Superconductivity

© Alexis Reymbaut

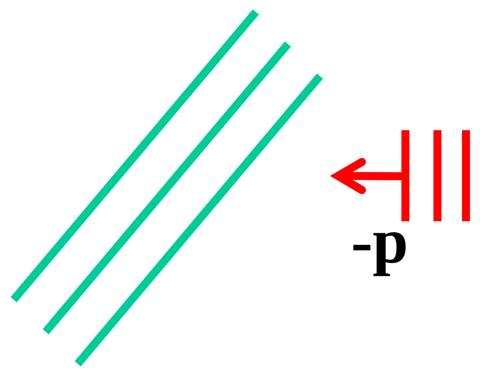
Attraction mechanism in the metallic state



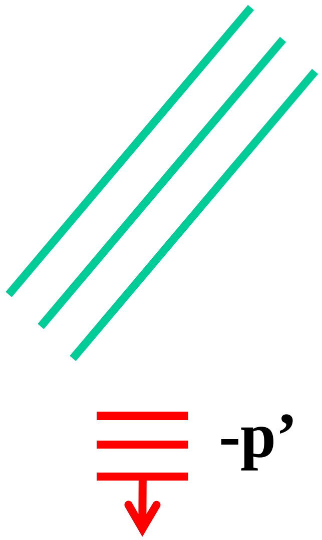
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



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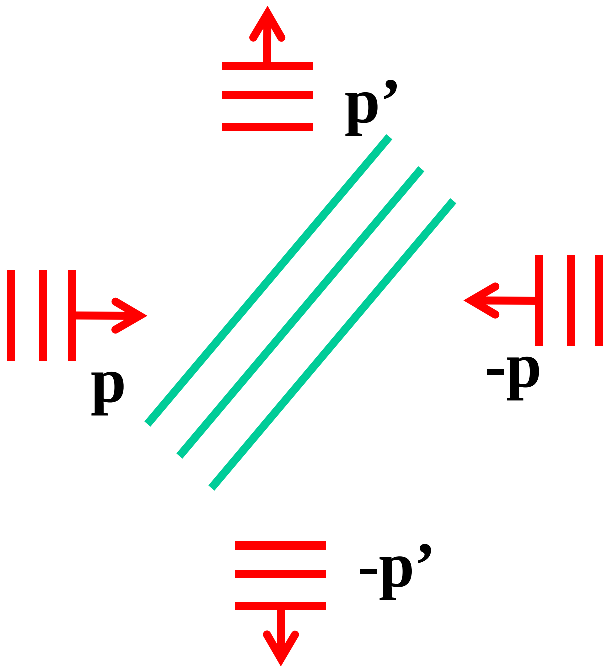
Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}$$

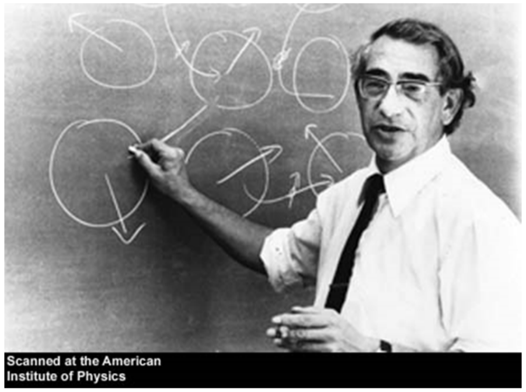
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left(\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \rangle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} + \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \right)$$

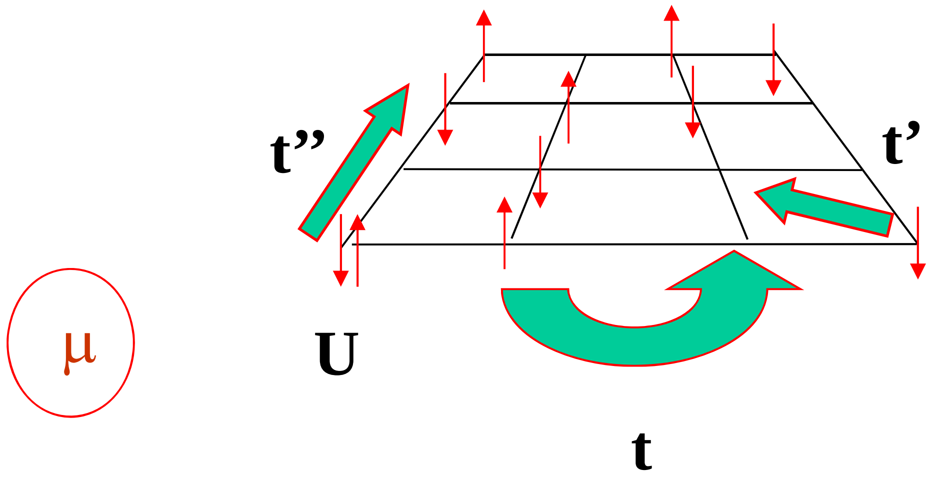
$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots.$$

Kinetic energy increases

Simplest Model for Mott insulator

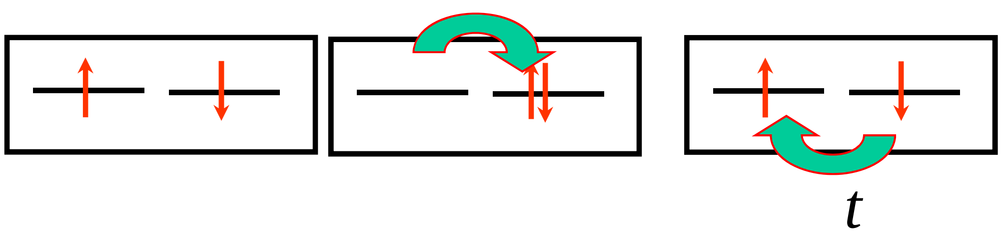
Hubbard model





1931-1980

$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



Effective model, Heisenberg: $J = 4t^2/U$

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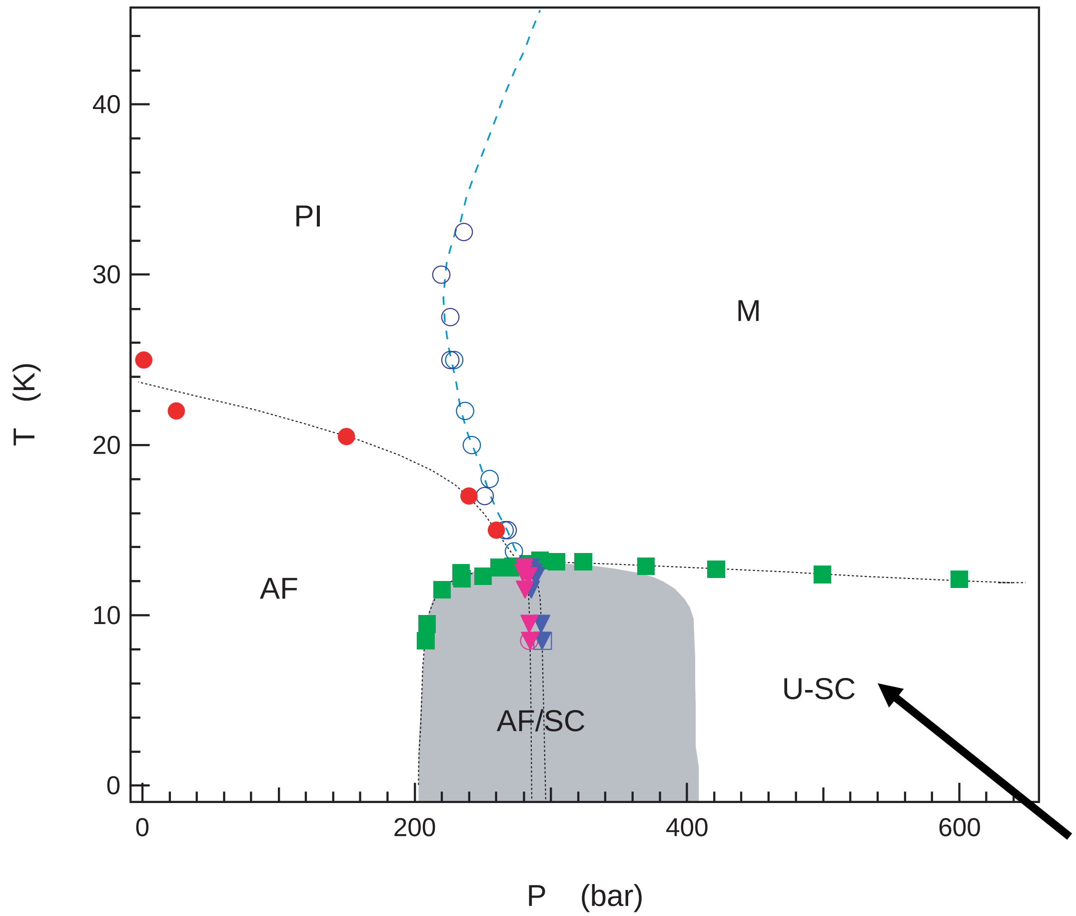
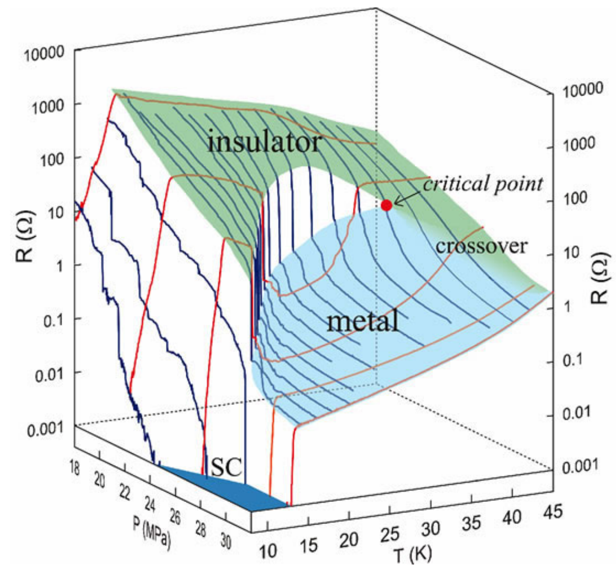
Superconductivity and attraction?

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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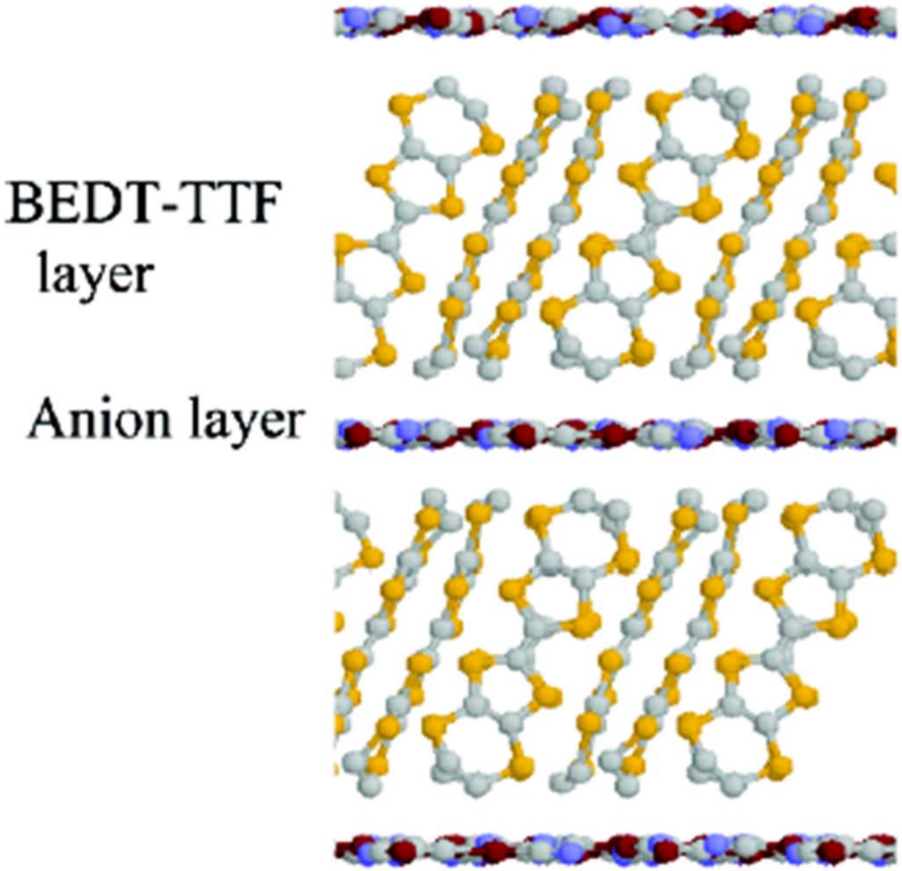
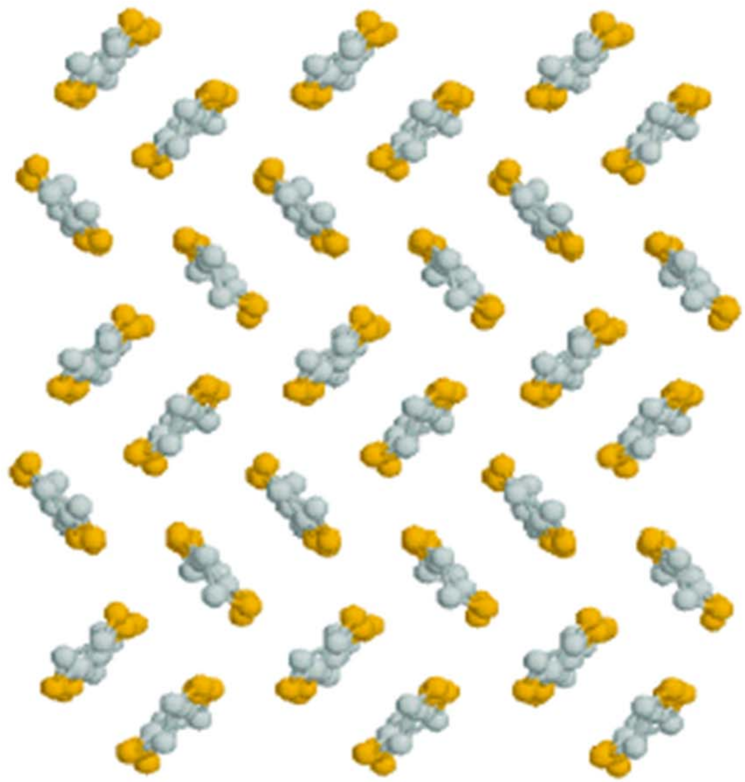
Layered organics (κ–BEDT-X family)





