Mott Physics in Strongly Correlated Superconductivity

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S. Okamoto, B. Kyung, M. Civelli

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

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Sousse, 6 November 2010

VERITATEM IN CHARITATE

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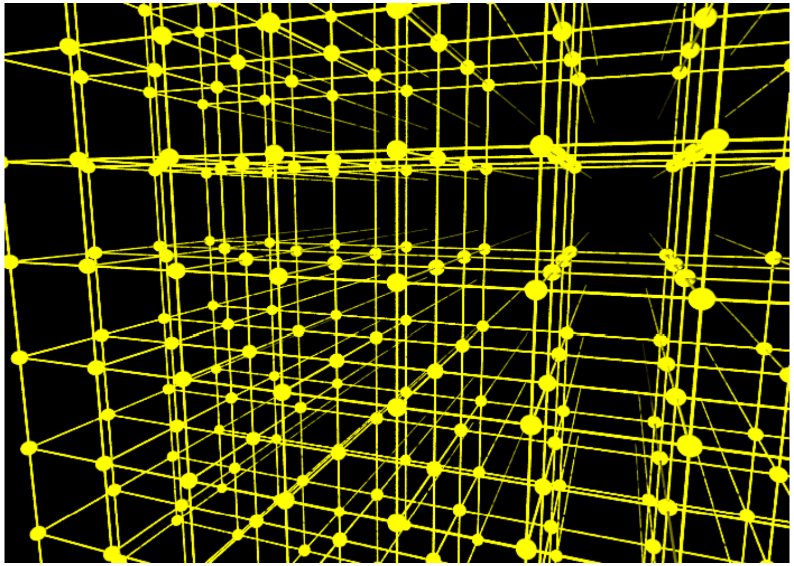
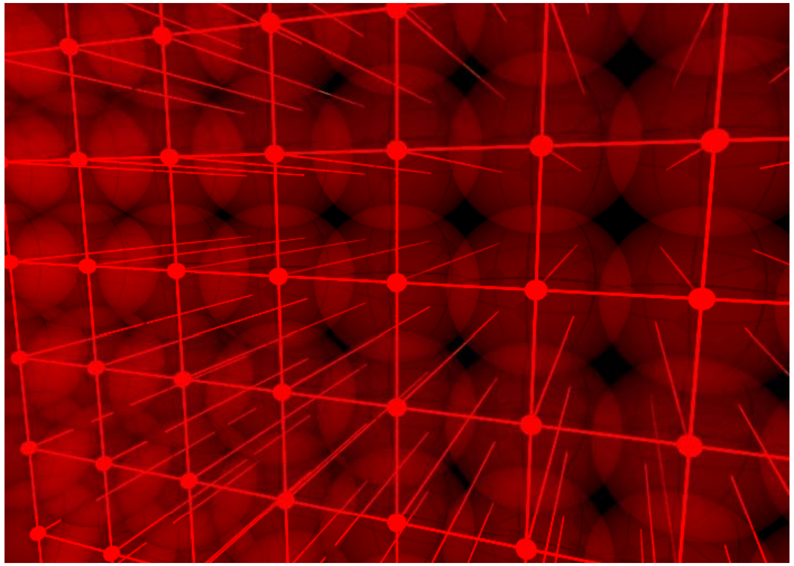
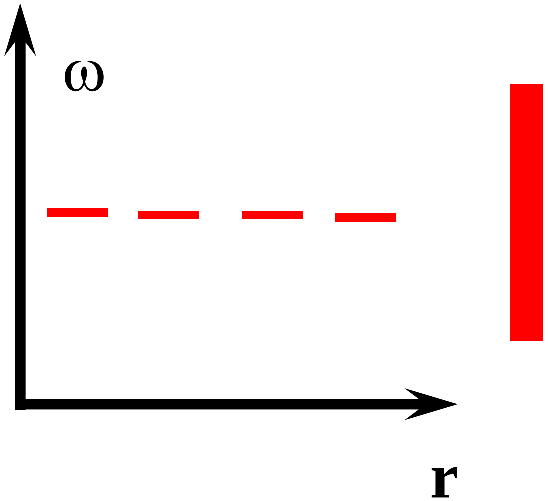
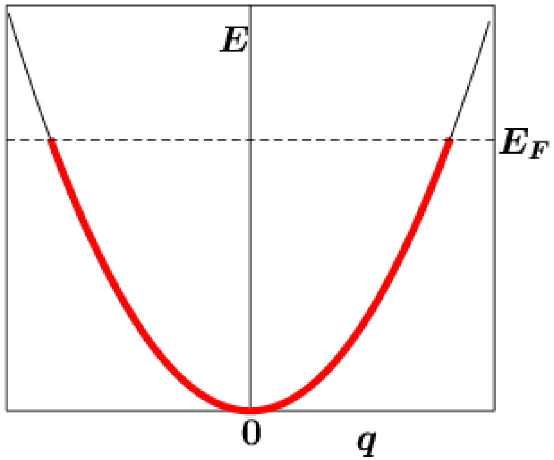
How to make a metal



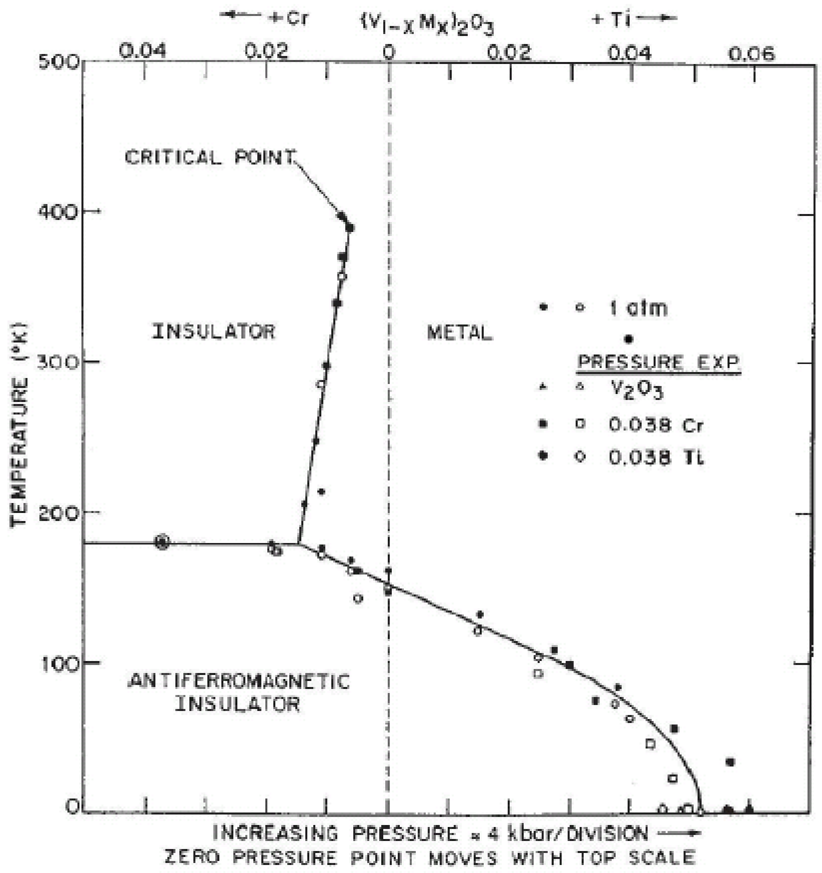






Courtesy, S. Julian

« Conventional » Mott transition



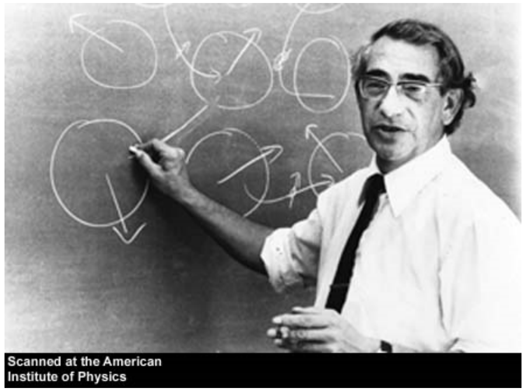
T

p

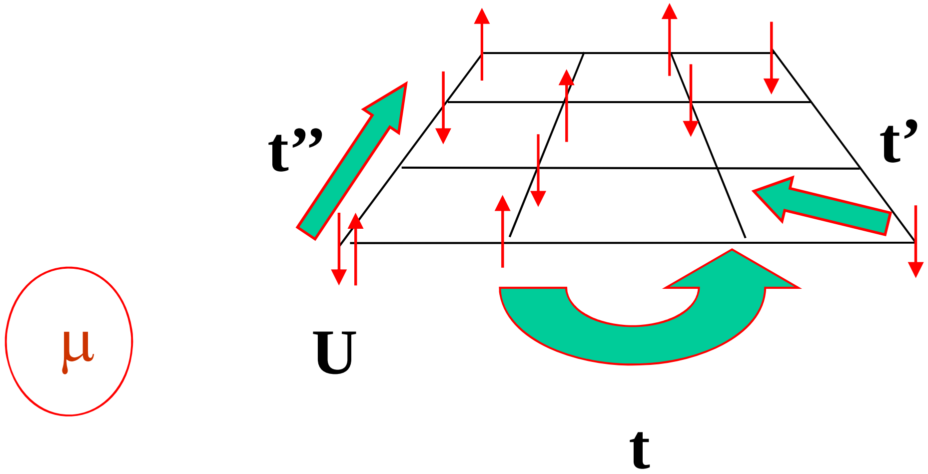
Understood from Hubbard model and dynamical mean field theory

Figure: McWhan, PRB 1970; Limelette, Science 2003

Hubbard model

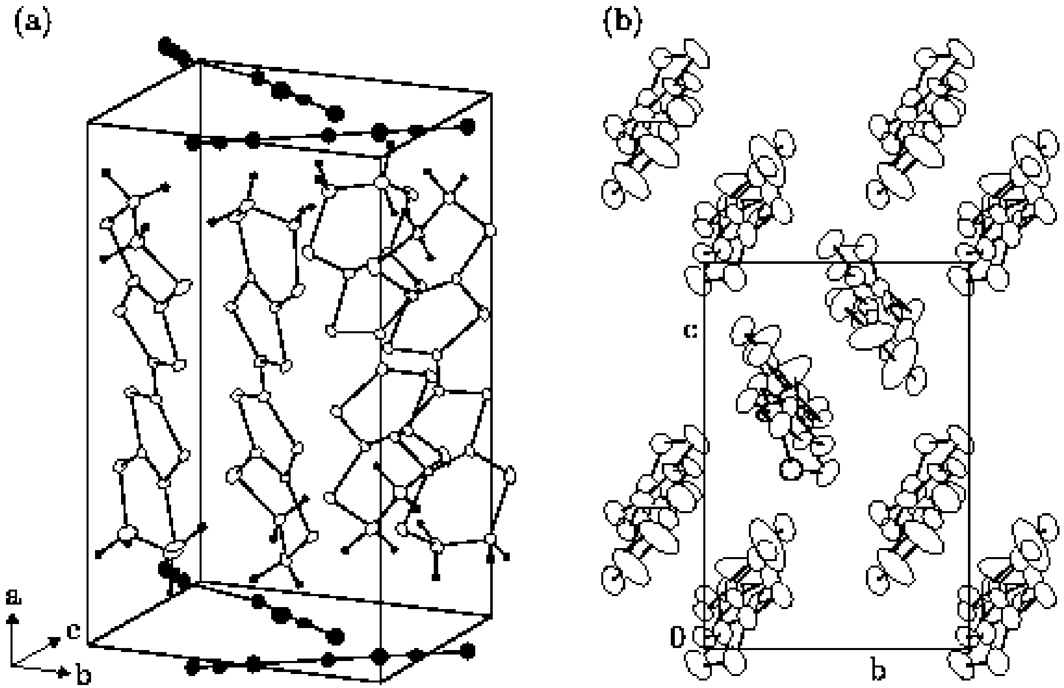


1931-1980



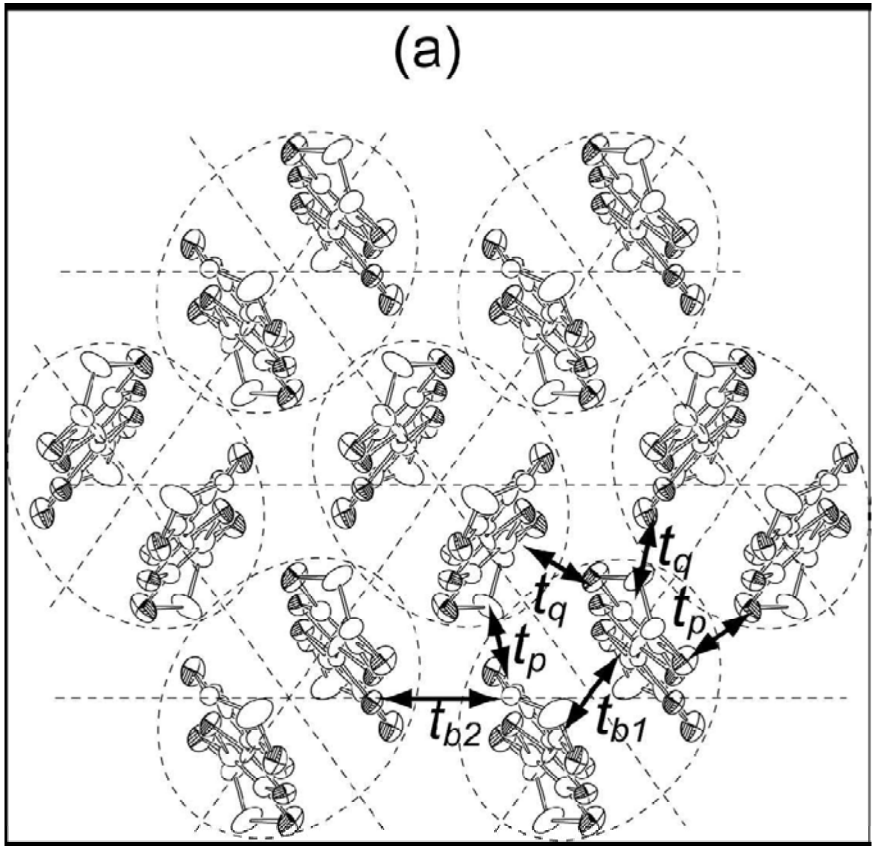
$$H = -\sum_{<ij>\sigma} t_{i,j} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Layered organic superconductors (κ–BEDT-X)

