Mott Physics in Strongly Correlated Superconductivity

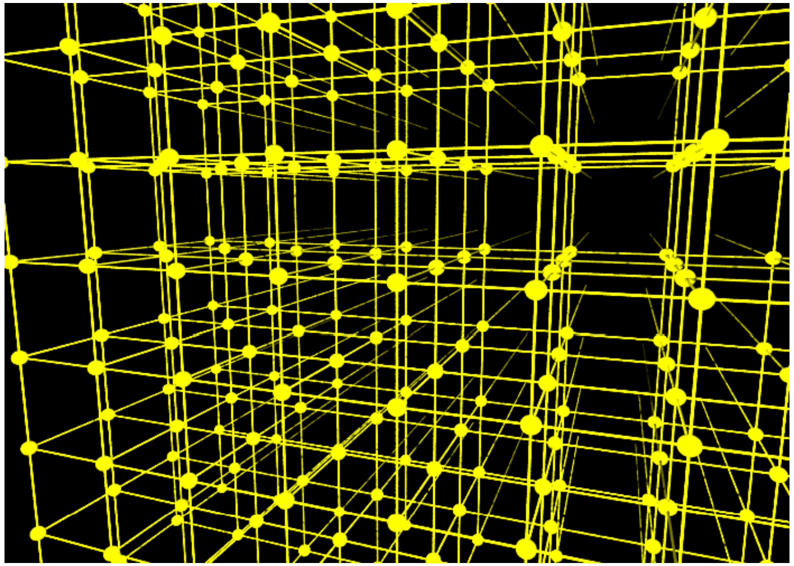
A.-M. Tremblay

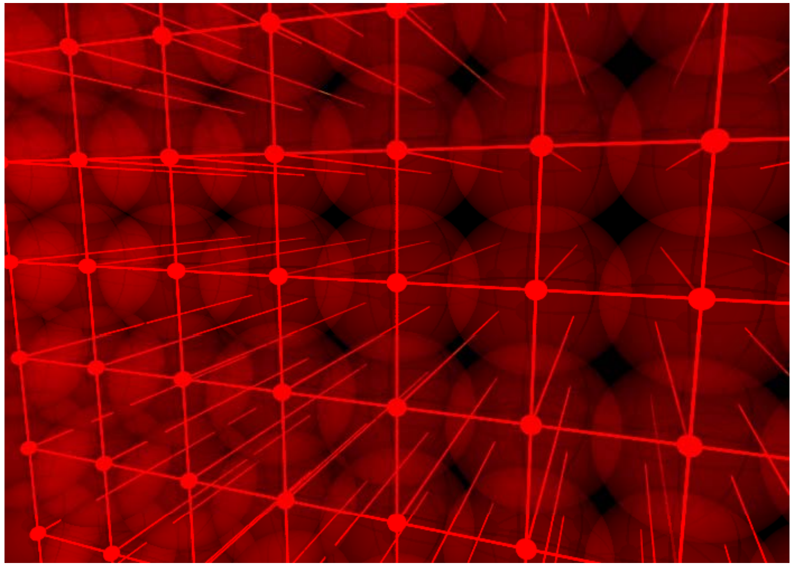
G. Sordi, D. Sénéchal, K. Haule,

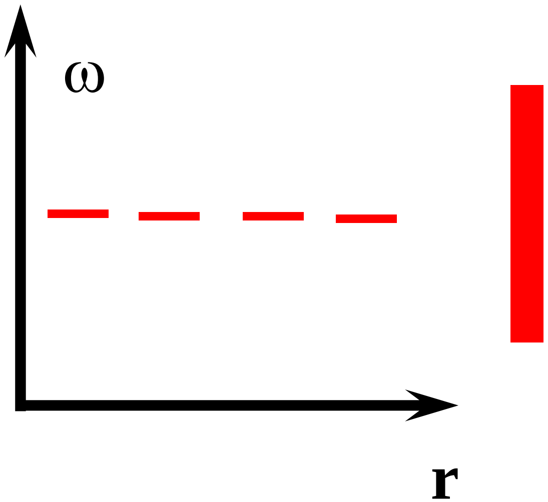
S. Okamoto, B. Kyung, M. Civelli

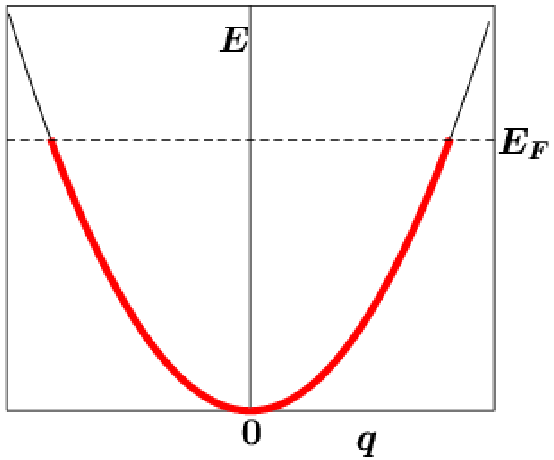
Los Alamos, 3 May 2011

How to make a metal



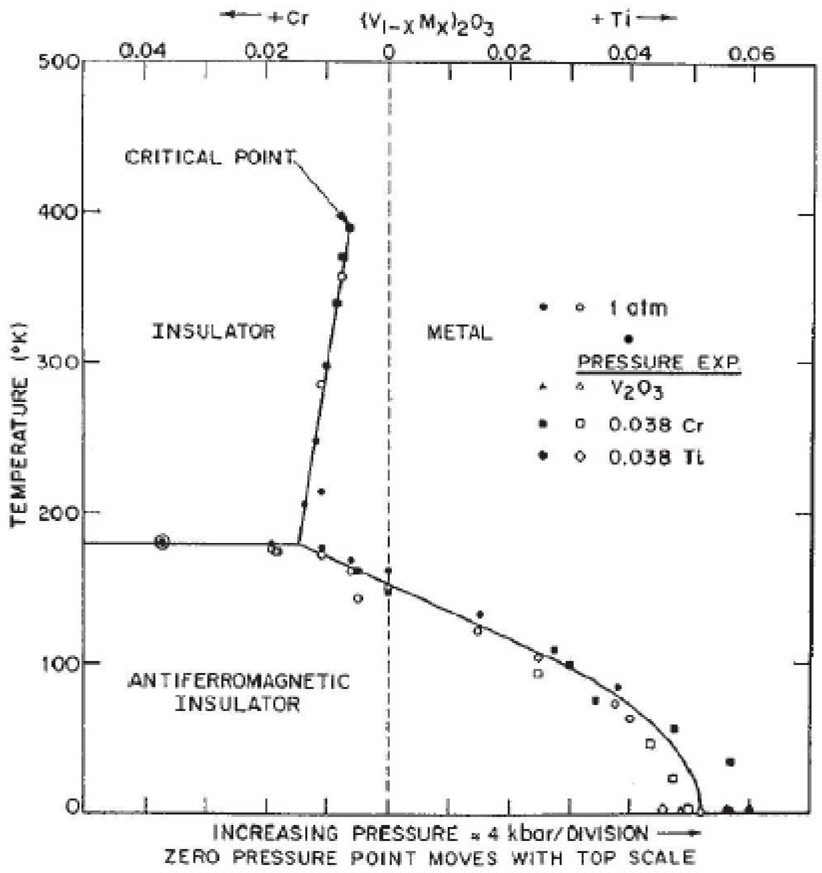






Courtesy, S. Julian

« Conventional » Mott transition



T

p

Understood from Hubbard model and dynamical mean field theory

Figure: McWhan, PRB 1970; Limelette, Science 2003

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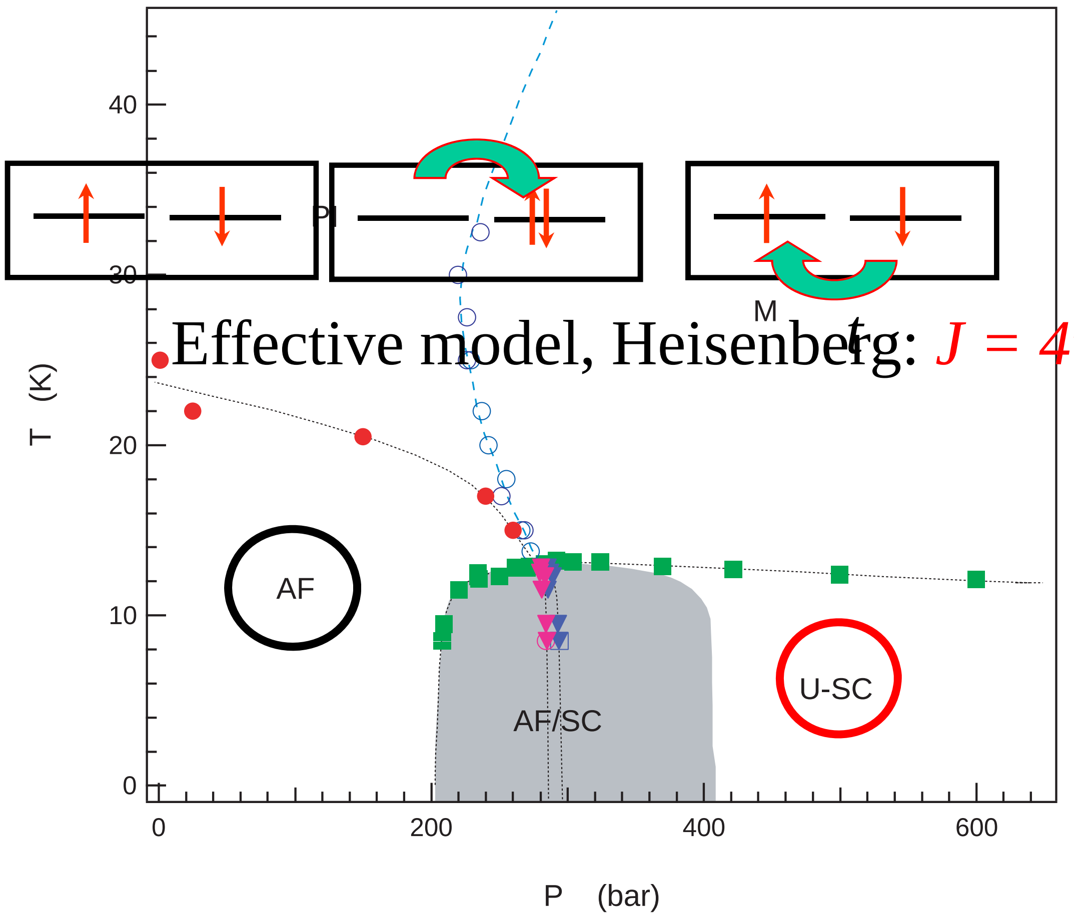
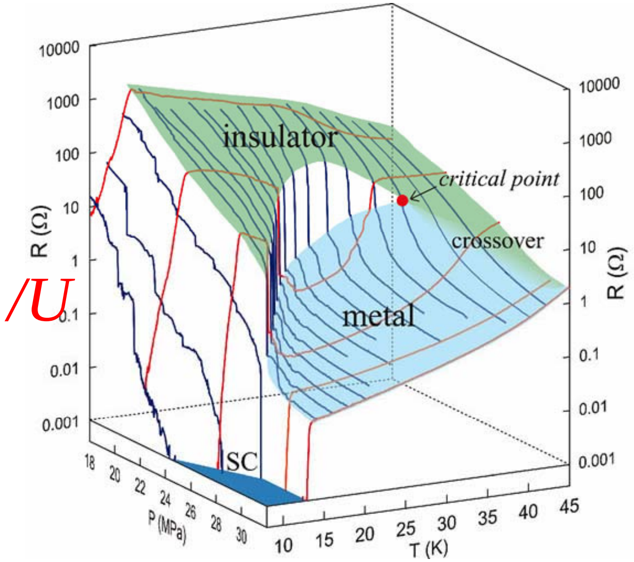
Bare Mott critical point in organics



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



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

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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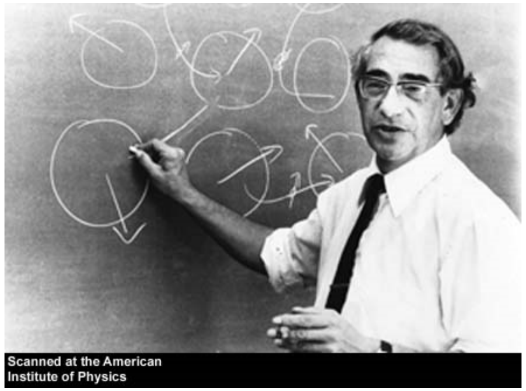
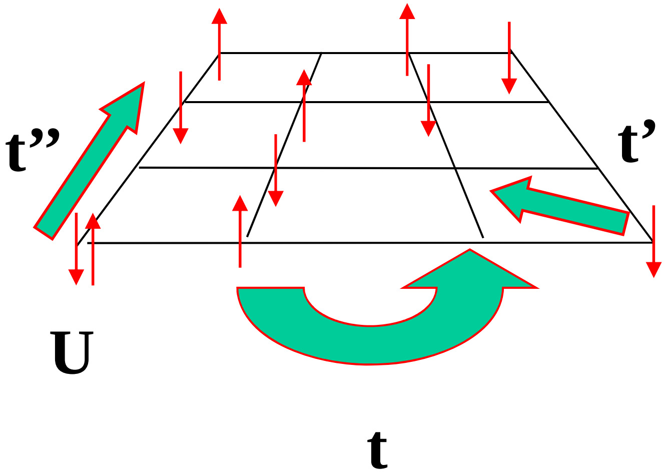
Hubbard model



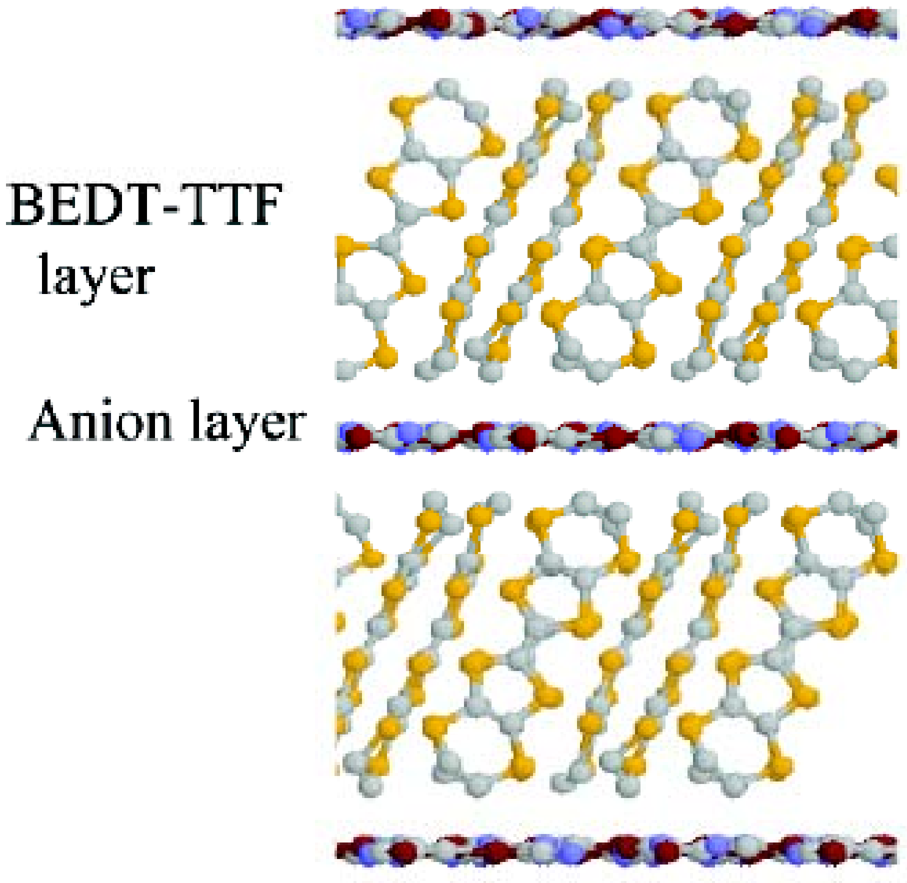
1931-1980

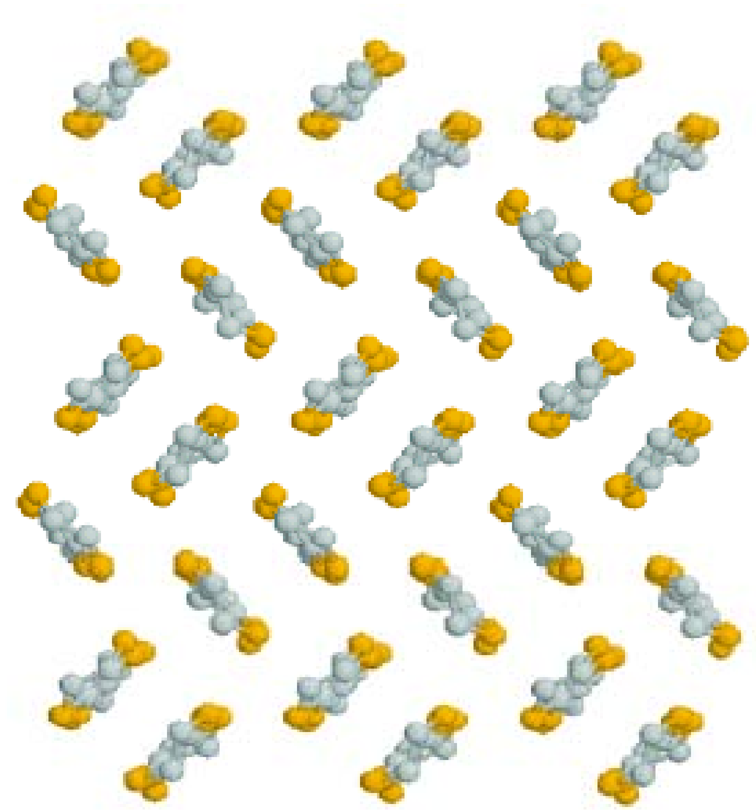
μ



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

Layered organics (κ–BEDT-X family)