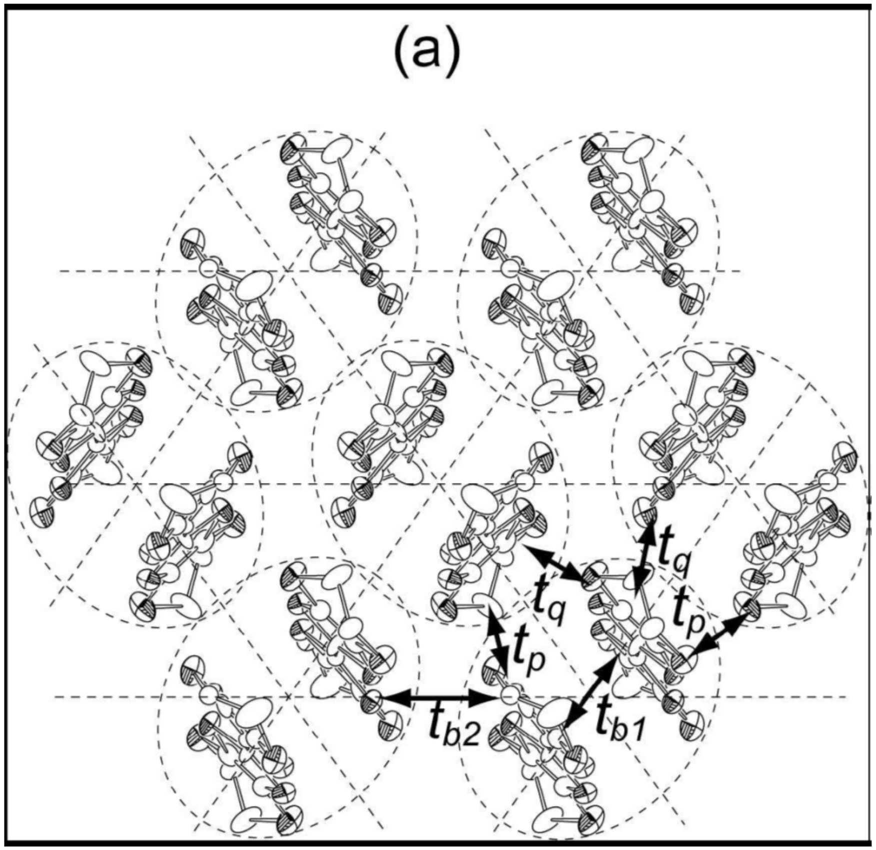
$$t \approx 50\,\text{meV}$$

$$\Rightarrow U \approx 400\,\text{meV}$$

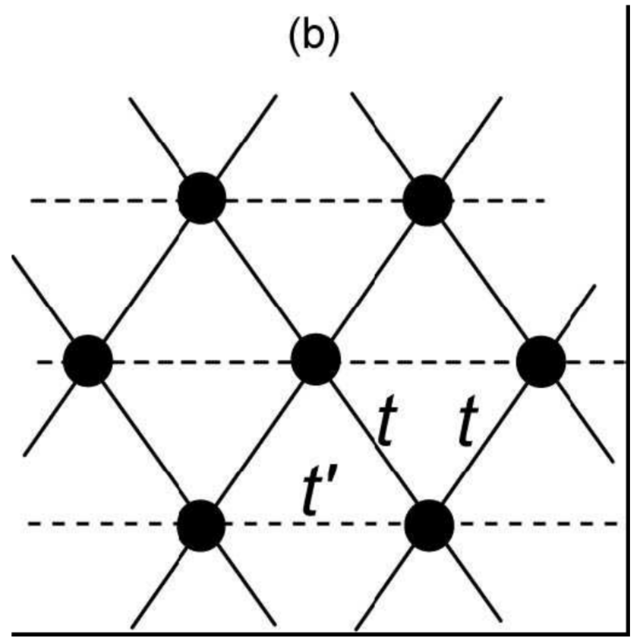
$$t'/t \sim 0.6 - 1.1$$

One-band Hubbard model of BEDT organics

H. Kino + H. Fukuyama, J. Phys. Soc. Jpn **65** 2158 (1996),
R.H. McKenzie, Comments Condens Mat Phys. **18**, 309 (1998)



Y. Shimizu, et al. Phys. Rev. Lett. **91**, 107001(2003)



$t \approx 50$ meV

$\Rightarrow U \approx 400$ meV

$t'/t \sim 0.6 - 1.1$

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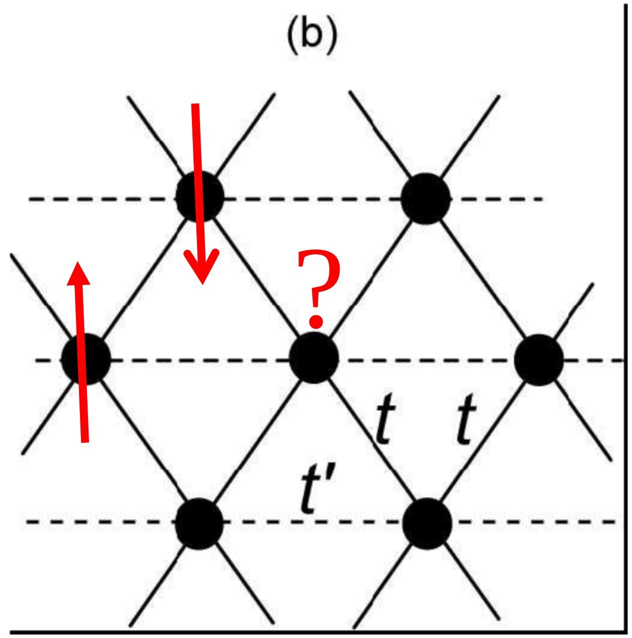
Magnetic frustration



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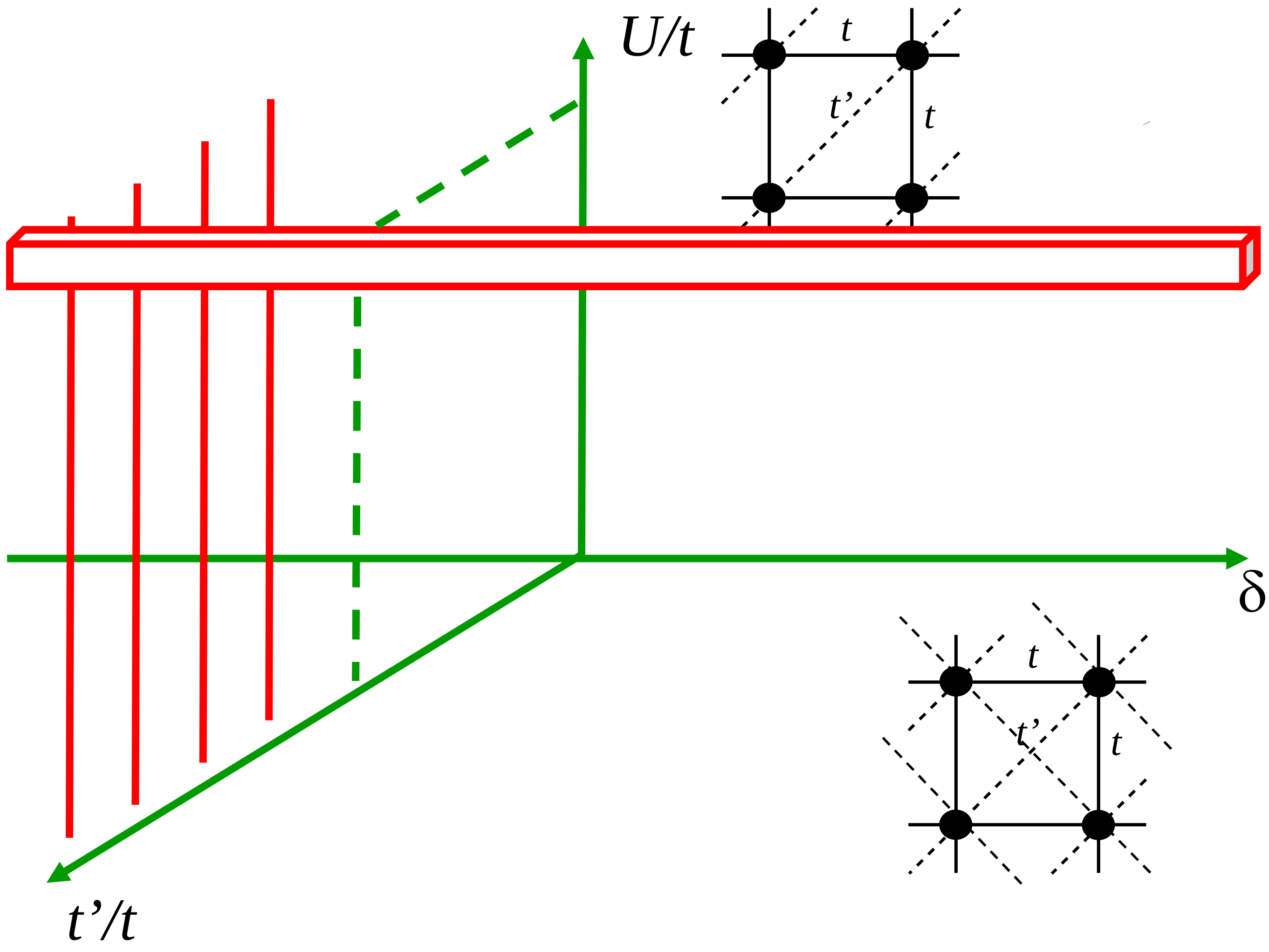
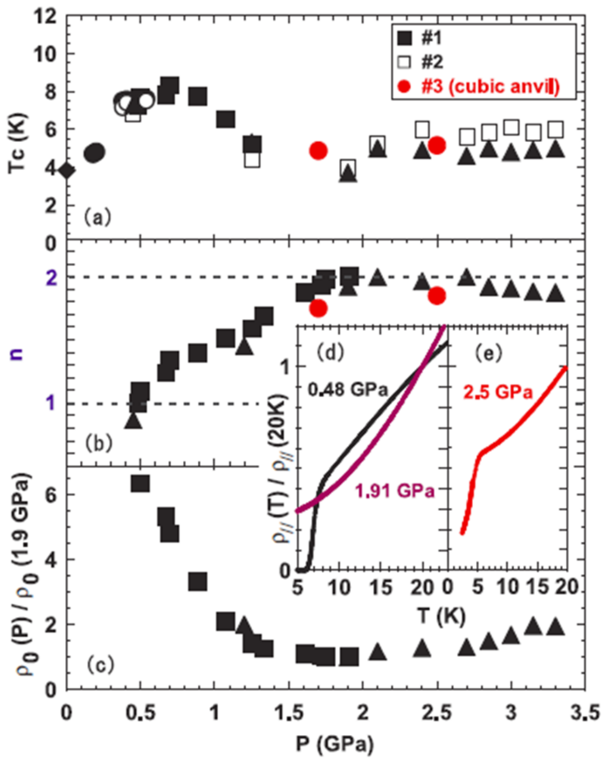
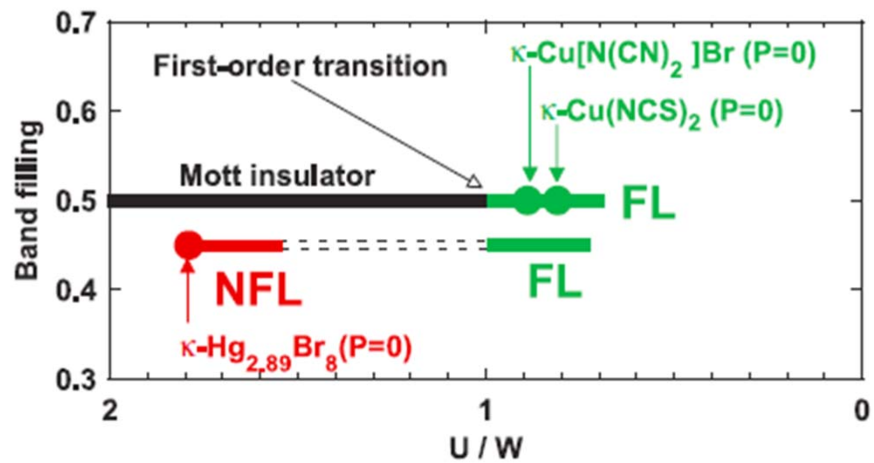
Perspective



A doped BEDT organic



	W (eV)	U (eV)	U/W	BF	T_c (K)
κ-Cu(NCS)$_2$ [a)]	0.57	0.46	0.81	0.50	10.4
κ-Cu[N(CN)$_2$]Br [a)]	0.55	0.49	0.89	0.50	11.8
κ-Hg$_{2.89}$Br$_8$ [b)]	0.26	0.465	1.79	0.45	4.3



Taniguchi et al. J. Phys. Soc. Japan, **76**, 113709 (2007)

R. N. Lyubovskaya et al. JETP Lett. **45,** 530 (1987)

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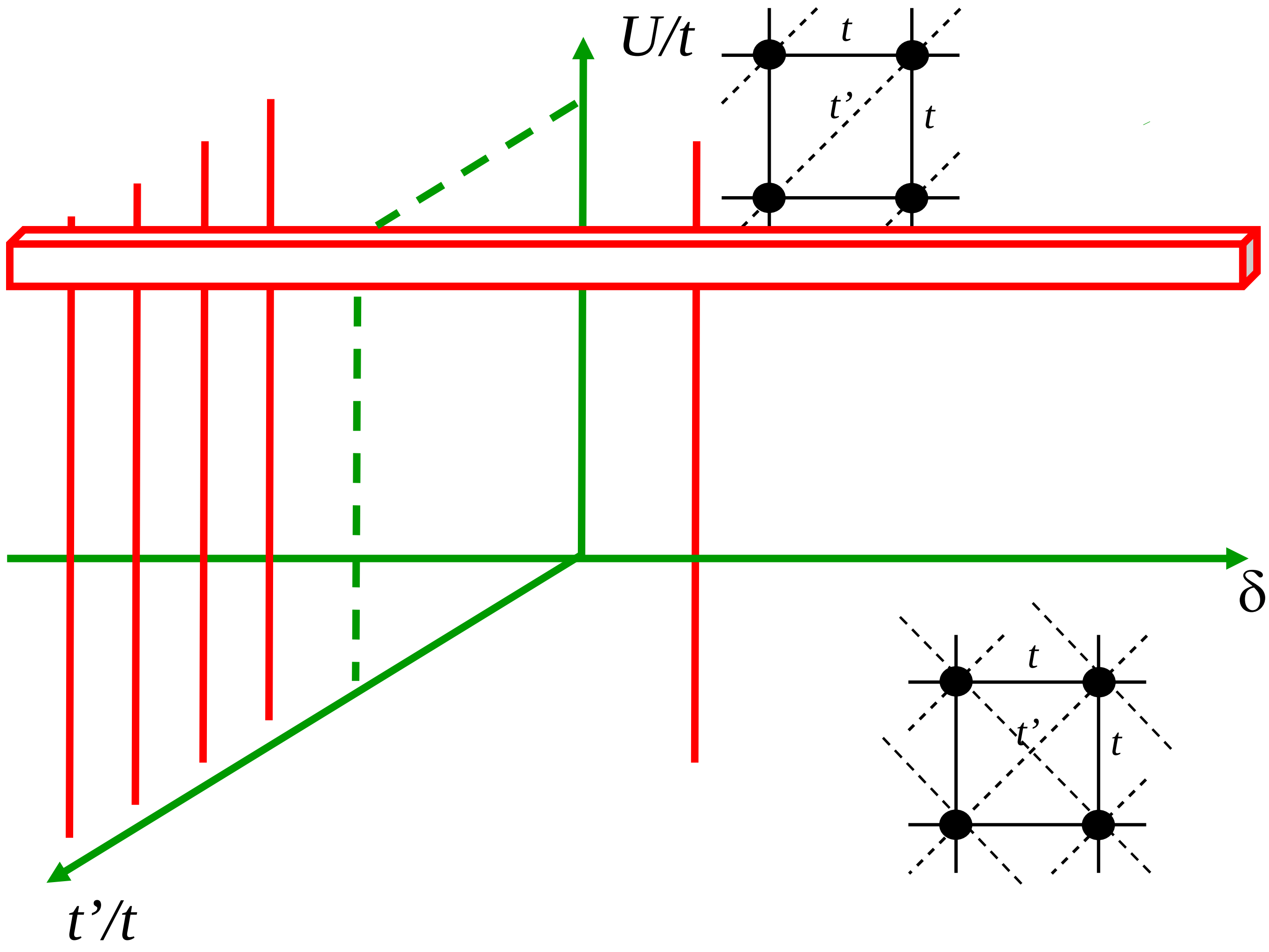
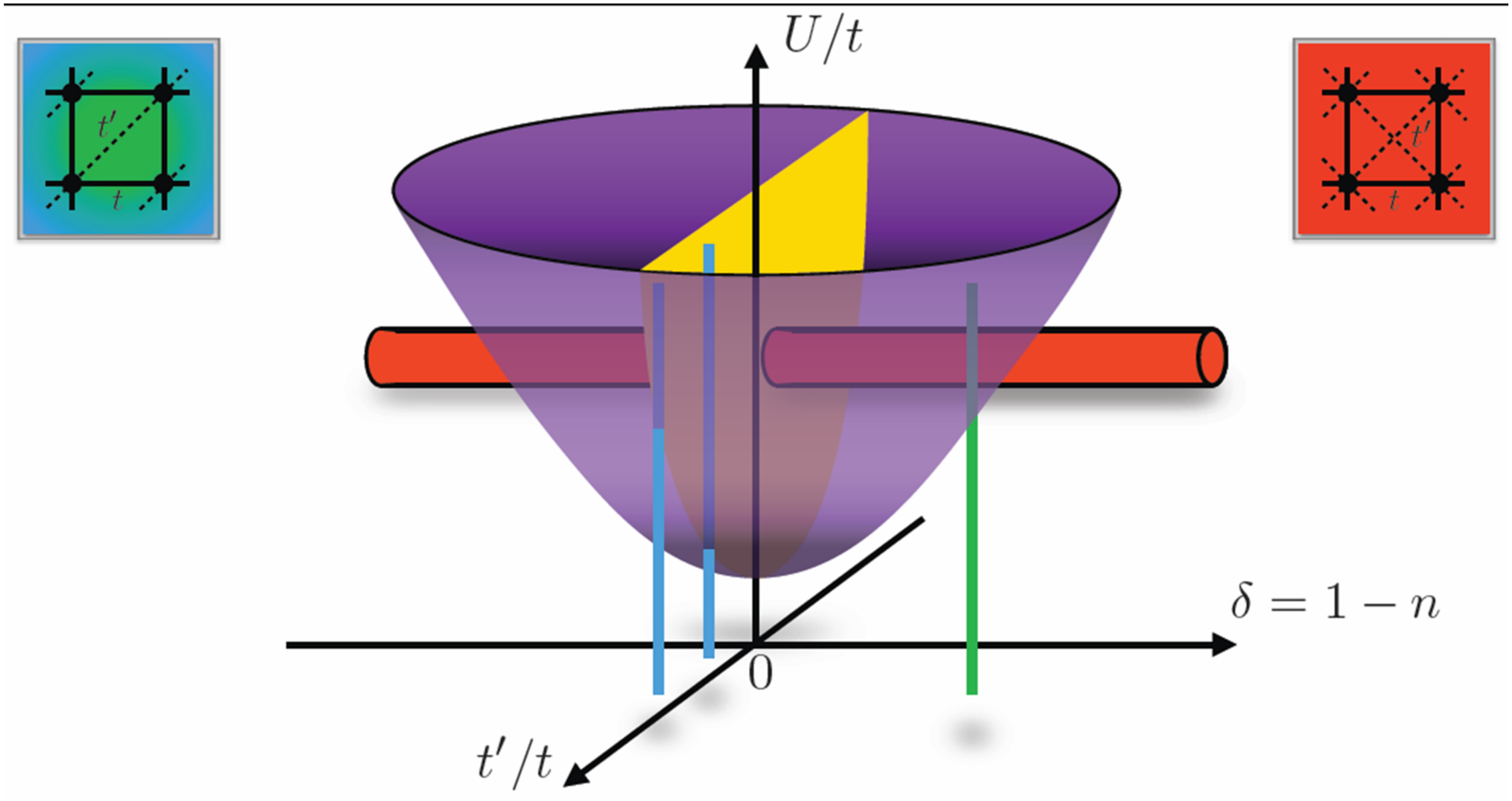
Perspective