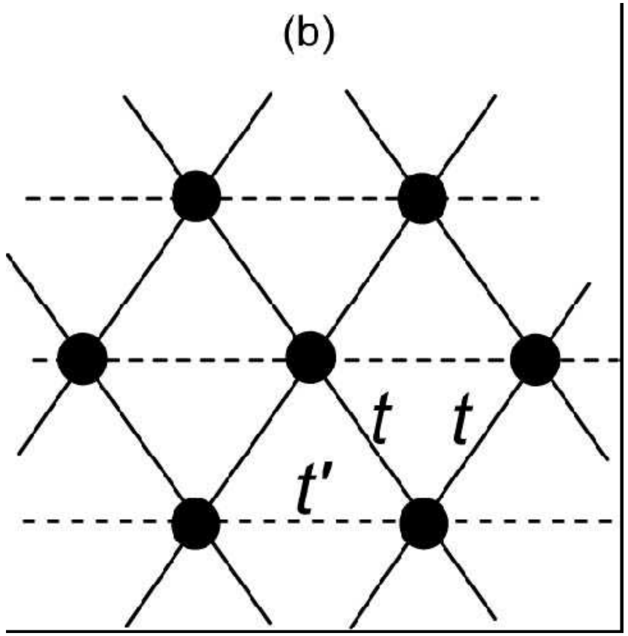


One-band Hubbard model of BEDT organics

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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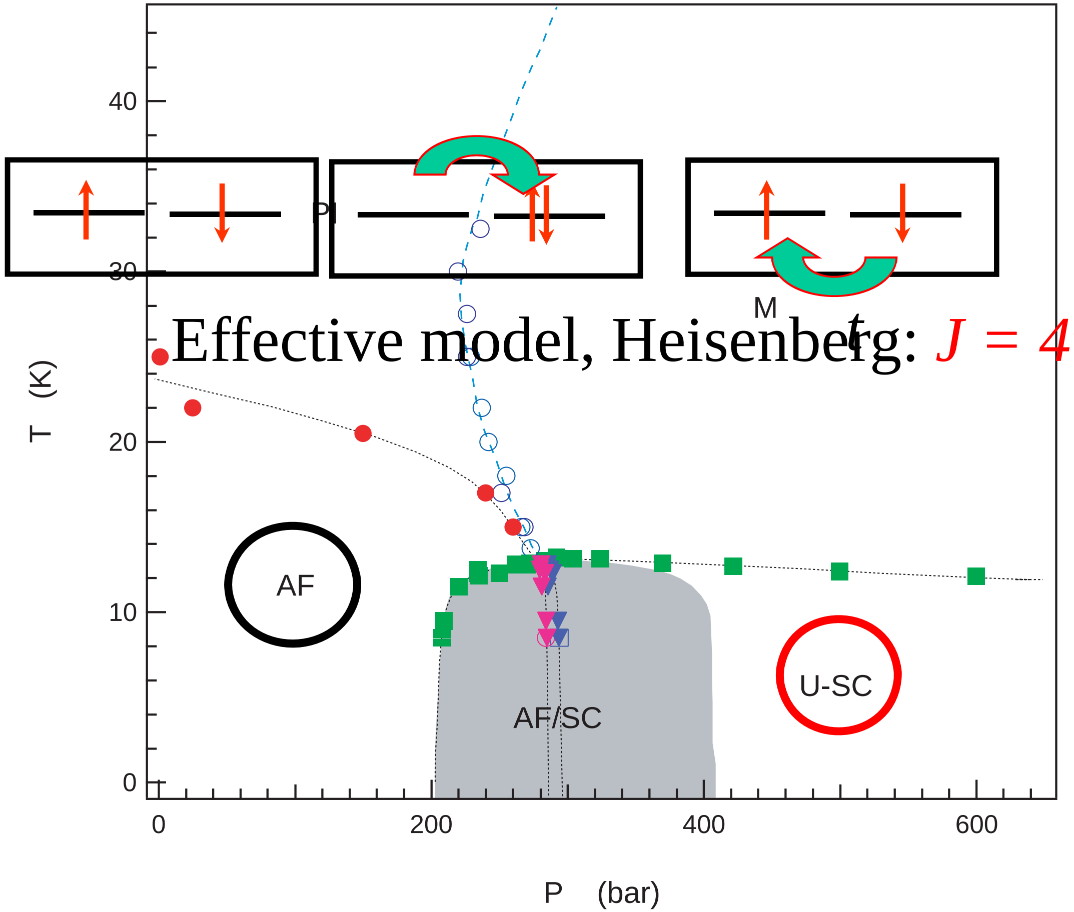
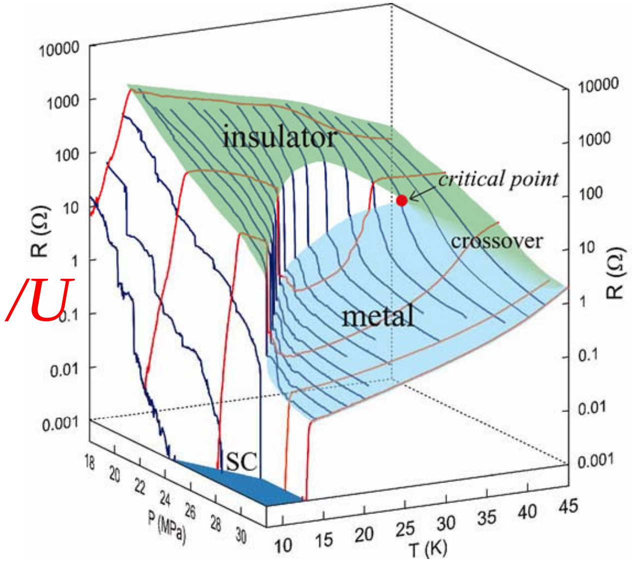
Bare Mott critical point in organics



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

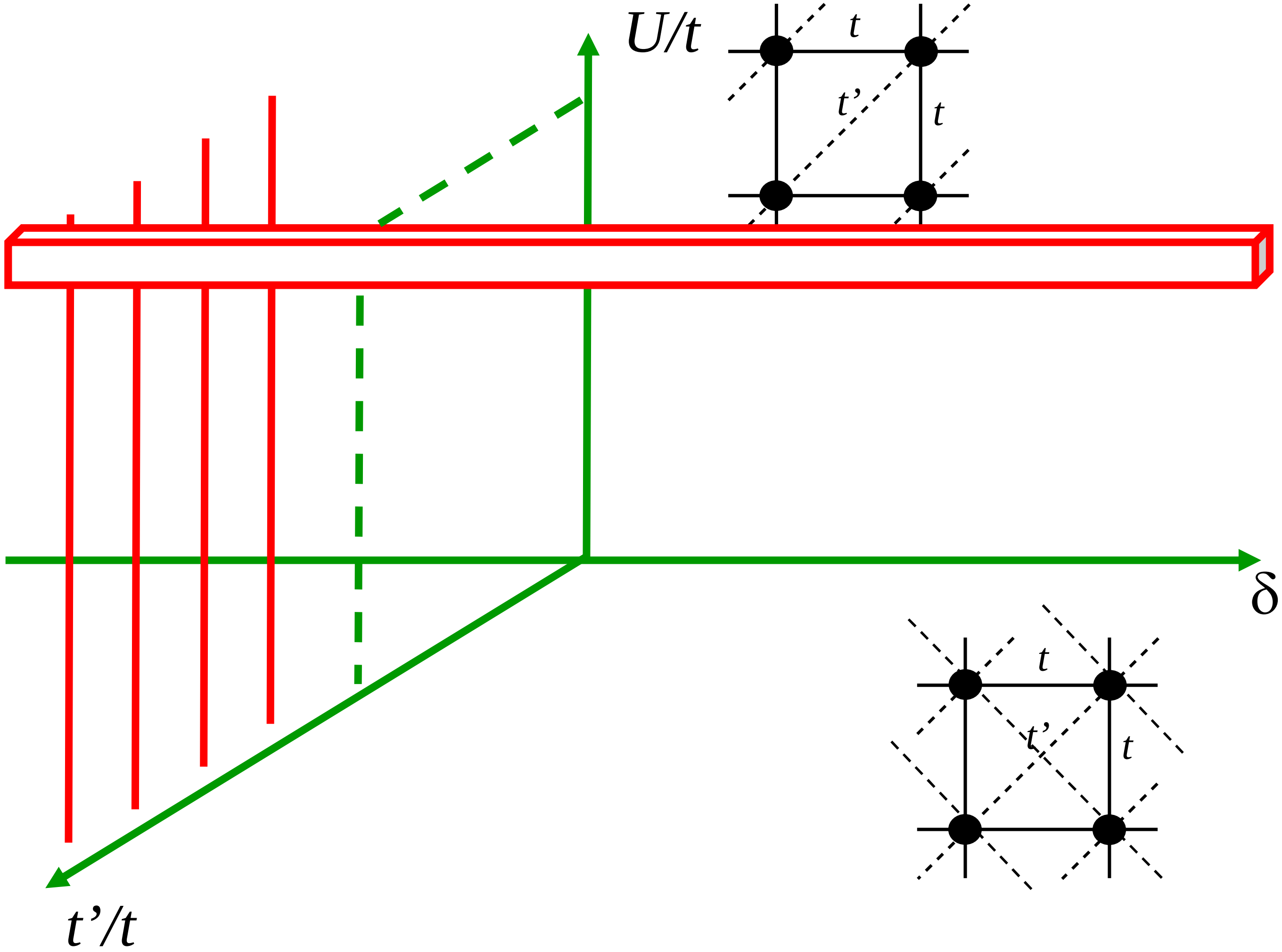


F. Kagawa, K. Miyagawa, + K. Kanoda
PRB **69** (2004) +Nature **436** (2005)

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

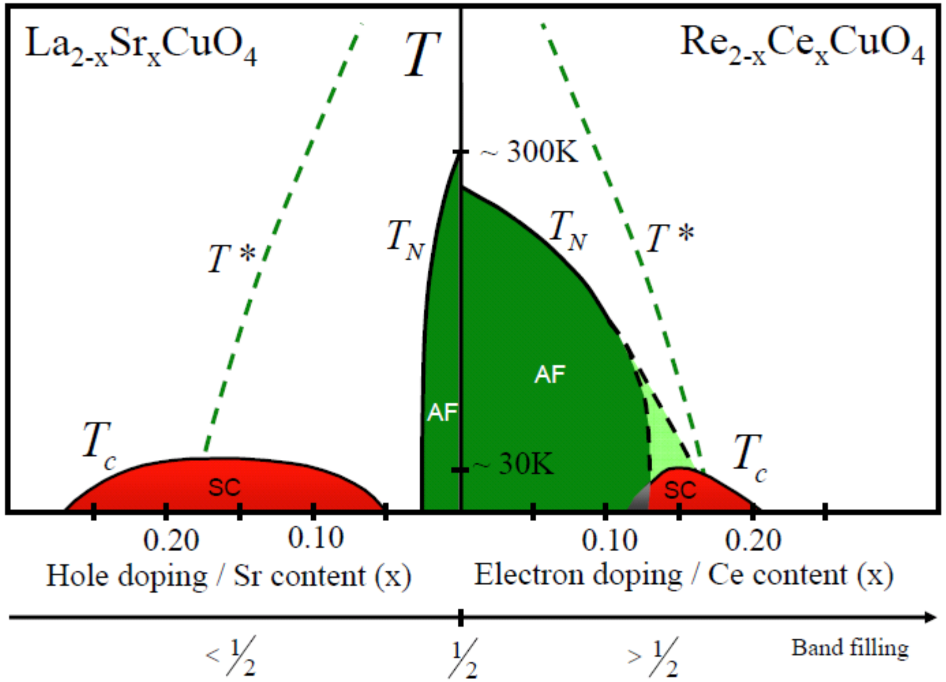
S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL **91** (2003)

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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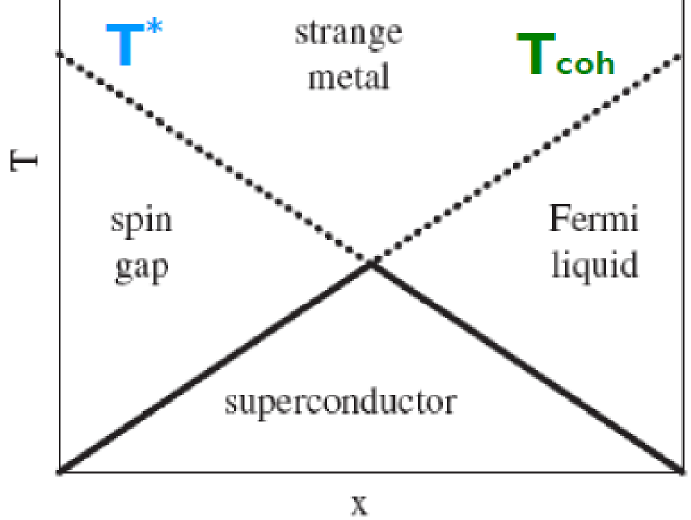
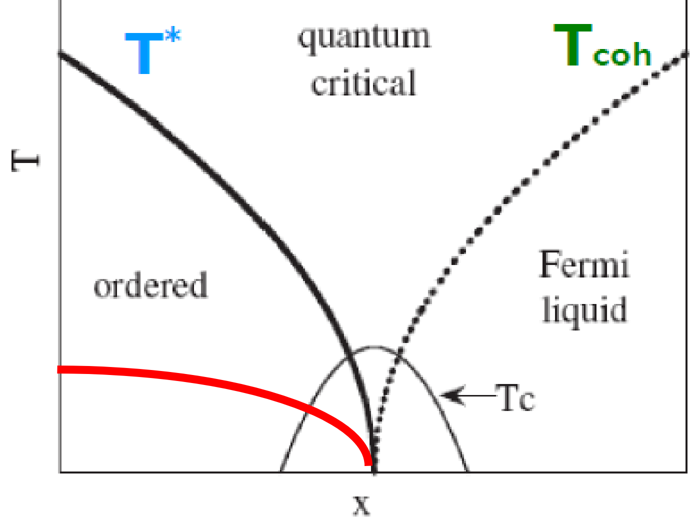
Two views (caricature)

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

RVB plain vanilla, YZR,



Competing order



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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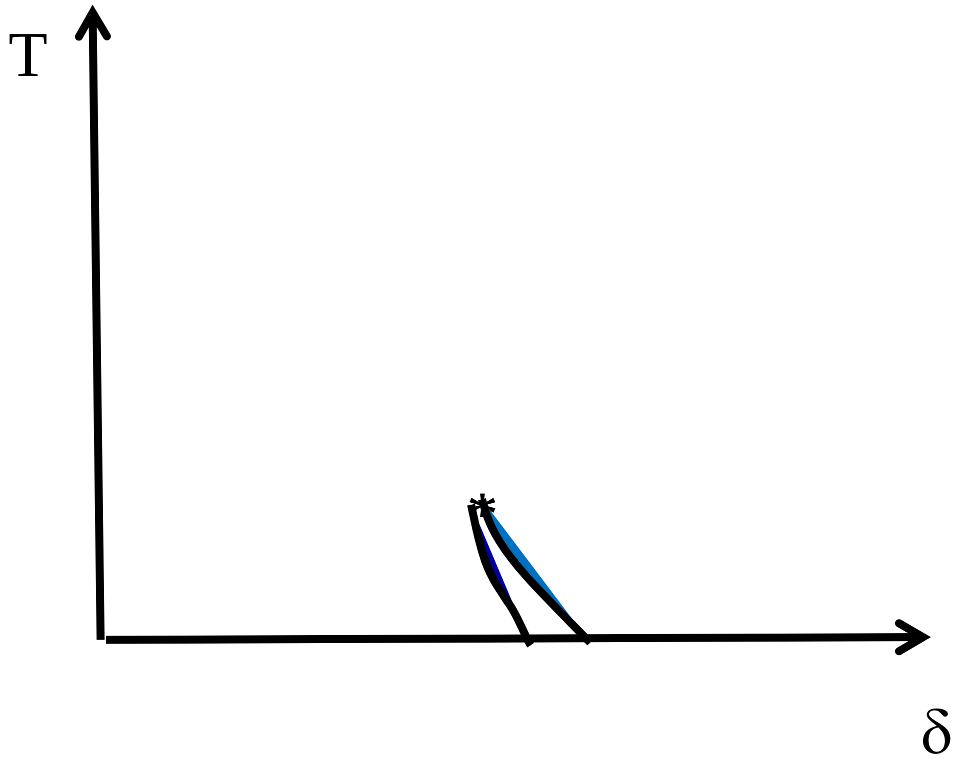
An alternate view (a bit of both)