$t \approx 50$ meV

$\Rightarrow U \approx 400$ meV

$t'/t \sim 0.6 - 1.1$

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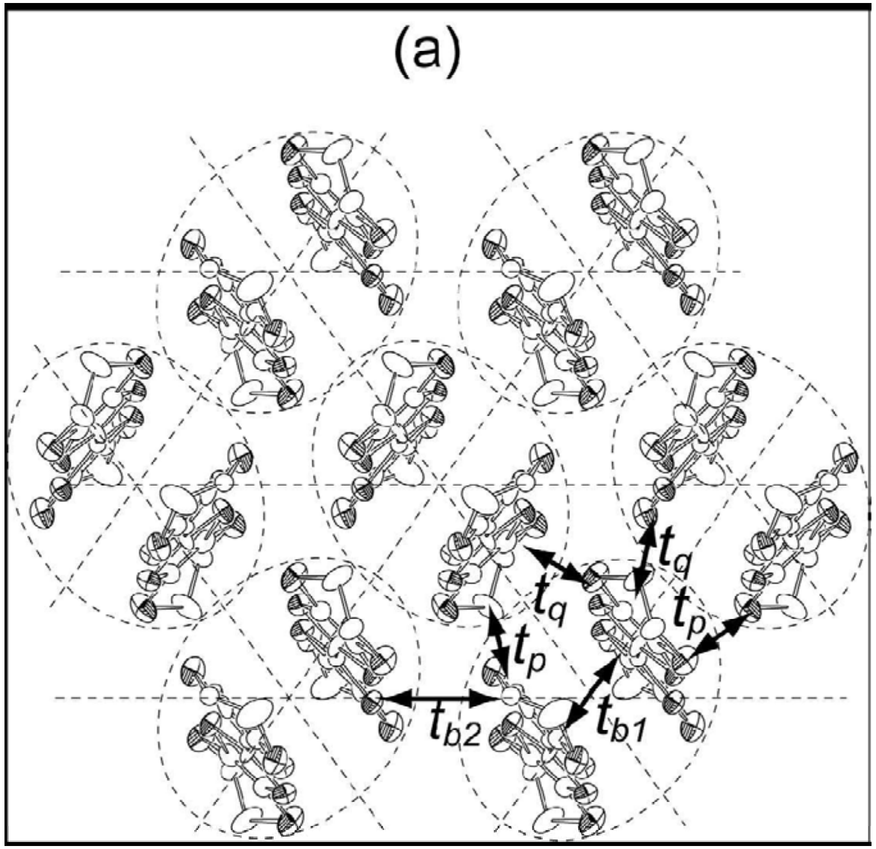
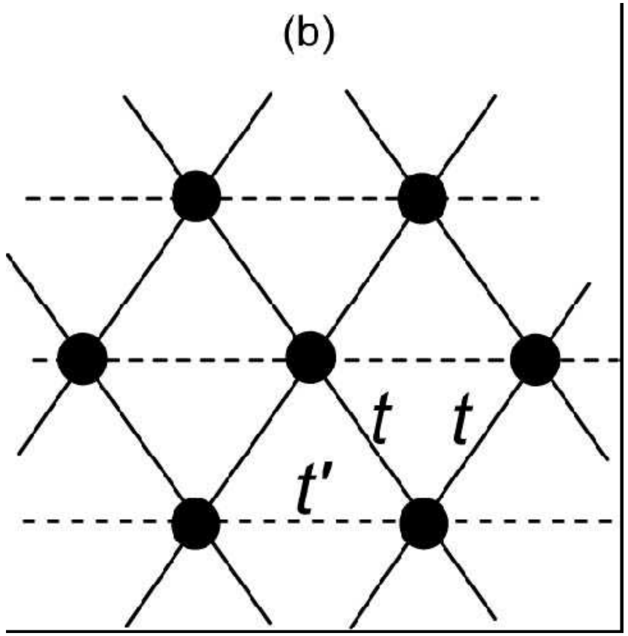
One-band Hubbard model of BEDT organics

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)

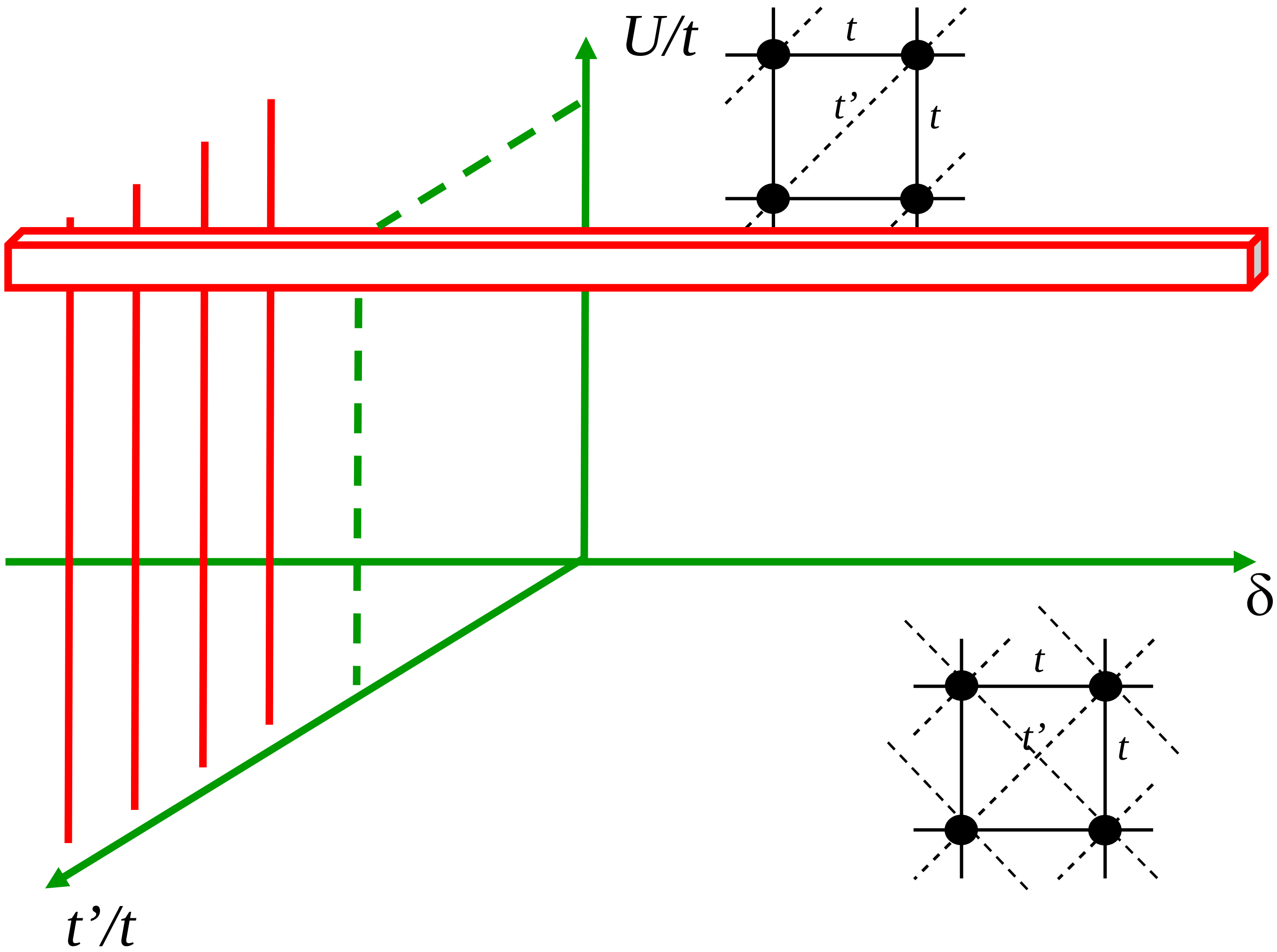


$$t \approx 50 \text{ meV}$$

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

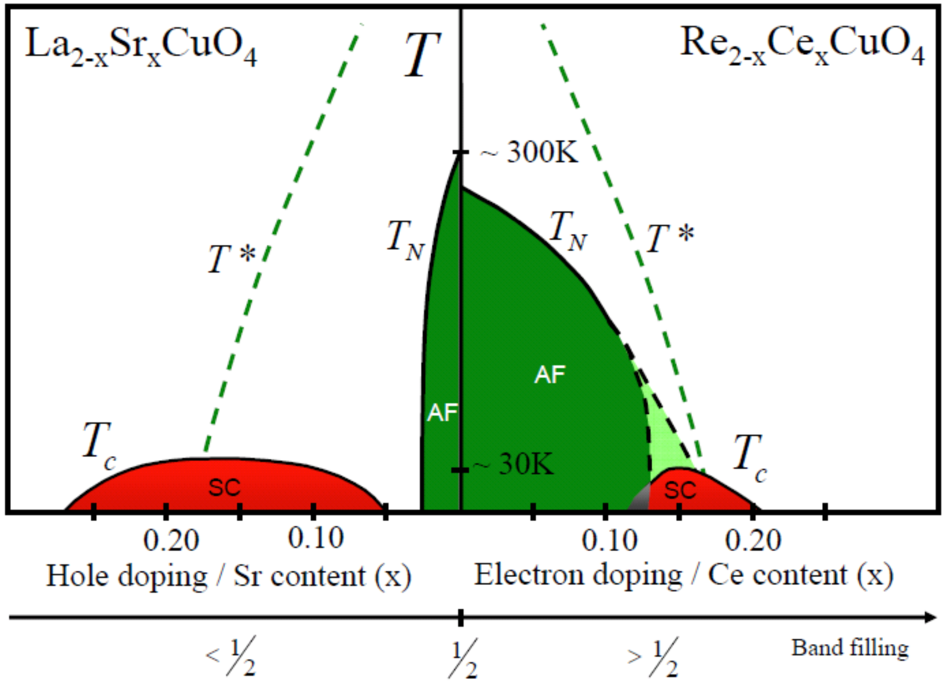
$t'/t \sim 0.6 - 1.1$

Perspective



Normal state of high-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)



What is under the dome?
Mott Physics away from $n = 1$

- Competing order
  - Current loops: Varma, PRB **81,** 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave : Chakravarty, Nayak, Phys. Rev. B **63**, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB **80**, 155129 (2009) ...
- Or Mott Physics?
  - RVB: P.A. Lee Rep. Prog. Phys. **71,** 012501 (2008)

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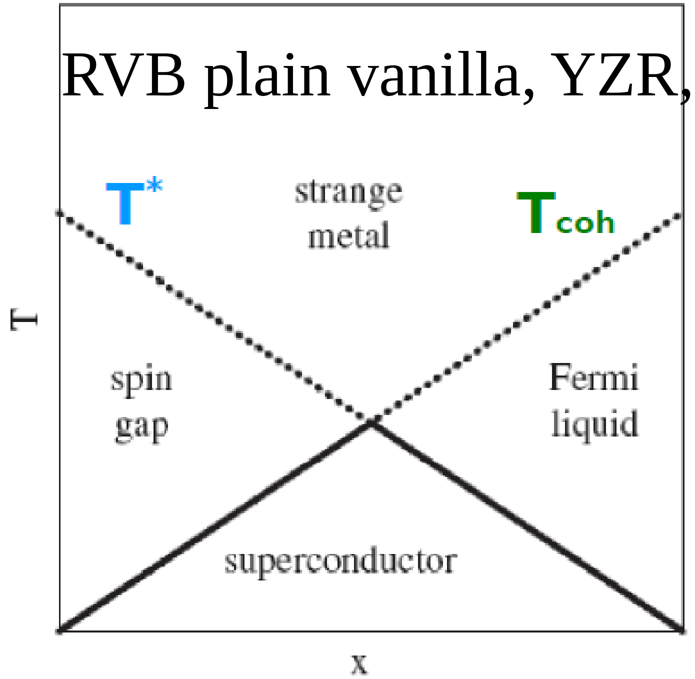
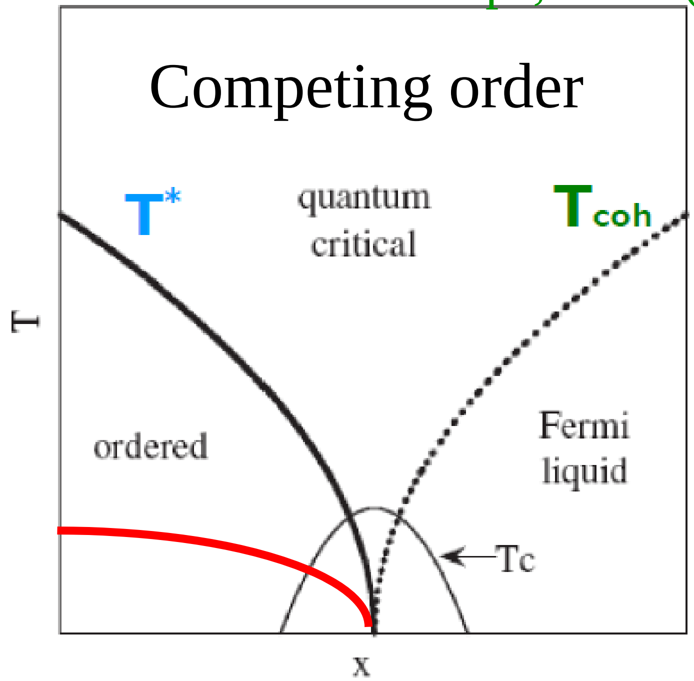
Two views (caricature)

Norman, Adv. Phys. (2005)
Broun, Nat. Phys. (2006)
Phillips, RMP (2010)





Why T_c decreases?
What is the origin of T^*?
What is the strange metal?

Long correlation length or not.
What lies beneath the dome.
Mott Physics away from $n = 1$

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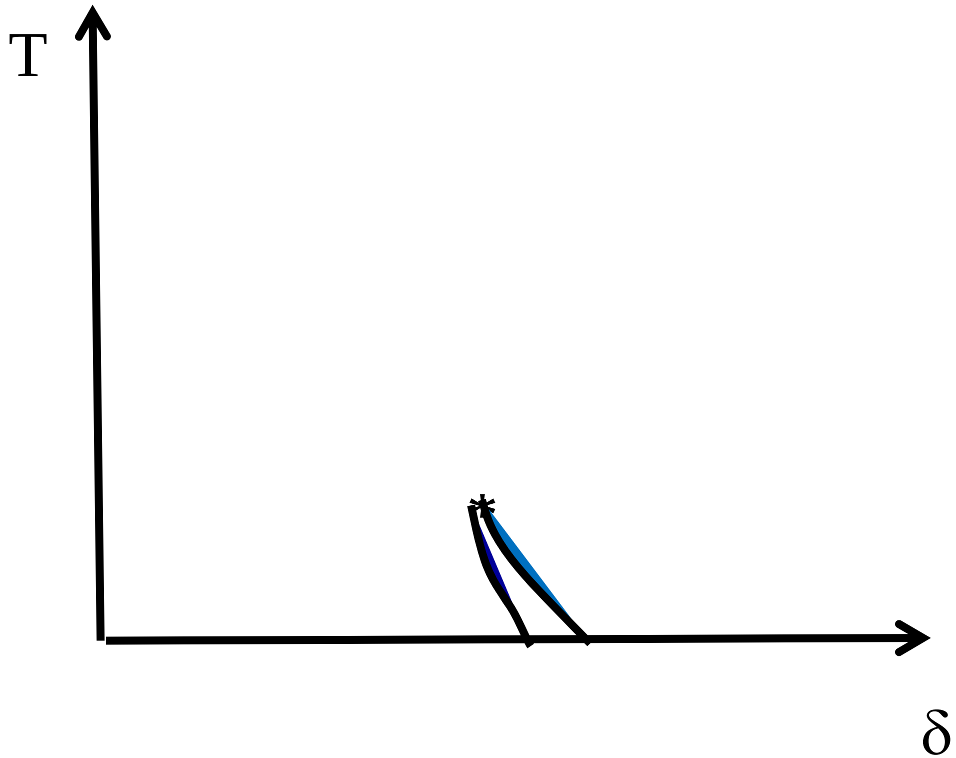
An alternate view (a bit of both)



G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
arXiv:1102.0463

Outline

- Method
- Normal state
- Superconducting state

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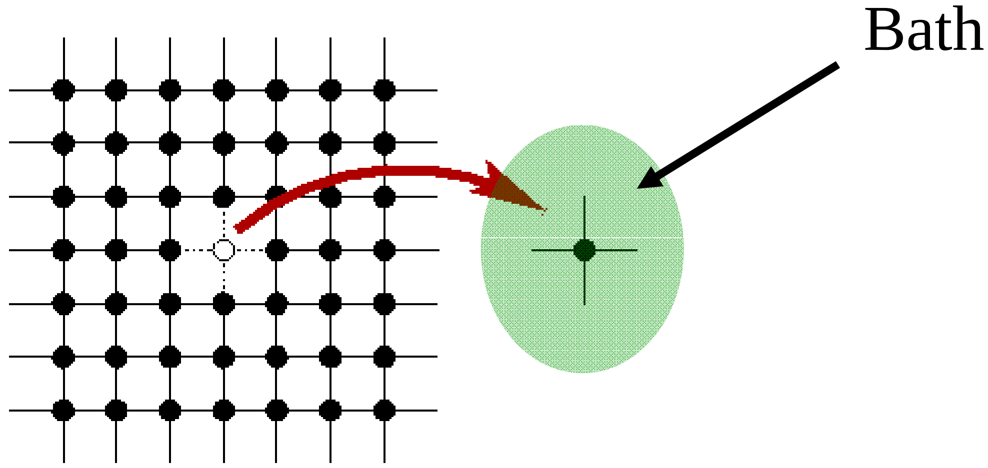
Method

Mott transition and Dynamical Mean-Field Theory. The beginnings in *d = infinity*

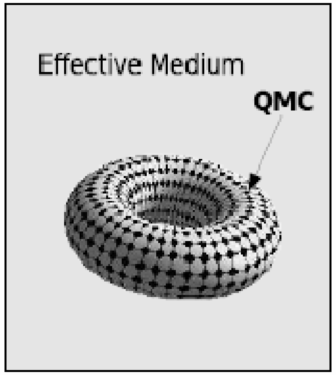
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

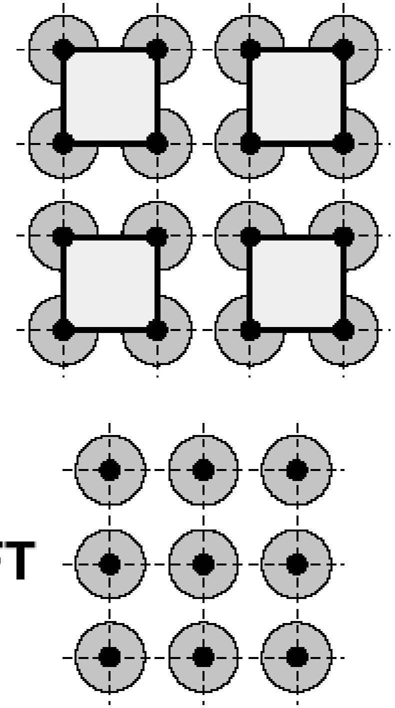
DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method



DCA

C-DMFT



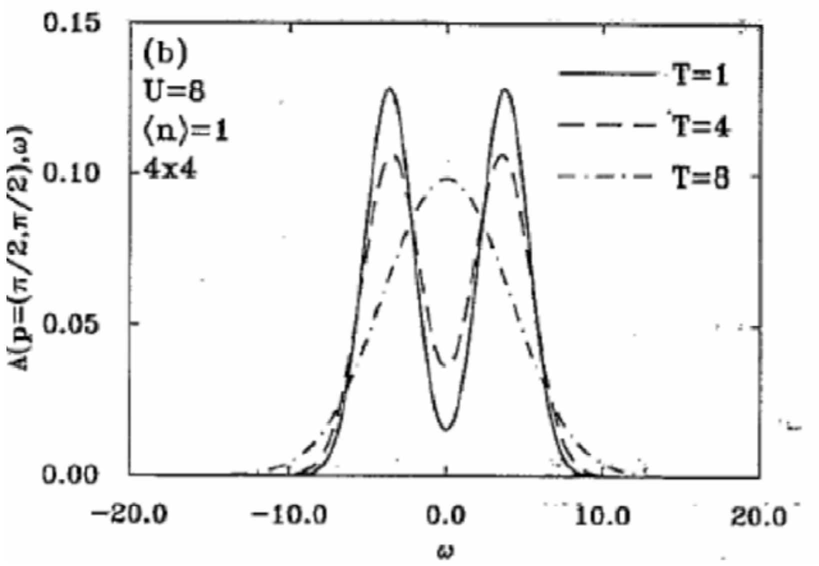
DMFT

Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).
Maier, Jarrell et al., Rev. Mod. Phys. **77**, 1027 (2005)

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

- Fermi liquid
  - Start from Fermi sea
  - Self-energy analytical
  - One to one correspondence of elementary excitations
  - Landau parameters
- Mott insulator
  - Hubbard model
  - Atomic limit
  - Self-energy singular
  - DMFT
  - How many sites in the cluster determines how low in temperature your description of the normal state is valid.