Generalized Phase Diagram



A. Reymbaut

Outline

- Method
- Weak vs strong correlations (AFM and SC)
- Phase diagram
  - $n = 1$
  - finite doping
- What controls maximum T_c ? (Quantum critical point?)

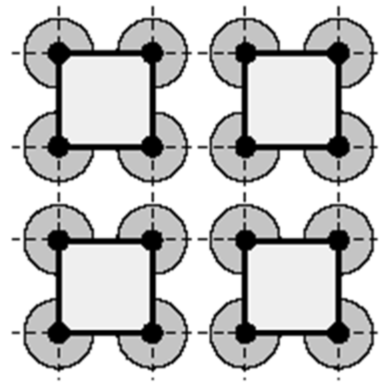
Method

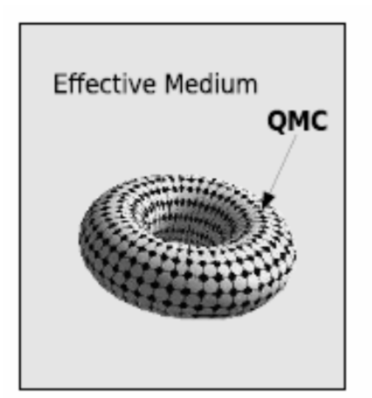
"The effect of concept-driven revolution is to explain old things in new ways. The effect of tool-driven revolution is to discover new things that have to be explained."

Freeman Dyson *Imagined Worlds*

2d Hubbard: Quantum cluster method

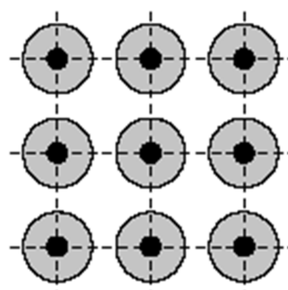
C-DMFT





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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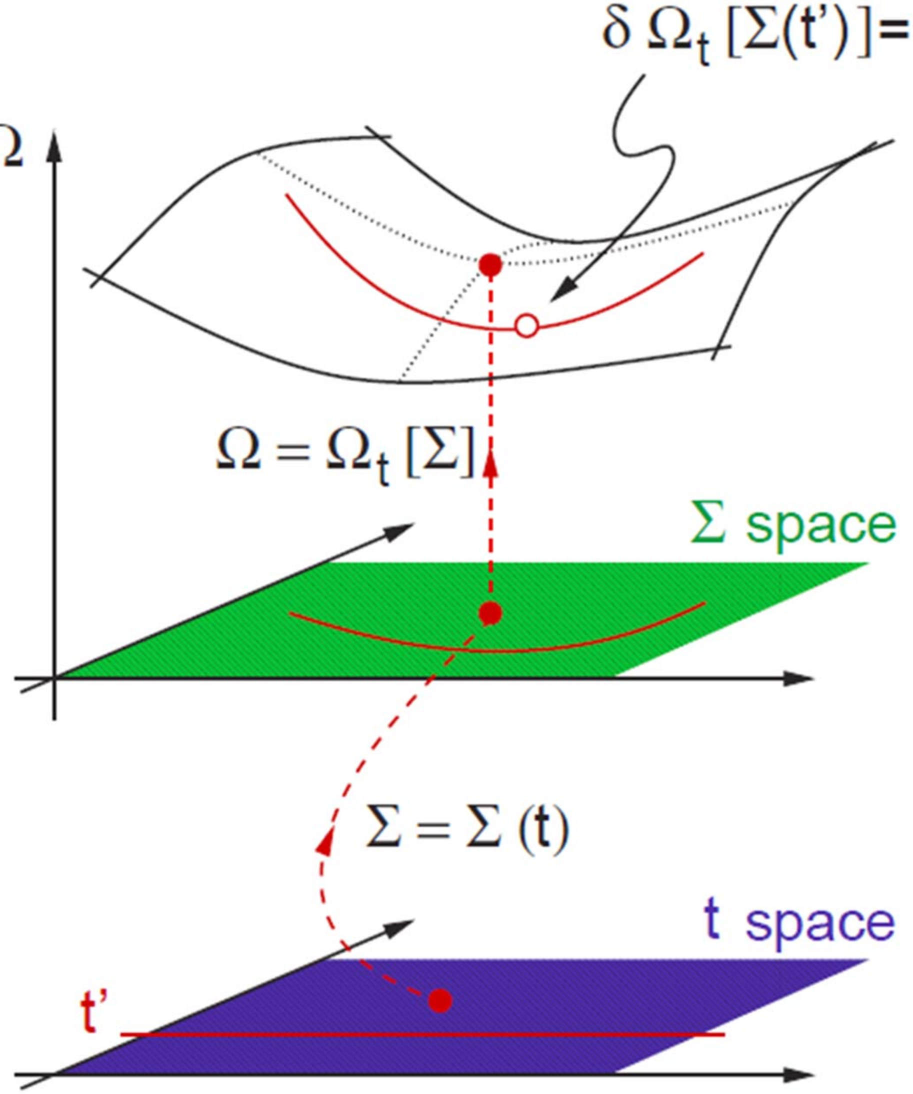
DMFT as a stationnary point



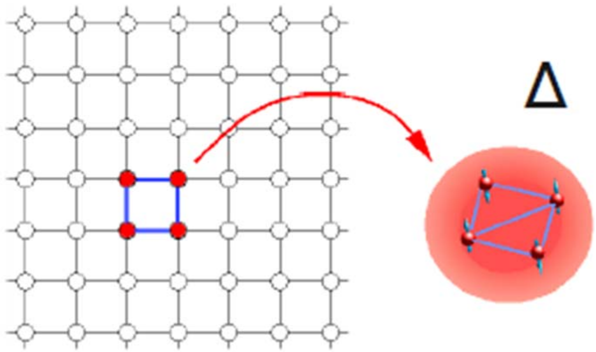
M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

+ and -

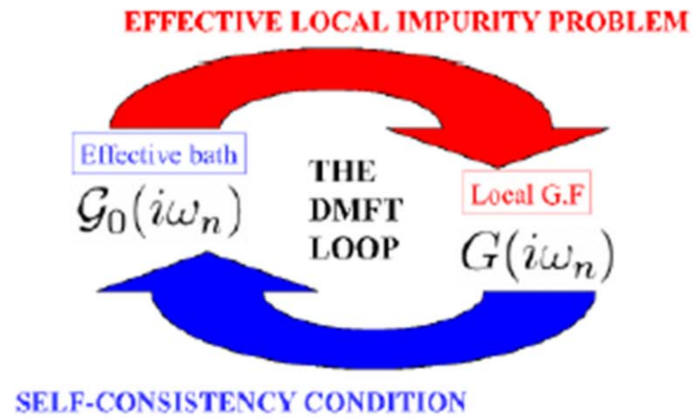
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

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

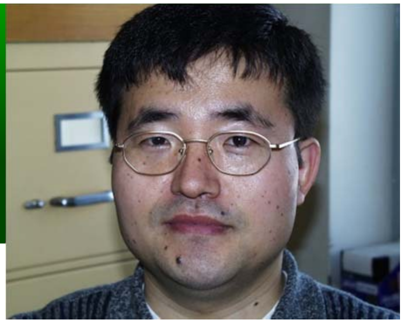
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)}\right]^{-1}$$

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

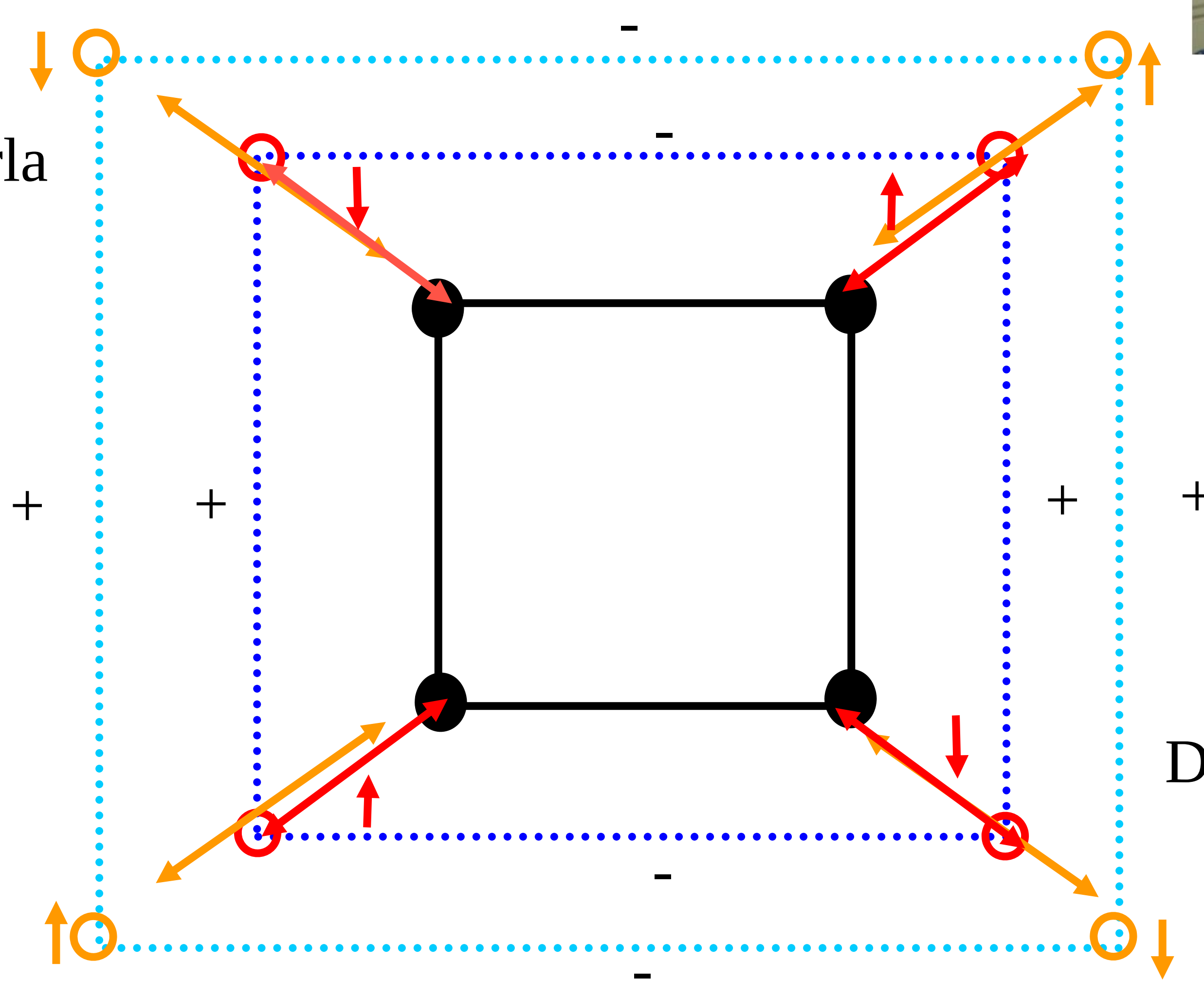
Exact diagonalization impurity solver

ED impurity solver (T = 0)

S. Kancharla



B. Kyung



David Sénéchal

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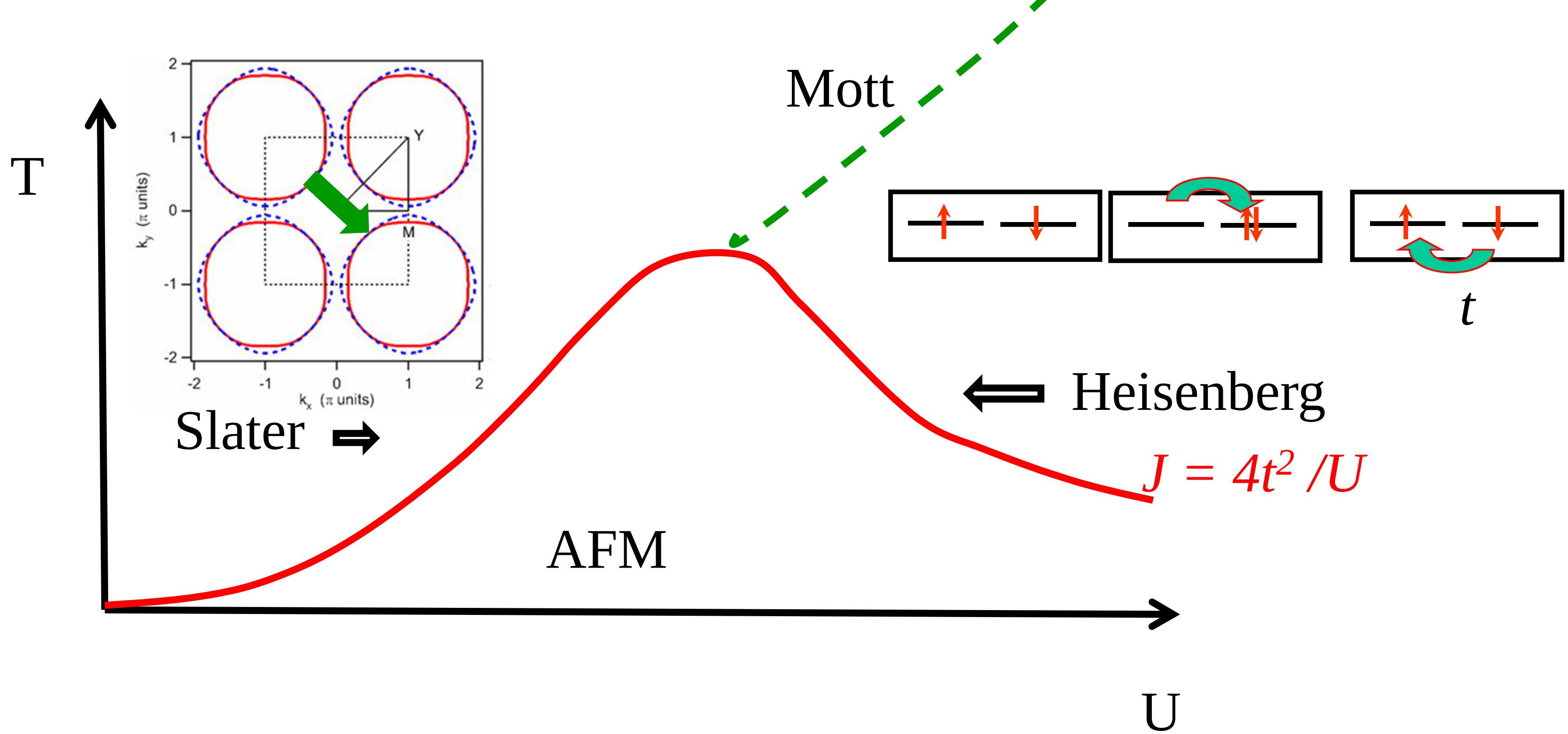
Weakly vs strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets