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

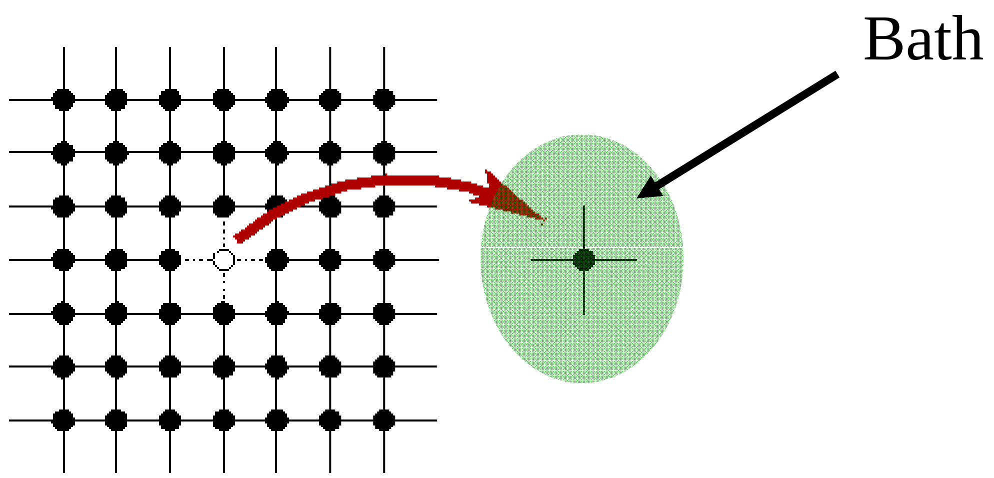
Outline

- Method
- Normal state
- Superconducting state

Method

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

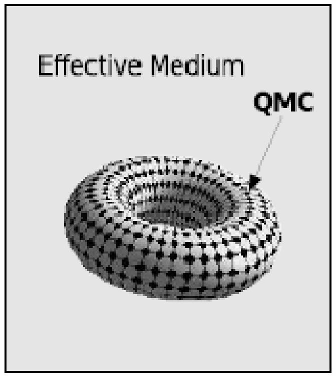
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

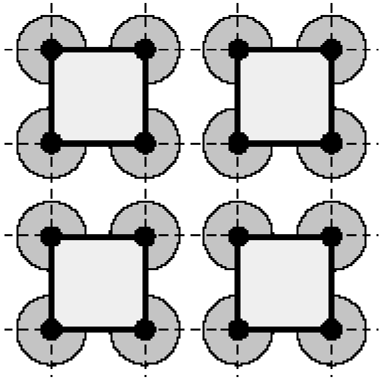
DMFT, (d = *3*)

2d Hubbard: Quantum cluster method

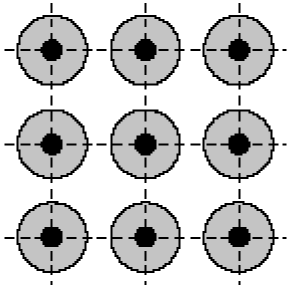


DCA

C-DMFT



DMFT

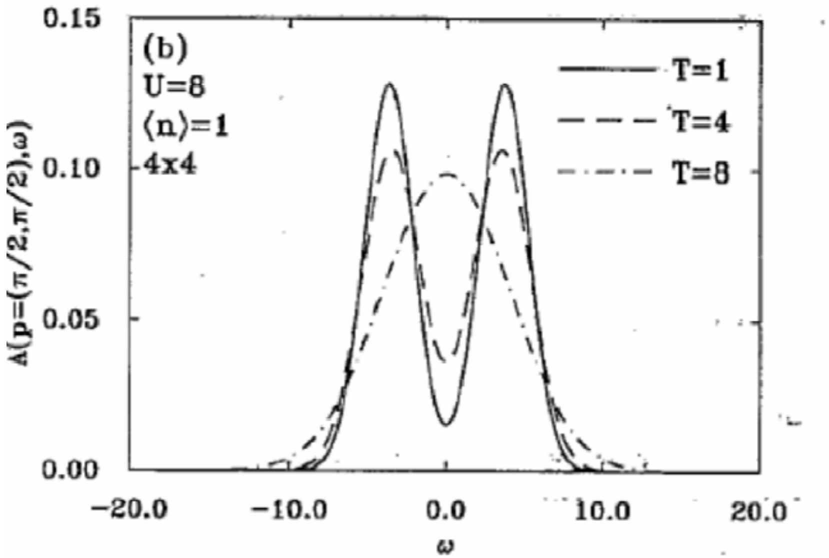


Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).
Maier, Jarrell et al., Rev. Mod. Phys. **77**, 1027 (2005)

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



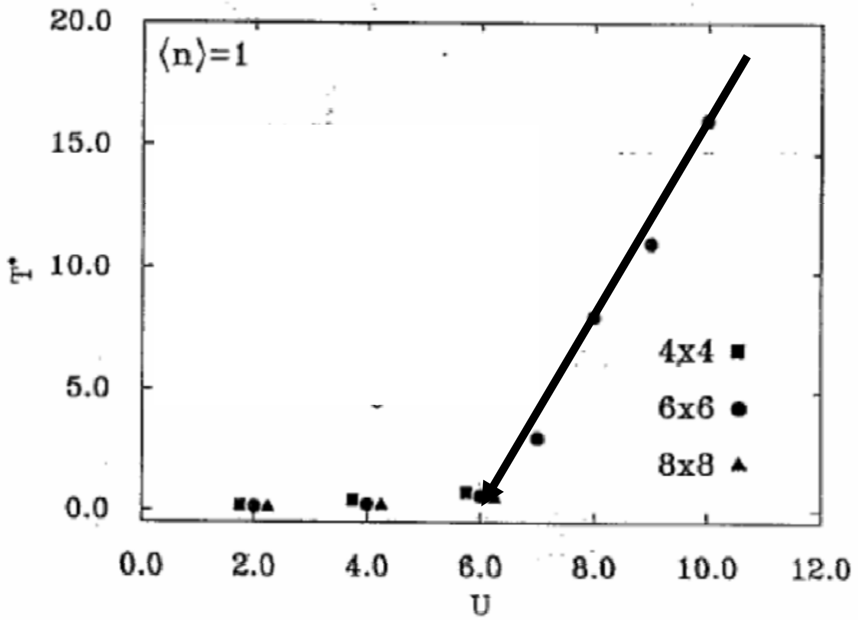


FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

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

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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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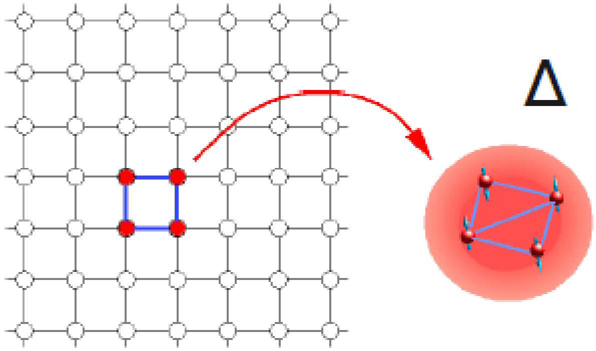
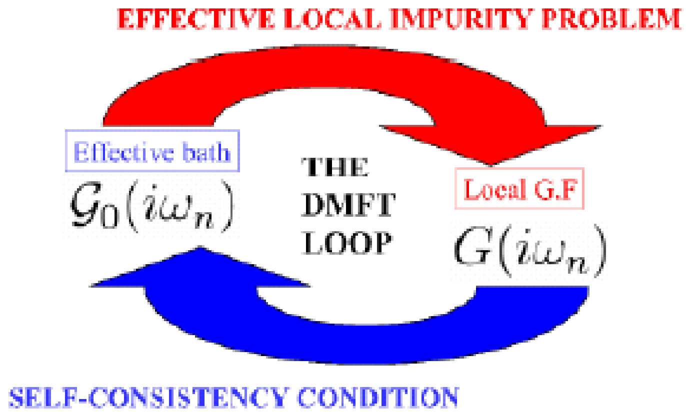
C-DMFT



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



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

Here: continuous time QMC

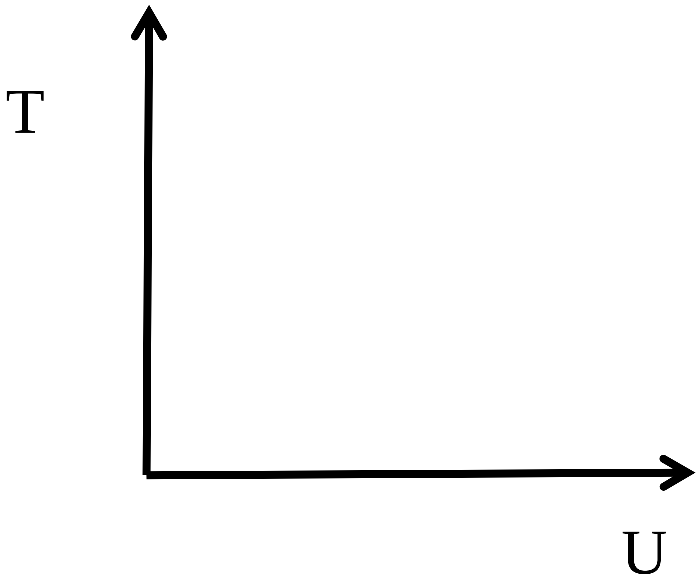
P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007

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

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



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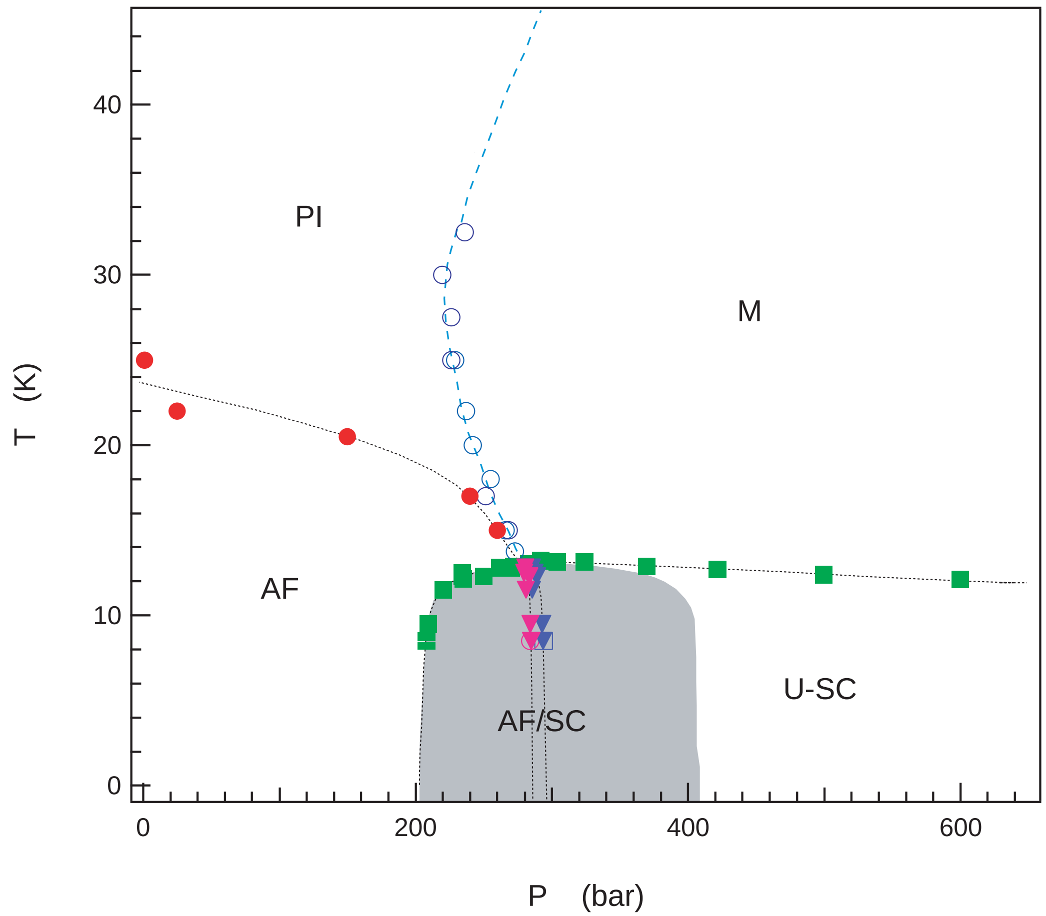
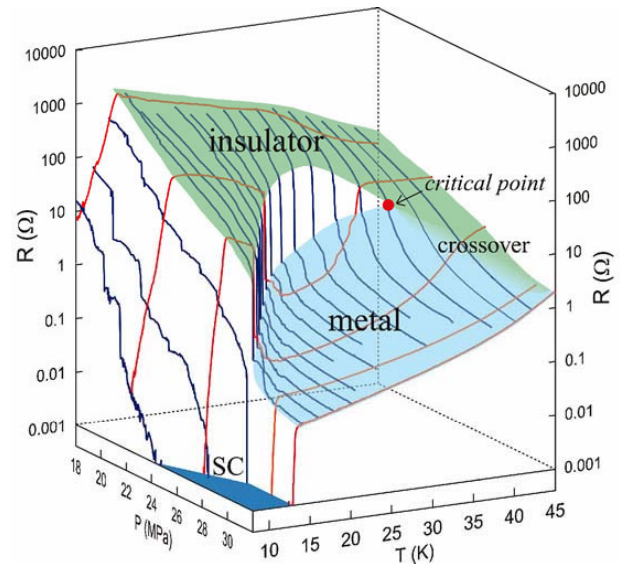
Bare Mott critical point in organics