Mott insulator at finite *T*



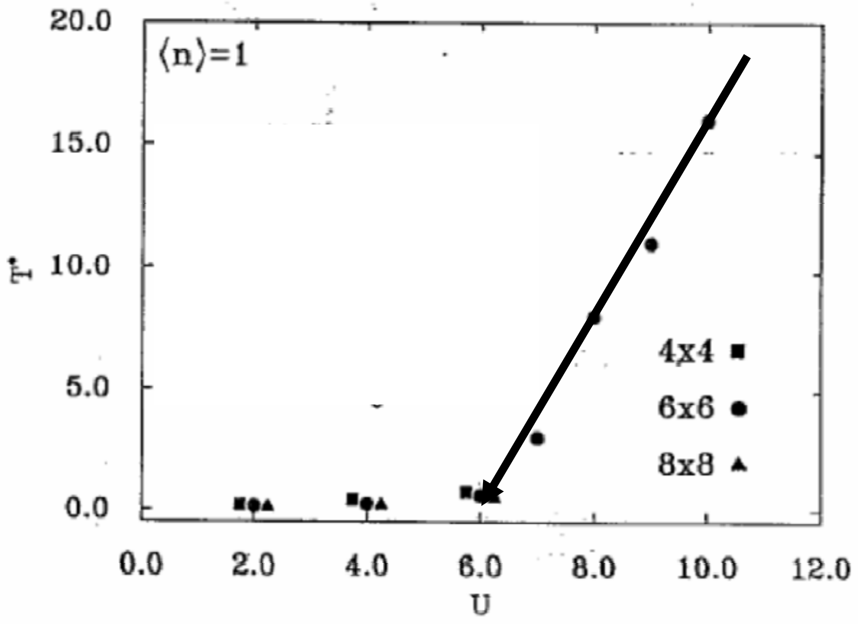


FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

M. Vekic and S.R. White, PRB 47, 1160 (1993)

Interaction-induced Mott transition, *n = 1*

Method	U_{c1}	U_c	U_{c2}	Ref.
VCA+ED 2 x 2 + 8b	5.25	5.5	6.37	Balzer et al. EPL (2009)
CDMFT+CTQMC+H 2 x 2	5.3		5.7	Park et al. PRL (2008)
DCA+CTQMC+H 8	5.7		6.4	Gull et al. cond-mat (2009)
DCA+CTQMC+H 4	!	~4.2	!	Gull et al. EPL (2008)
Dual fermions	!	~6.5	!	Hafermann et al. (2008)
CDMFT+ED 2 x 2 + 8b 15 parameters	?	~5.6	?	Liebsch, Merino… (2008)
CDMFT+ED 2,3,4		~4		Zhang et al. PRB (2007) (3d also)
QMC 6 x 6		6		Vekic et al. (1993)

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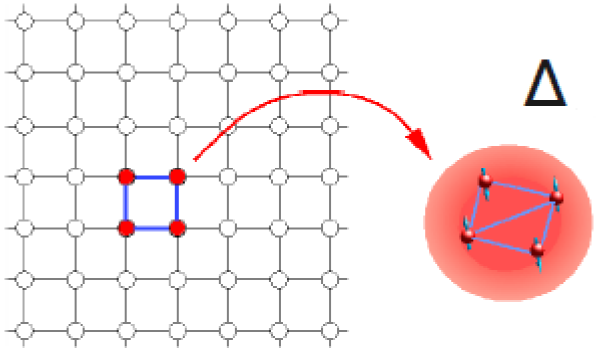
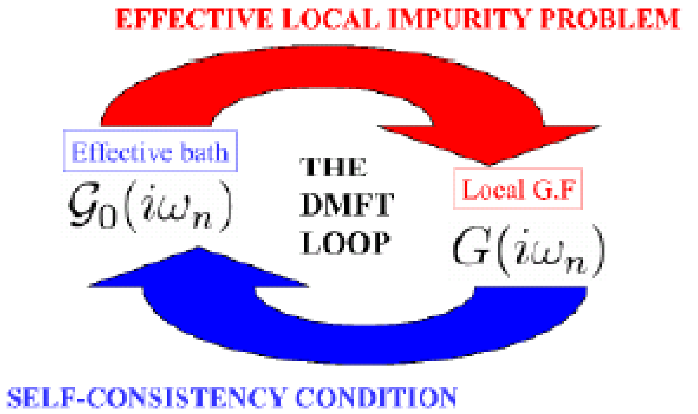
C-DMFT



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



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

Here: continuous time QMC

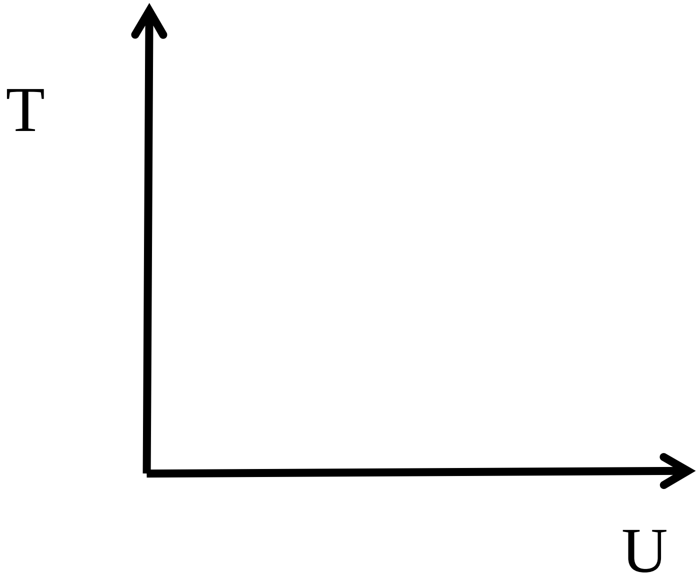
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

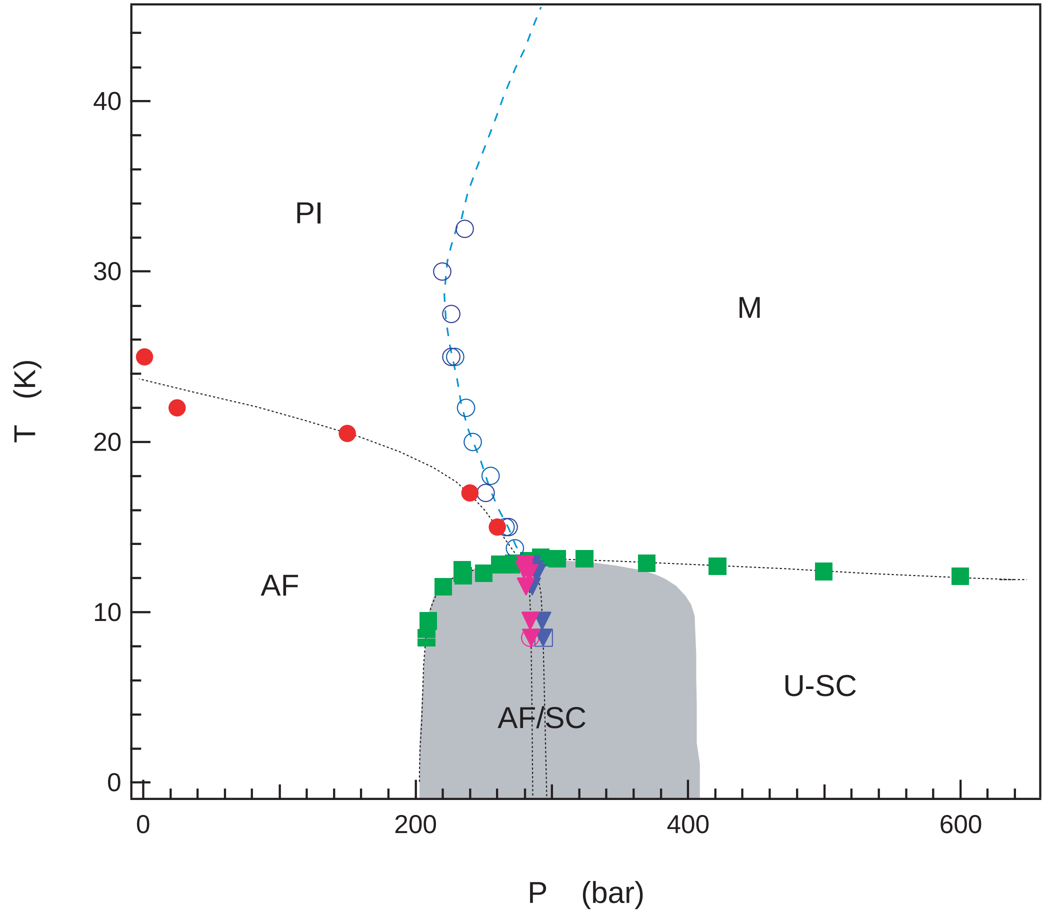
Solving cluster in a bath problem

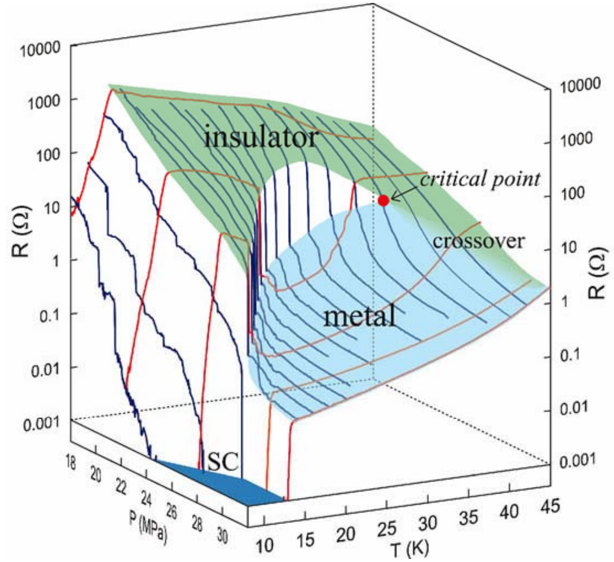
- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
  - P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).
  - K. Haule, Phys. Rev. B **75**, 155113 (2007).

Interaction-induced Mott transition $d = 2$



Bare Mott critical point in organics





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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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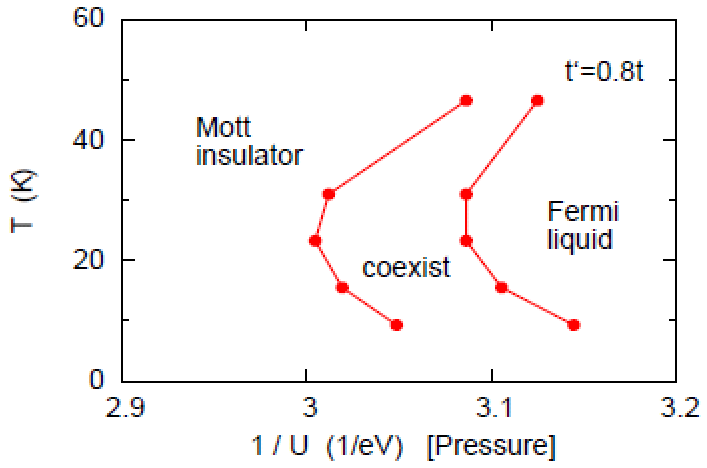
Interaction-induced Mott transition theory



κ–BEDT-Cl

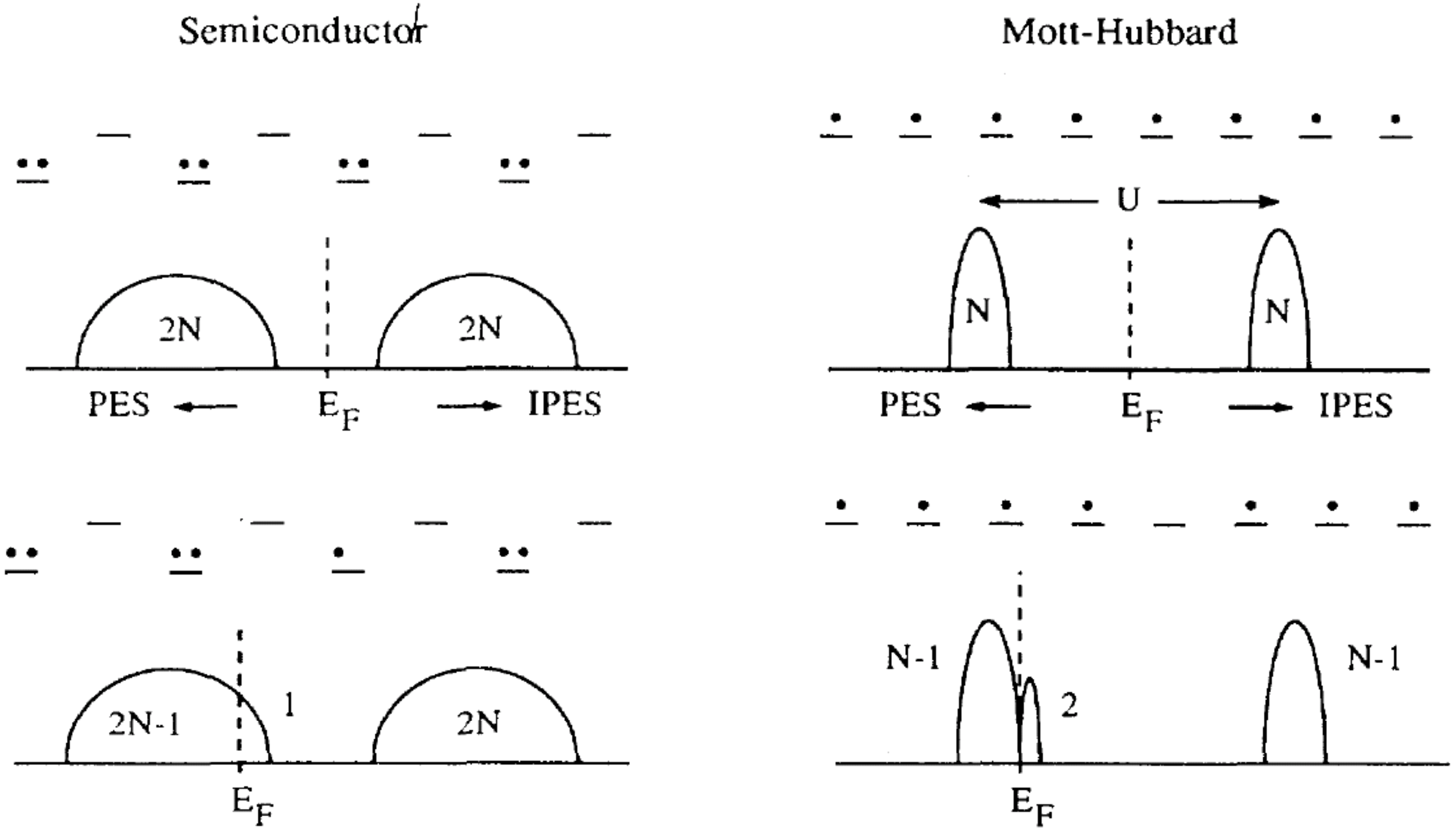
κ–BEDT-CN

Liebsch Phys. Rev. B **79**, 195108 (2009)

See also: Ohashi et al. PRL **100**, 076402 (2008)

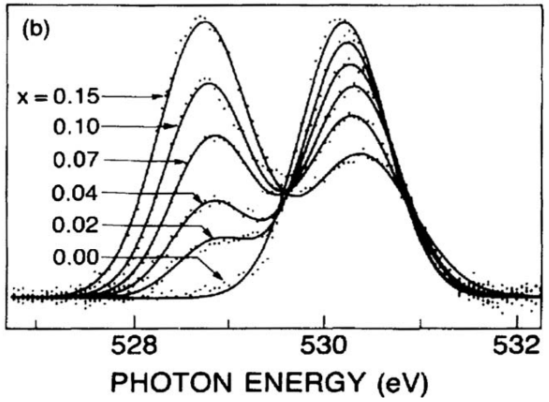
Cuprates as doped Mott insulators

Spectral weight transfer

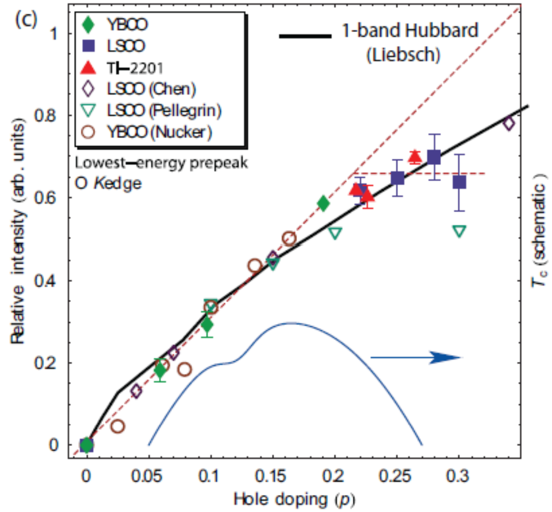


Meinders *et al.* PRB **48**, 3916 (1993)

Experiment: X-Ray absorption



Chen et al. PRL **66**, 104 (1991)



Peets et al. PRL **103**, (2009), Phillips, Jarrell arXiv

Number of low energy states above $\omega = 0$ scales as $2x$ +

Not as 1+x as in Fermi liquid

Meinders *et al.* PRB **48**, 3916 (1993)

Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
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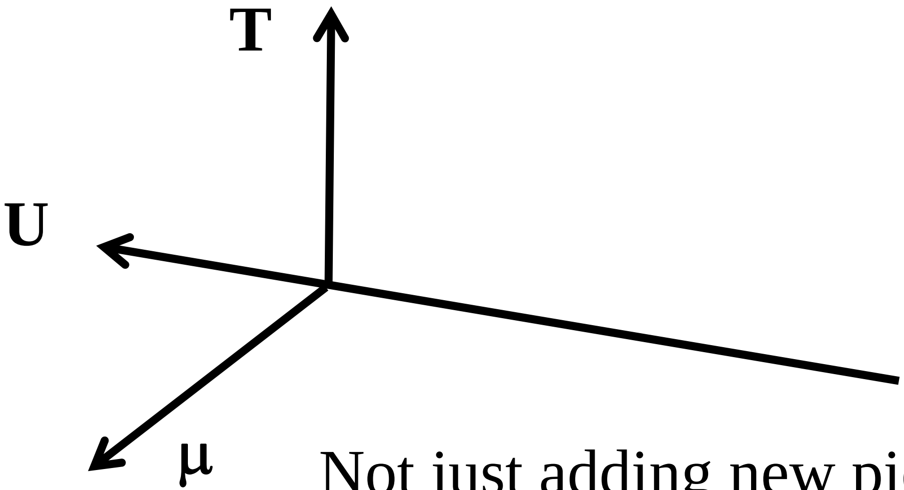
Doping-induced Mott transition (*t'=0*)