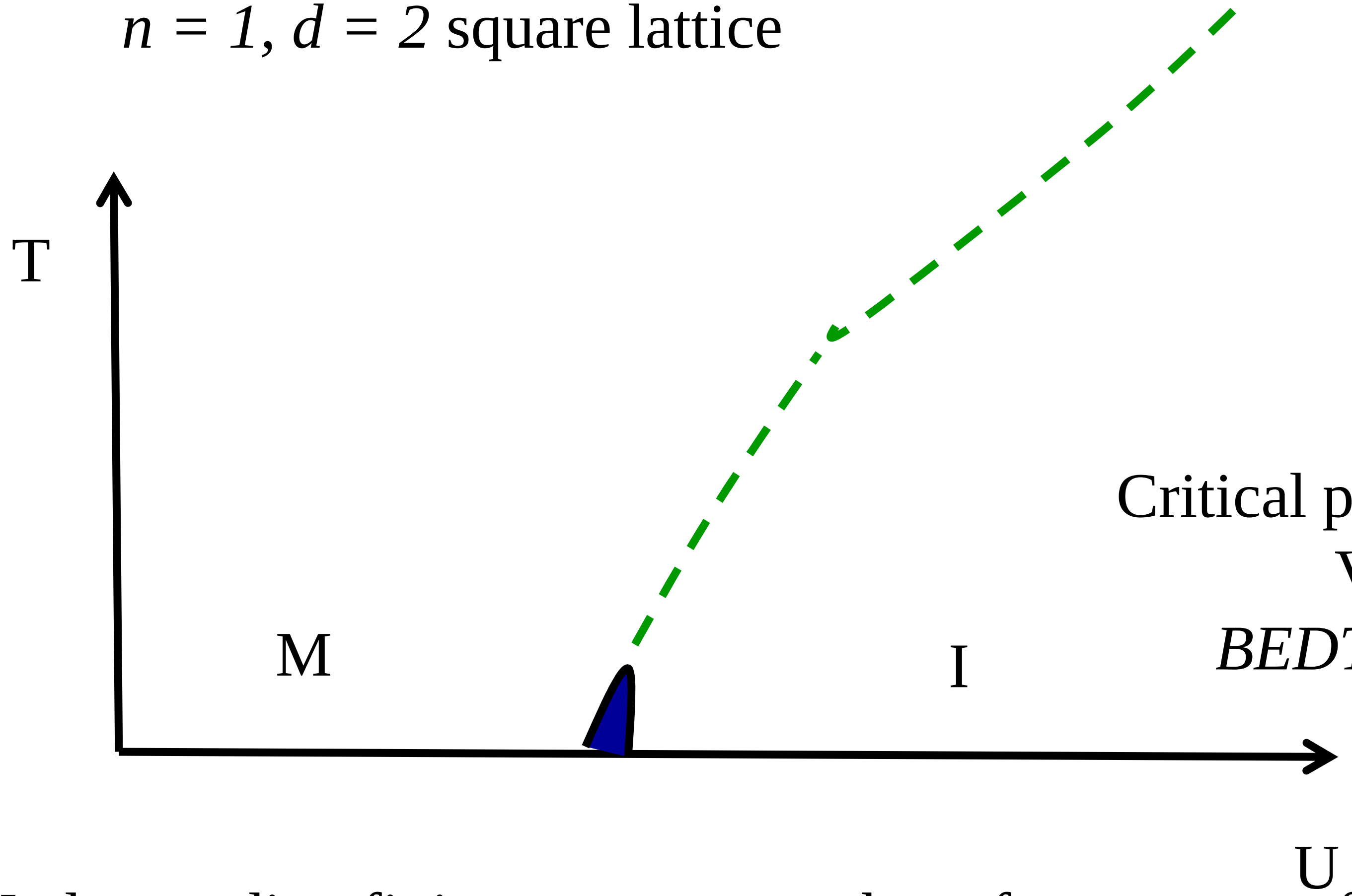
Weak vs Strong correlations

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



Local moment and Mott transition

n = 1, d = 2 square lattice



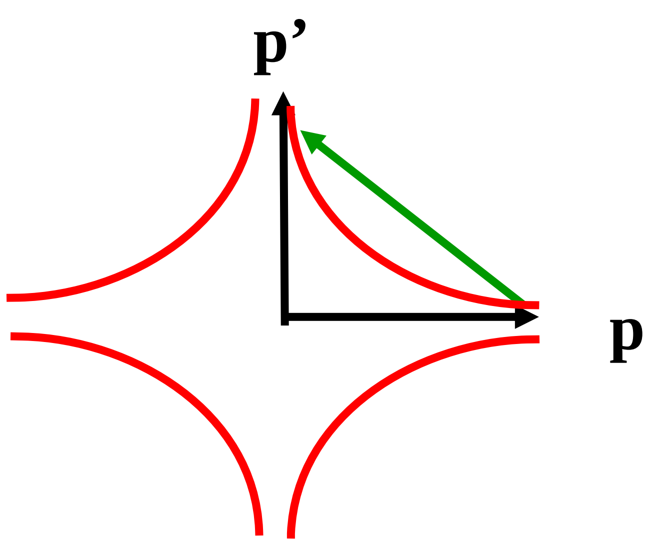
Critical point visible in
V_2O_3,
BEDT organics

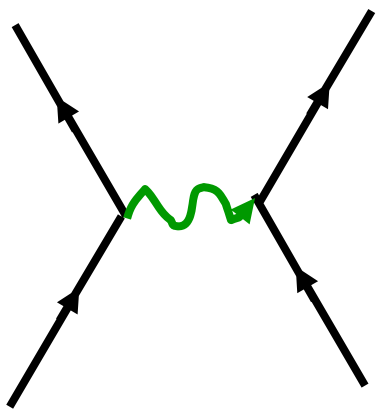
Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

Weakly vs strongly correlated superconductivity

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)

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#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow}$$

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left(\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \rangle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} + \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \right)$$

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots .$$

Kinetic energy increases

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)

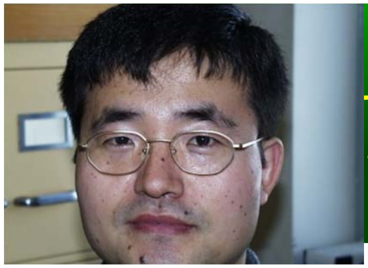
Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

T = 0 phase diagram $n = 1$

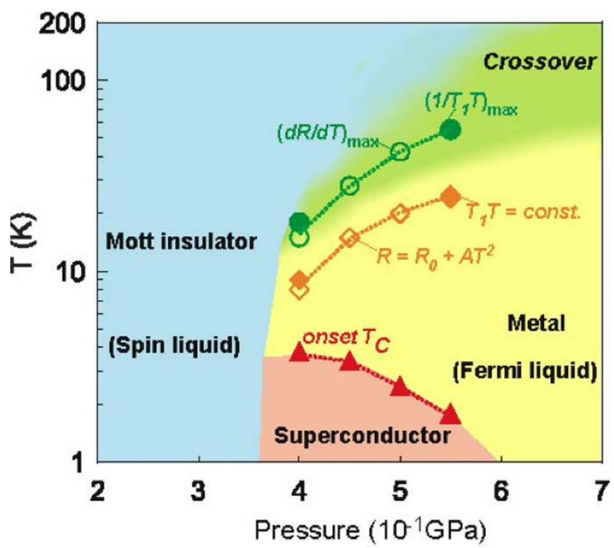
Phase diagram

Exact diagonalization as impurity solver ($T=0$).

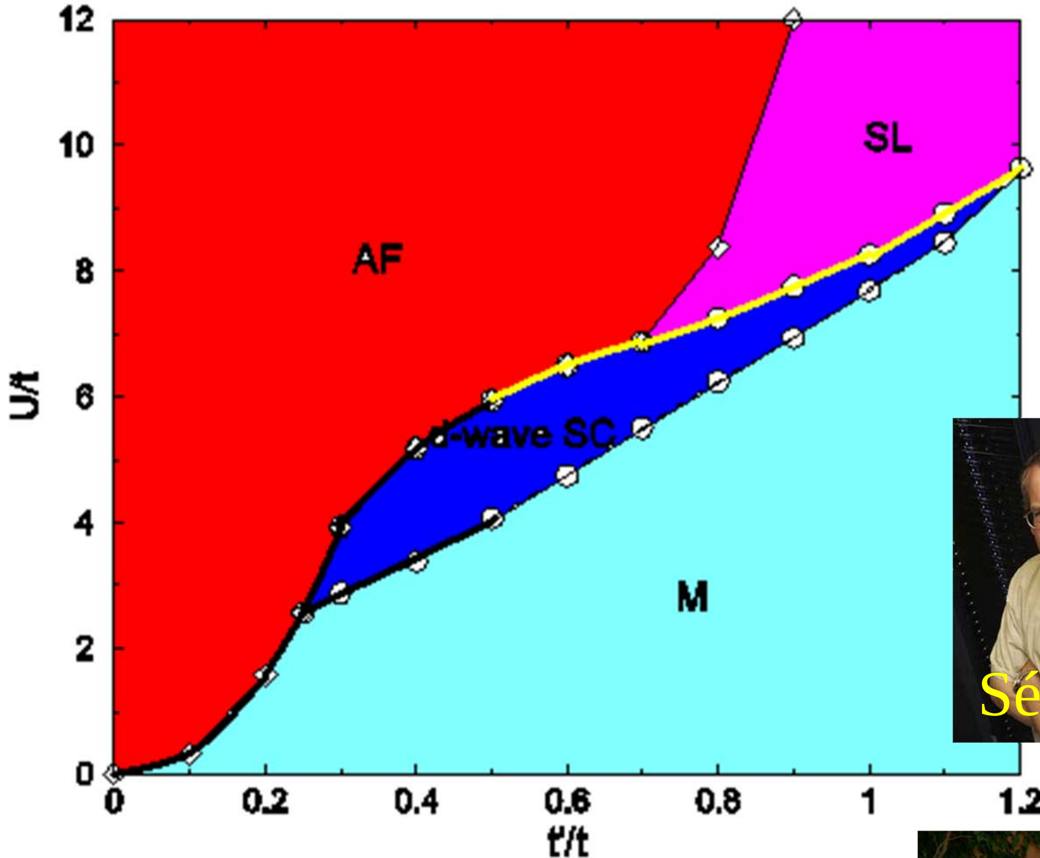


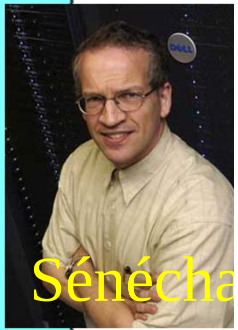
Theoretical phase diagram BEDT

X= $Cu_2(CN)_3$ (t'~ t)



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





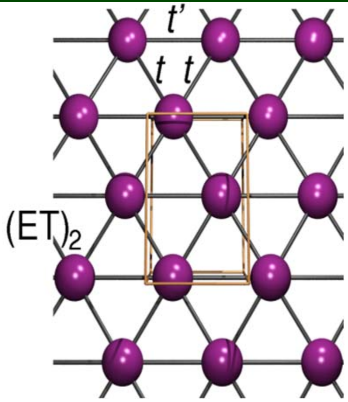
Kyung, A.-M.S.T. PRL 97, 046402 (2006)

Sénéchal, Sahebsara, Phys. Rev. Lett. **97**, 257004

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

Other compounds (R. Valenti et al.)

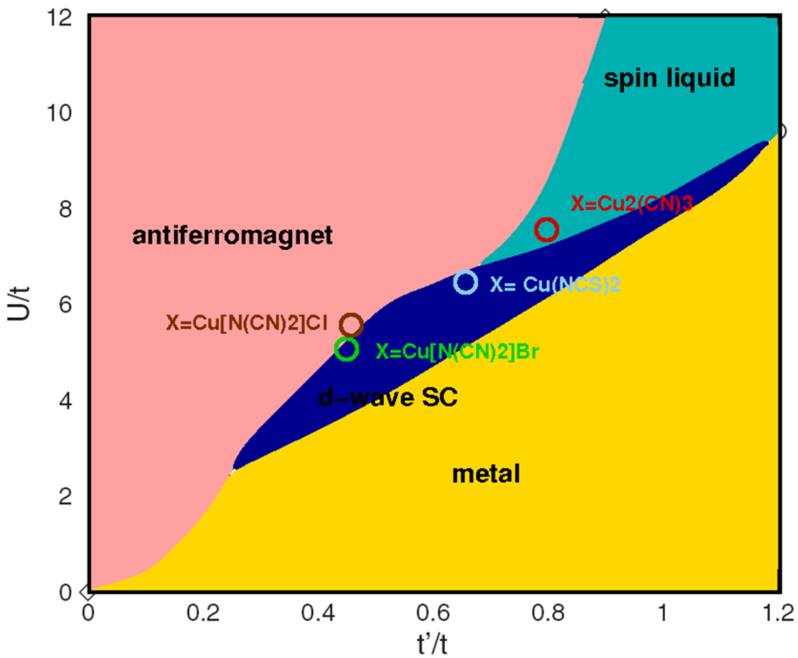
	Hueckel		DFT	
X	t'/t	U/t	t'/t	U/t
CN	1.06	8.2	0.83 (0.85)	7.3 (12)
SCN	0.84	6.8	0.58 (0.83)	6.0
Cl	0.75	7.5	0.44	7.5
Br	0.68	7.2	0.42	5.1



Kandpal et al. PRL (2009)

Nakamura et al. JPSJ (2009)

Komatsu et al. JPSJ (1996)



Kyung, Tremblay PRL (2006)

Tocchio, Parola, Gros, Becca PRB (2009)

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Analogous results with other methods

H. Morita et al., J. Phys. Soc. Jpn. 71, 2109 (2002).

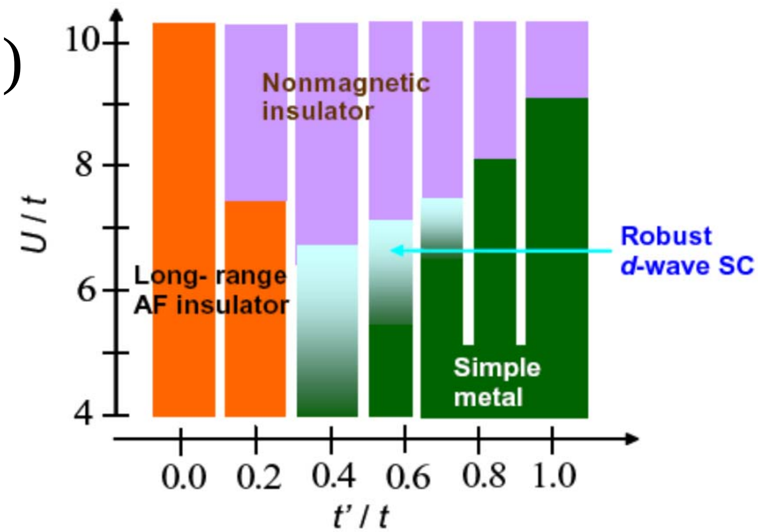
J. Liu et al., Phys. Rev. Lett. 94, 127003 (2005).

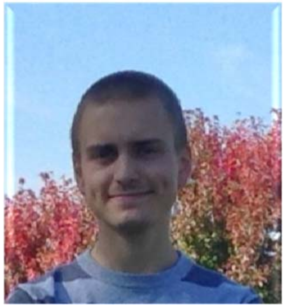
S.S. Lee et al., Phys. Rev. Lett. 95, 036403 (2005).

B. Powell et al., Phys. Rev. Lett. 94, 047004 (2005).

J.Y. Gan et al., Phys. Rev. Lett. 94, 067005 (2005).

