Pseudogap T* along the Widom line of a first-order transition in doped Mott insulators

A.-M. Tremblay

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ICSM 2012, 30 avril 2012

VERITATEM IN CHARITATE

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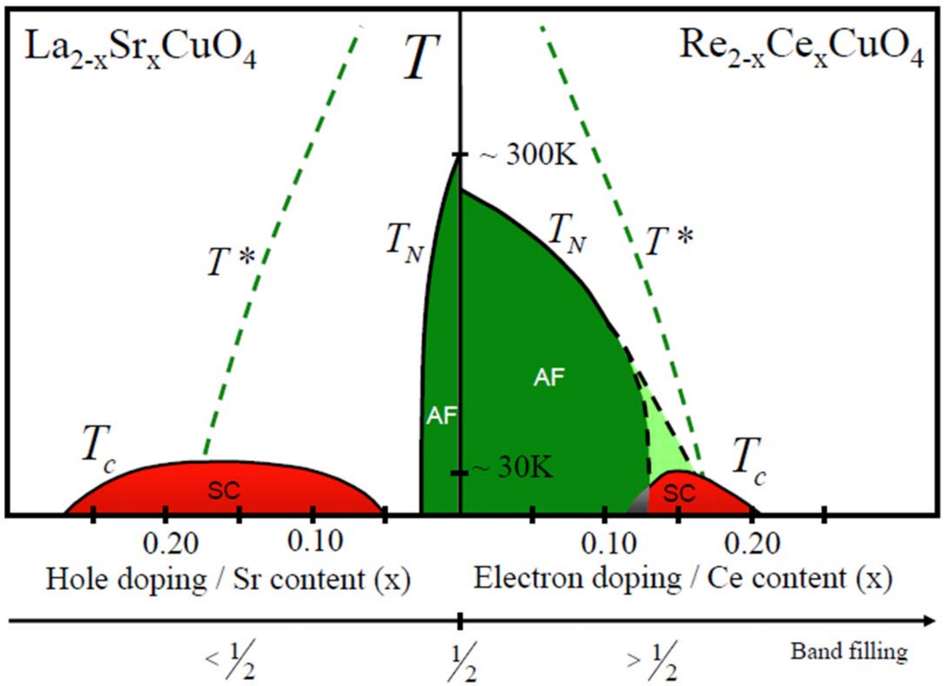
High-temperature superconductors

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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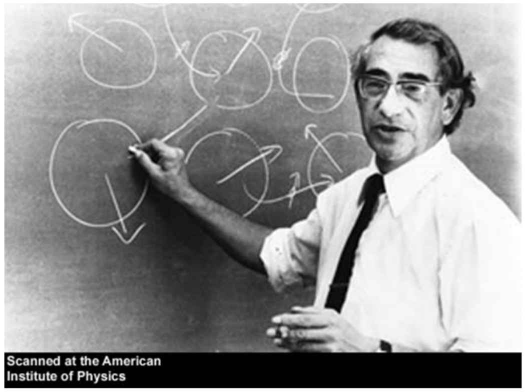
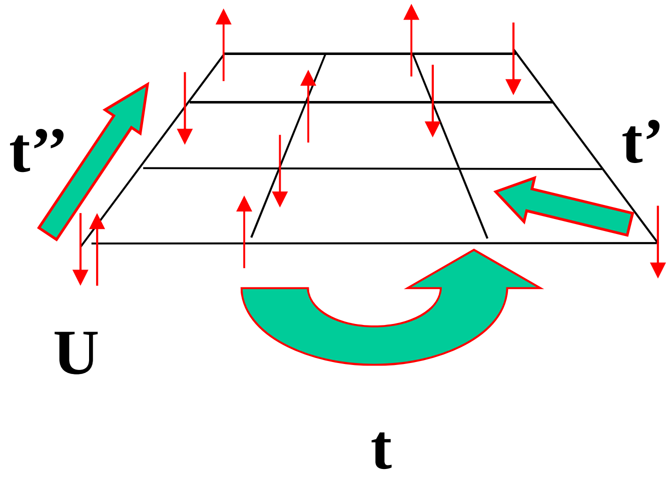
Hubbard model