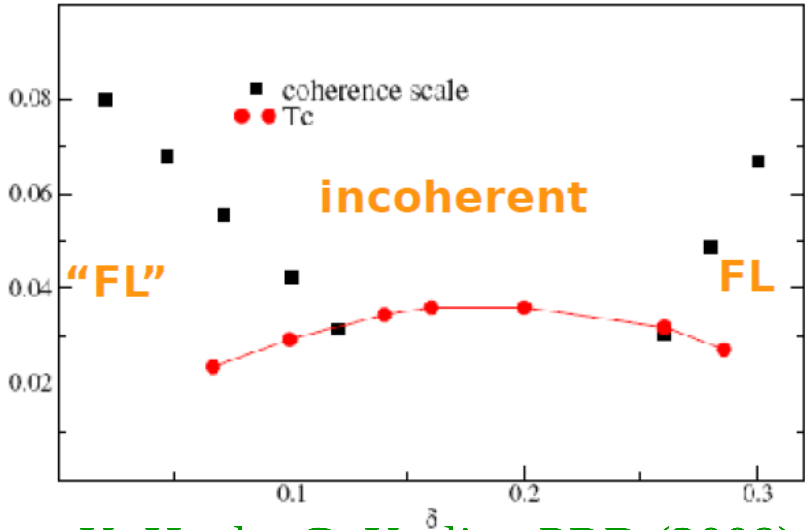


Kristjan Haule

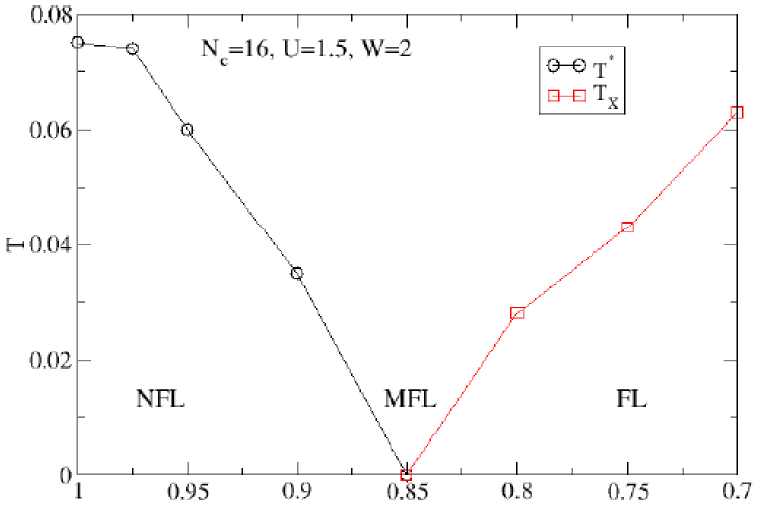
Not just adding new piece:
Lesson from DMFT, first order transition + critical point governs phase diagram

Doping driven Mott transition, *t' = 0*

Method	t'	Orbital selective	U	Critical point	Ref.
D+C+H 8			7		Werner et al. cond-mat (2009)
D+C+H 4					Gull et al. EPL (2008)
	-0.3		10,6		Liebsch, Merino… (2008)
					Ferrero et al. PRB (2009)
D+C+H 8			7		Gull, et al. PRB (2009)

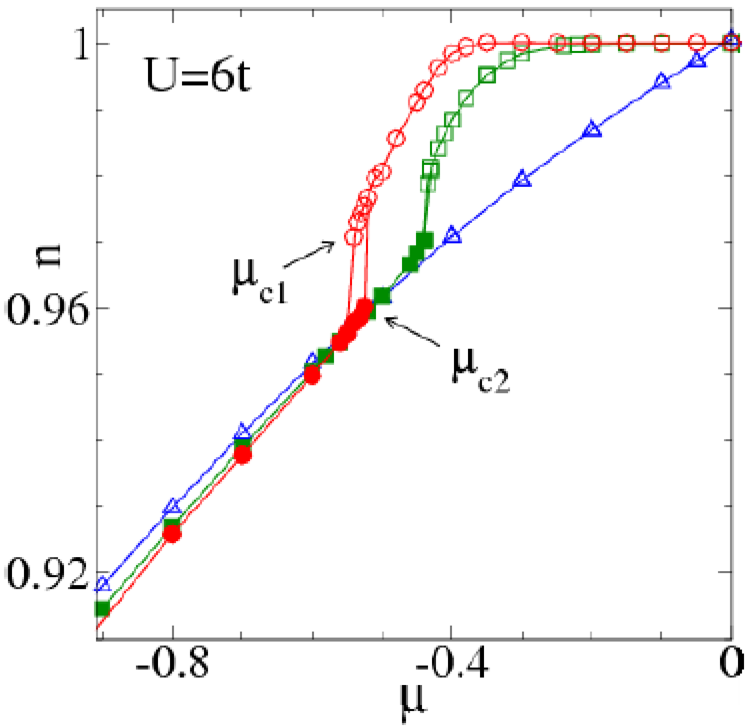


K. Haule, G. Kotliar, PRB (2008)



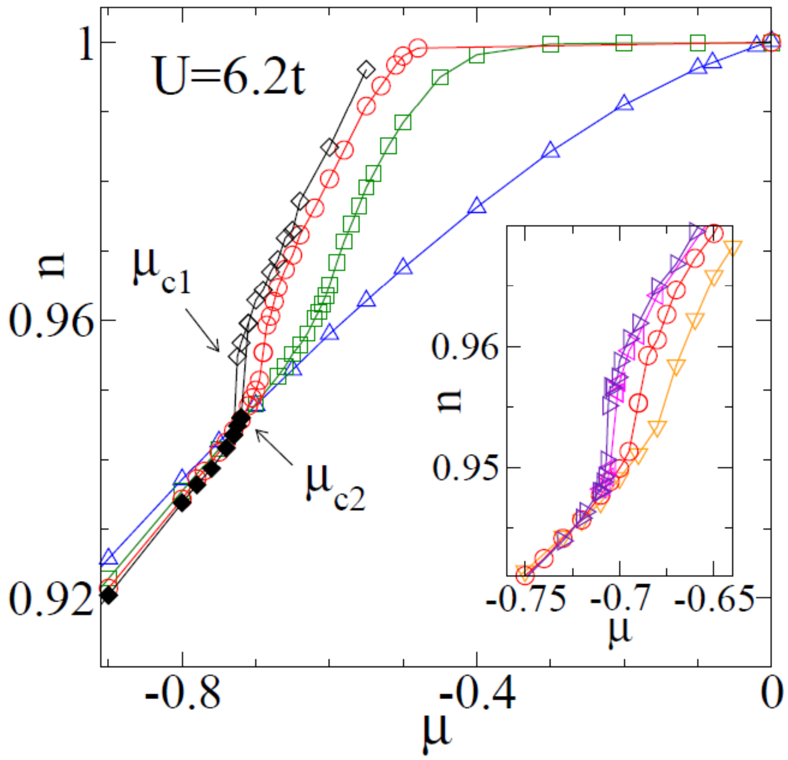
Vildhyadhiraja, PRL (2009)

First order transition at finite doping

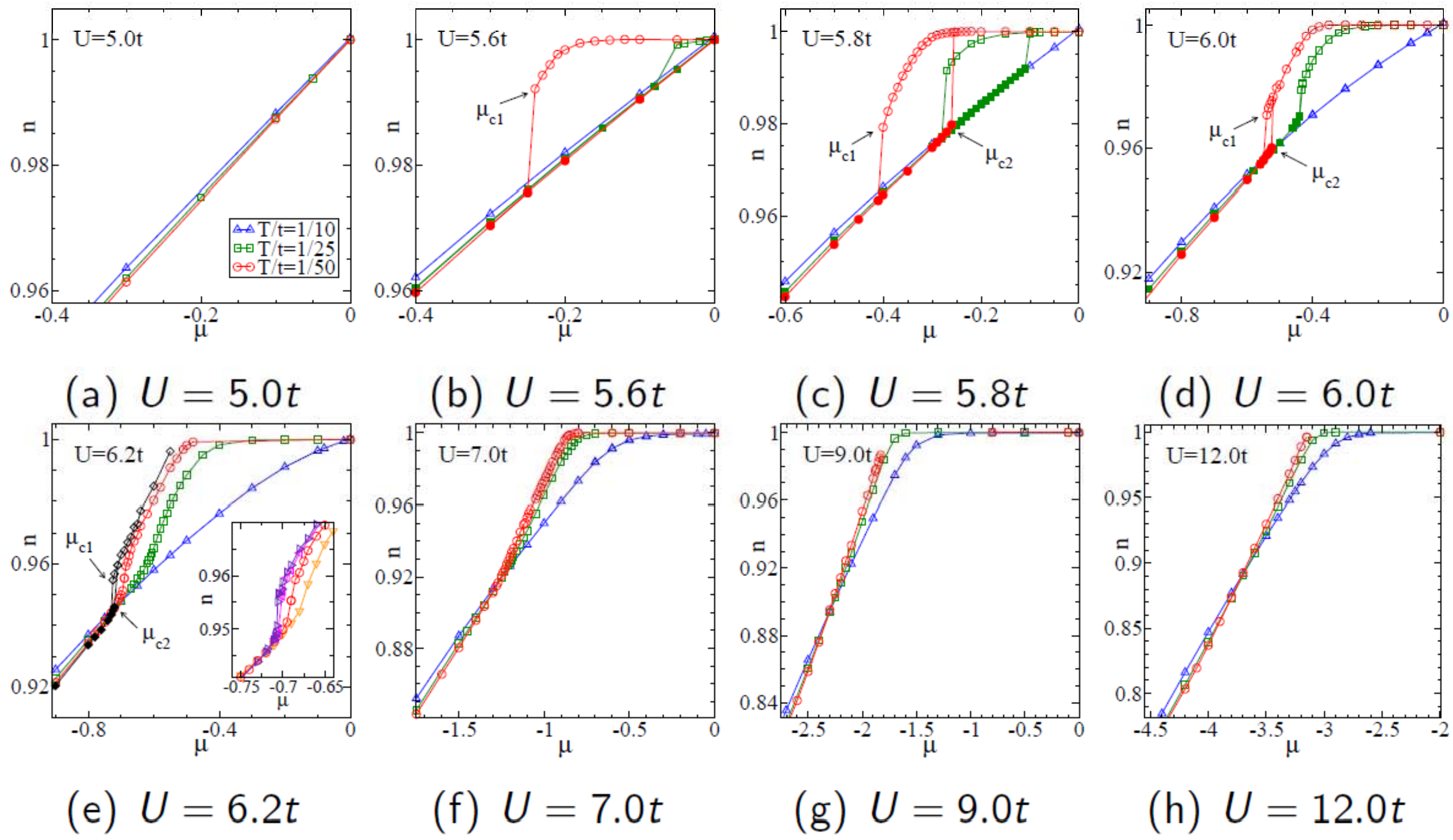


$n(\mu)$ for several temperatures:
$T/t = 1/10$, $1/25$, $1/50$

The critical point



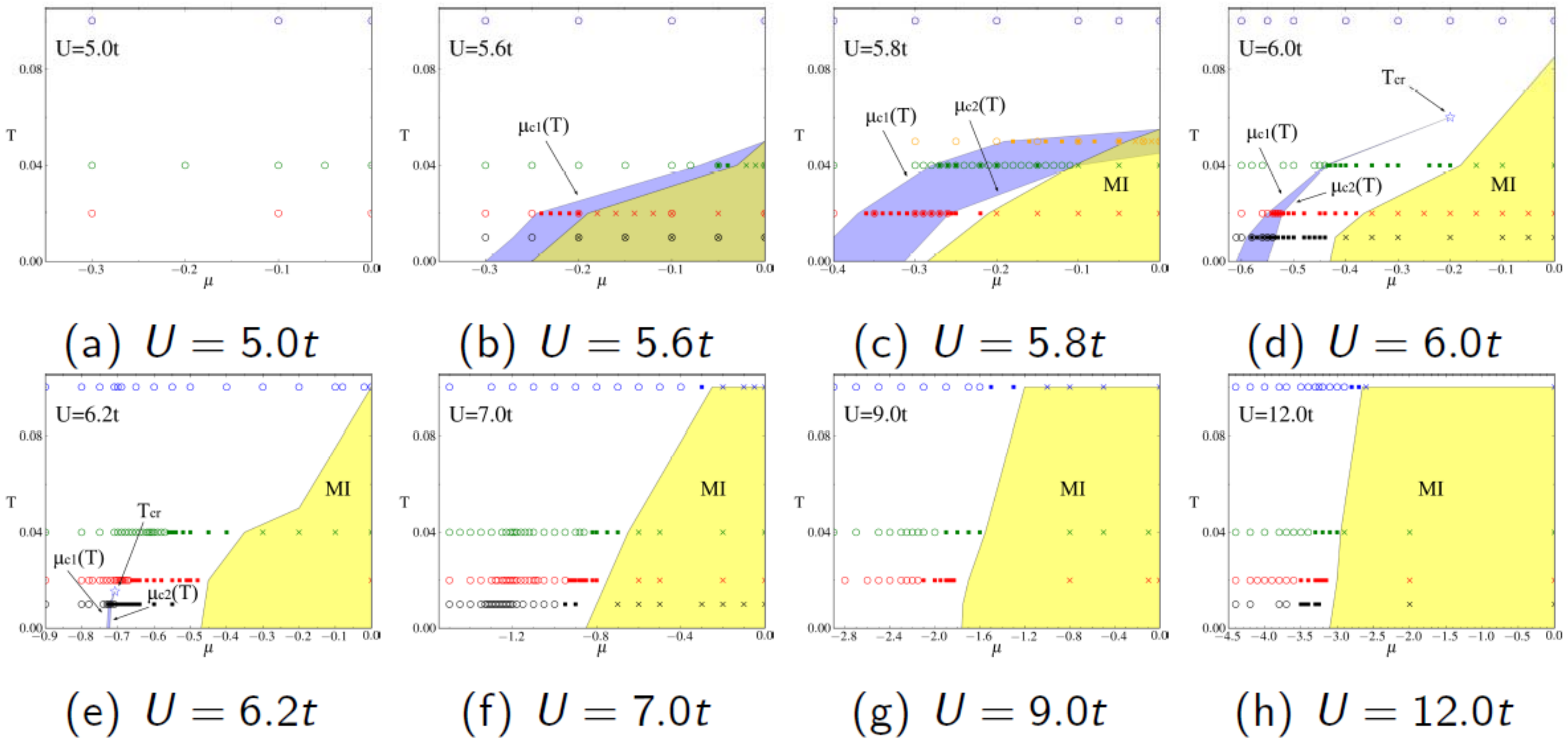
Systematic exploration $n(\mu)$



(a) $U = 5.0t$ (b) $U = 5.6t$ (c) $U = 5.8t$ (d) $U = 6.0t$

(e) $U = 6.2t$ (f) $U = 7.0t$ (g) $U = 9.0t$ (h) $U = 12.0t$

Systematic exploration of the phase diagram



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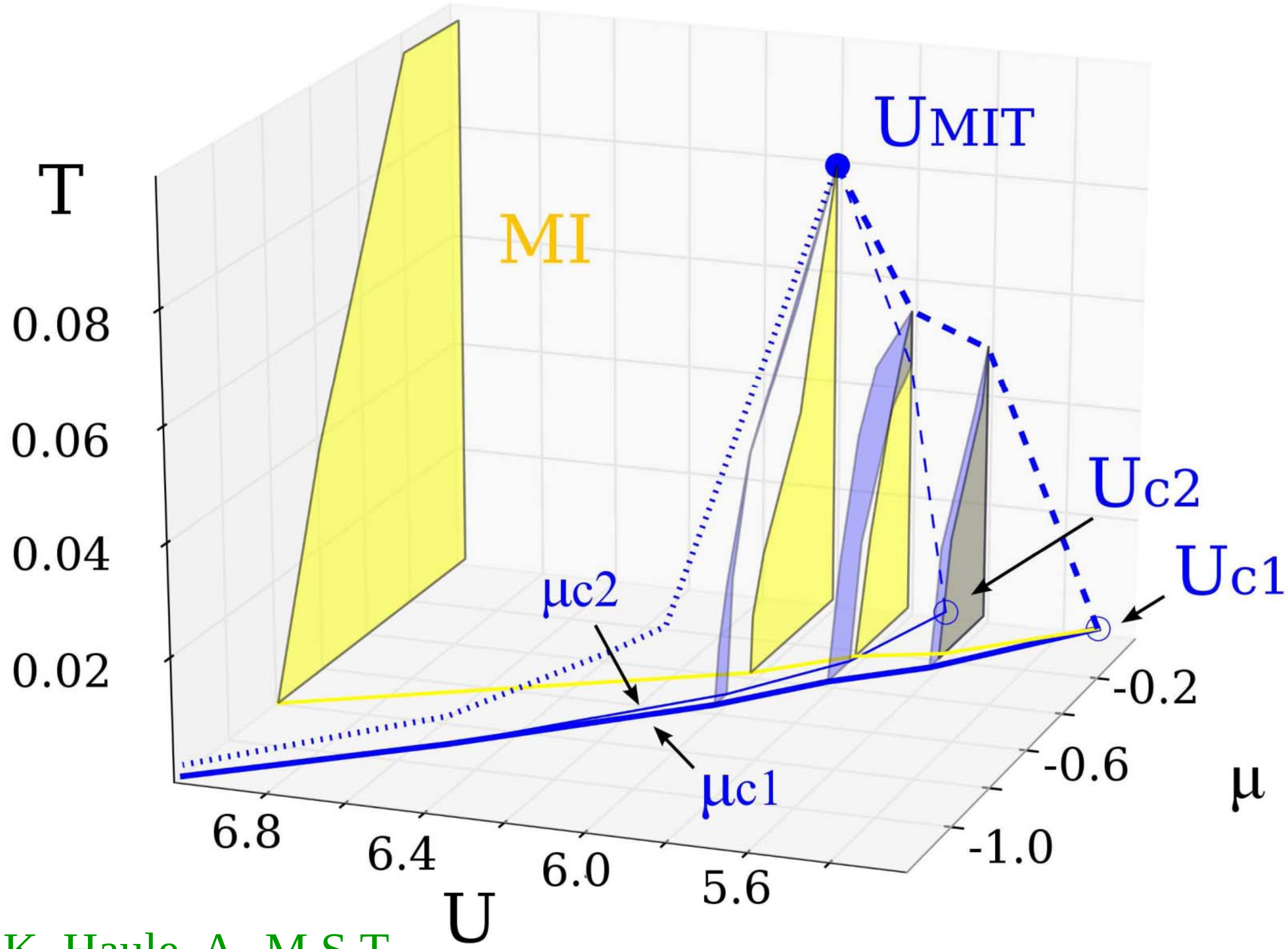
(e) $U = 6.2t$ (f) $U = 7.0t$ (g) $U = 9.0t$ (h) $U = 12.0t$

Yellow region: Mott insulator ($n(\mu) = 1$, $dn/d\mu = 0$)
White region: metal ($dn/d\mu = 0$)
Blue region: coexistence region