T. Watanabe et J. Phys. Soc. Japan (2006)





Charles-David Hébert

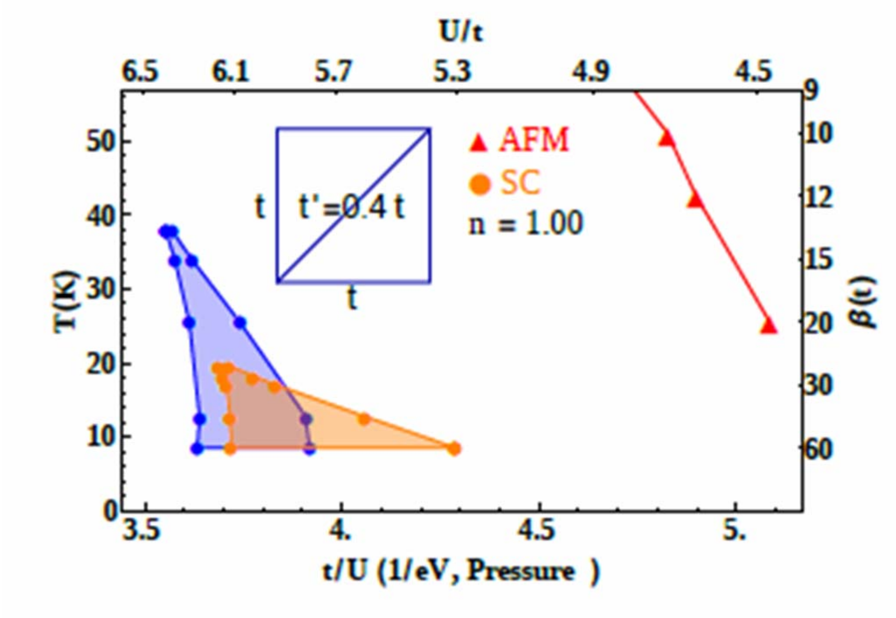
Patrick Sémon

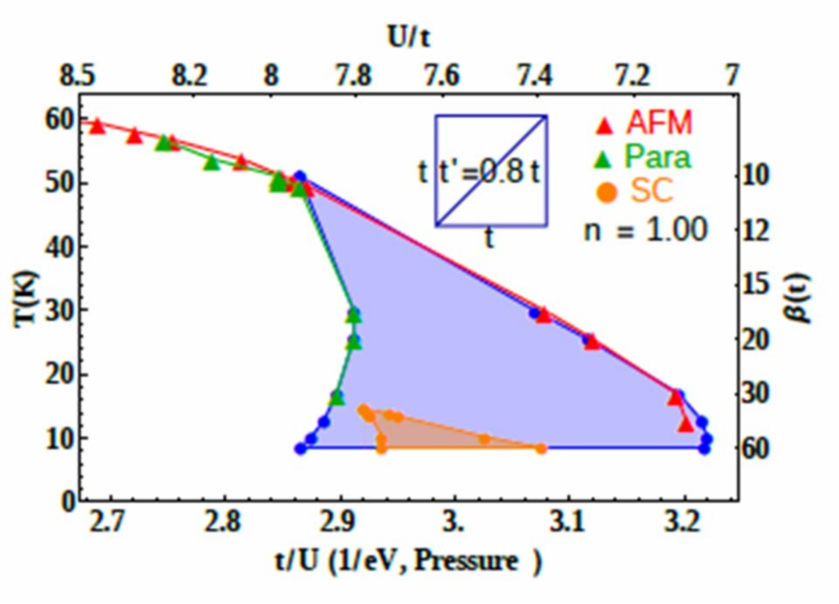
$n = 1$, finite T

Made possible by

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

Effect of frustration ($n = 1$)





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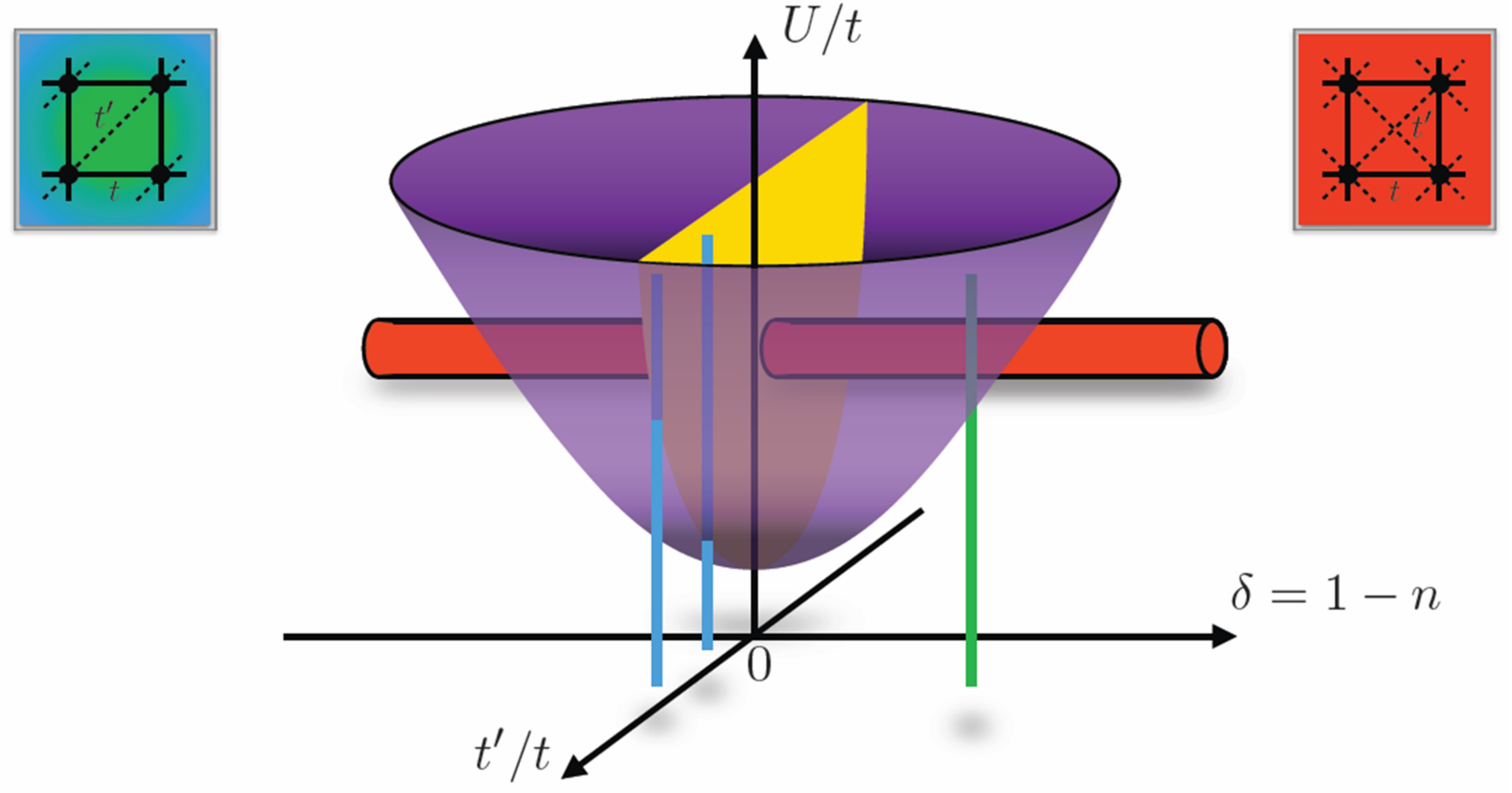
Generalized Phase Diagram



Doped Organics: normal state

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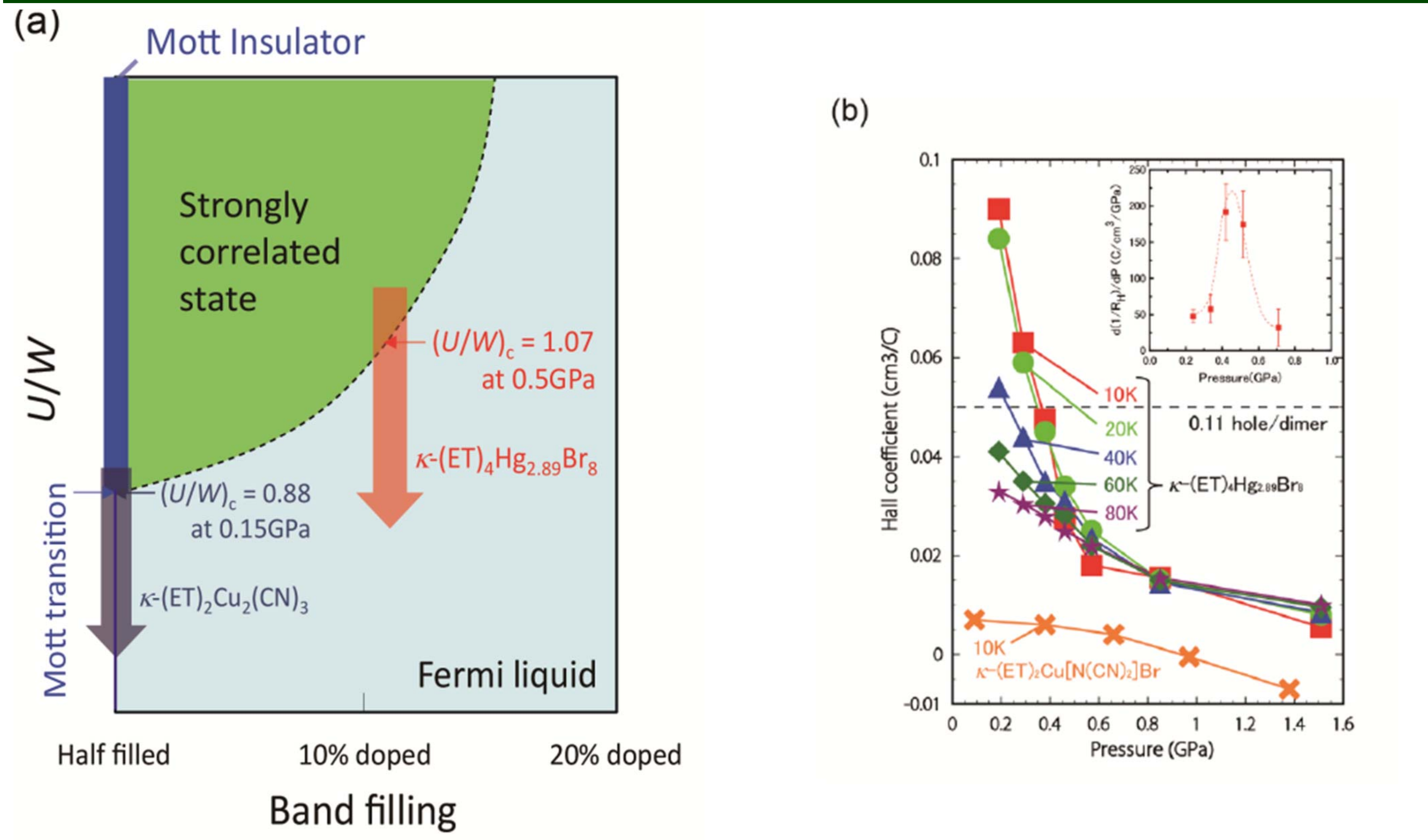
Doped BEDT



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

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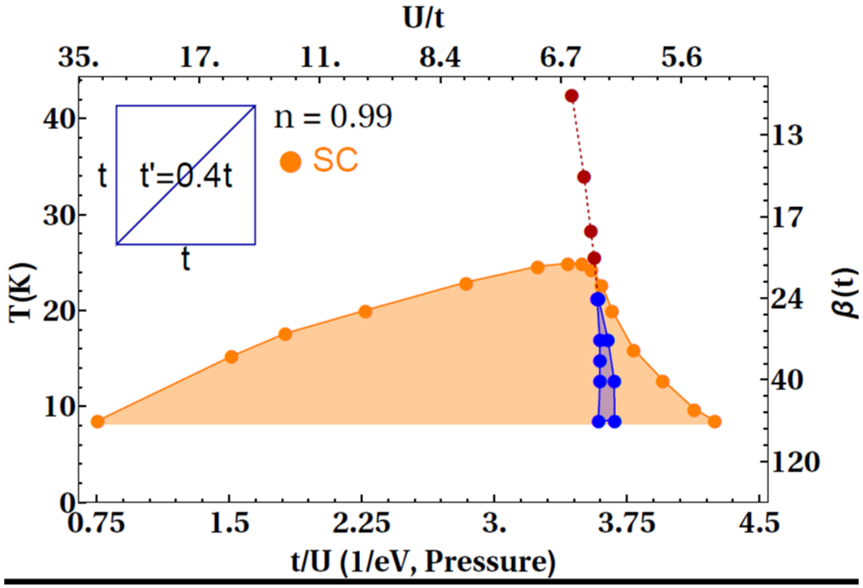
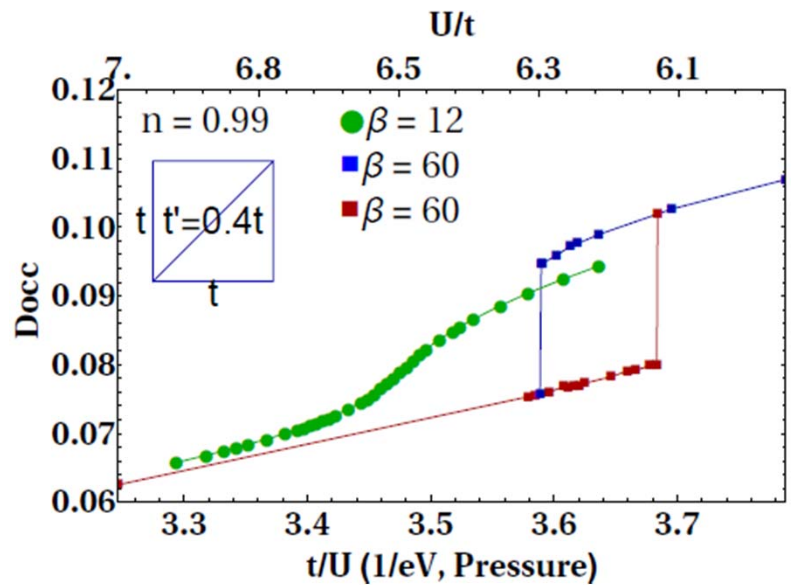
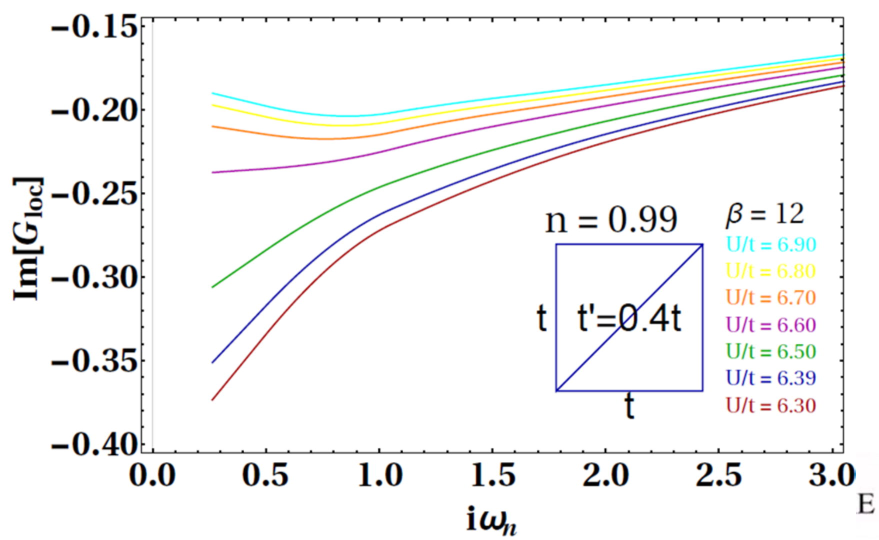
Widom line in organics