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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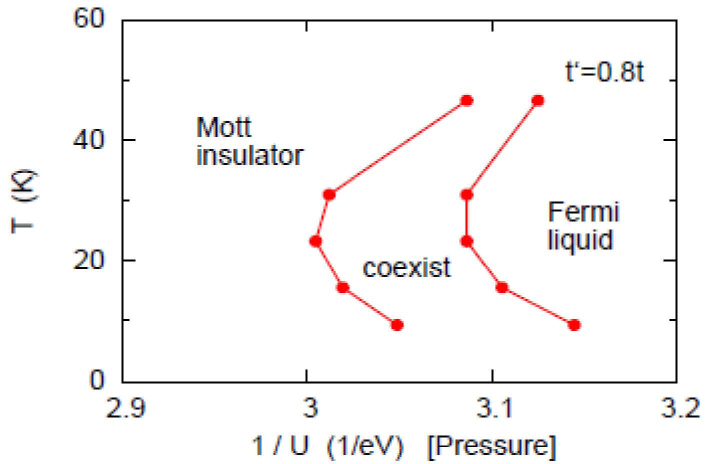
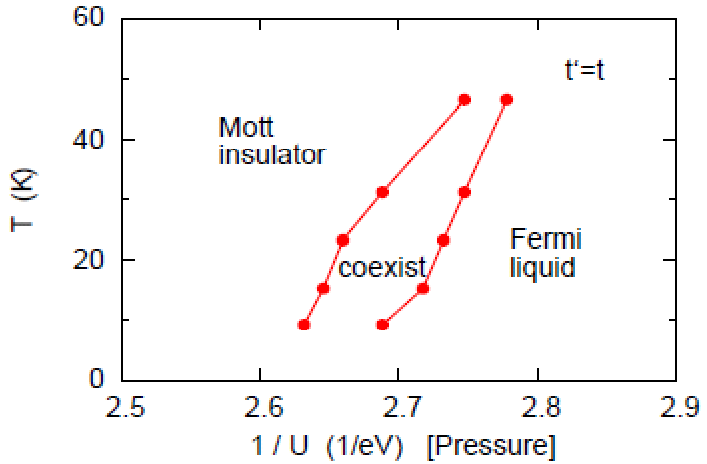
Interaction-induced Mott transition theory



κ–BEDT-Cl



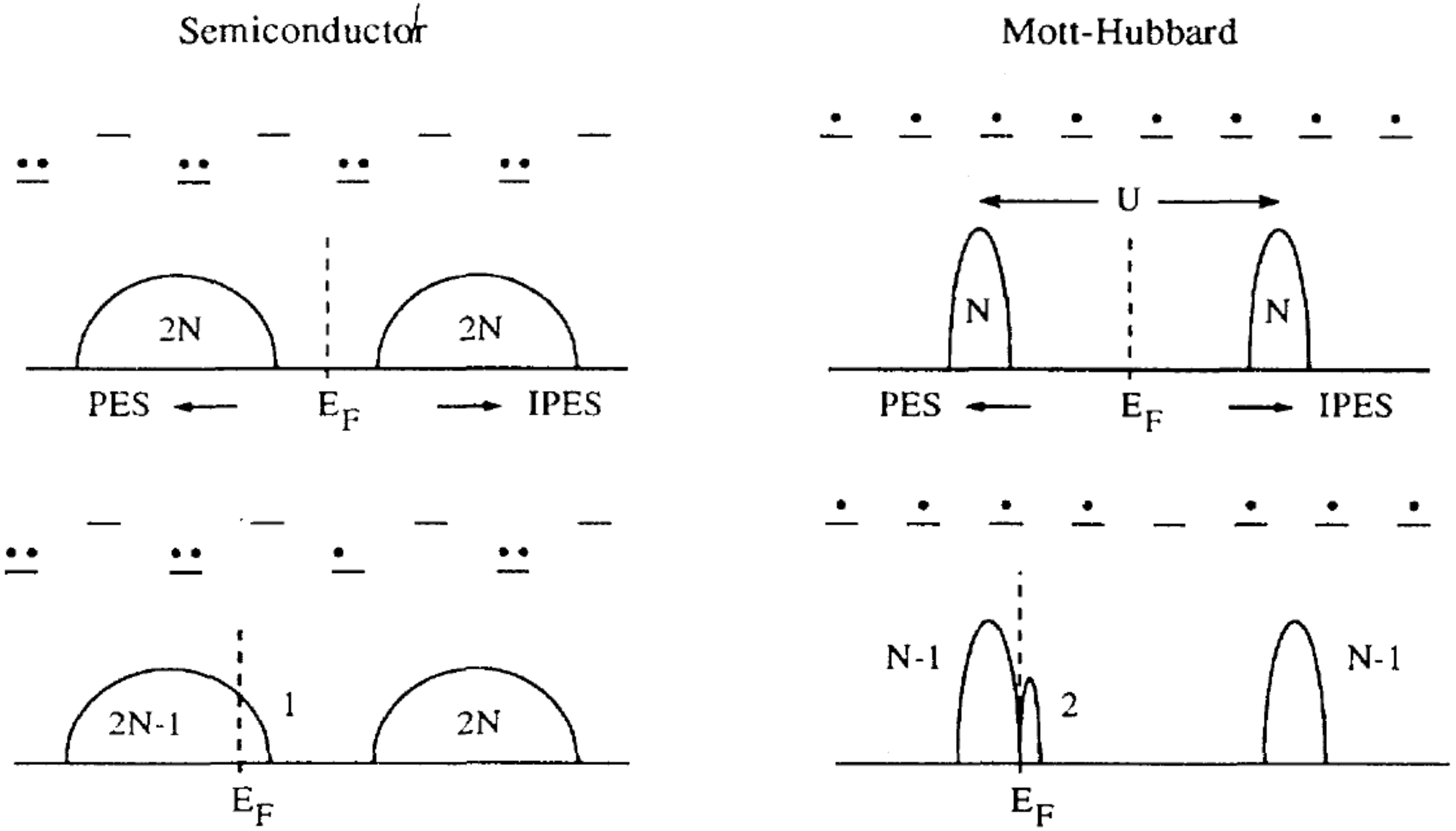
κ–BEDT-CN

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

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

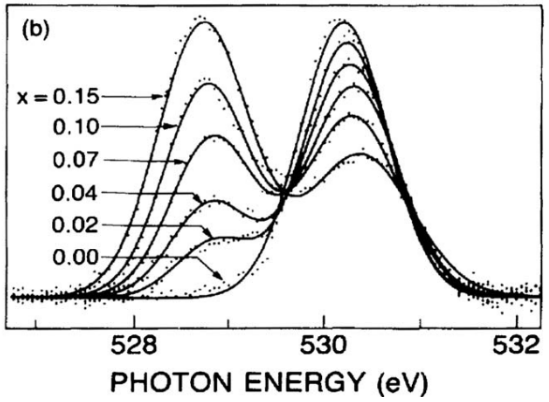
Cuprates as doped Mott insulators

Spectral weight transfer

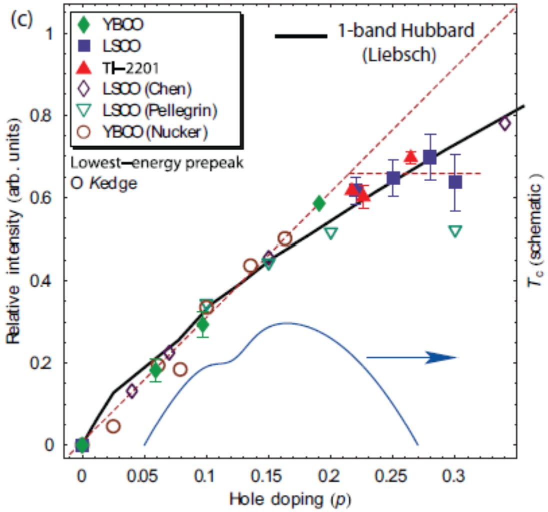


Meinders *et al.* PRB **48**, 3916 (1993)

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 ω = 0 scales as *2x* +

Not as 1+x as in Fermi liquid

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

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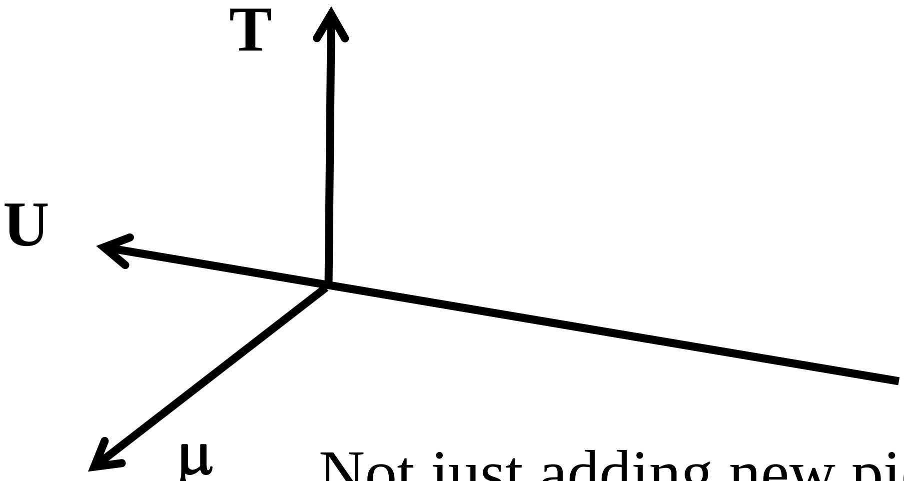
PRL, **104**, 226402 (2010)

Doping-induced Mott transition (*t’=0*)



Kristjan Haule

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

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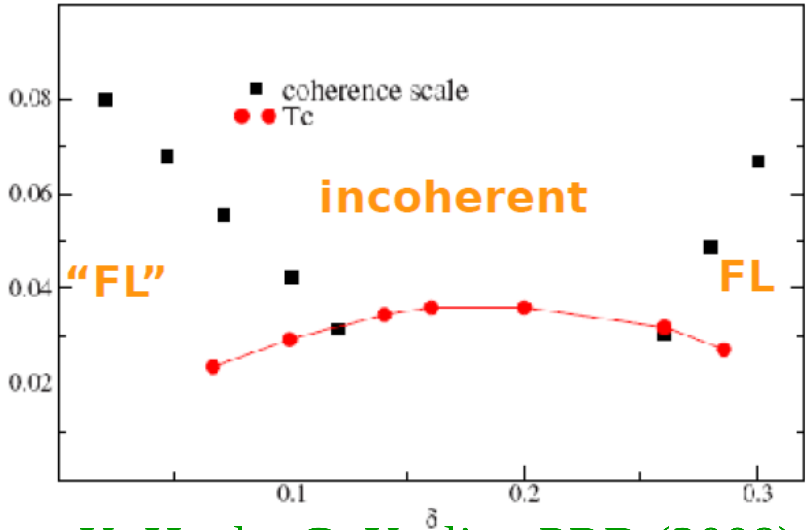
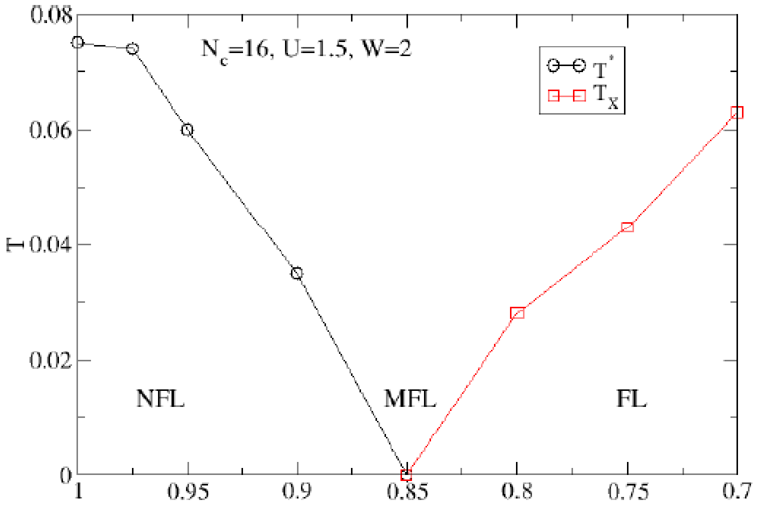
Doping driven Mott transition, *t' = 0*

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)

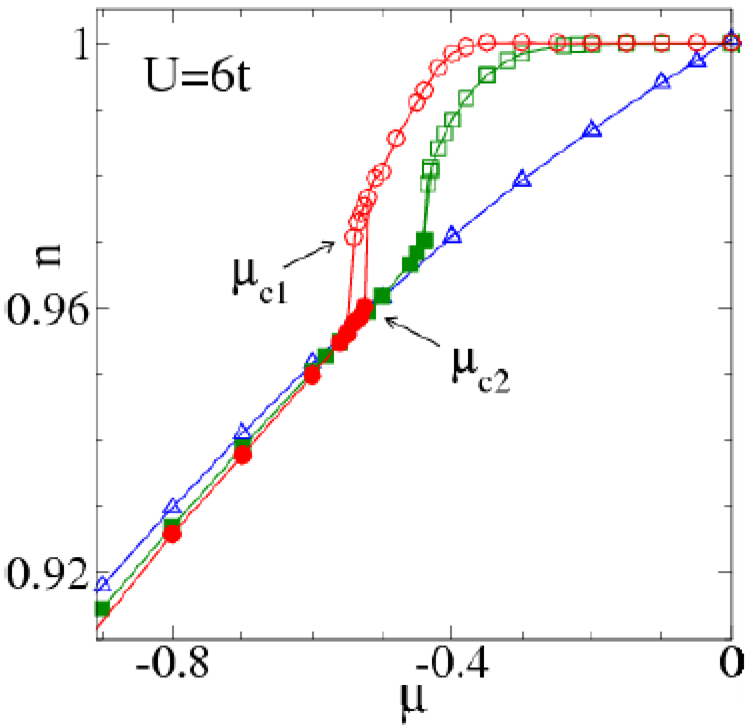


K. Haule, G. Kotliar, PRB (2008)

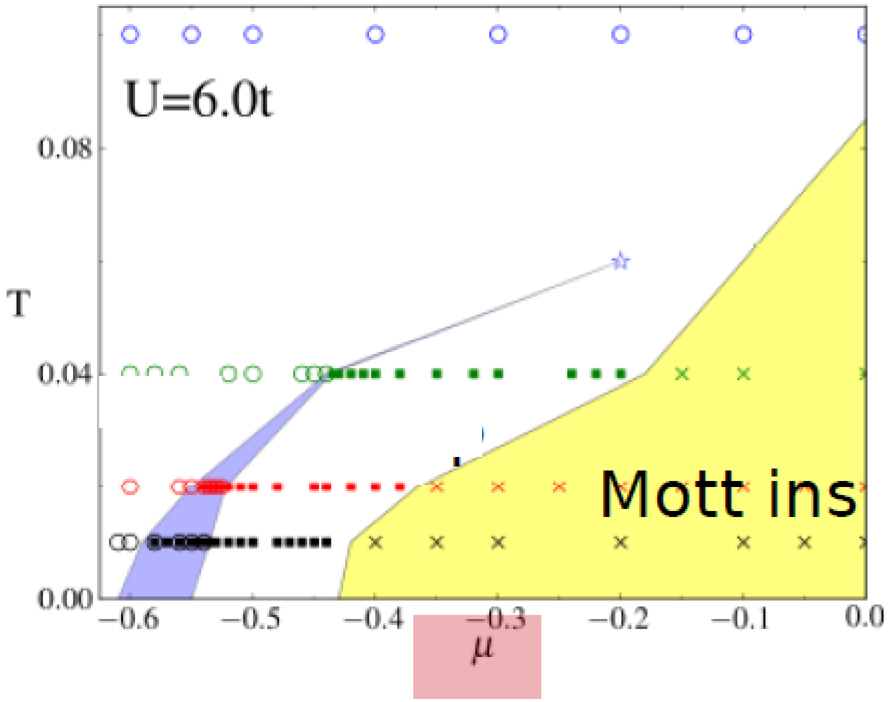


Vildhyadhiraja, PRL (2009)