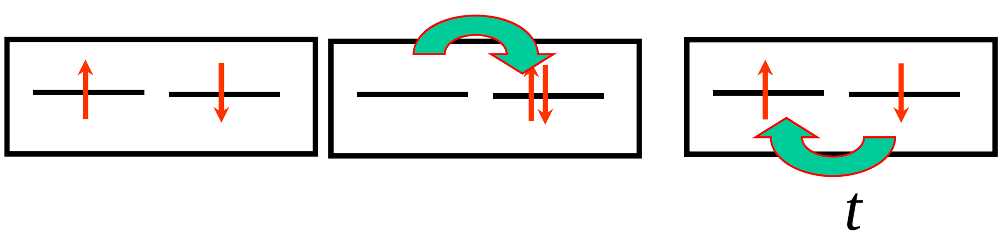


1931-1980

μ



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



$t = 1$

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

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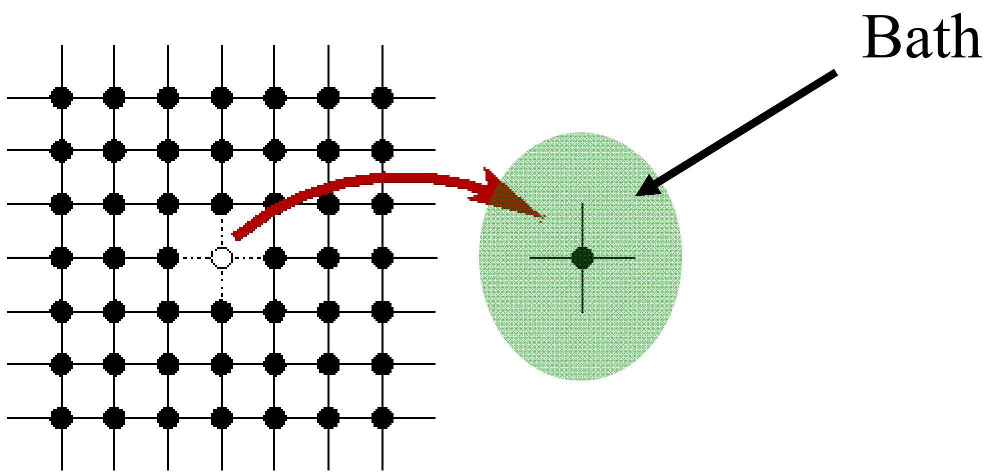
Method

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

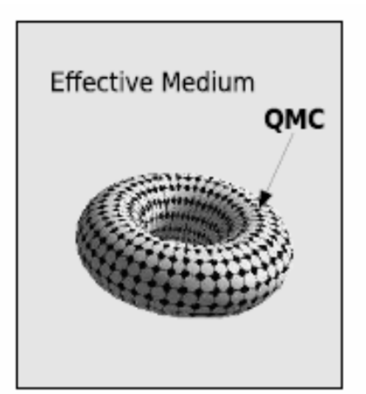
- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



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

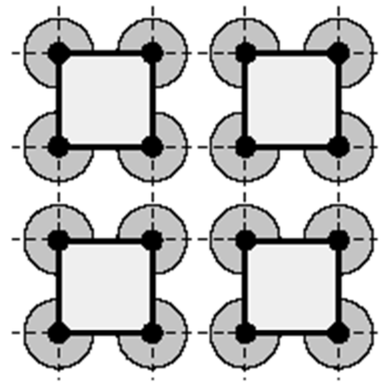
DMFT, (d = 3)