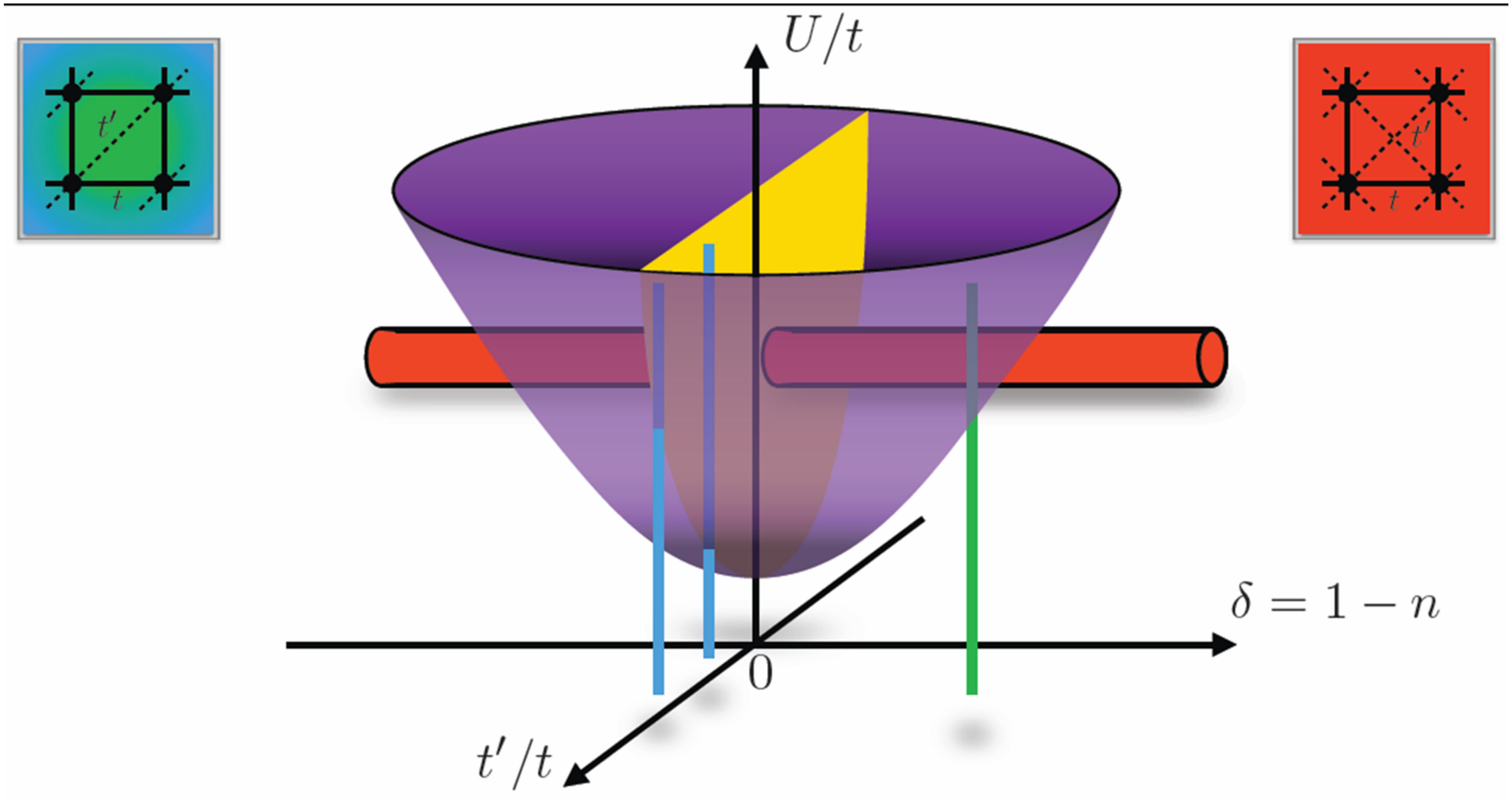






Charles-David Hébert, Patrick Sémon , AMT

Generalized Phase Diagram



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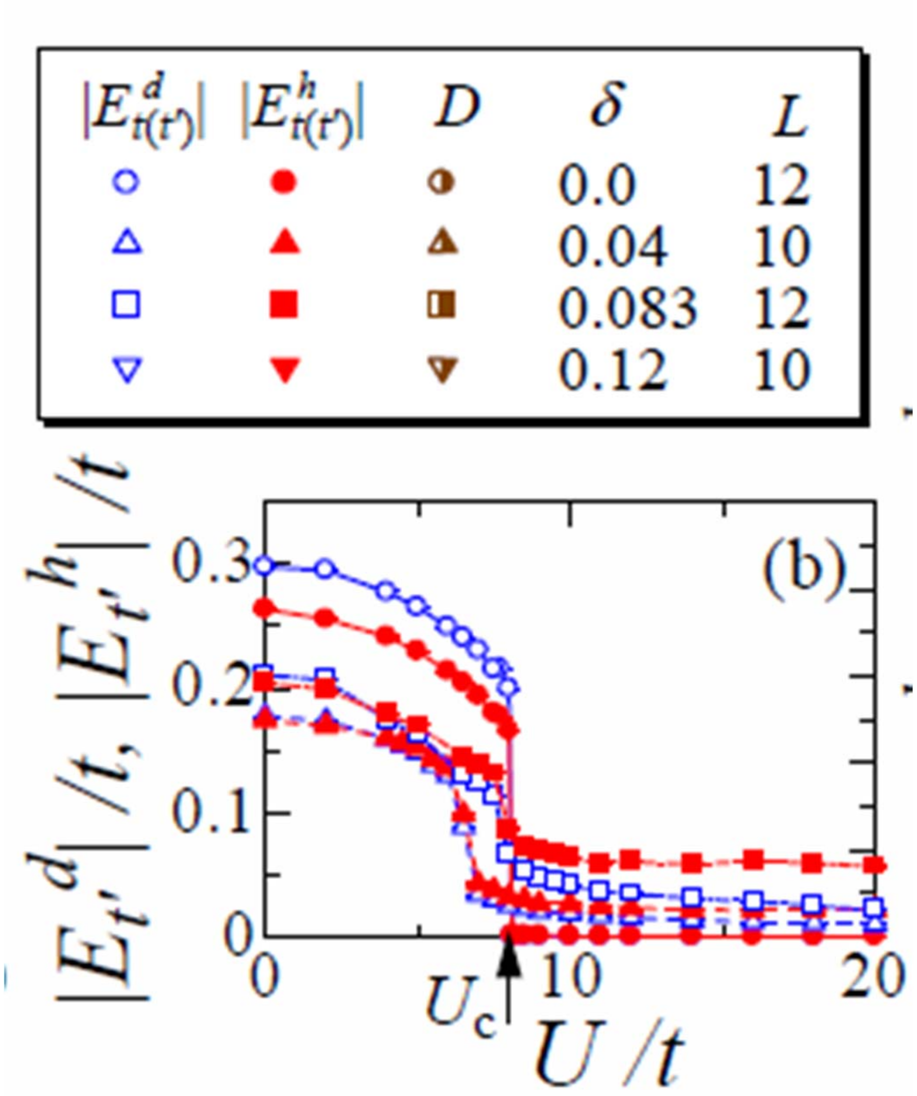
Results from variational MC



t'/t = 0.8

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

Superconductivity in the organics at finite T

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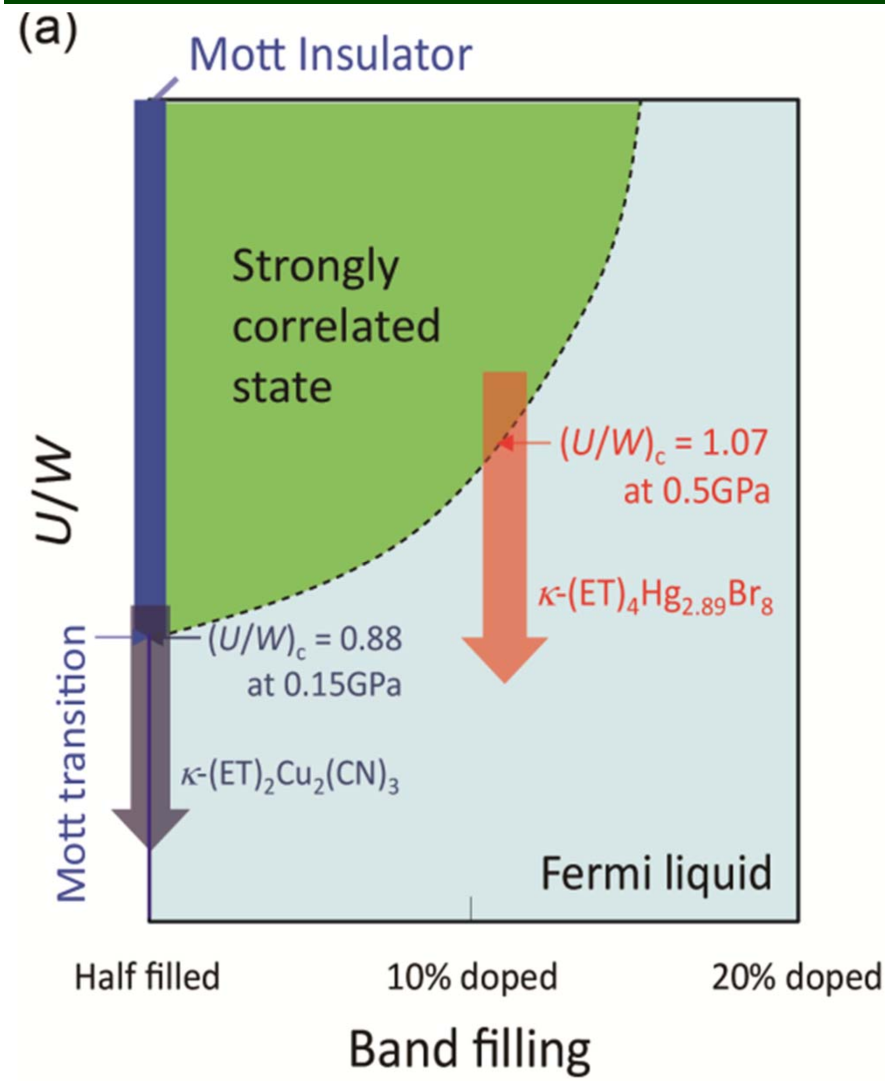
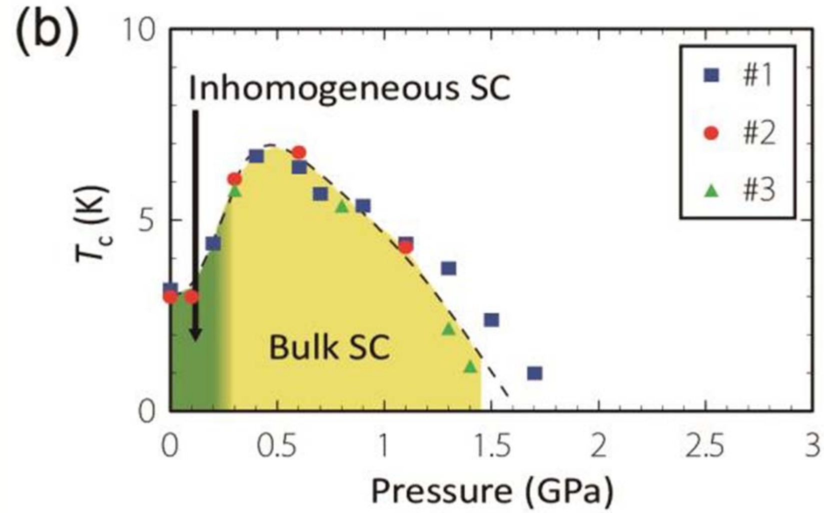
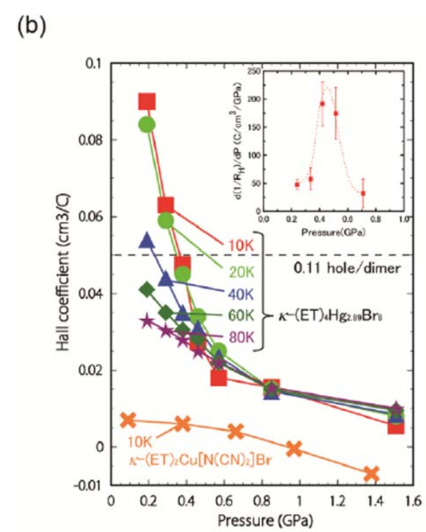
Doped BEDT







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

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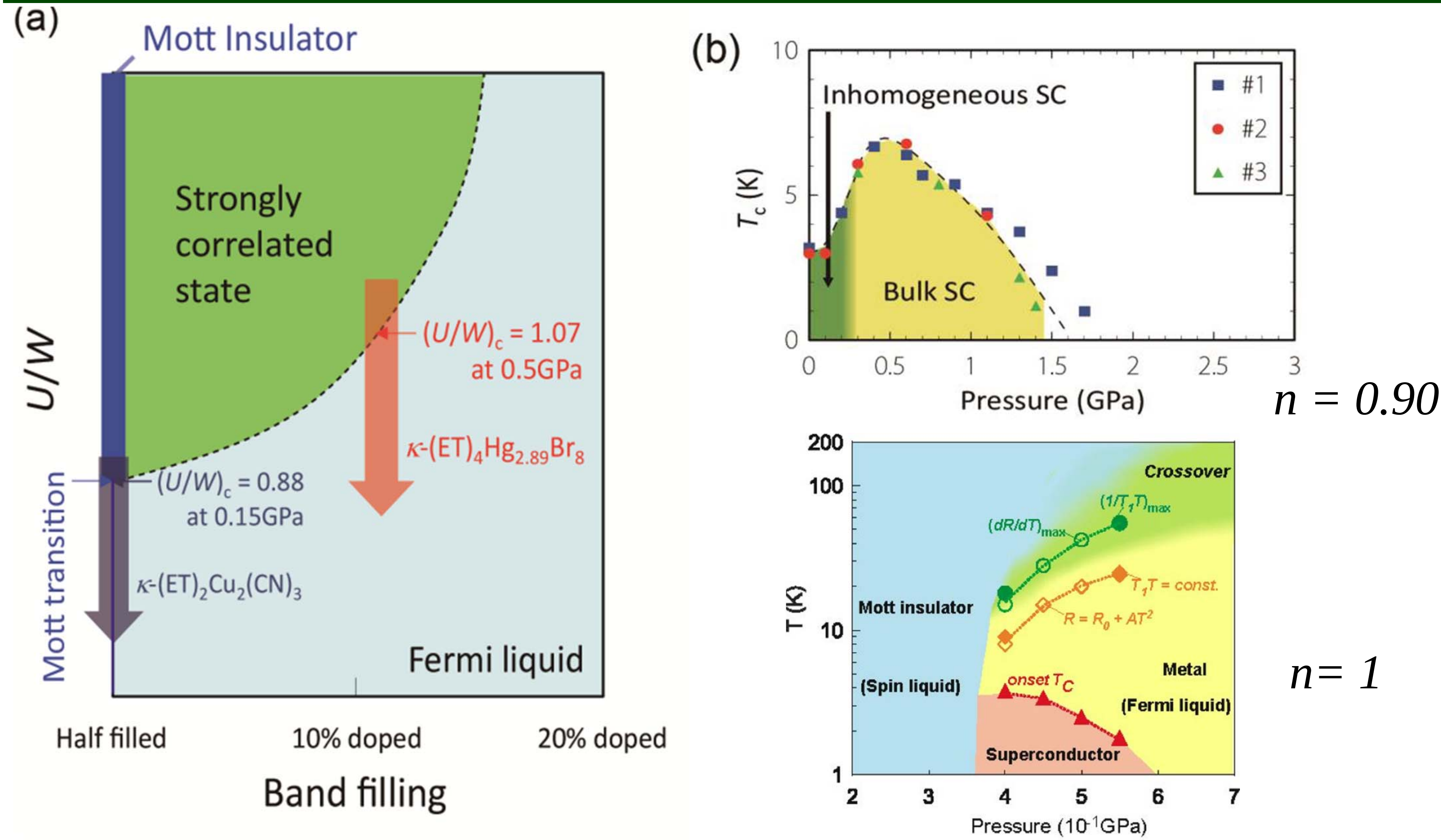
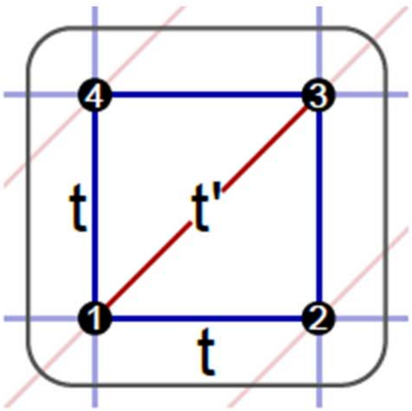
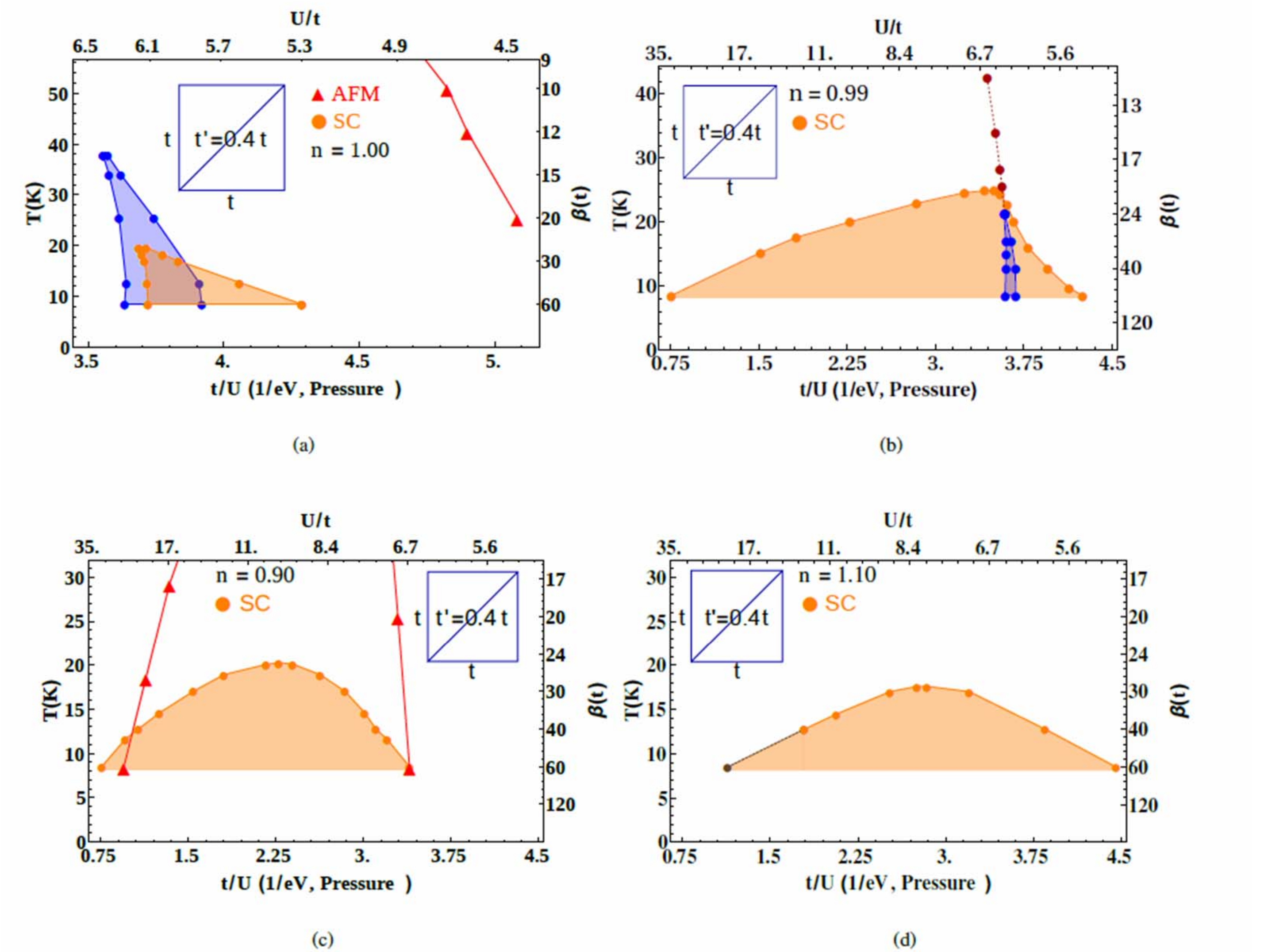