First order transition at finite doping

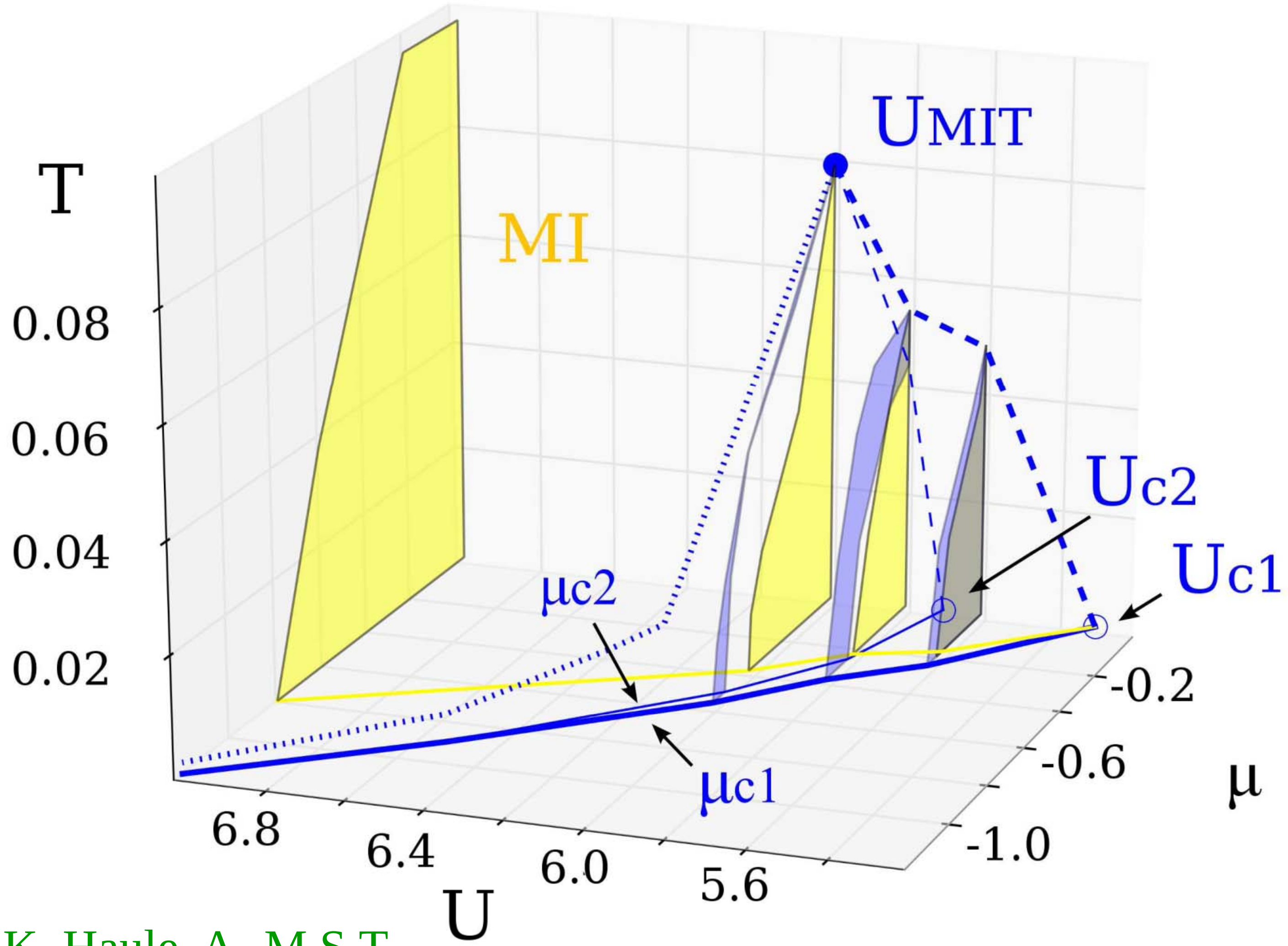


$n(\mu)$ for several temperatures: $T/t = 1/10,\ 1/25,\ 1/50$



Hysteretic behavior: fingerprint first order transition!

Normal state phase diagram



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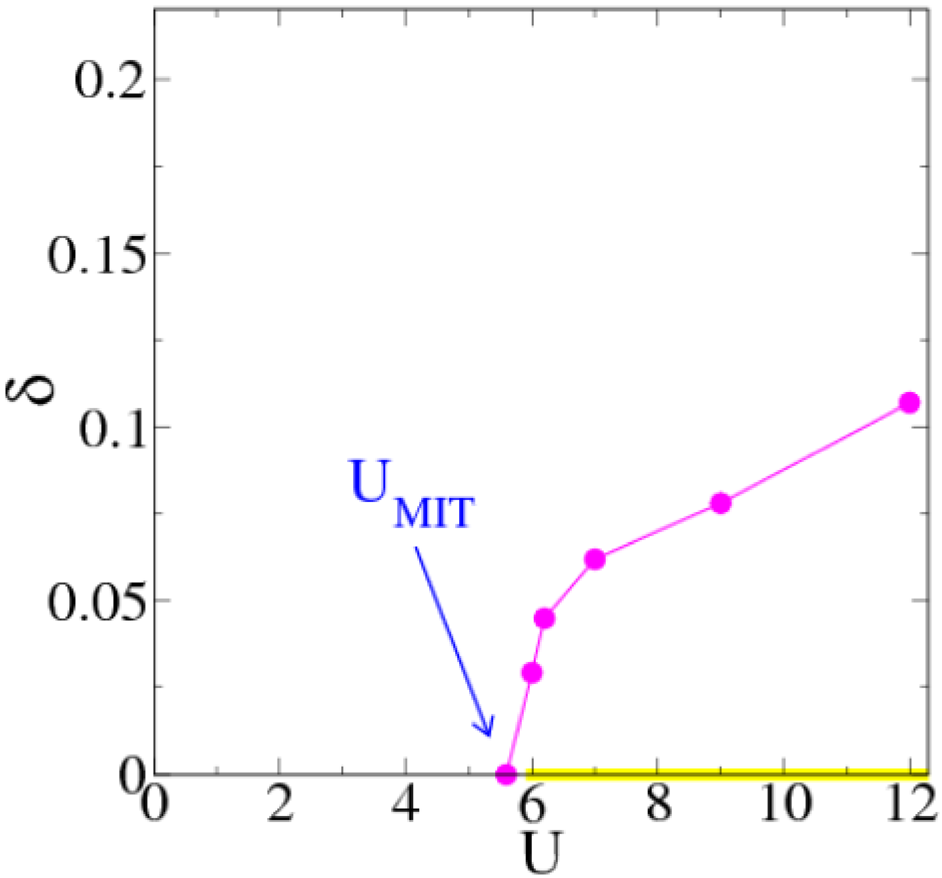
Link to Mott transition up to optimal doping

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



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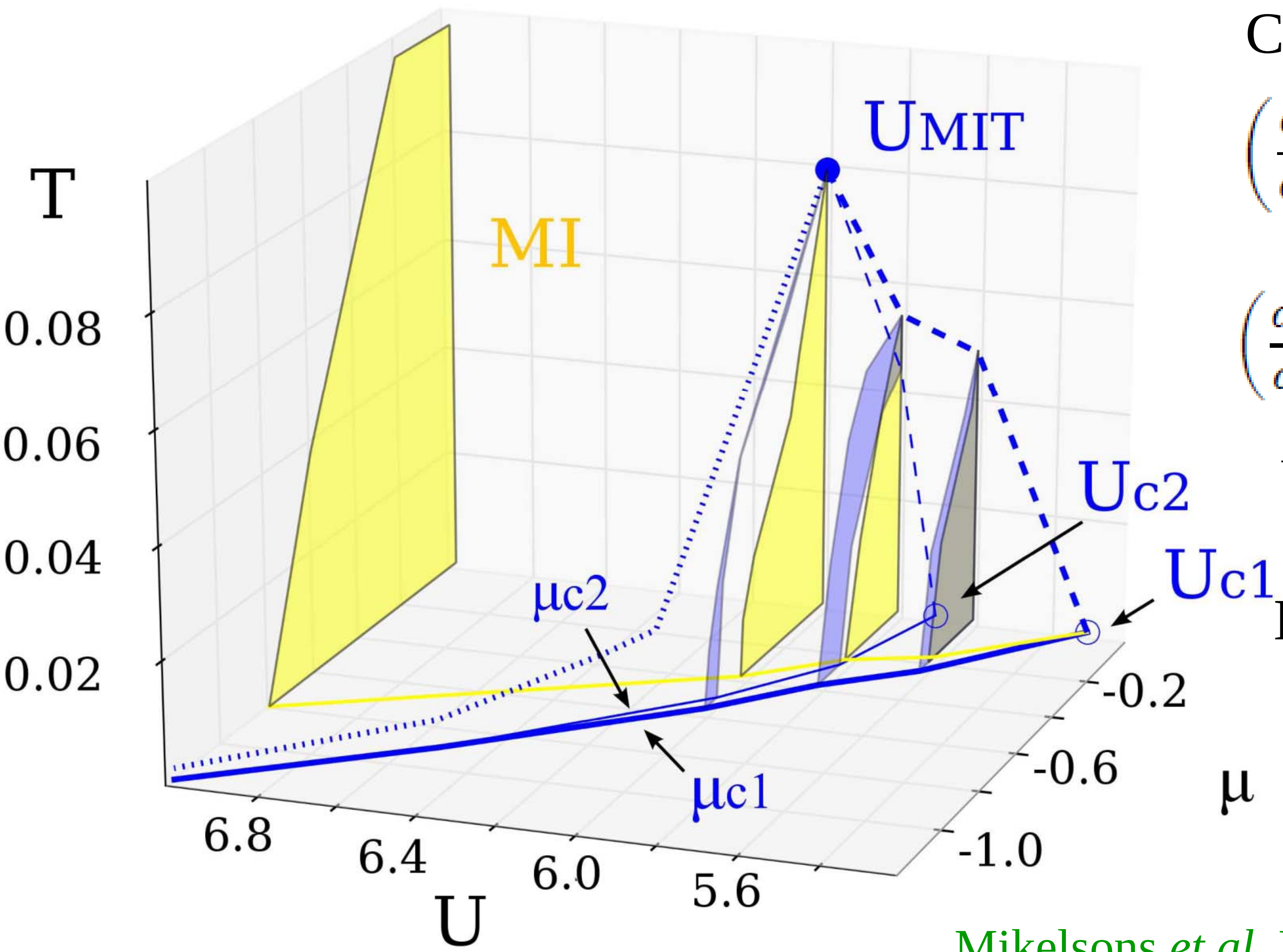
Thermodynamic properties



Clausius-Clapeyron

$$\left(\frac{dT_c}{d\mu_c}\right)_U = \frac{(n_1 - n_2)}{(S_2 - S_1)}$$

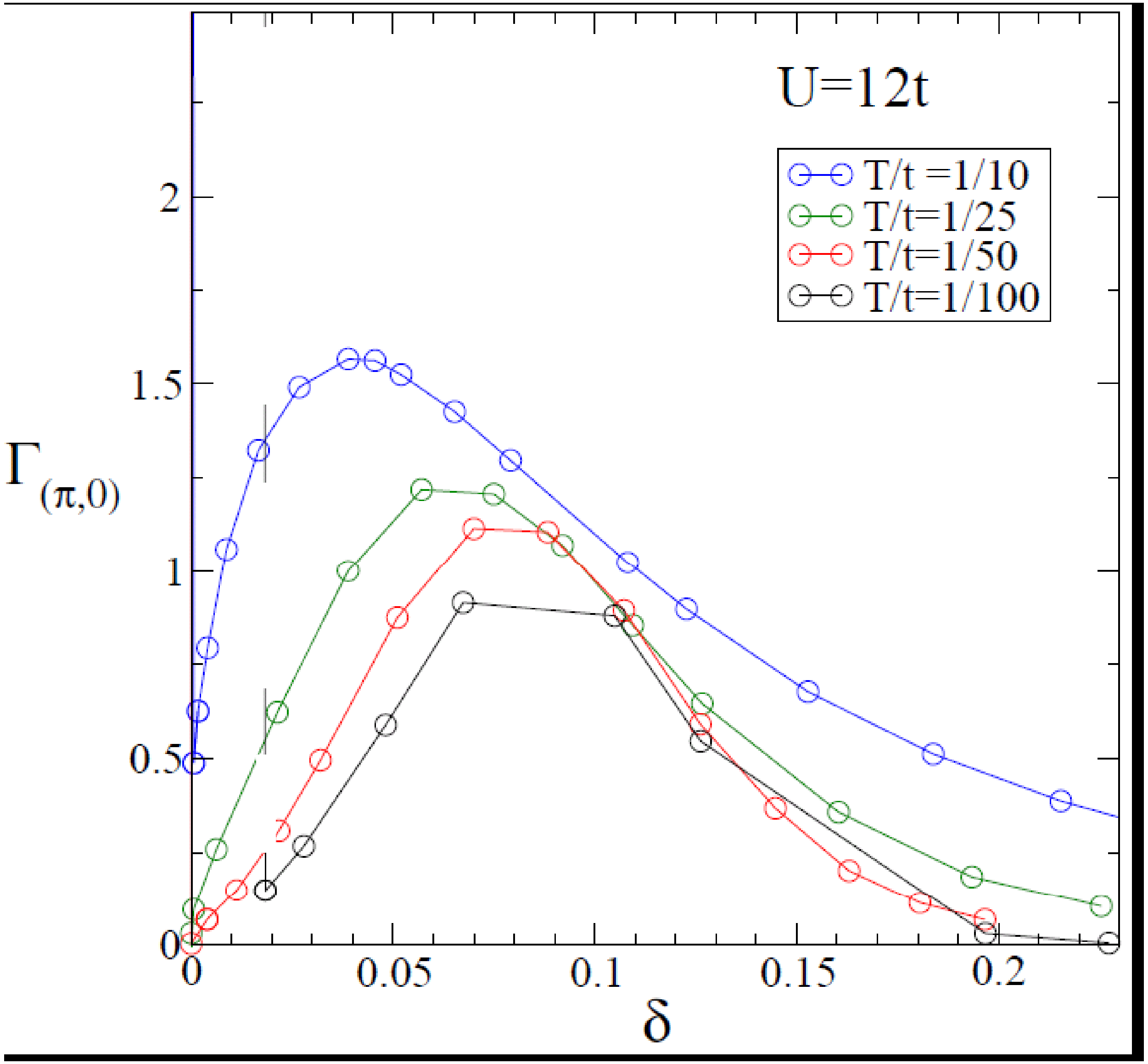
$$\left(\frac{dU_c}{d\mu_c}\right)_T = \frac{(n_1 - n_2)}{(D_1 - D_2)}$$