2d Hubbard: Quantum cluster method

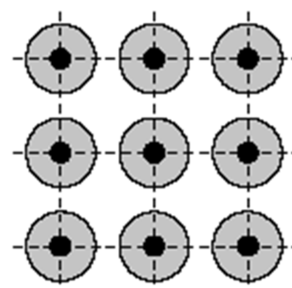


DCA

C-DMFT



DMFT



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

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

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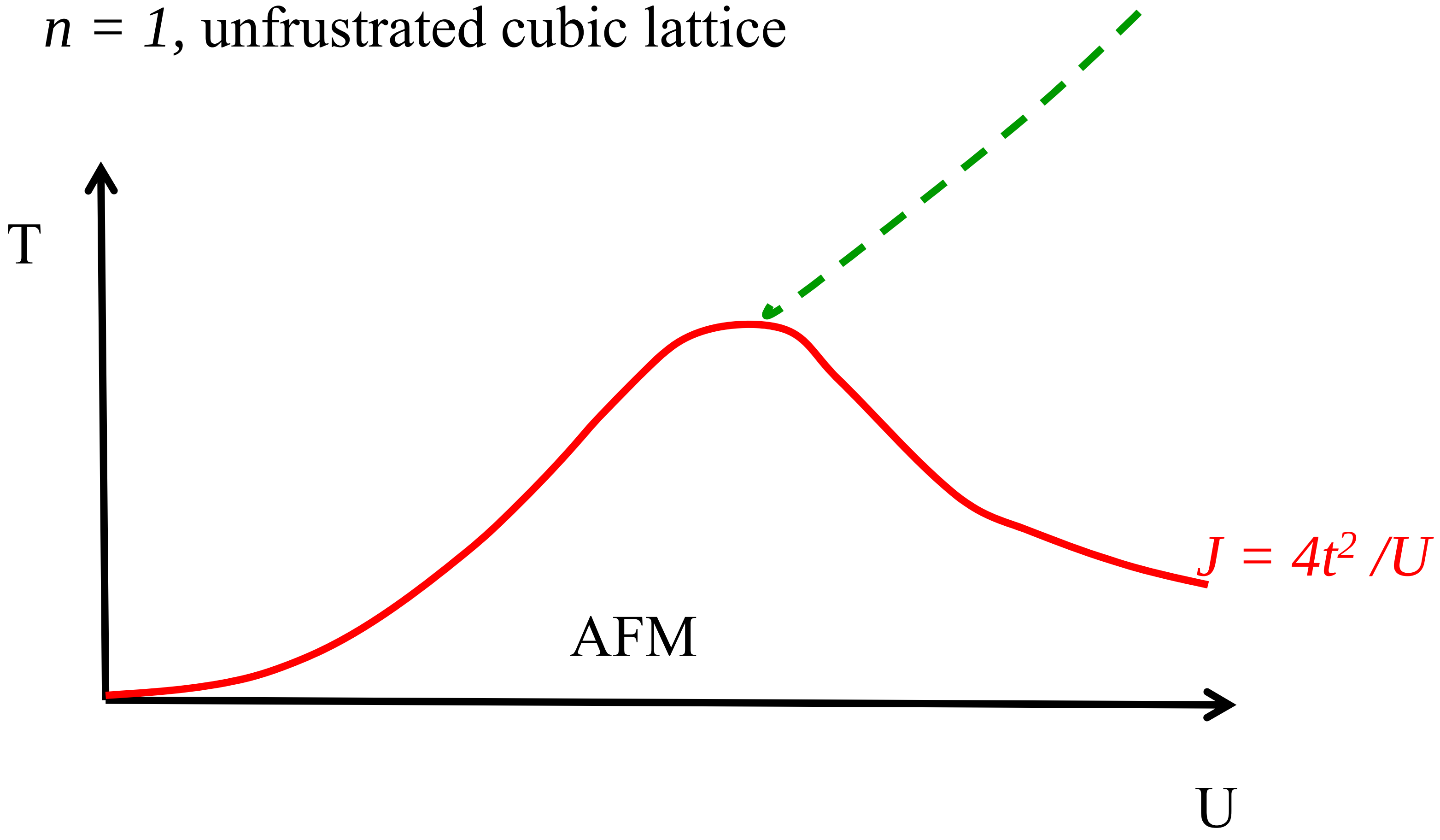
Not perfect!

- Missing:
  - Long wavelength fluctuations
- Included:
  - Short-range dynamical and spatial correlations

- Long range order:
  - Allow symmetry breaking in the bath (mean-field)