H. Oike, K. Miyagawa, H. Taniguchi, K. Kanoda PRL **114**, 067002 (2015)

t'=0.4t

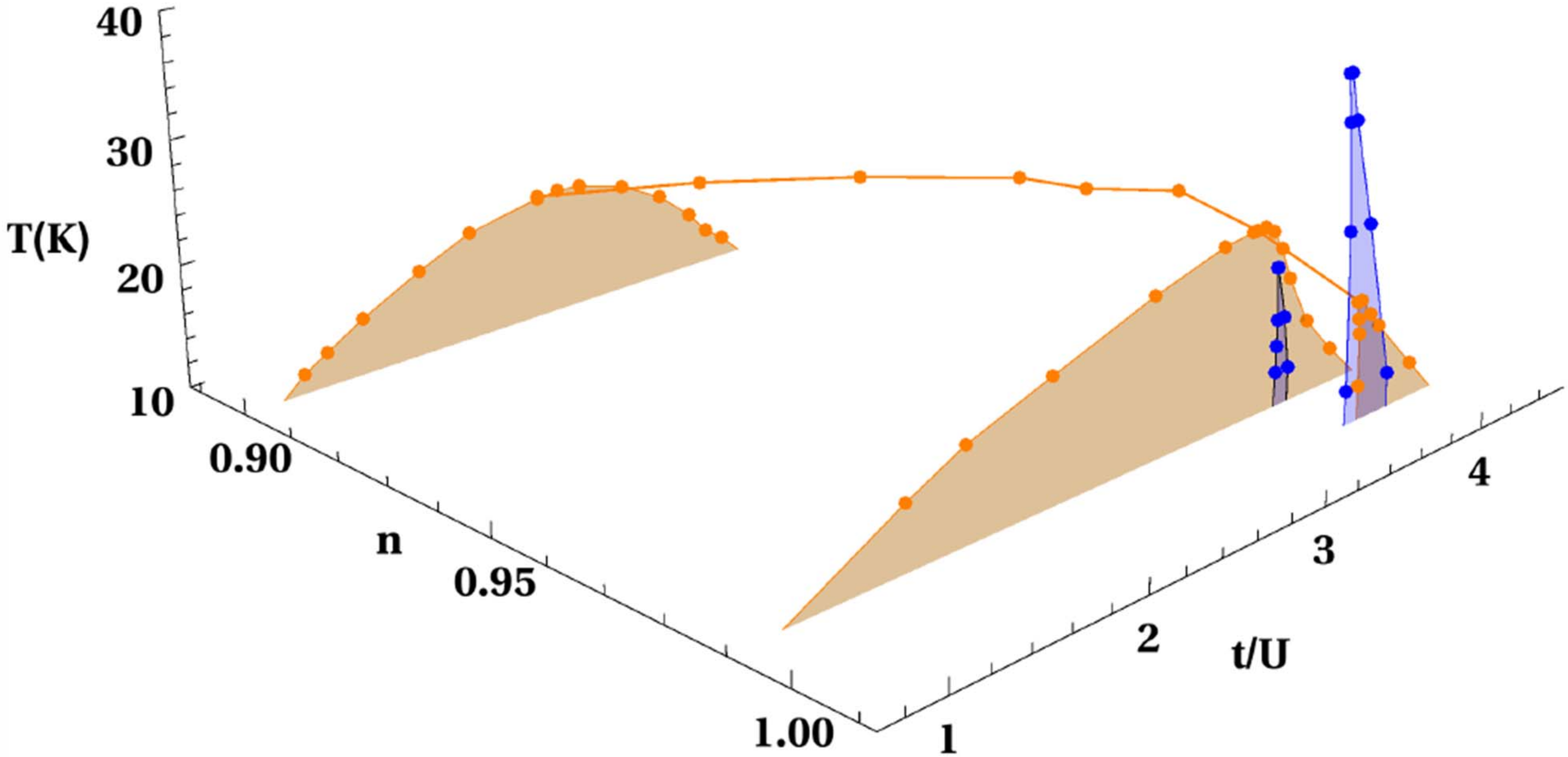


t
t'
t

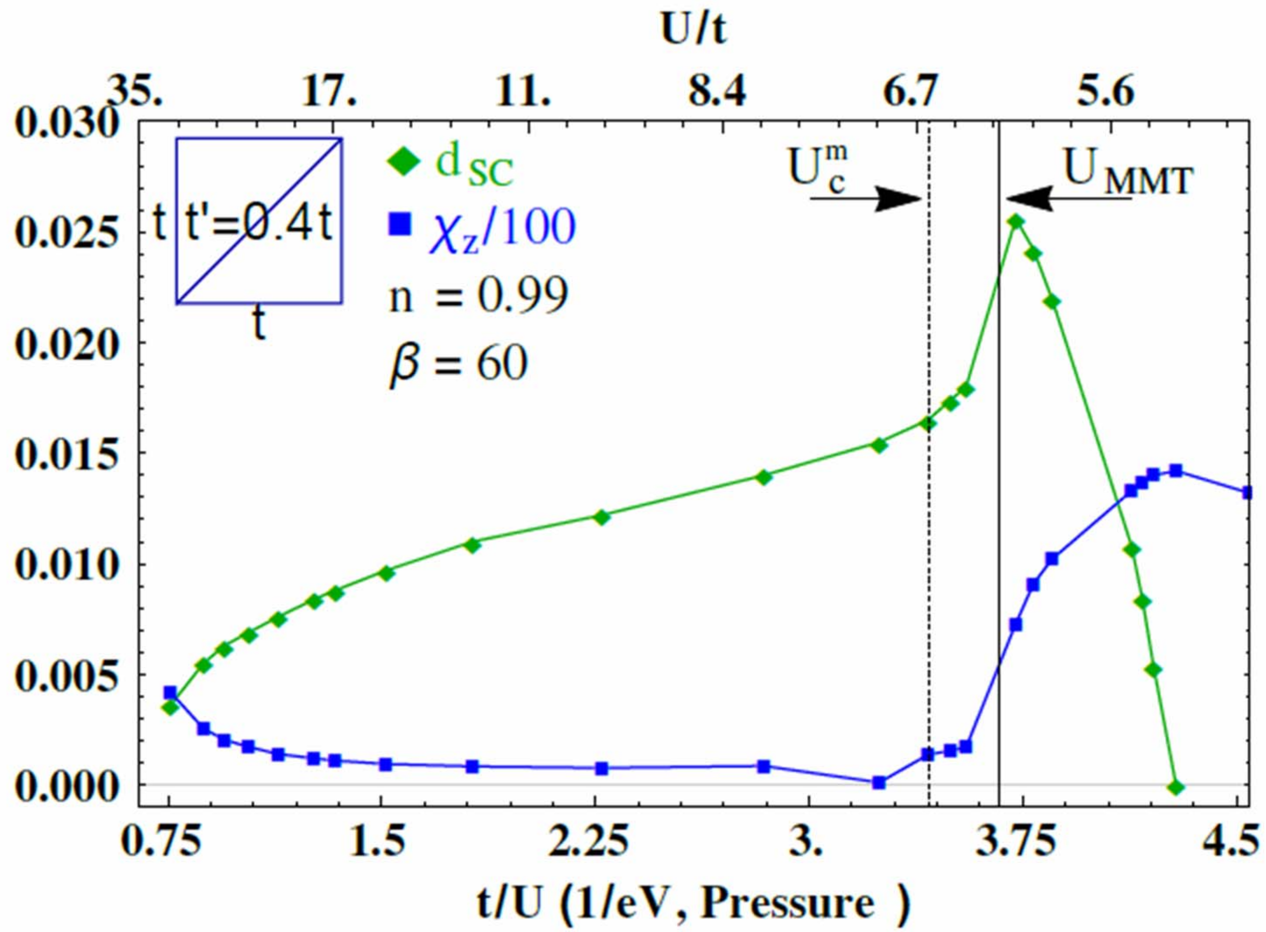


U/t
t/U (1/eV, Pressure)
T(K)
β(t)
AFM
SC
n = 1.00
t'=0.4 t
(a)
n = 0.99
(b)
n = 0.90
(c)
n = 1.10
(d)

t' = 0.4t overview



Signatures of Widom line in the superconducting state



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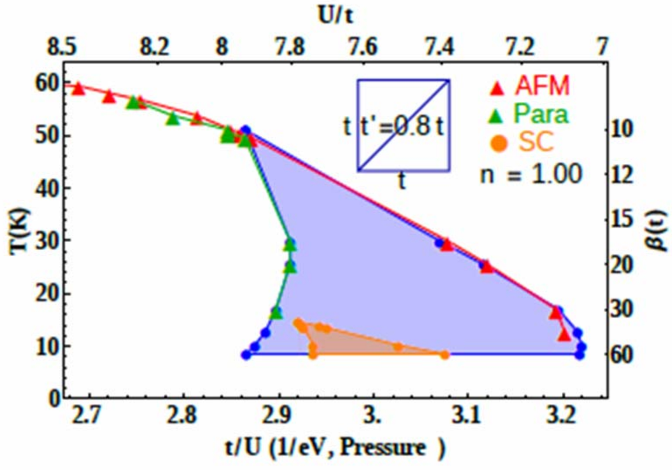
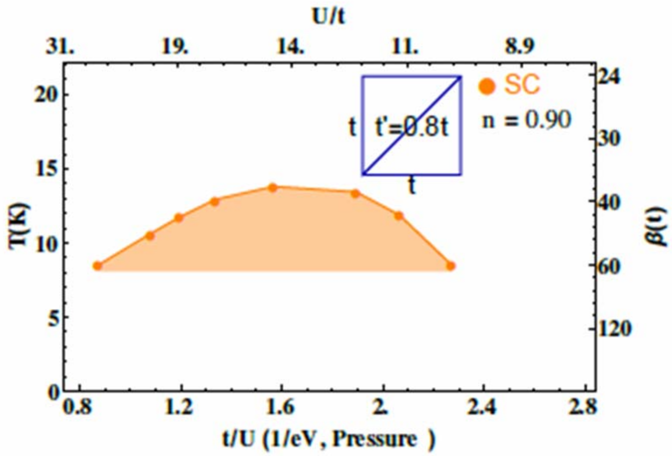
t’ = 0.8 t



U/t
8.5
8.2
8
7.8
7.6
7.4
7.2
7
AFM
Para
SC
t
t'=0.8 t
t
n = 1.00
T(K)
β(t)
t/U (1/eV, Pressure)

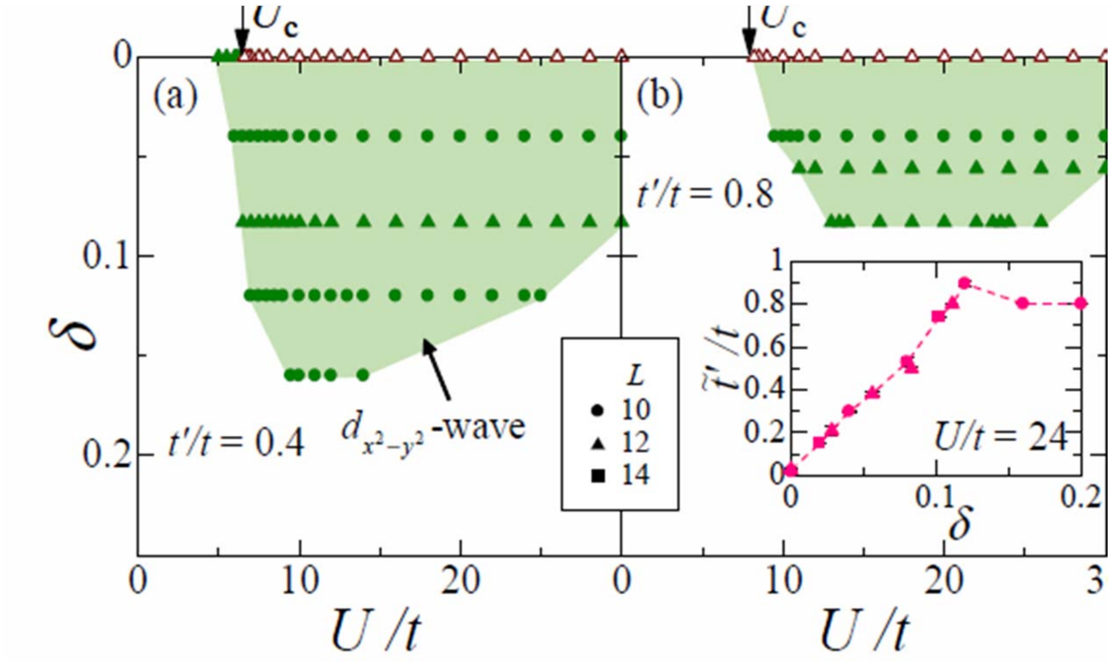
(a)



U/t
31.
19.
14.
11.
8.9
SC
n = 0.90
t
t'=0.8t
t
T(K)
β(t)
t/U (1/eV, Pressure)