Underdoped phase
lower *D* and *S*
More compressible

$$\left(\frac{\partial S}{\partial n}\right)_T = 0$$

Mikelsons *et al.* PRB **80**, (2009)

Maximum scattering rate



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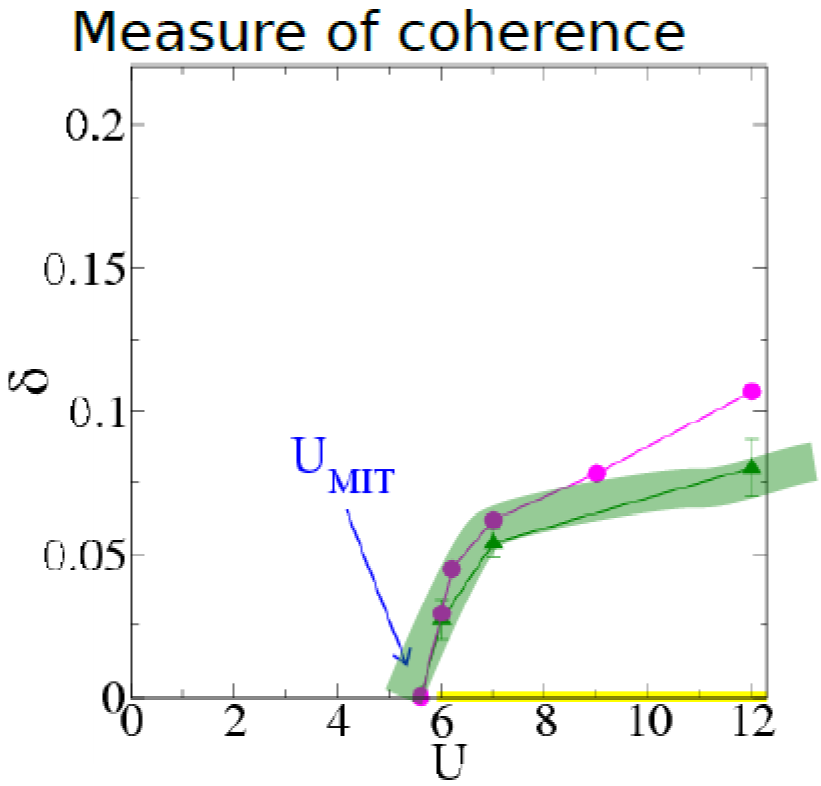
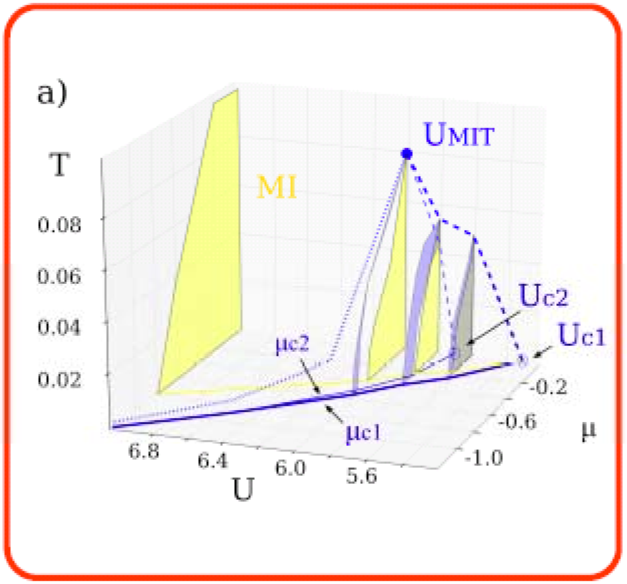
Maximum scattering rate from Mott Physics

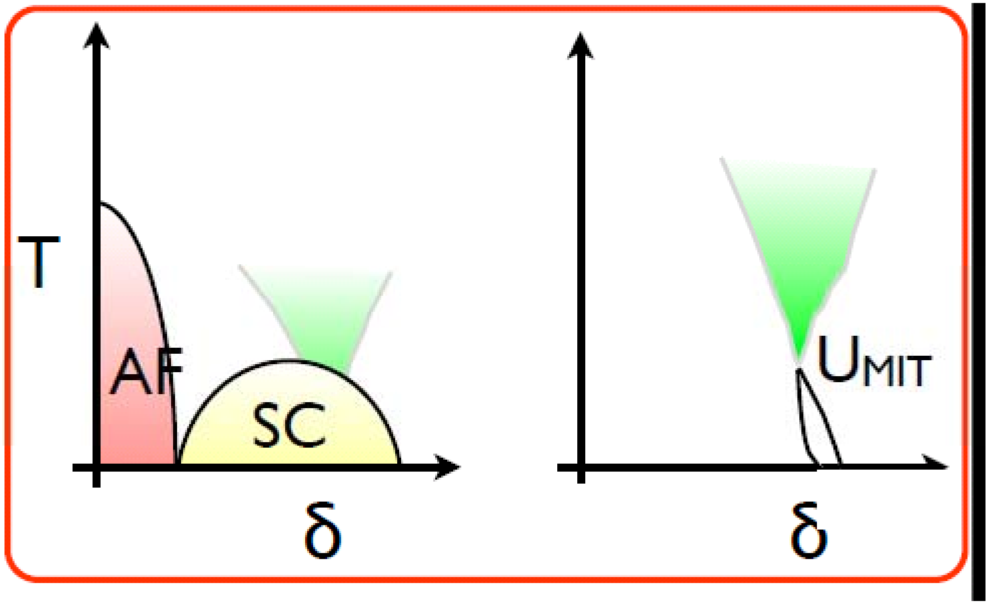


δ

Max [$\mathrm{Im}\Sigma_K$(w->0)] originate at U_{MIT}

What is under the dome





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Underdoped metal very sensitive to anisotropy

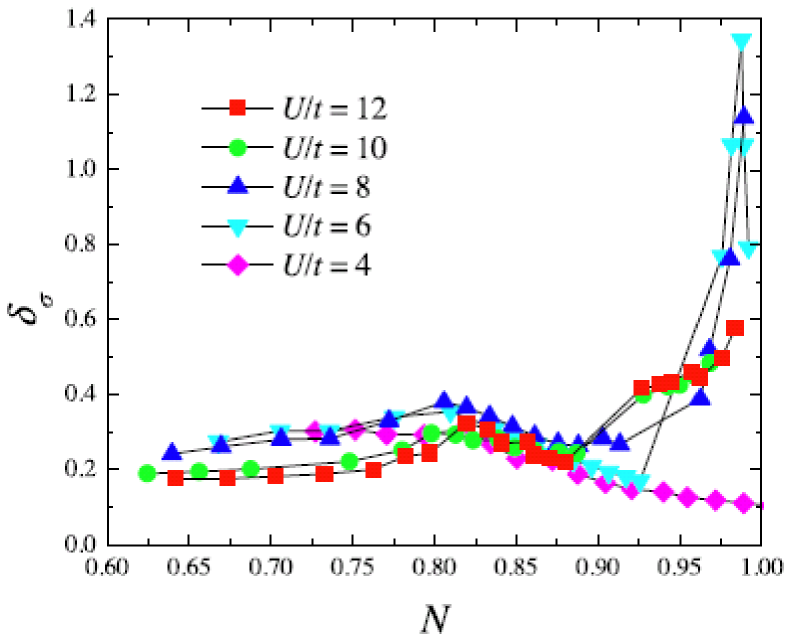
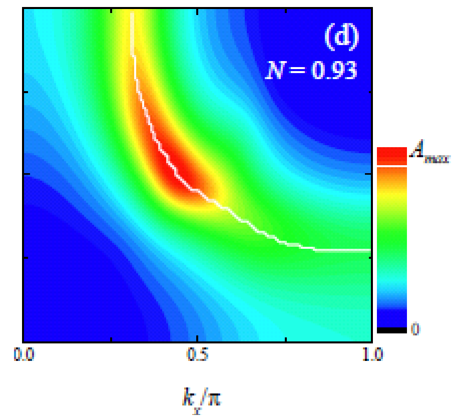
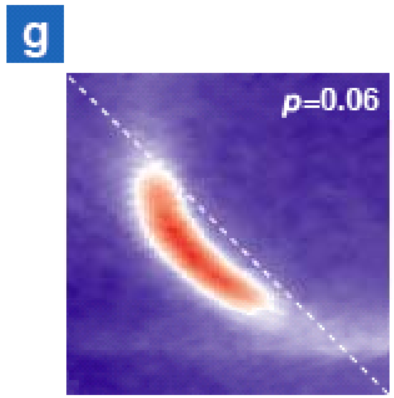


FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2\left[\sigma_x(0) - \sigma_y(0)\right] / \left[\sigma_x(0) + \sigma_y(0)\right]$ as a function of filling N for various values of U and $\eta = 0.1$, $\delta_0 = 0.04$.