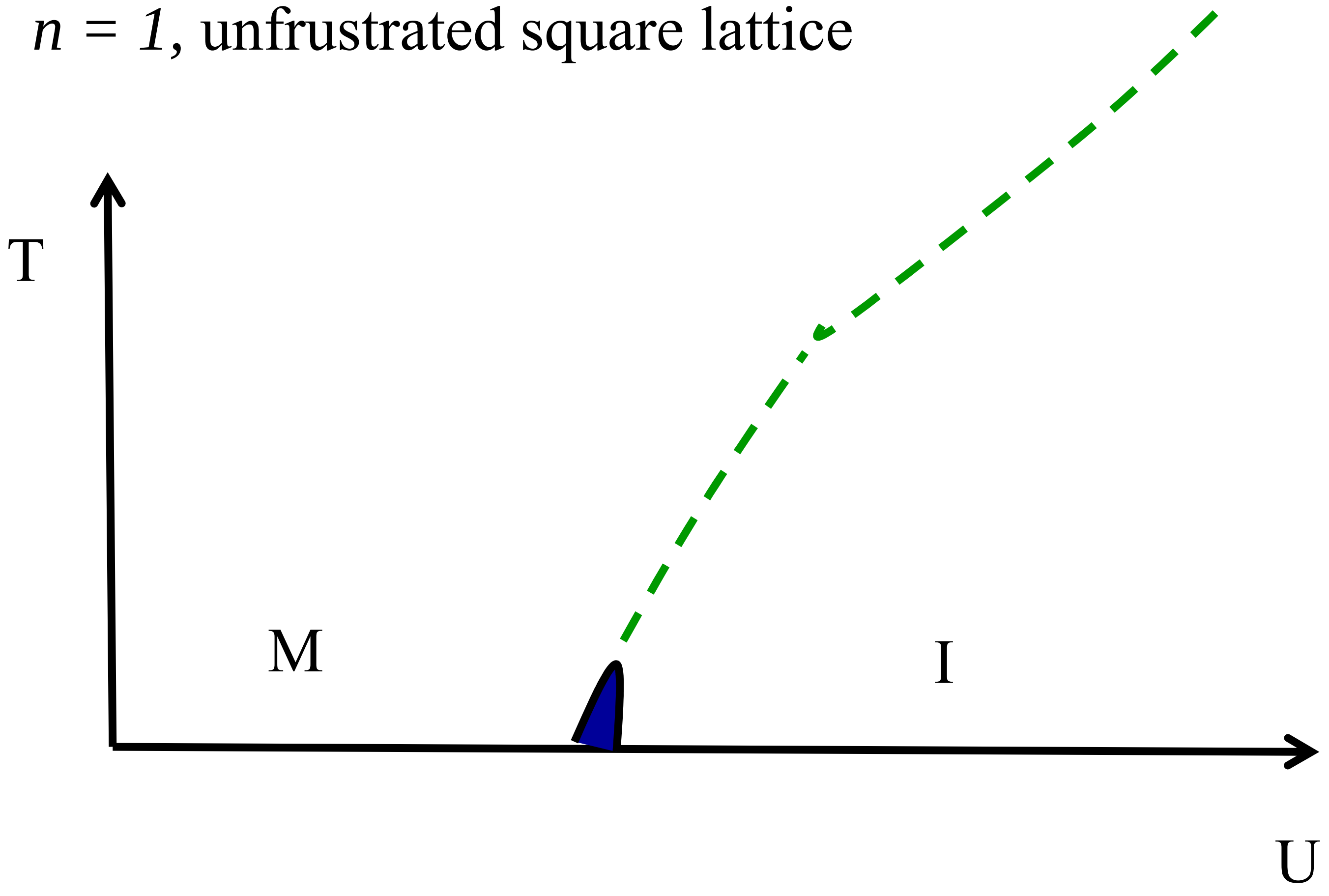
Local moment and Mott transition

$n = 1$, unfrustrated cubic lattice



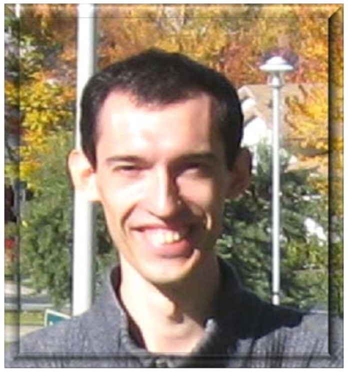
Local moment and Mott transition

n = *1*, unfrustrated square lattice



Outline

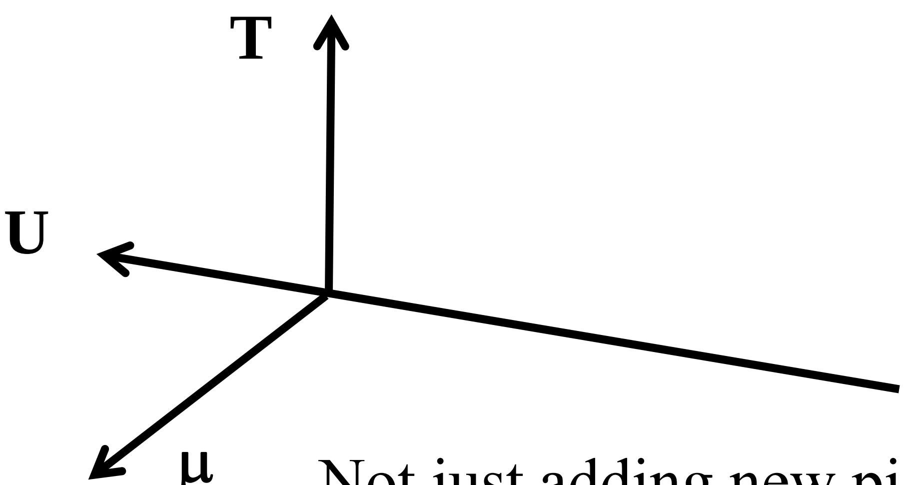
- Method
- Finite *T* phase diagram
  - Normal state (no LRO, what is below the dome)
    - First order transition
    - Widom line and pseudogap