Normal state phase diagram



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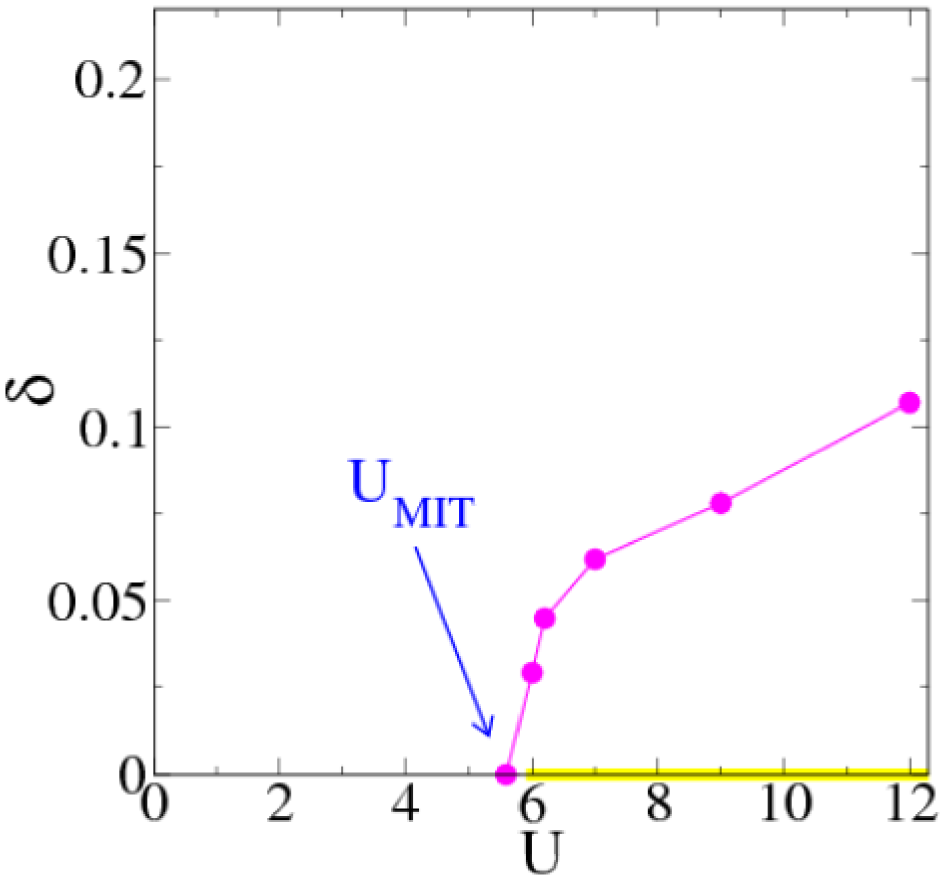
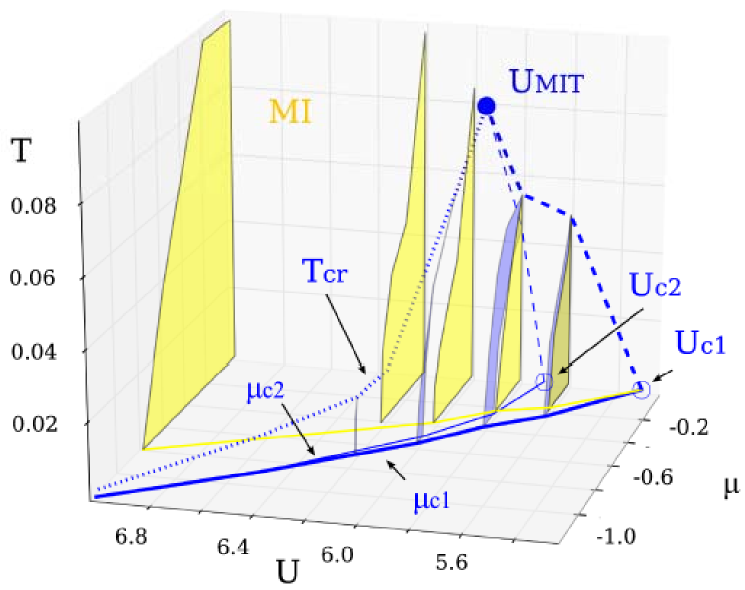
PRL, **104**, 226402 (2010)

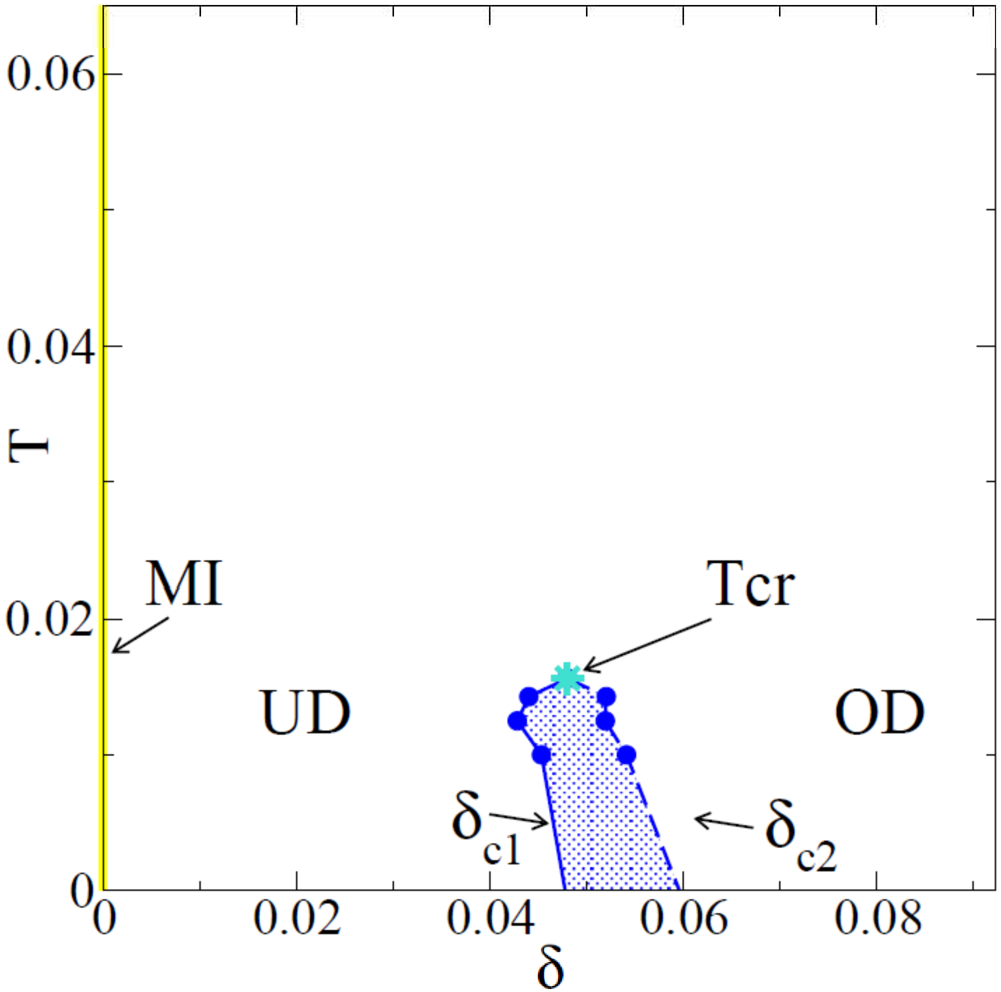
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of *U*





Characterisation of the phases ($U=6.2t$)



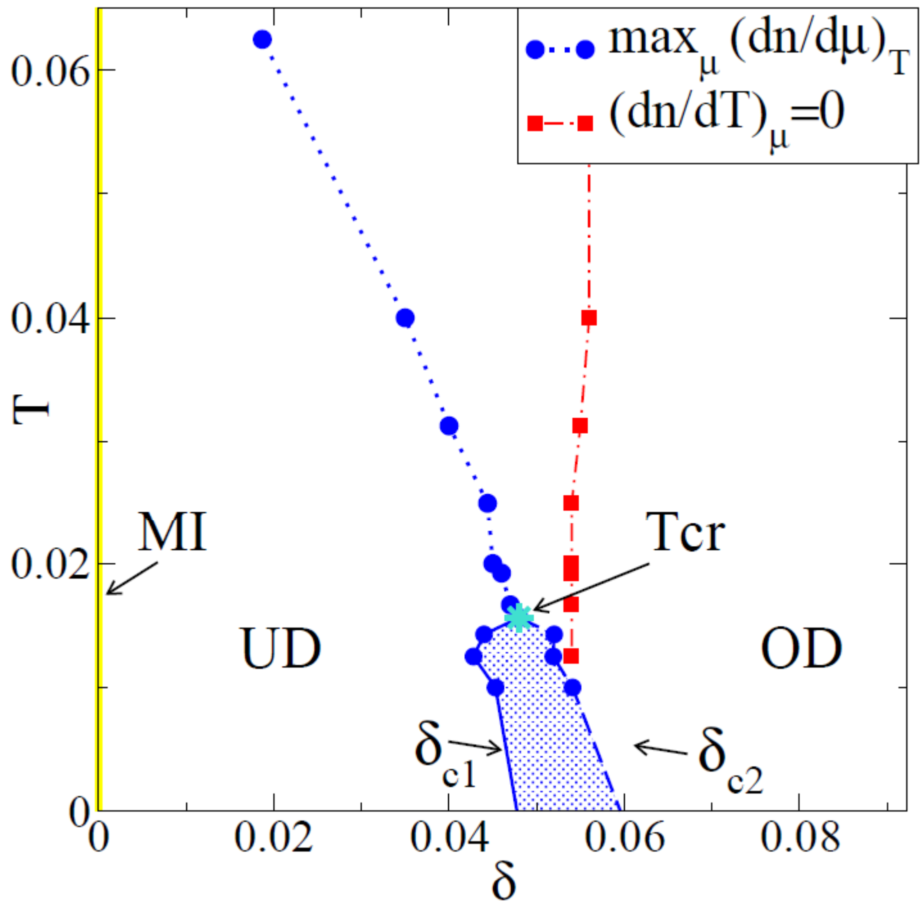
$U > U_{\mathrm{MIT}}$:

1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

Here "optimal doping" δ_c = doping at which the 1st order transition occurs

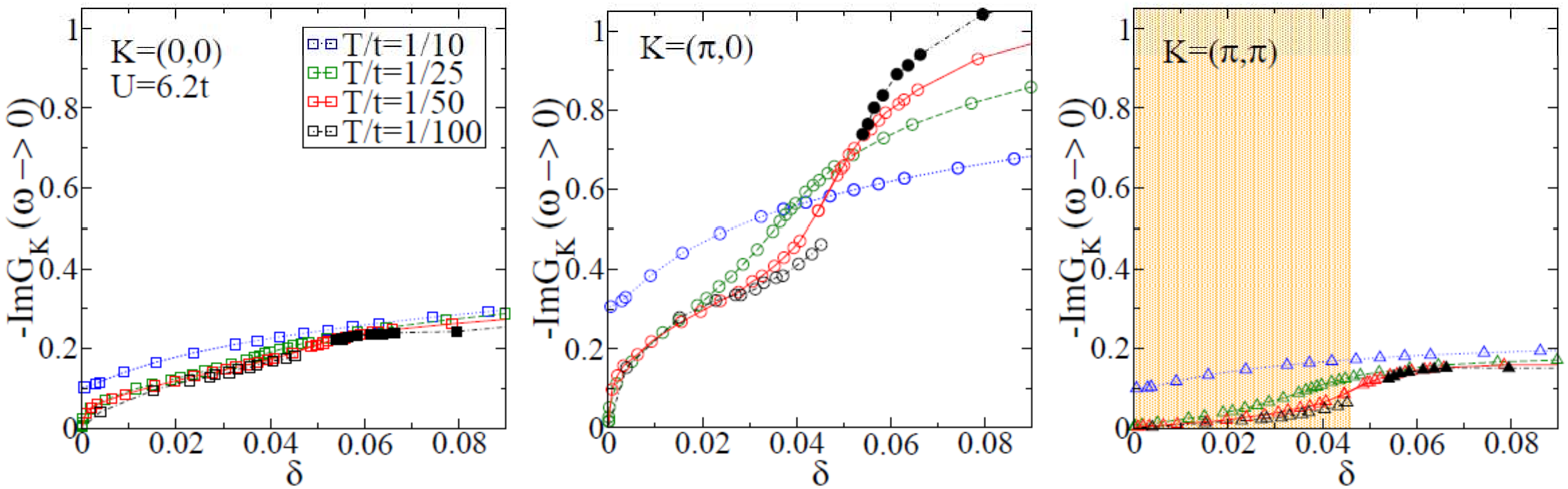
How does the UD phase differ from the OD phase?

Phase characterisation: thermodynamics



- UD and OD phases are stable ($d^2\Omega < 0$)
- UD and OD phases have a different filling
- UD has smaller entropy and smaller double occupation than the OD phase
- maximum of compressibility $\max_\mu(dn/d\mu)_T$
- near the 1st order transition: crossing of isotherms $dn/dT|_\mu = 0$
  $\Rightarrow$ maximum of entropy ($dS/d\mu = 0$) (cf Khatami PRB 2010)

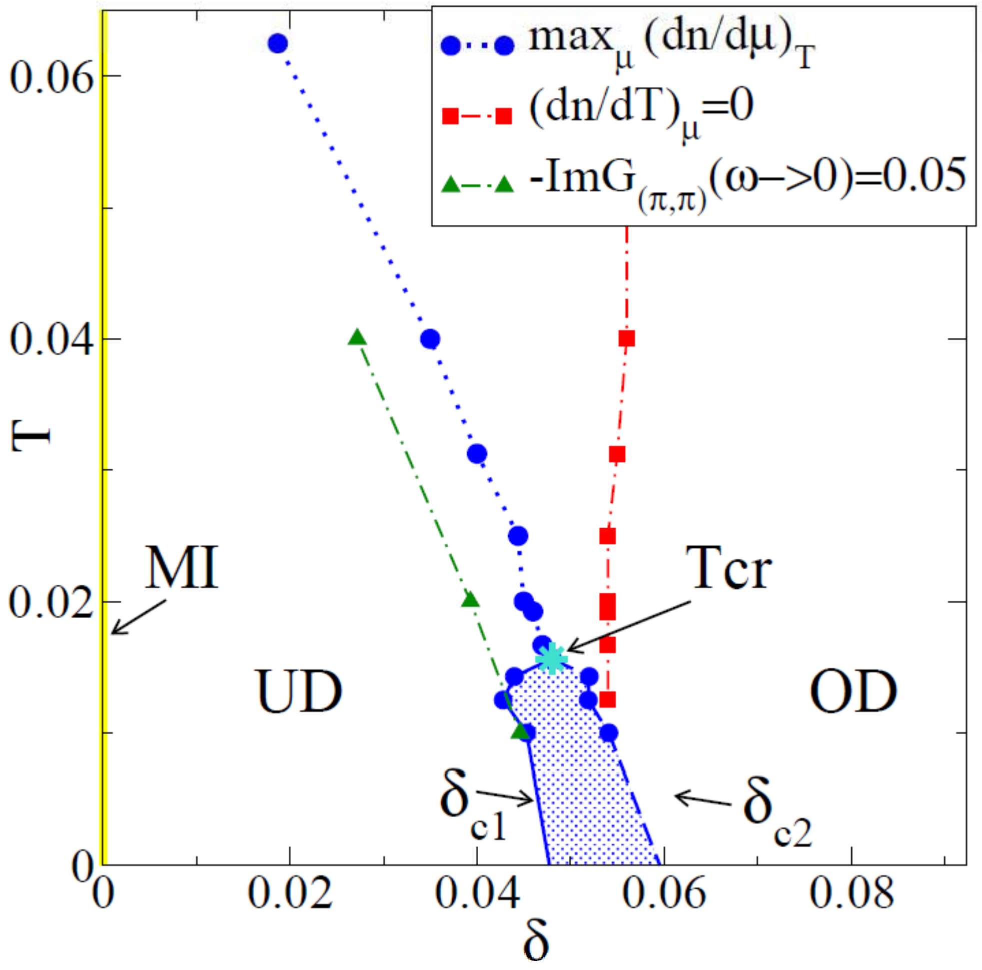
Phase characterisation: DOS at E_F



(a) $K = (0, 0)$ (b) $K = (\pi, 0)$ (c) $K = (\pi, \pi)$

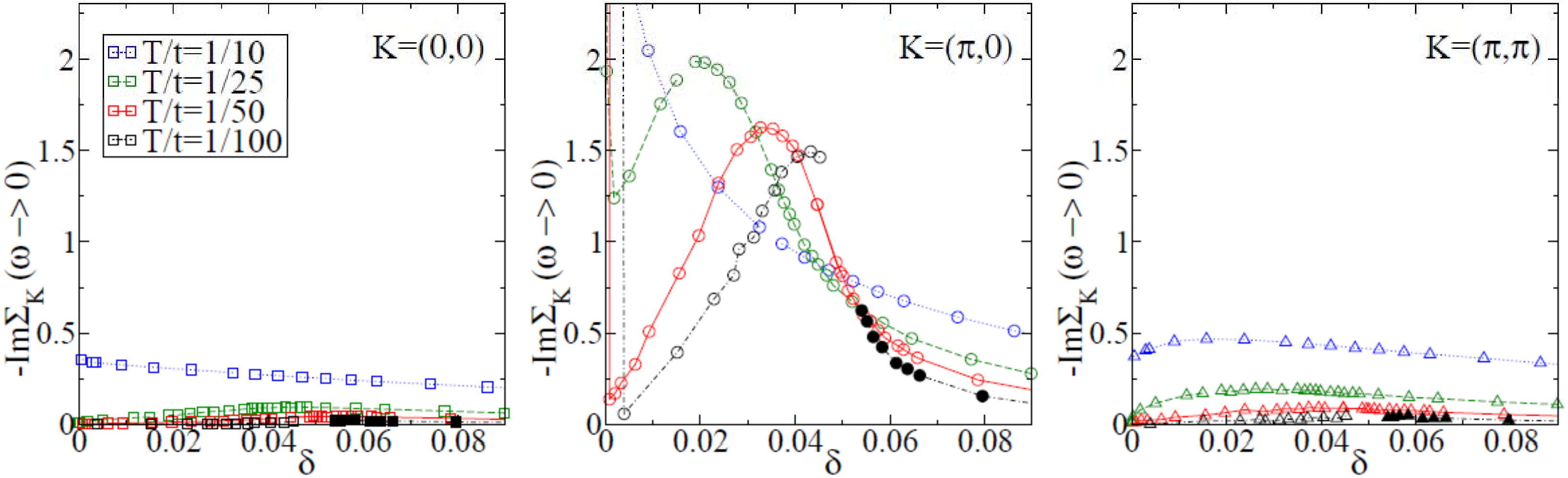
- MI: all cluster momenta are insulating
- UD: strong cluster momentum differentiation: $K = (\pi, \pi)$ insulator, $K = (\pi, 0), (0, 0)$ metallic
- OD: all cluster momenta are metallic

Momentum differentiation at the transition



- UD phase: strong cluster momentum differentiation (cf Ferrero et al, EPL 2009, PRB 2009, Gull et al, PRB 2010)
- our contribution: phenomenon linked to first order transition at finite doping