Okamoto, Sénéchal, Civelli, AMST
PRB (R) in press,





Satoshi Okamoto

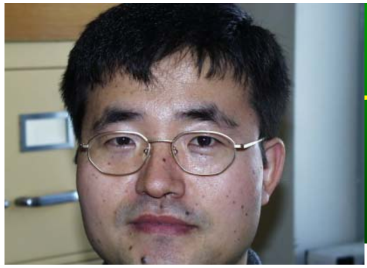
David Sénéchal

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

Superconductivity

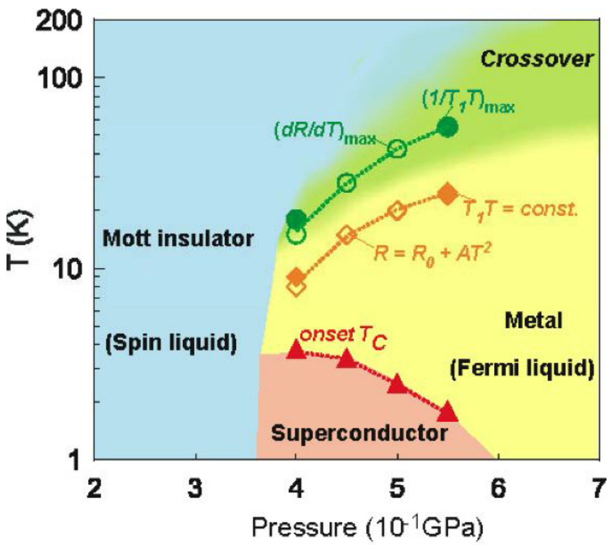
Phase diagram

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

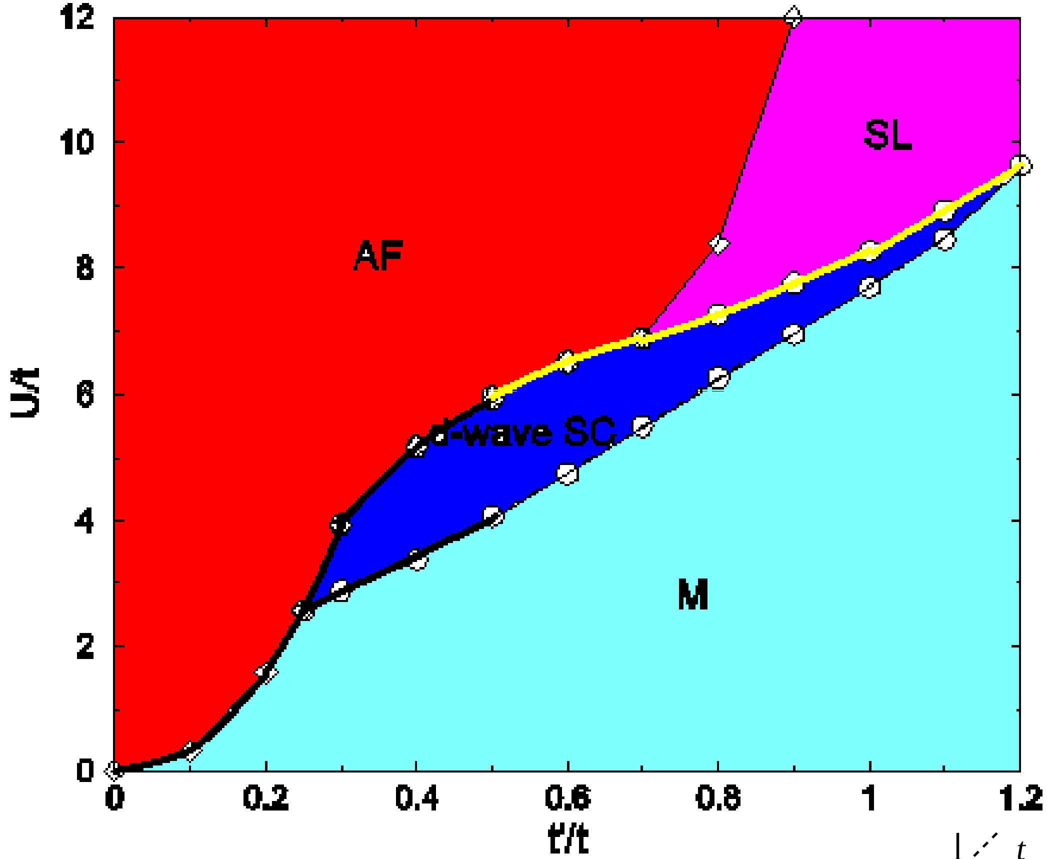


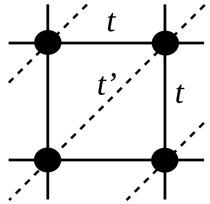
Theoretical phase diagram BEDT

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



Y. Kurisaki, et al.





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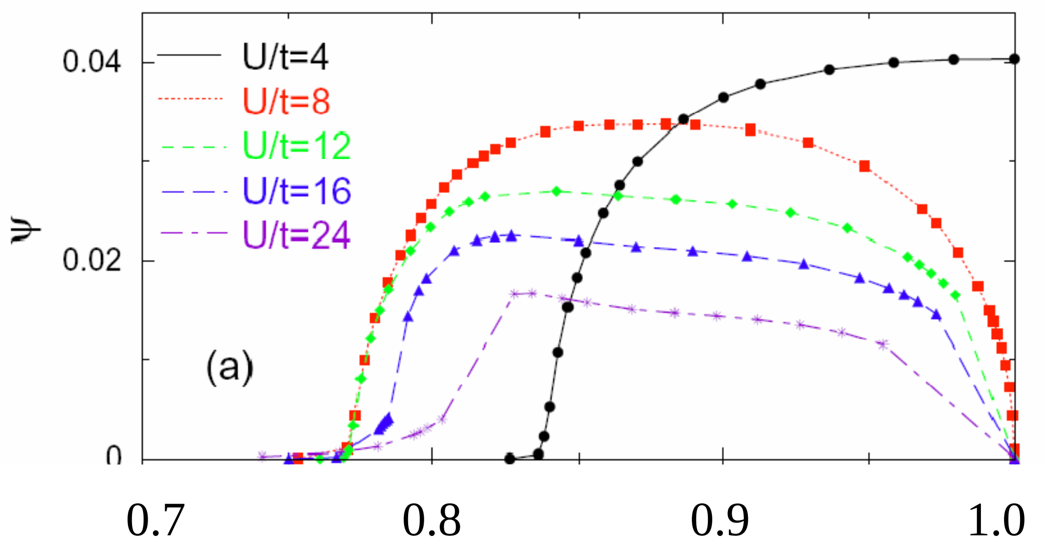
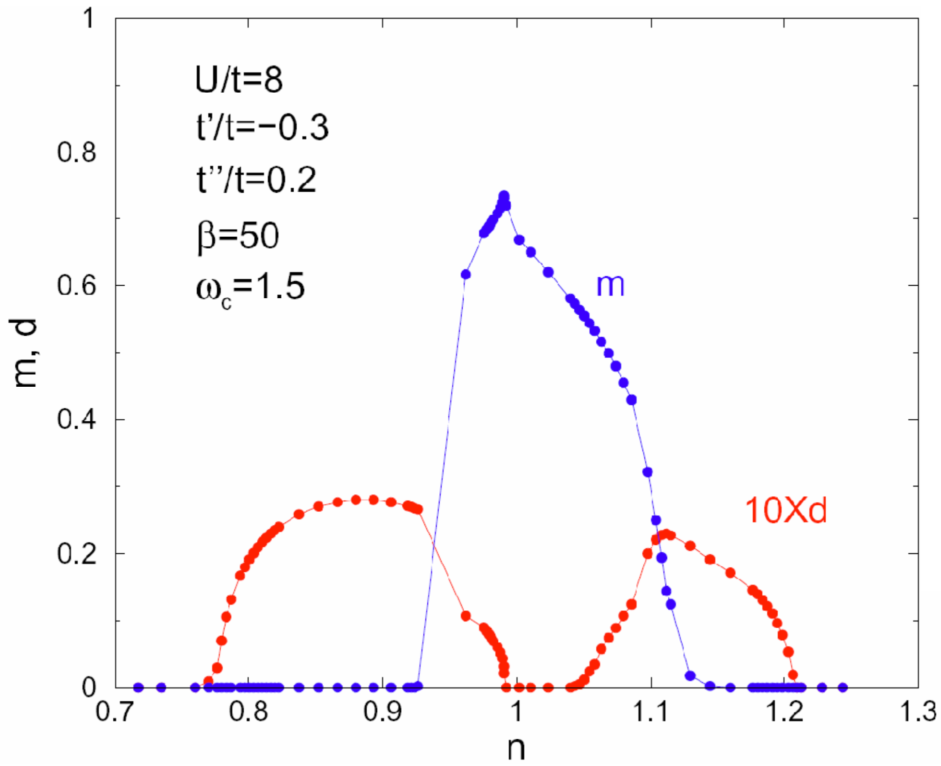
Phys. Rev. Lett. **95**, 177001(2005)   Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

Dome vs Mott (CDMFT)

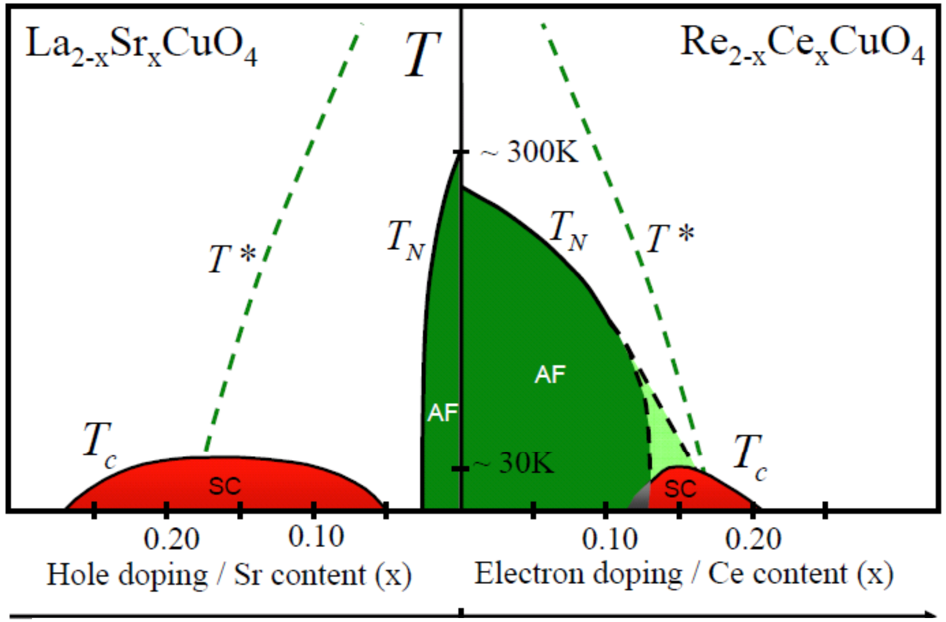


Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST Phys. Rev. B (2008)

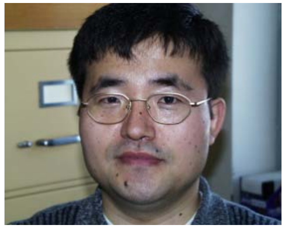
CDMFT global phase diagram



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



Armitage, Fournier, Greene, RMP (2009)



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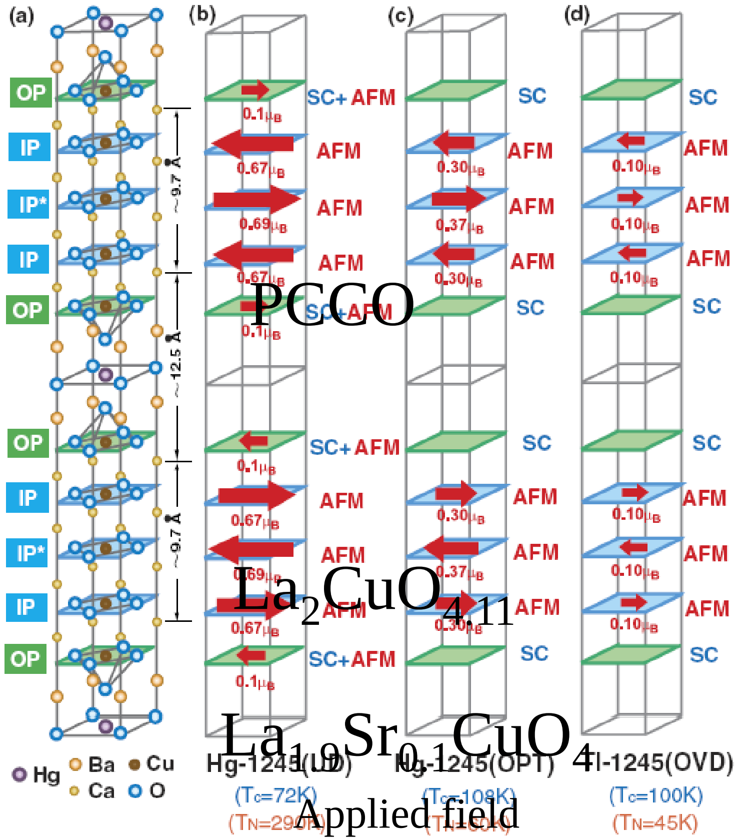
Homogeneous coexistence (experimental)



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Consistent with following experiment

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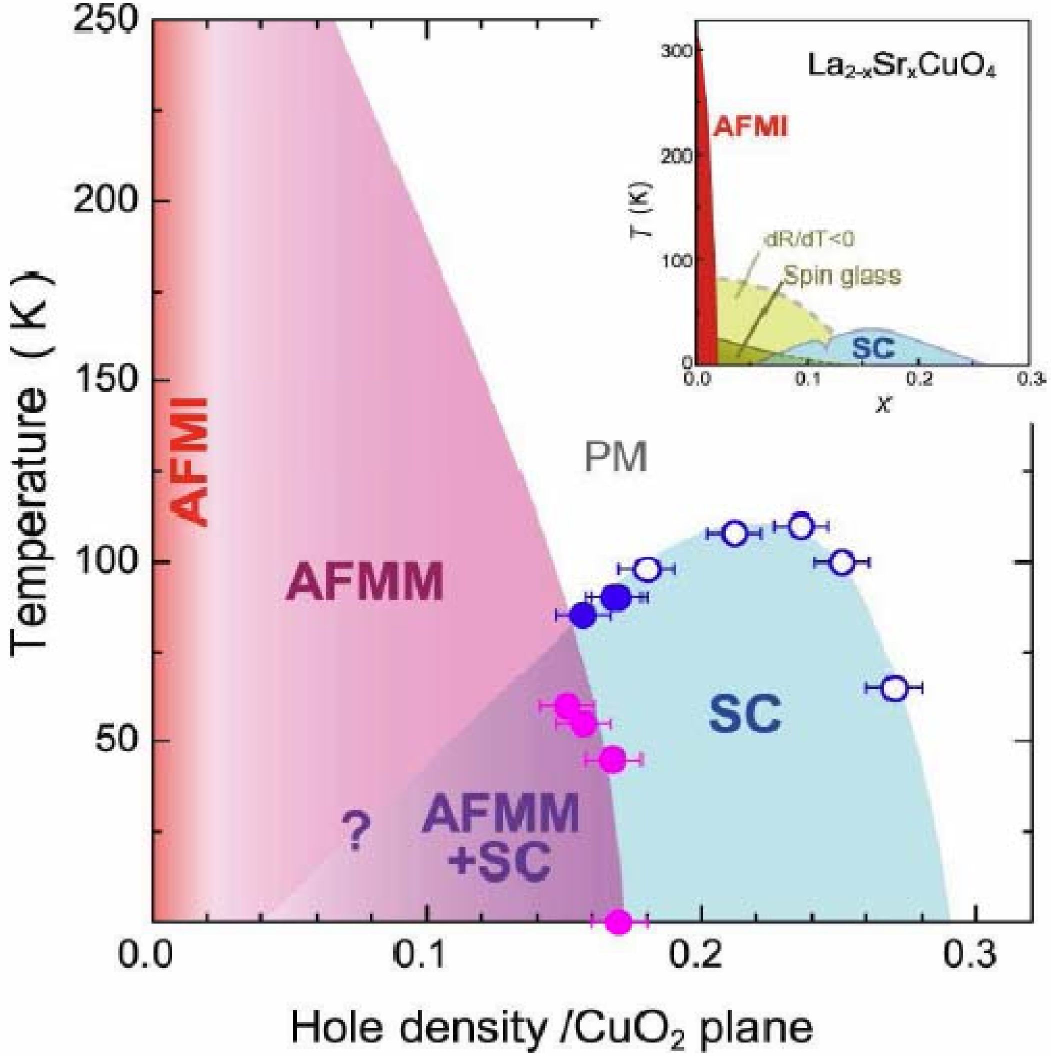

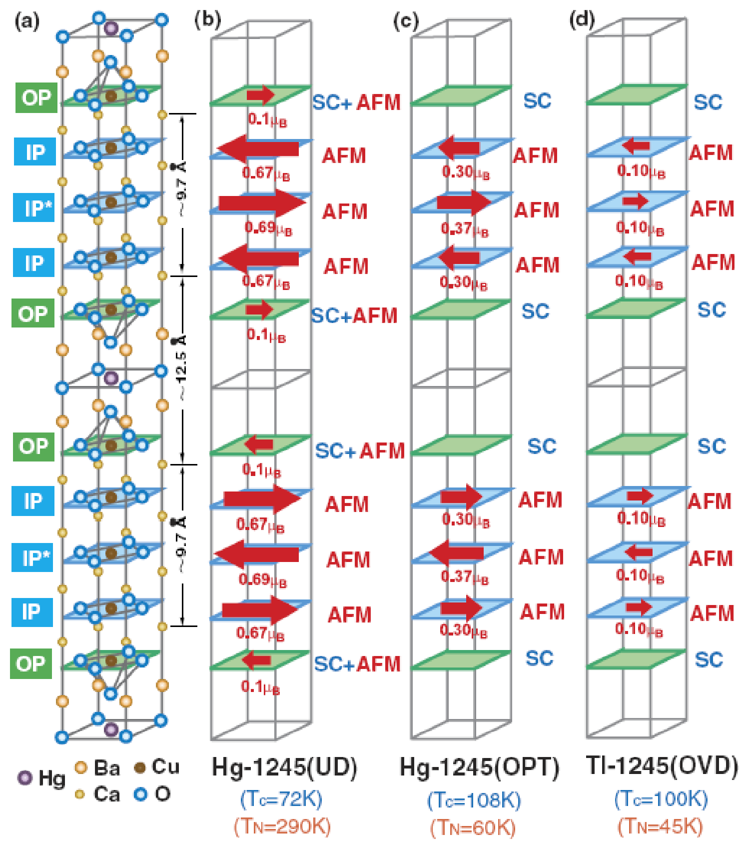

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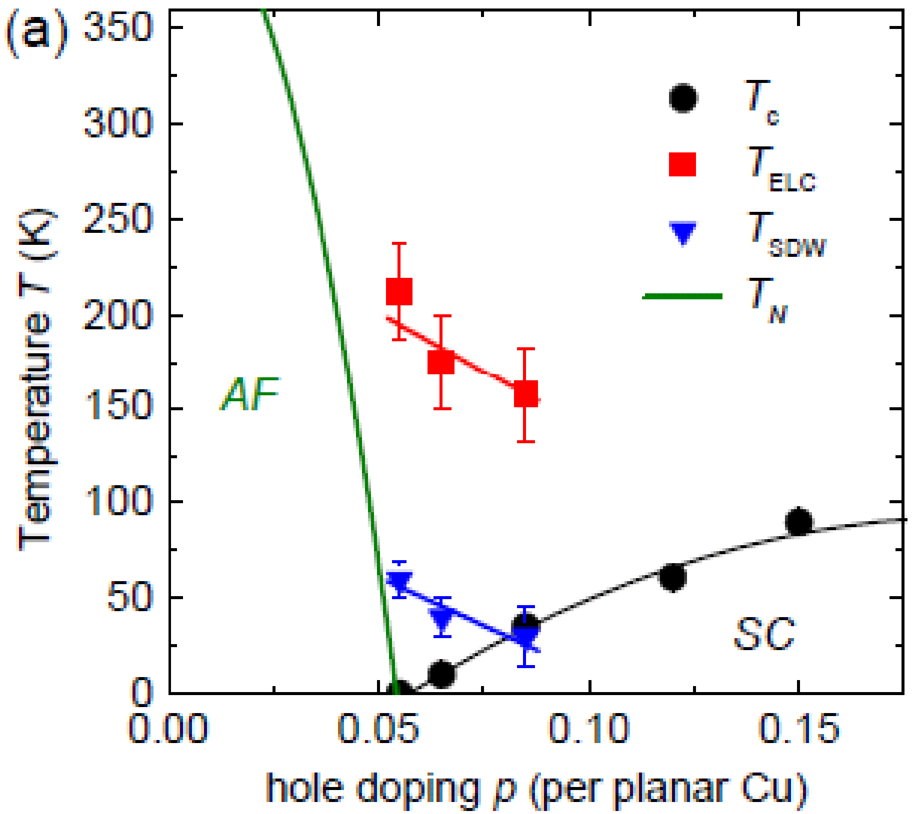
Magnetic phase diagram of YBCO