(b)

Results from variational MC



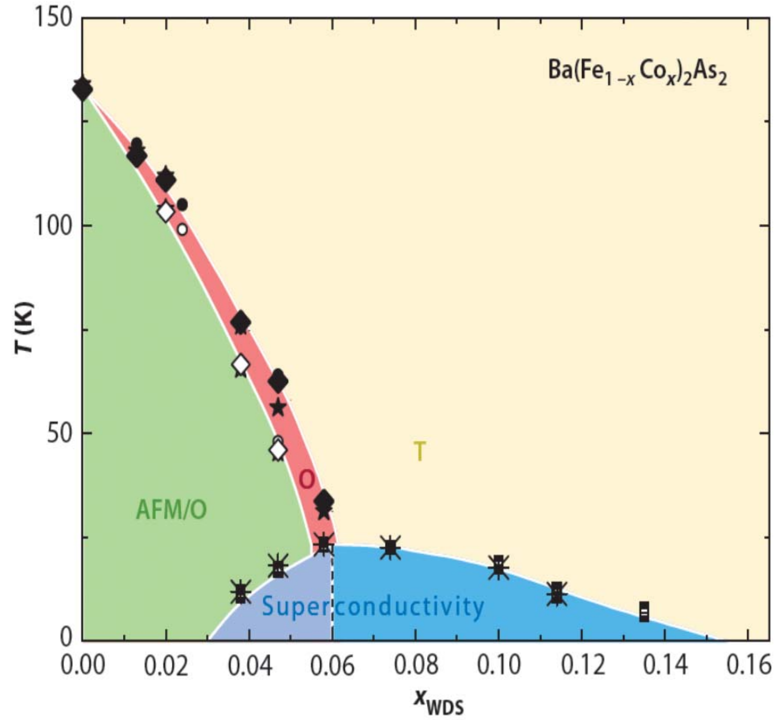
T. Watanabe, H. Yokoyama and M. Ogata
JPS Conf. Proc. **3**, 013004 (2014)

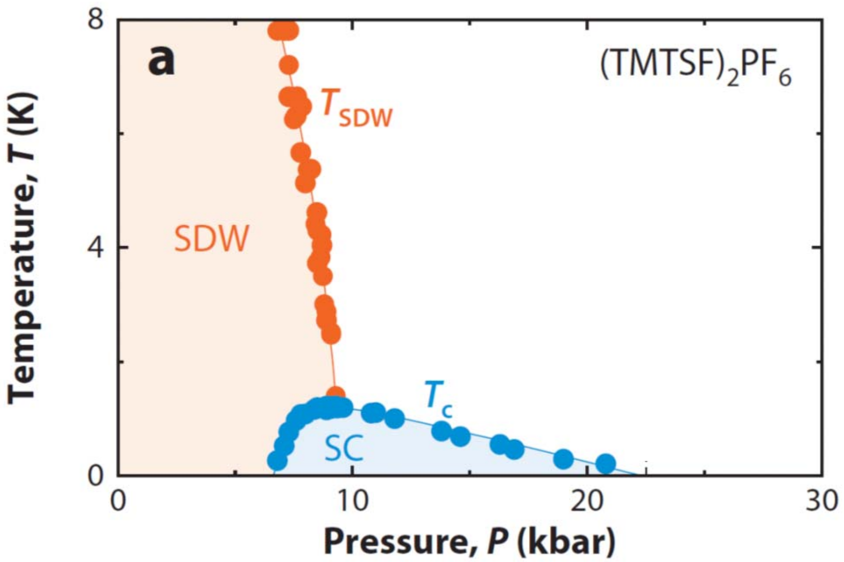
Antiferromagnetic quantum critical point scenario (weakly correlated)

Pnictides and organics

Pnictides

Organics





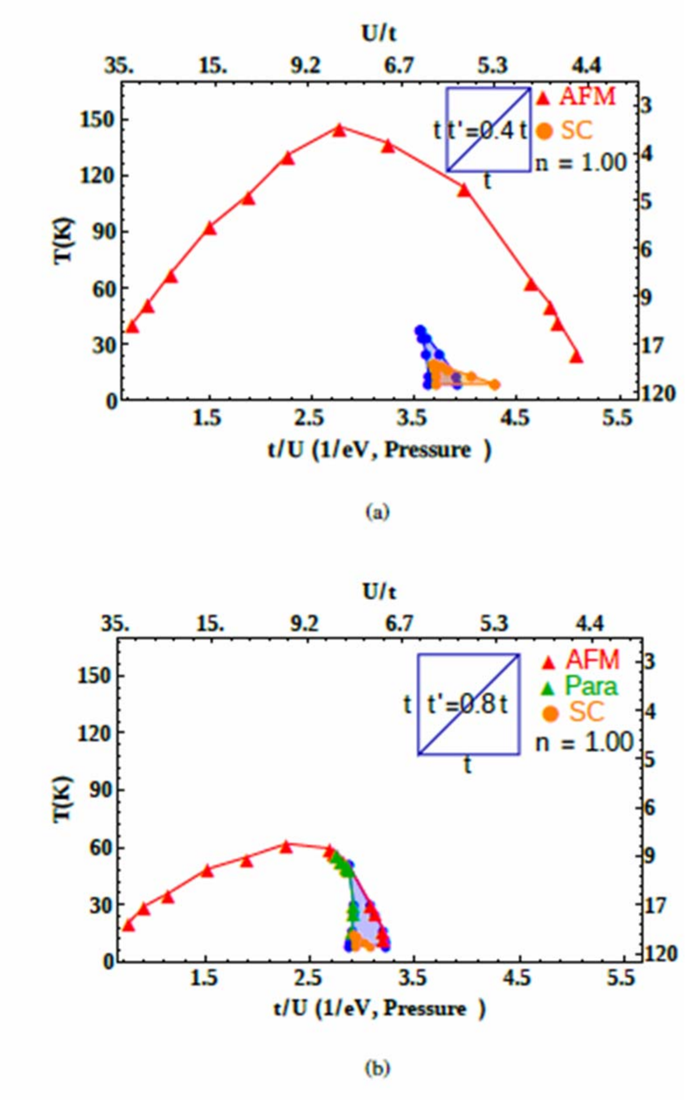
The Archetype

Magnetic superconductivity

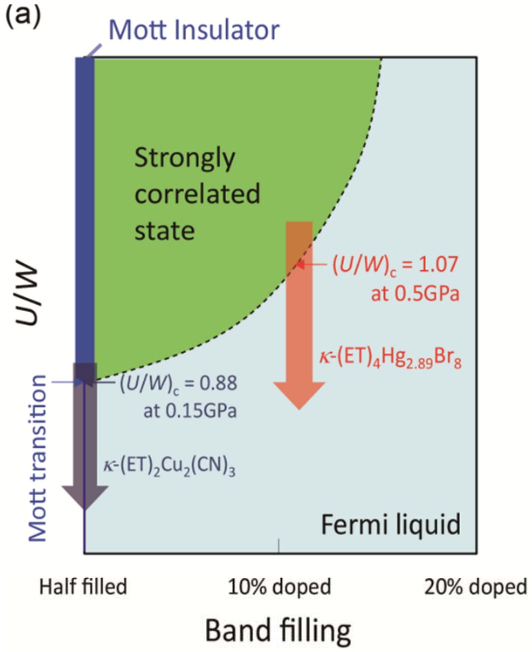
Nicolas Doiron-Leyraud, Bourbonnais, Taillefer 2010

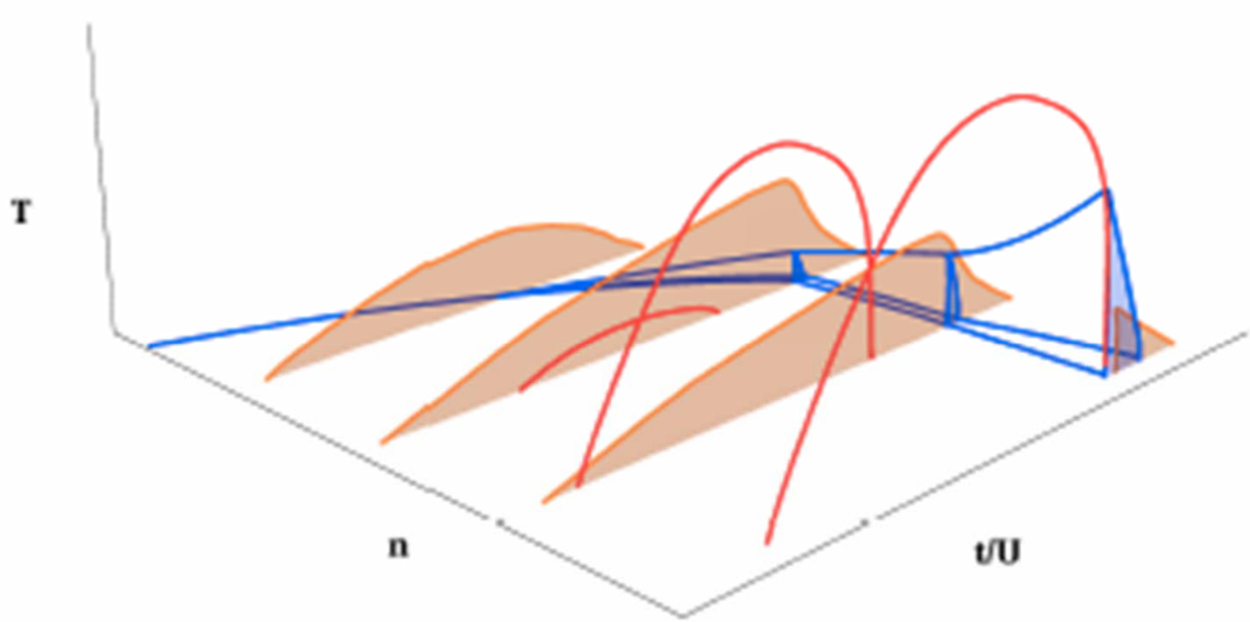
Canfield et al. (2010)

AFM not related to maximum T_c



Generic case highly frustrated case





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Wei Wu

AFM quantum critical point in heavy fermions (with same methods)

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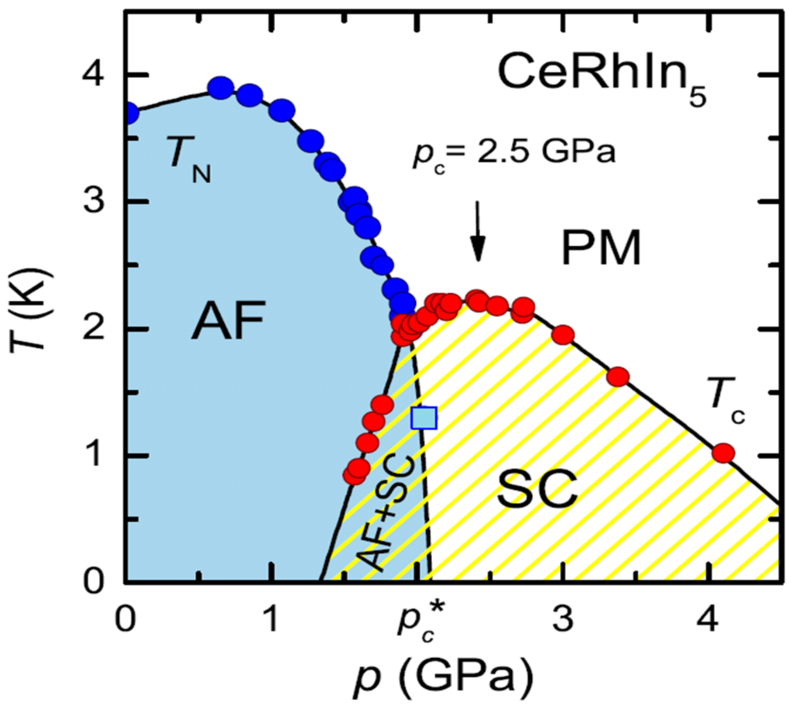
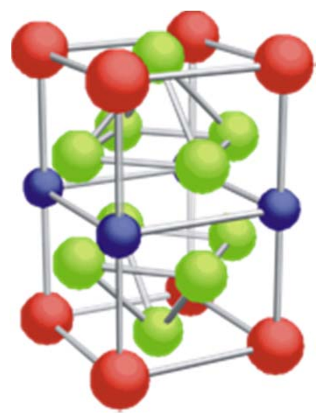
Heavy fermions

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



Knebel et al. (2009)

$CeRhIn_5$



Magnetic superconductivity

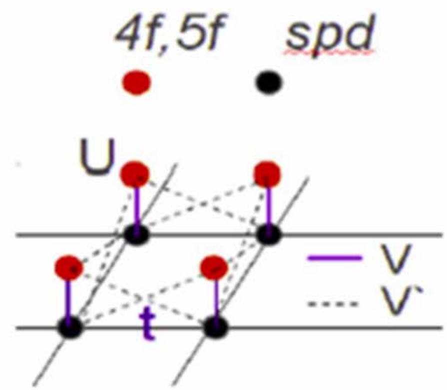
Quantum criticality

Mathur et al., Nature 1998

Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$

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

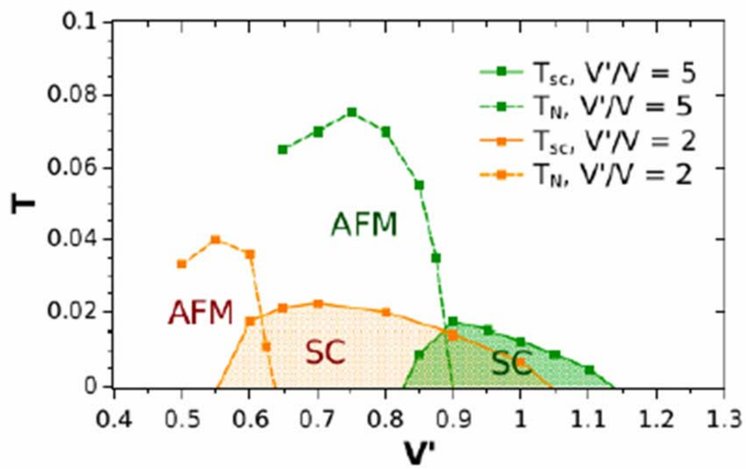


$$V_k = V + 2V'[cos(k_x) + cos(k_y)]$$

U=4

AFM: antiferro-magnetism
SC: superconducting

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



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

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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
    - (or remnants in SC state) (also T_c decreases in e-doped)
- Physics
  - SC dome without an AFM QCP. Extension of Mott
  - SC from short range J.
  - T_c decreases at Widom line

Main collaborators

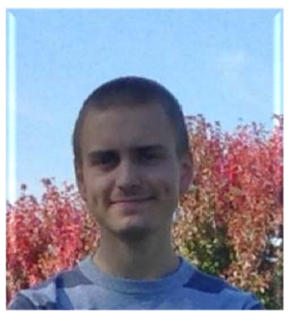
David Sénéchal

Patrick Sémon

Giovanni Sordi

Kristjan Haule

Bumsoo Kyung



Charles-David Hébert

Wei Wu

Lorenzo Fratino

Team

Tremblay, Reymbaut, Gagnon, Verret, Hébert, Charlebois, Nourafkan

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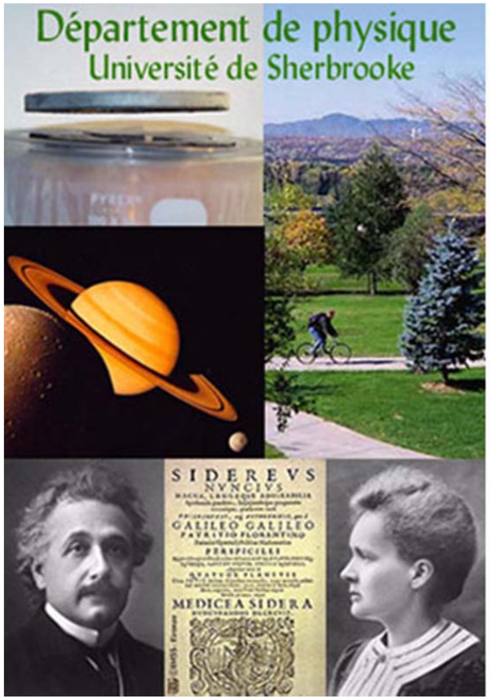

André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Le regroupement québécois sur les matériaux de pointe

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Le calcul de haute performance
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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