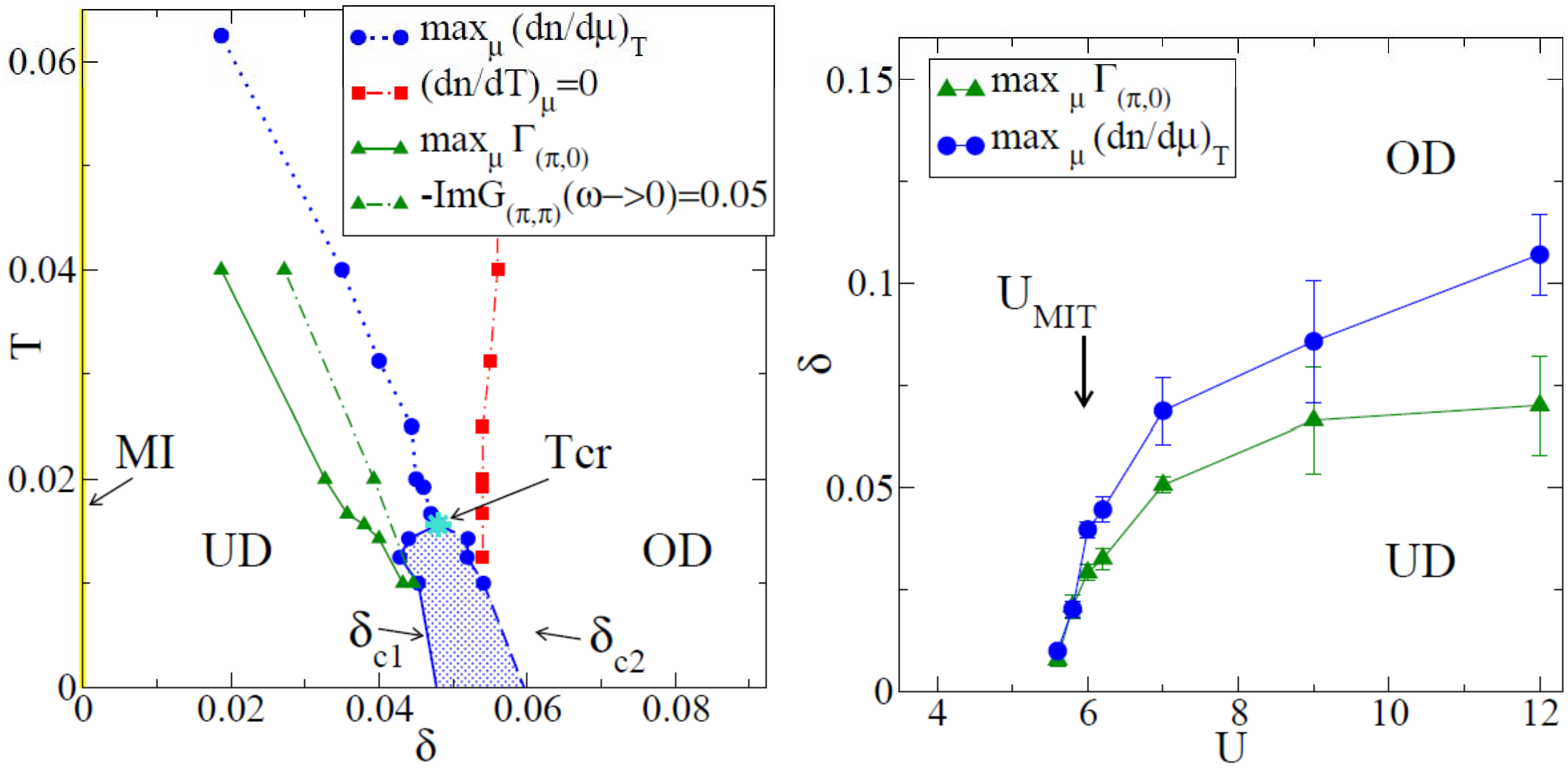
Phase characterisation: scattering rate



(a) $K = (0, 0)$ (b) $K = (\pi, 0)$ (c) $K = (\pi, \pi)$

- $\text{Im}\Sigma_{K=(\pi,0)}(\omega \to 0)$ shows a maximum at UD/OD transition
- OD: coherent, FL
- UD: coherent, NFL: coherence does NOT result from QP propagations, but from another mechanism

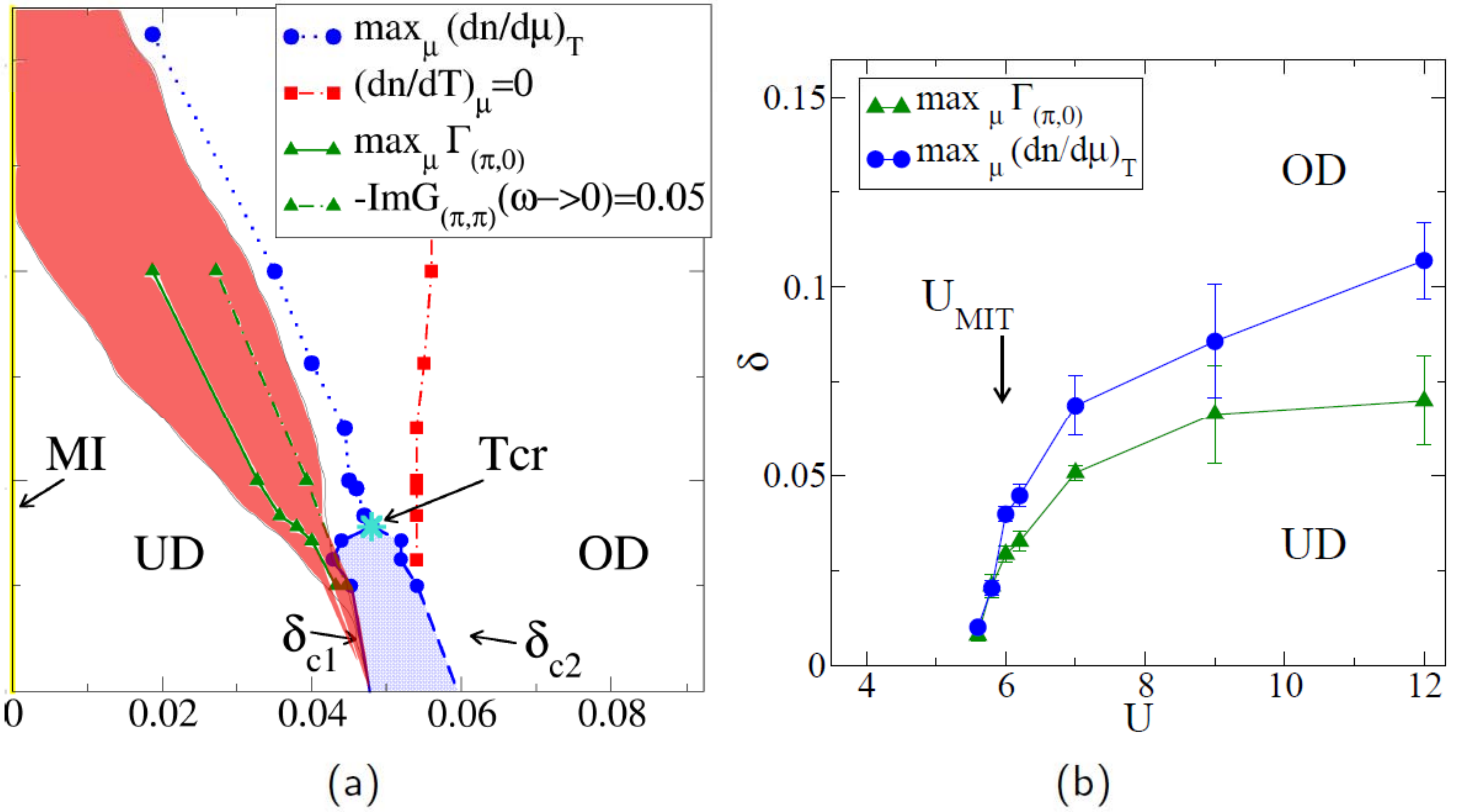
Maximum originates at the UD/OD transition



(a) (b)

- Mott physics far away from half filling

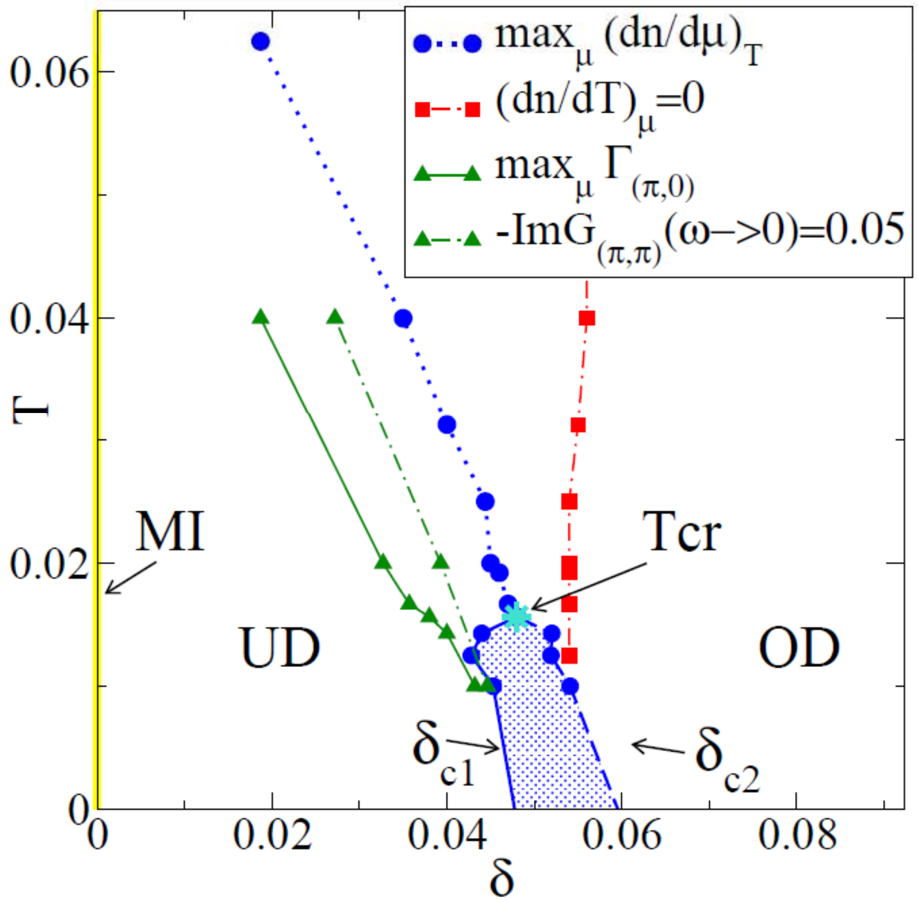
Maximum originates at the UD/OD transition



- Mott physics far away from half filling
- "Strange metal" between the UD/OD trasition

Emerging physical picture

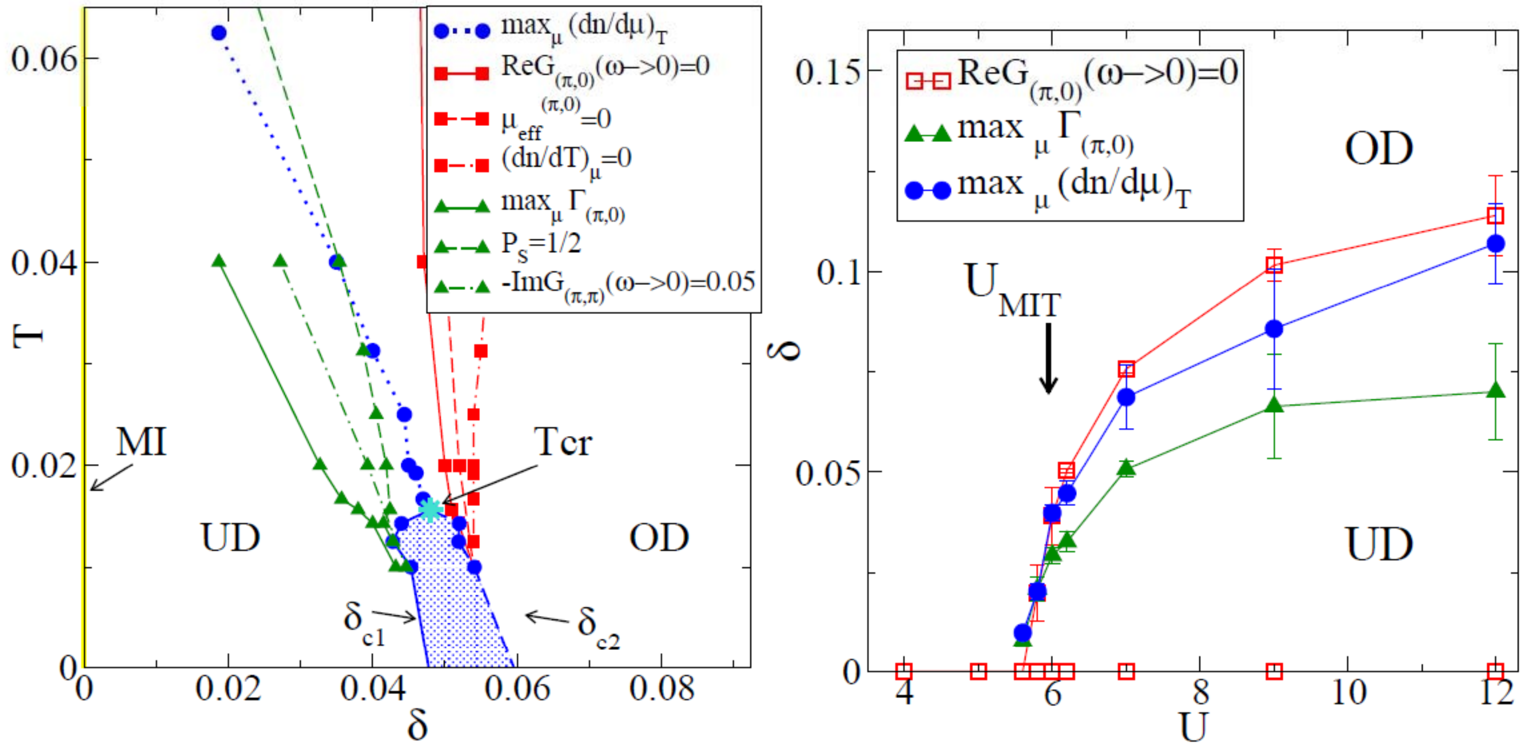
UD: coherent, NFL, holes propagating in a sea of singlets



OD: coherent, FL, Landau quasiparticles

Lev Tolstoj, AK: All Fermi liquids are all alike, each Non Fermi liquid is Non Fermi in its own way (© Shastry)

Summary



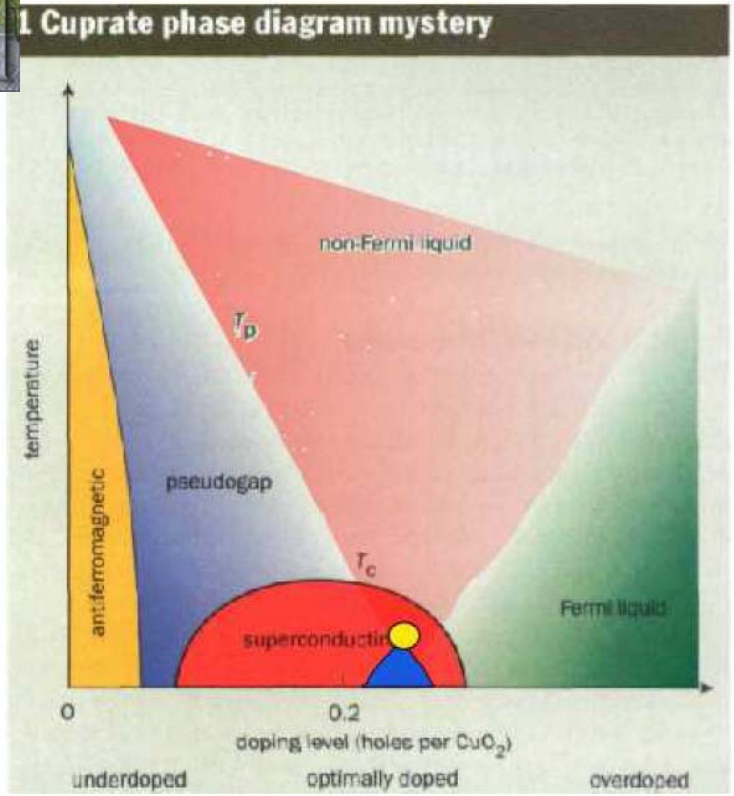
- first order transition at finite doping between two metals
- it is associated to Mott physics: all signatures of the first order transition can be traced back to Mott critical point

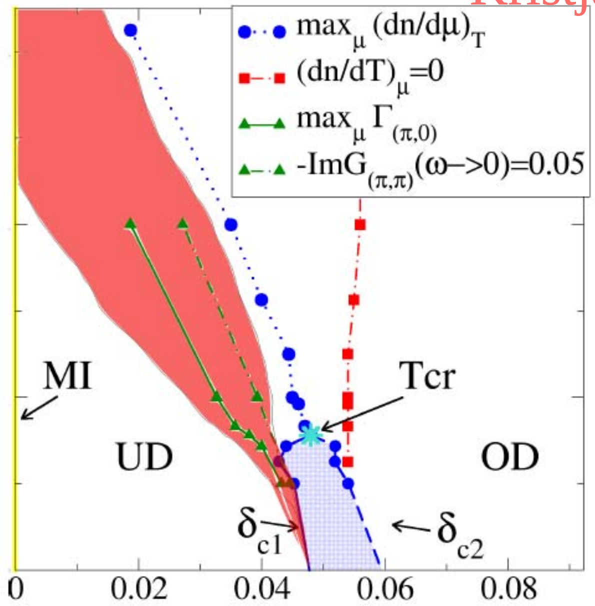
⇒ signature of the Mott transition in the 2D Hubbard model extends way beyond half filling!

Beneath the dome

Giovanni Sordi

Kristjan Haul





criticality originates from
first order transition at finite doping
coming from influence of Mott physics well beyond half filling!

G. Sordi, K. Haule, A.-M.S.T PRL, **104**, 226402 (2010)
and arXiv:1102.0463

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Another property of the UD phase

Underdoped metal very sensitive to anisotropy

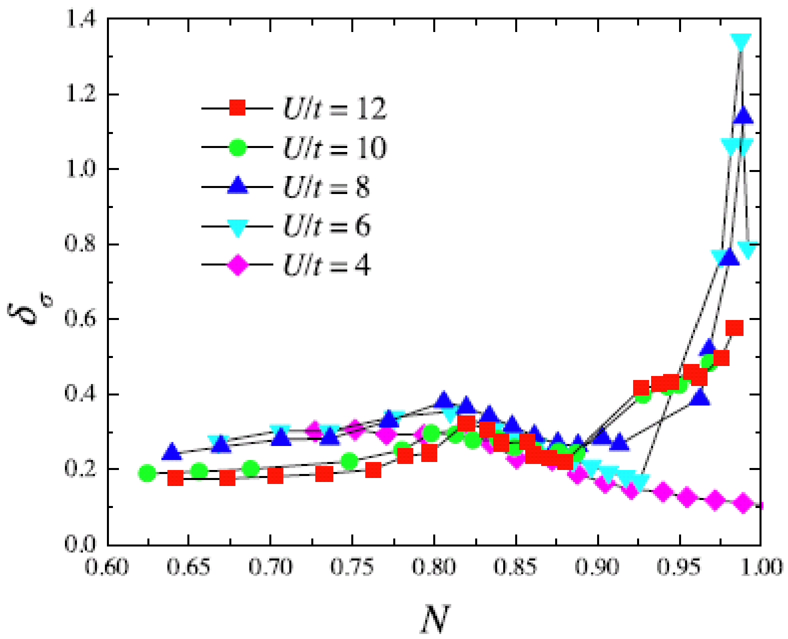
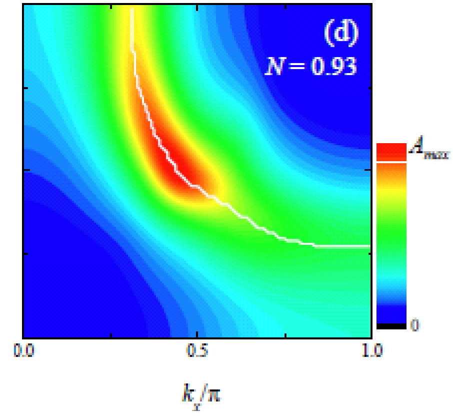
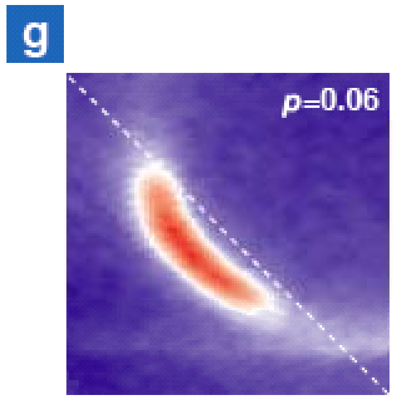


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\,[\sigma_x(0) - \sigma_y(0)]\,/\,[\sigma_x(0) + \sigma_y(0)]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.

Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B **82**, 180511R 2010





Satoshi Okamoto

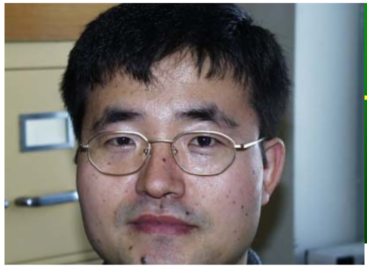
David Sénéchal

D. Fournier *et al.* Nature Physics (Marcello Civelli

Superconductivity

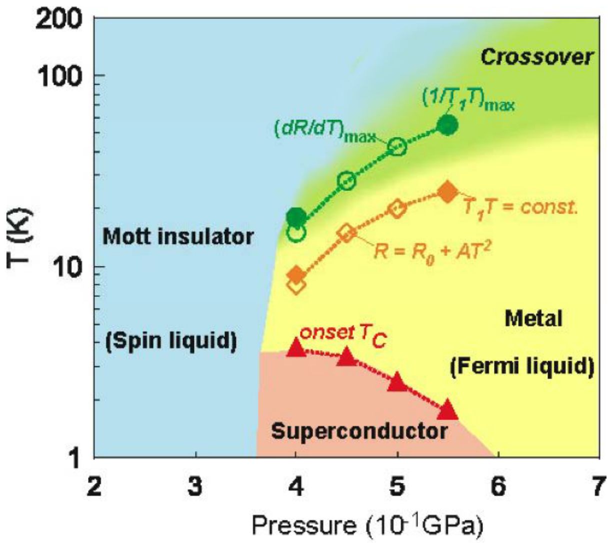
Phase diagram

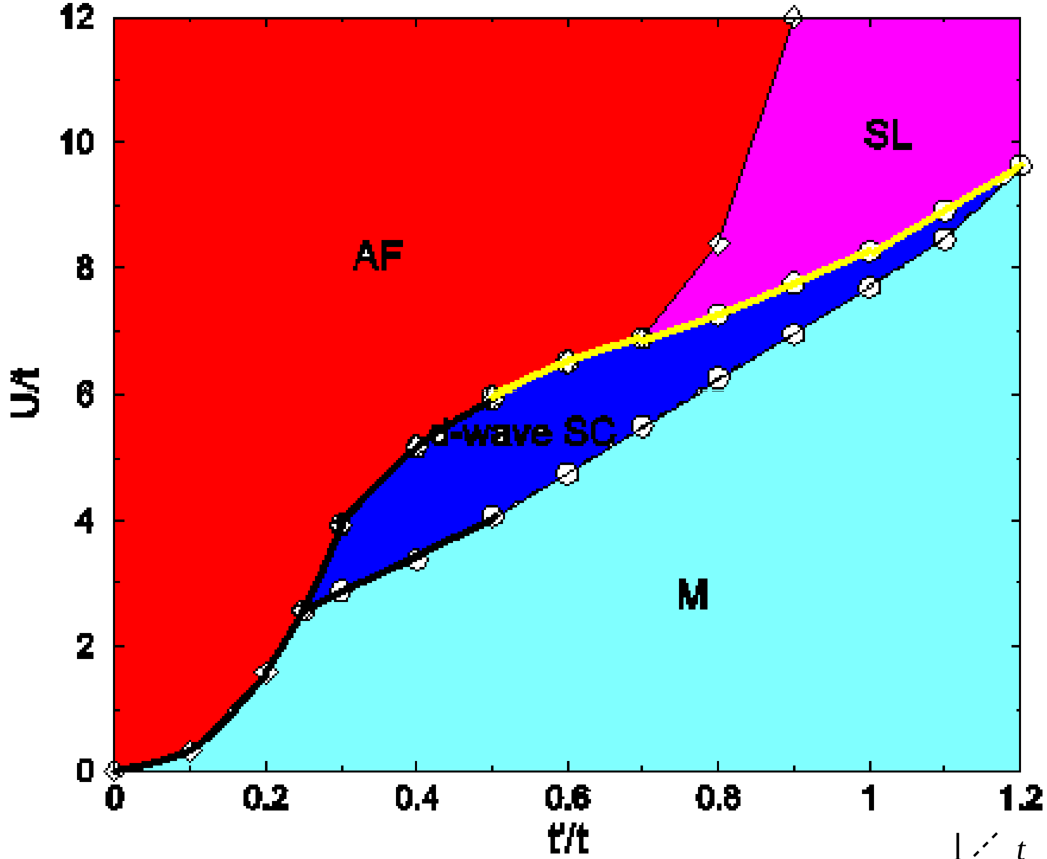
Exact diagonalization as impurity solver ($T=0$).

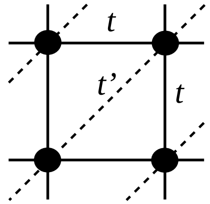


Theoretical phase diagram BEDT

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





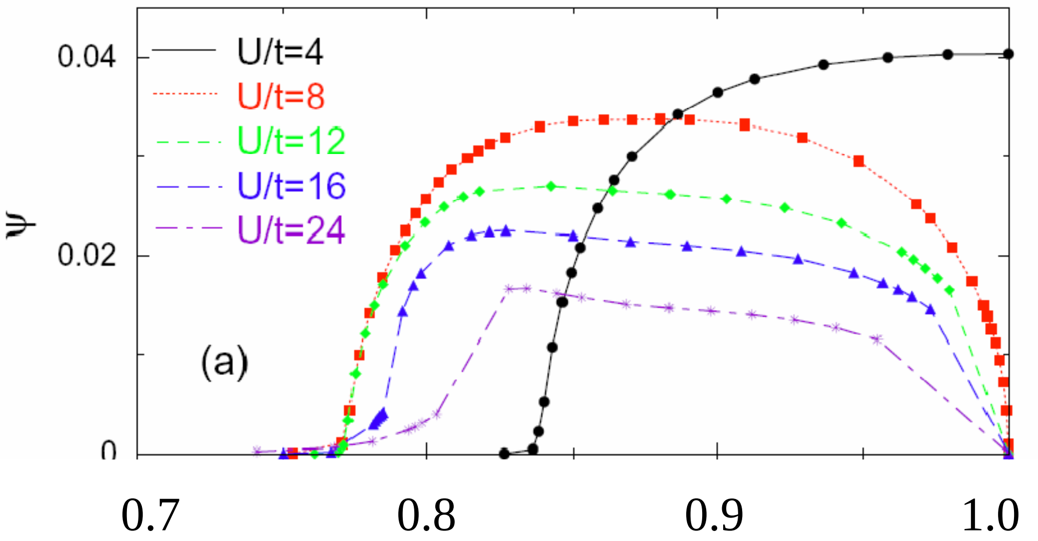


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

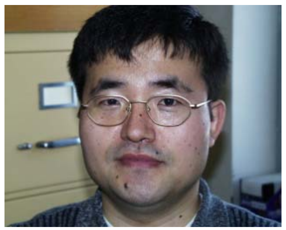
Y. Kurisaki, et al.

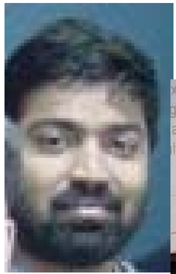
Phys. Rev. Lett. **95**, 177001(2005) Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

Dome vs Mott (CDMFT)



Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)





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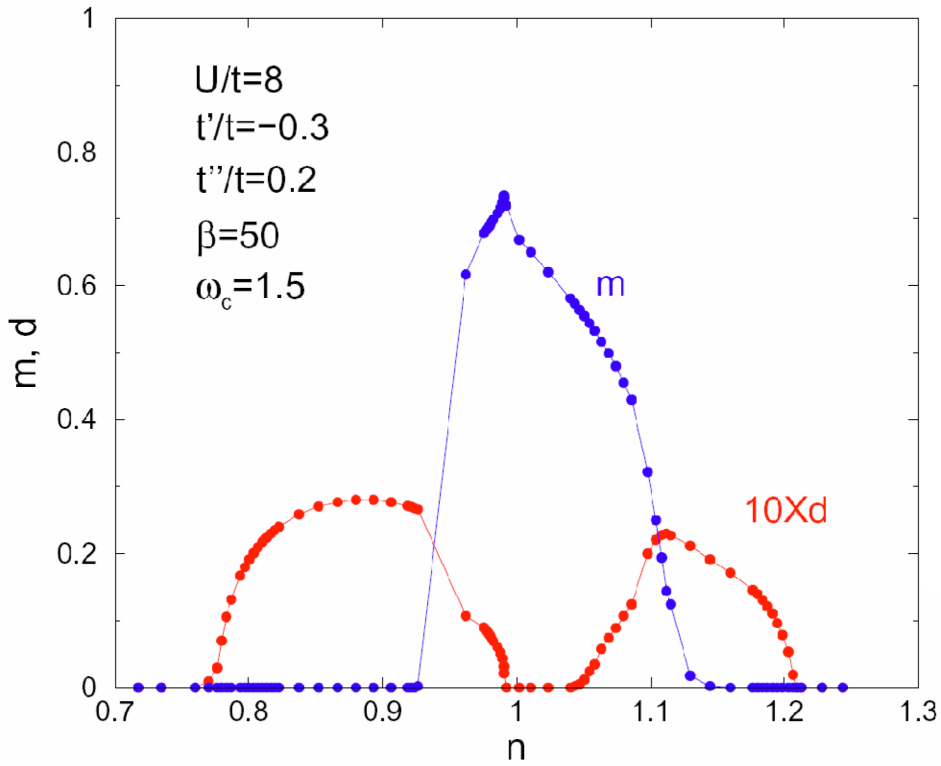
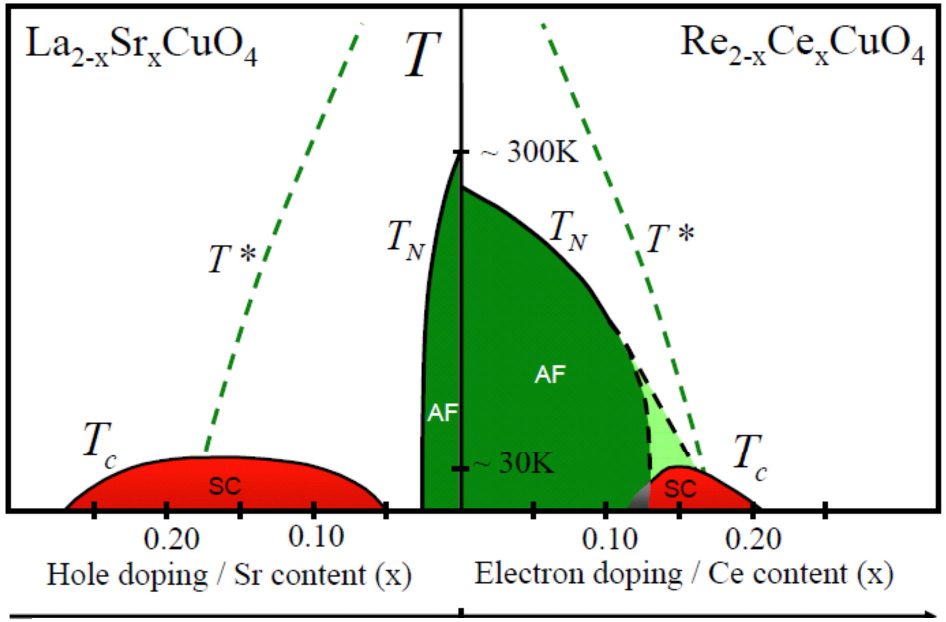
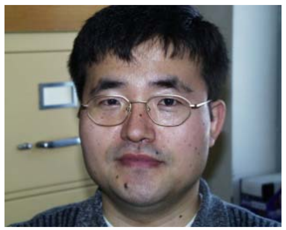
CDMFT global phase diagram



Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)



Armitage, Fournier, Greene, RMP (2009)



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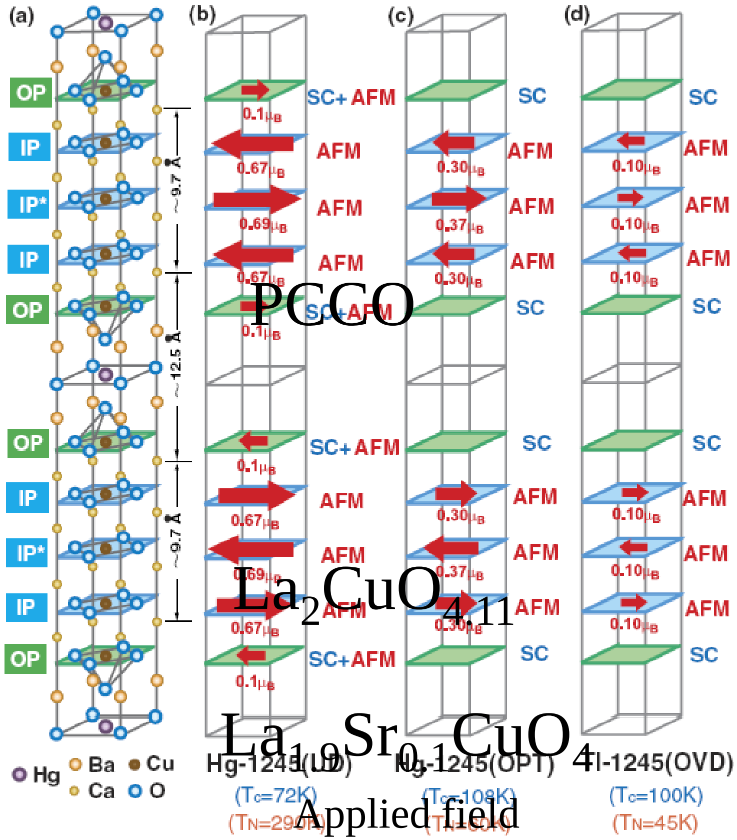
Homogeneous coexistence (experimental)



- H. Mukuda, M. Abe, Y. Araki, Y. Kitaoka, K. Tokiwa, T. Watanabe, A. Iyo, H. Kito, and Y. Tanaka, Phys. Rev. Lett. **96**, 087001 (2006).
- Pengcheng Dai, H. J. Kang, H. A. Mook, M. Matsuura, J. W. Lynn, Y. Kurita, Seiki Komiya, and Yoichi Ando, Phys. Rev. B **71**, 100502 R (2005).
- Robert J. Birgeneau, Chris Stock, John M. Tranquada and Kazuyoshi Yamada, J. Phys. Soc. Japan, **75**, 111003 (2006).
- Chang, … Mesot PRB **78**, 104525 (2008).

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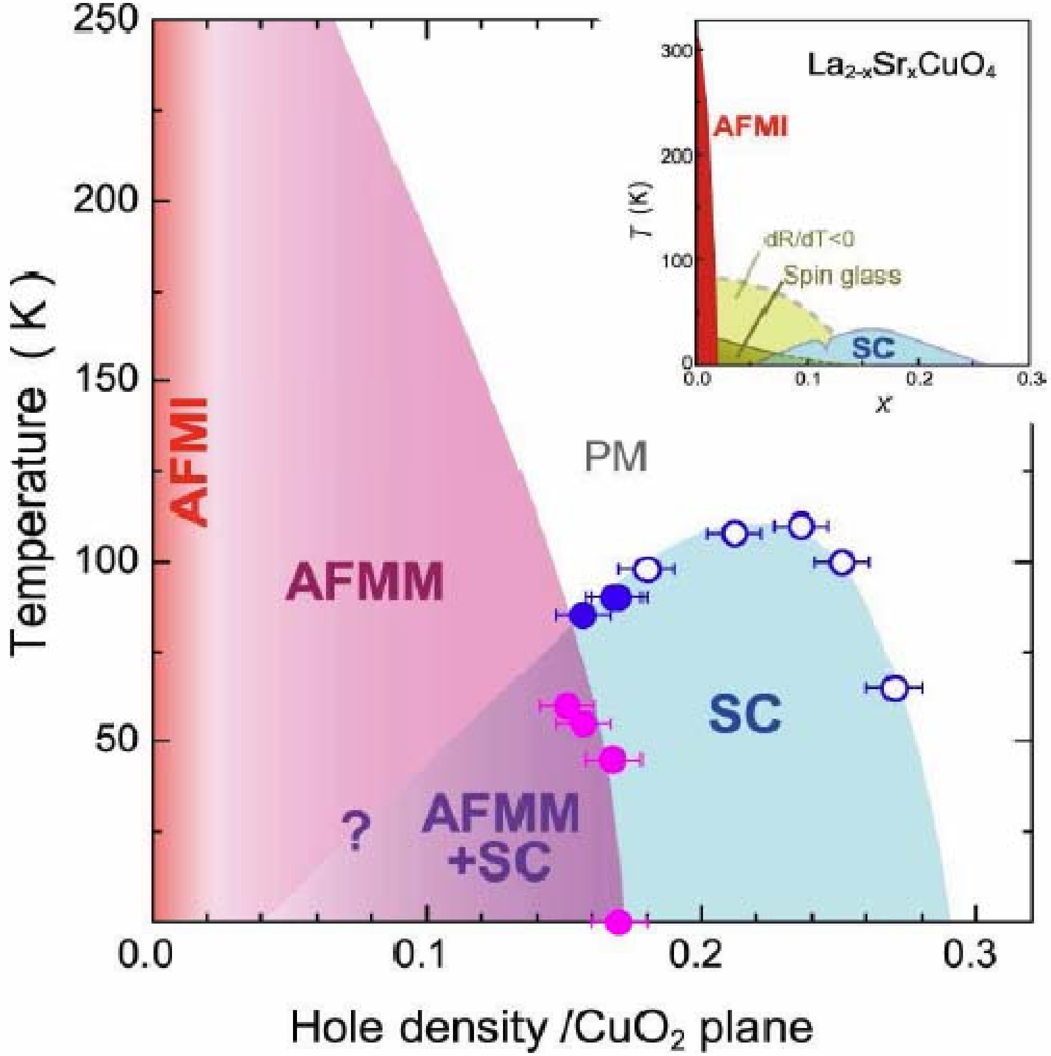
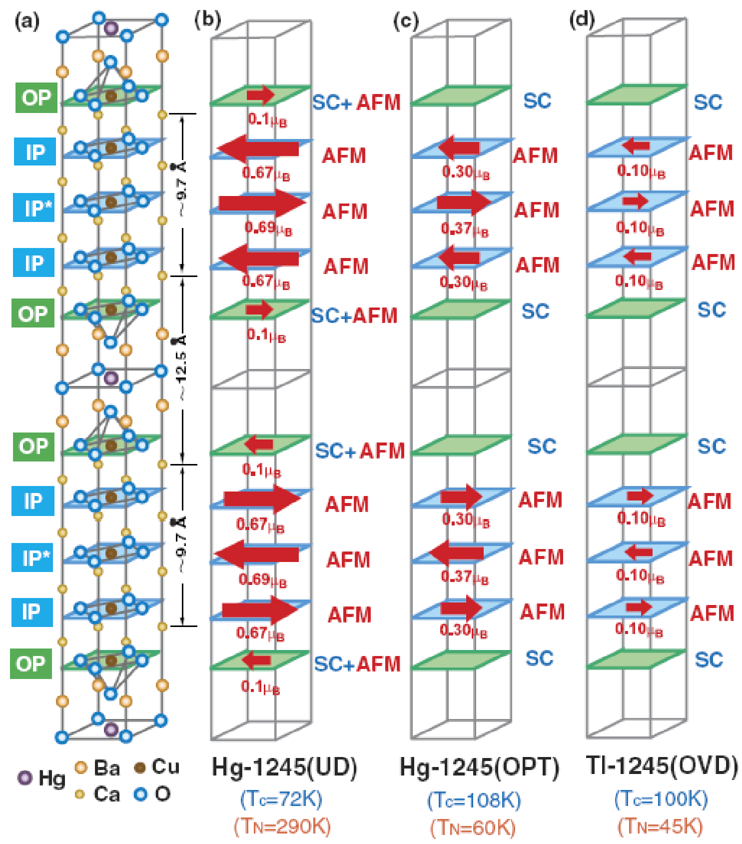
Consistent with following experiment