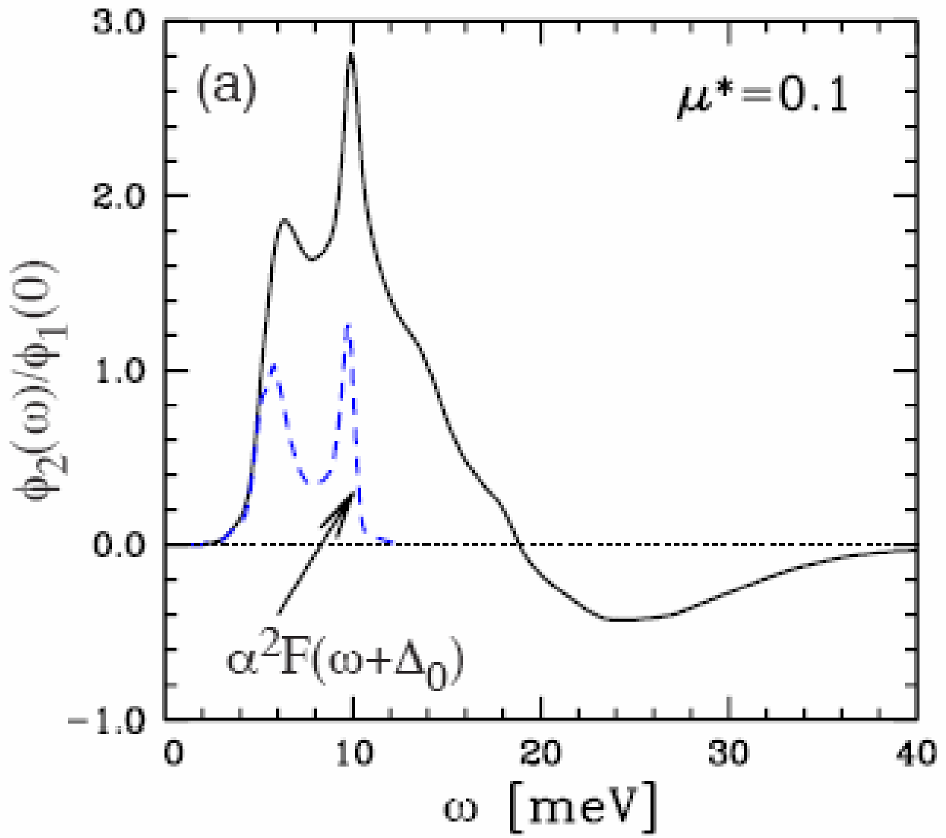


Haug, … Keimer, arXiv:1008.4298

The glue

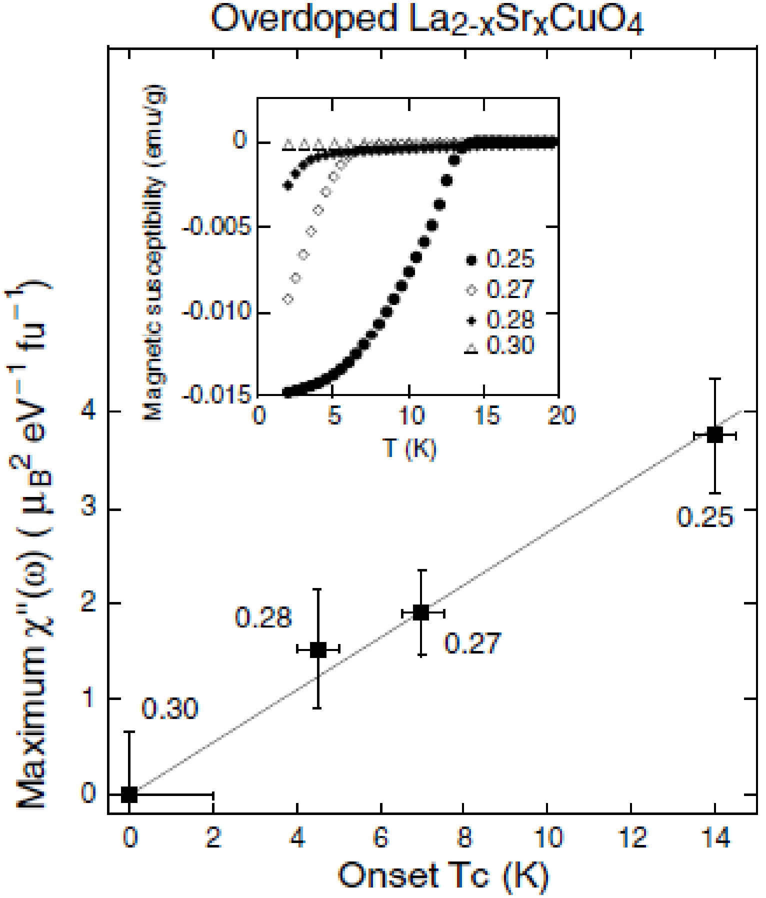
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

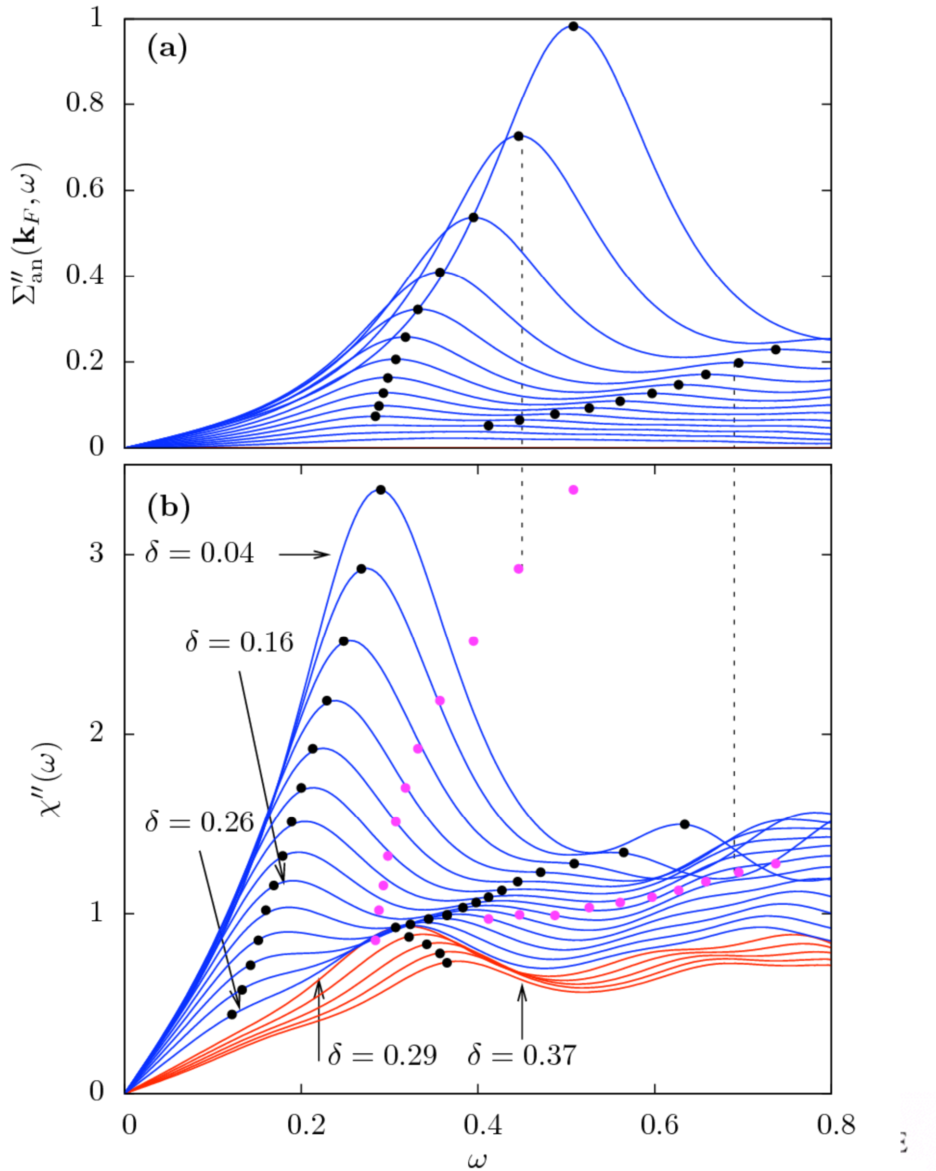


The glue

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



Wakimoto … Birgeneau PRL (2004)



The glue and neutrons

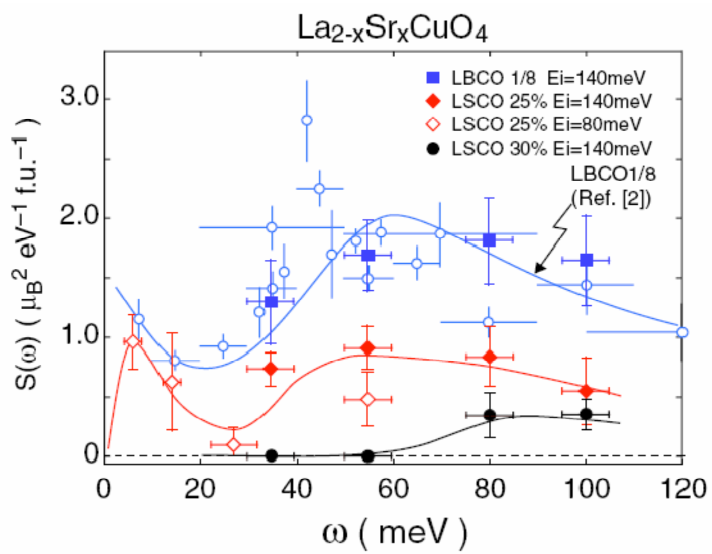
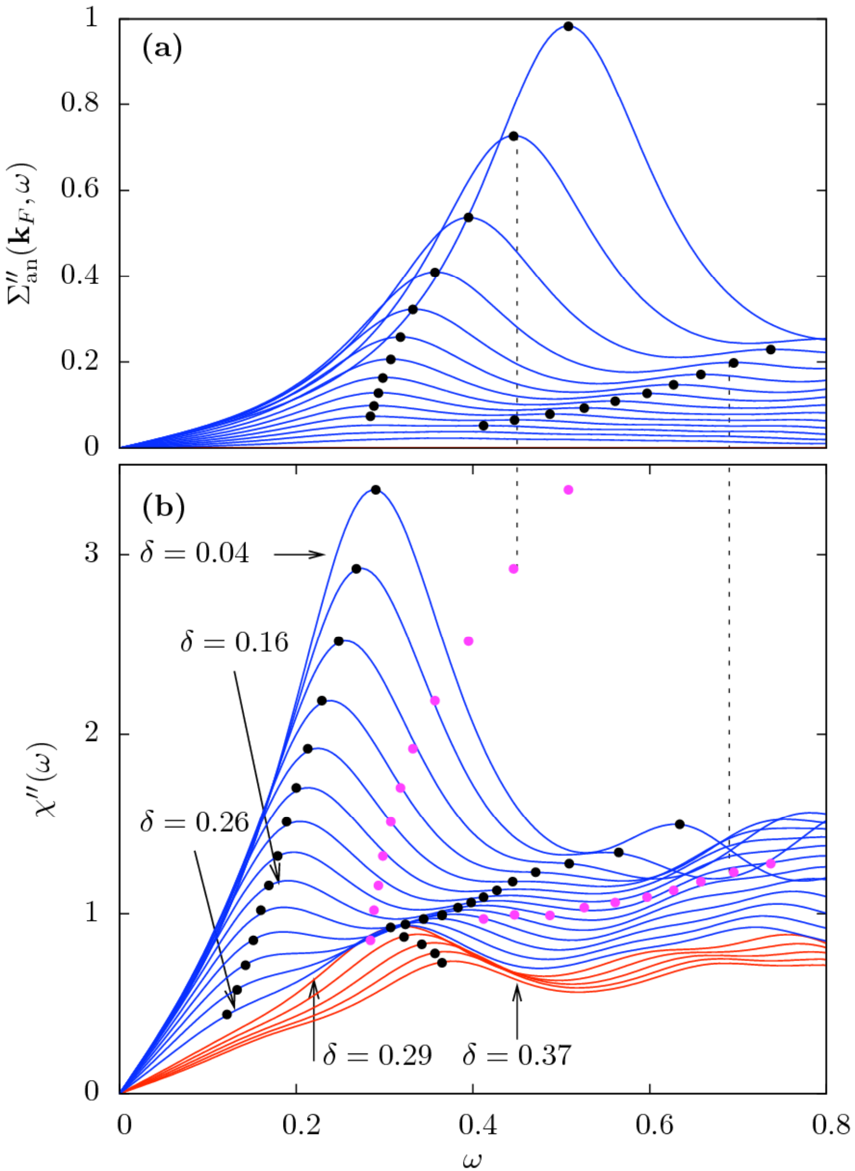


FIG. 3 (color online). **Q**-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-H integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i =$ 140 meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 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.

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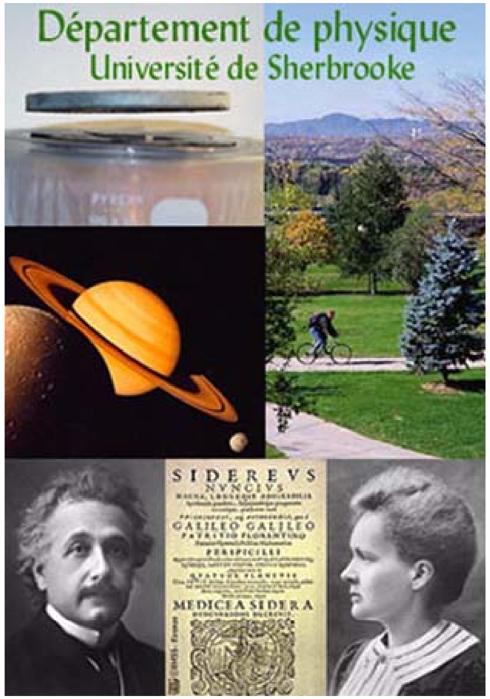

André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP
Le regroupement québécois sur les matériaux de pointe

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Merci

Arigato

Thank you