H. Mukuda, Y. Yamaguchi, S. Shimizu, … A. Iyo JPSJ **77**, 124706 (2008)





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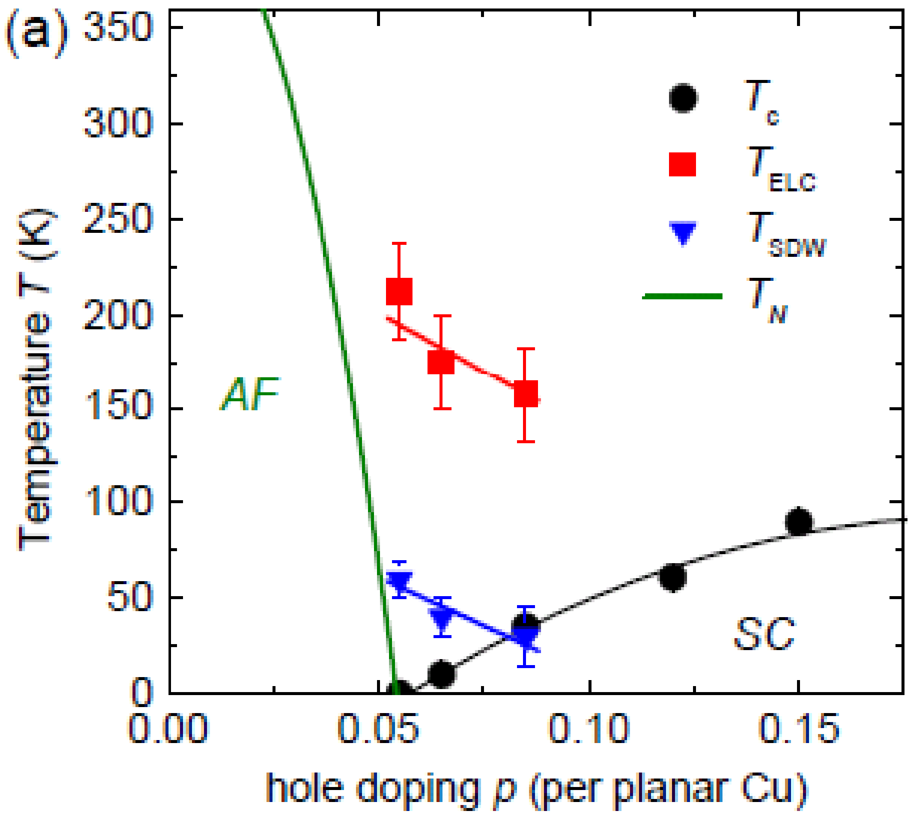
Magnetic phase diagram of YBCO

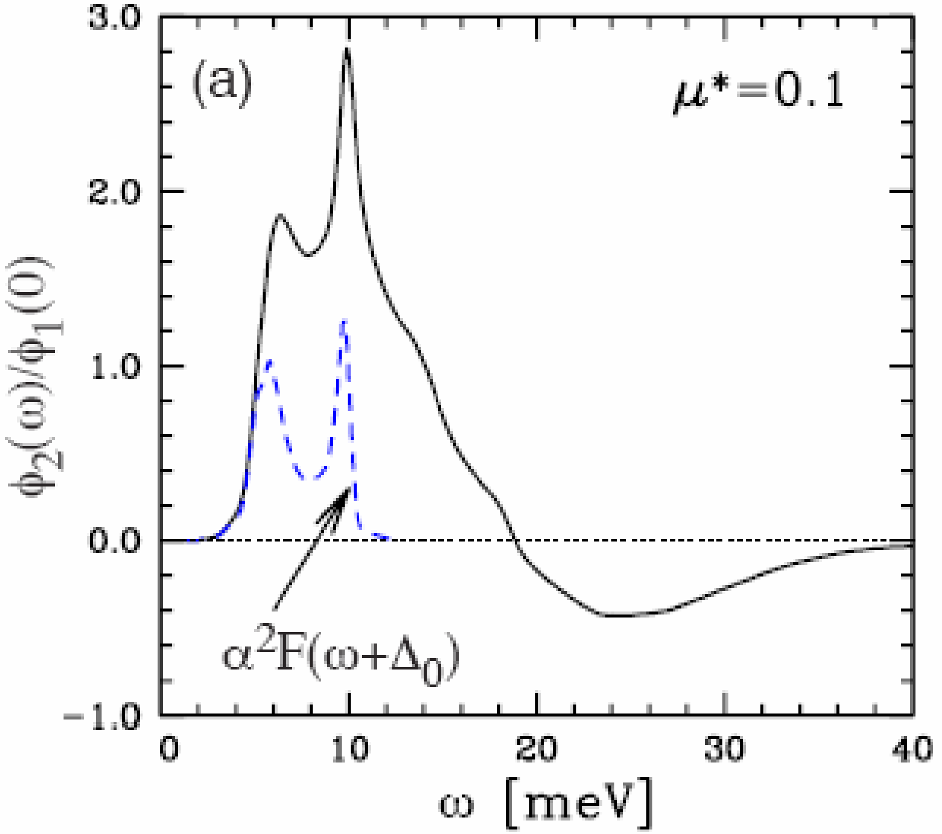


Haug, … Keimer, arXiv:1008.4298

The glue

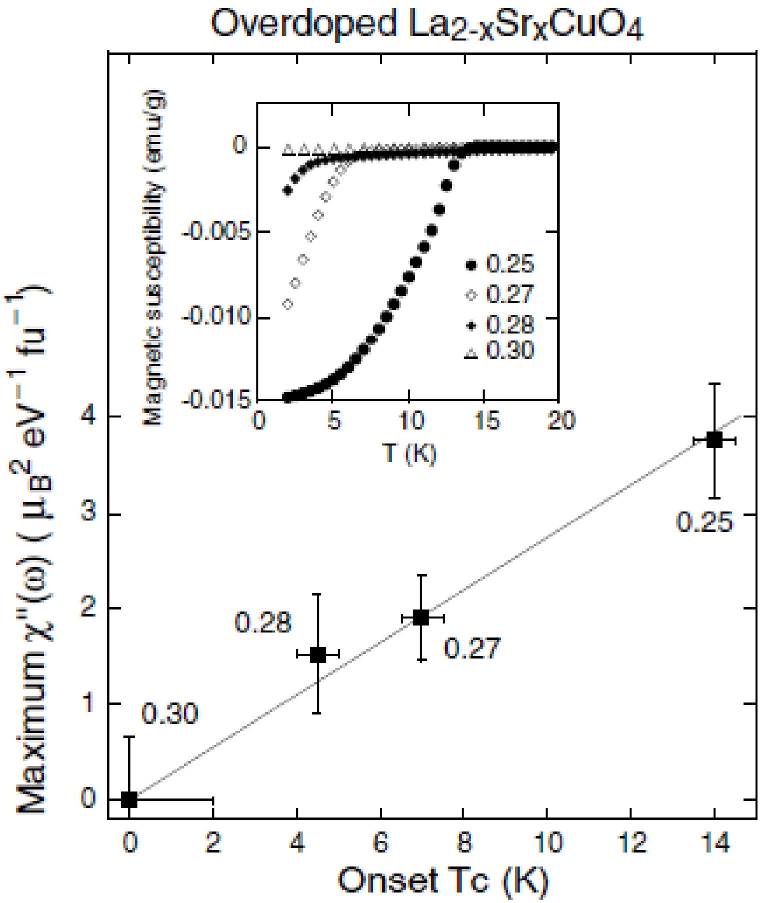
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

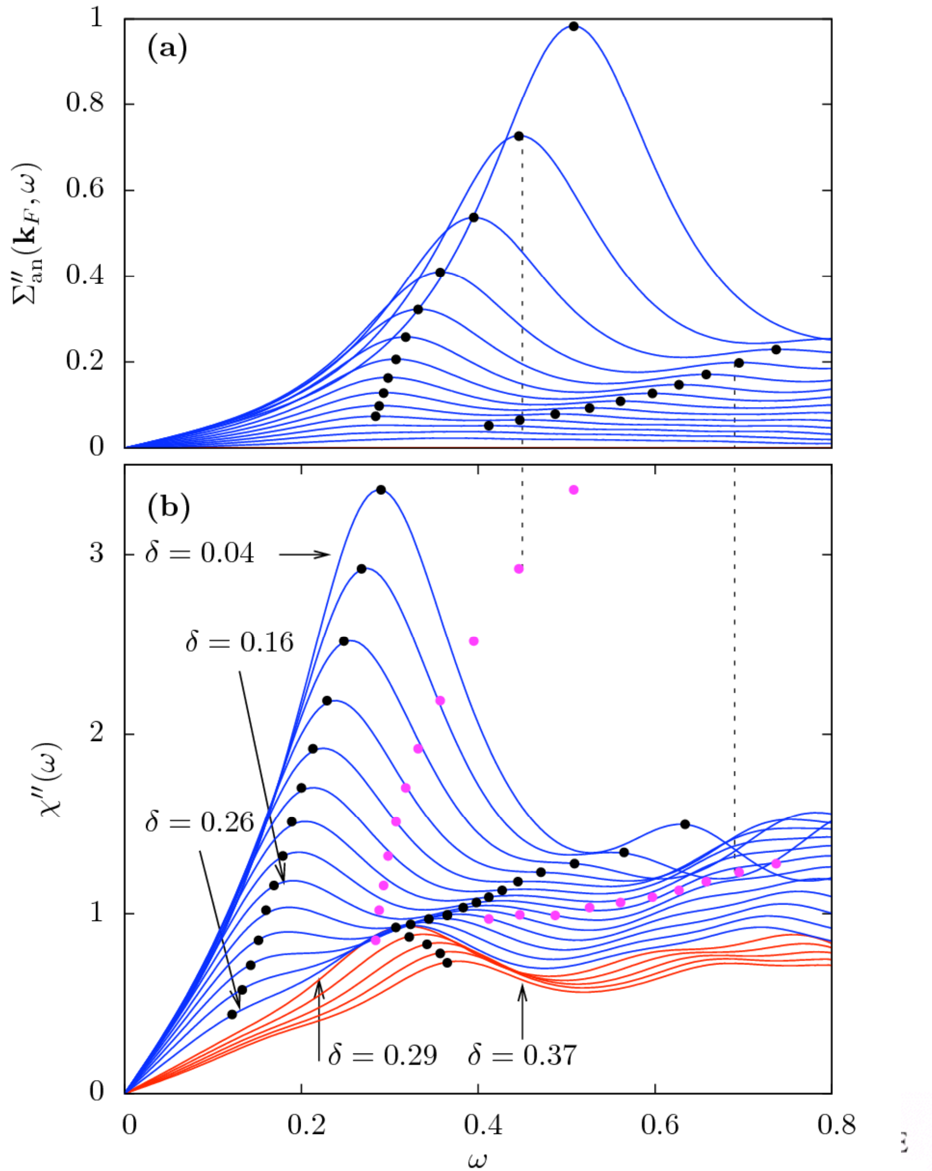


The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

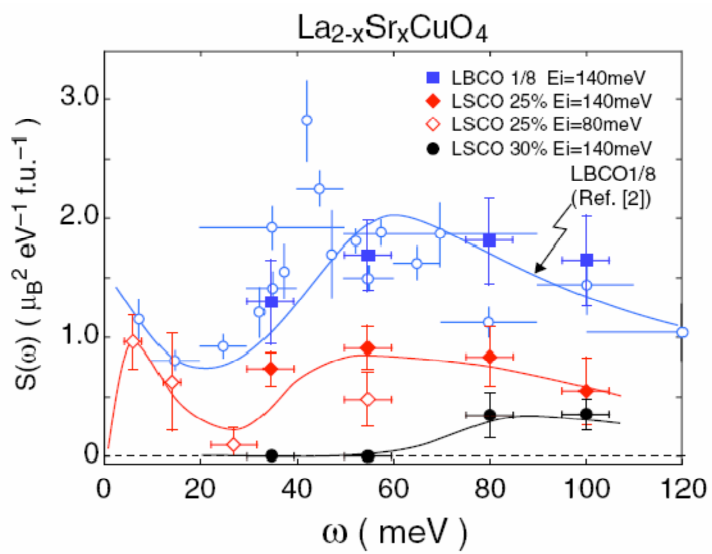
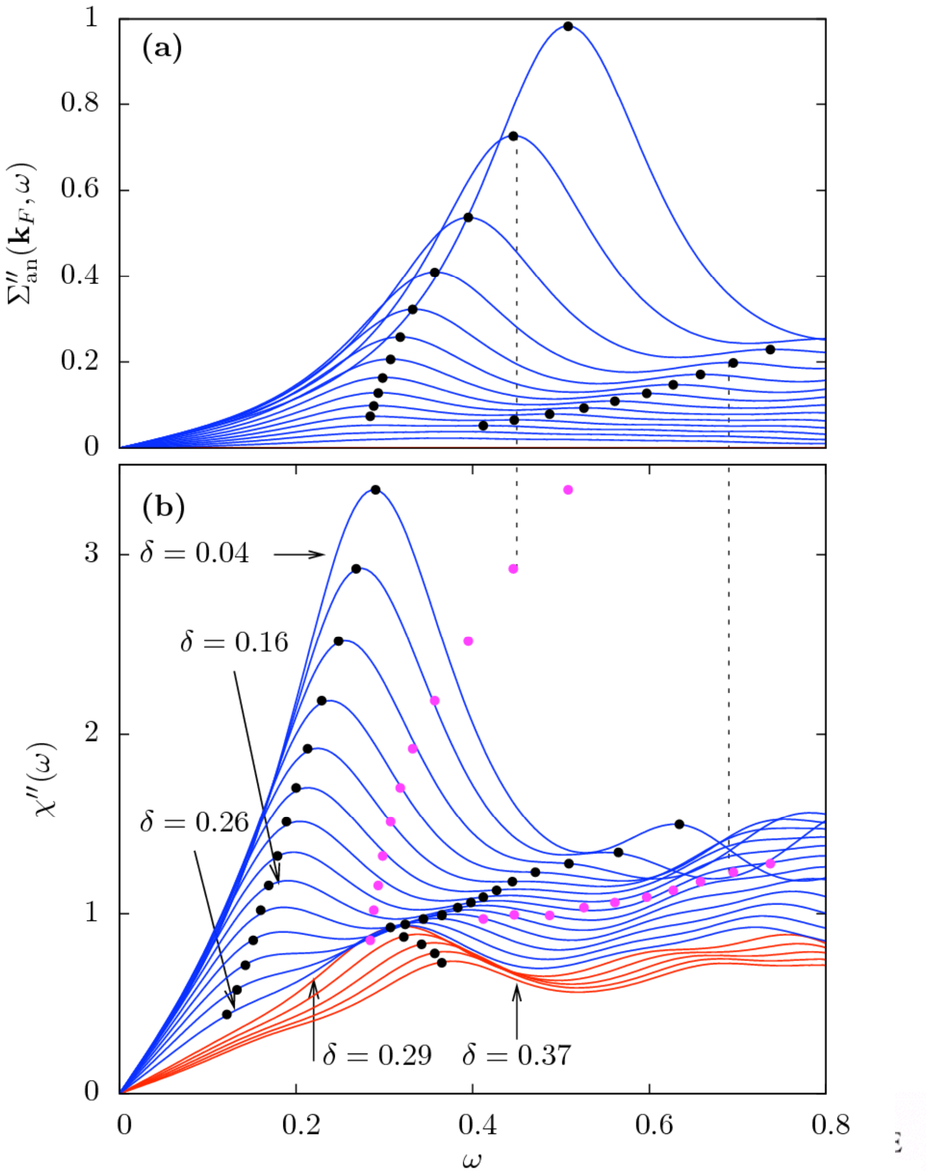


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i =$ 140 meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Wakimoto … Birgeneau PRL (2007);
PRL (2004)



Main collaborators

Giovanni Sordi

David Sénéchal

Kristjan Haule

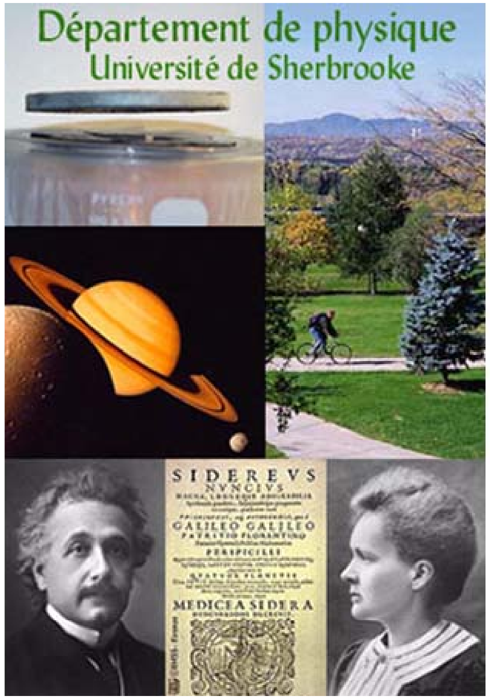
Bumsoo Kyung

Marcello Civelli

Satoshi Okamoto

Conclusions

- The influence of Mott Physics extends way beyond half-filling
- Conjecture that quantum-critical like behavior is constant U cut of our phase diagram, i.e. very low T critical point.
- Superconductivity follows naturally and retardation effects in pairing come from spin fluctuations.



André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Merci

Arigato

Thank you