Giovanni Sordi

G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)
and
Phys. Rev. B. **84**, 075161 (2011)

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



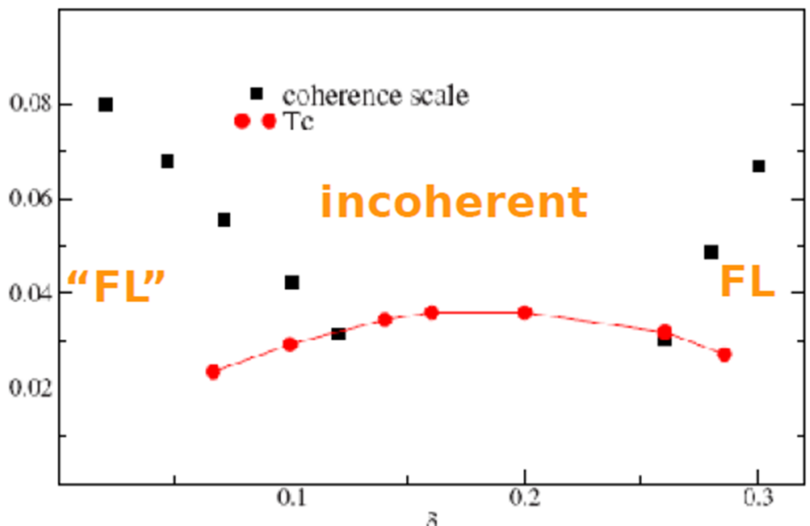
Kristjan Haule

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

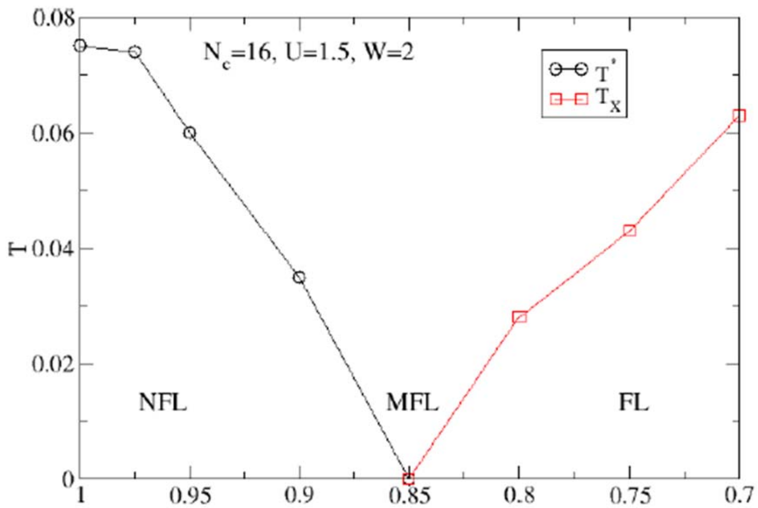
Université de Sherbrooke

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)

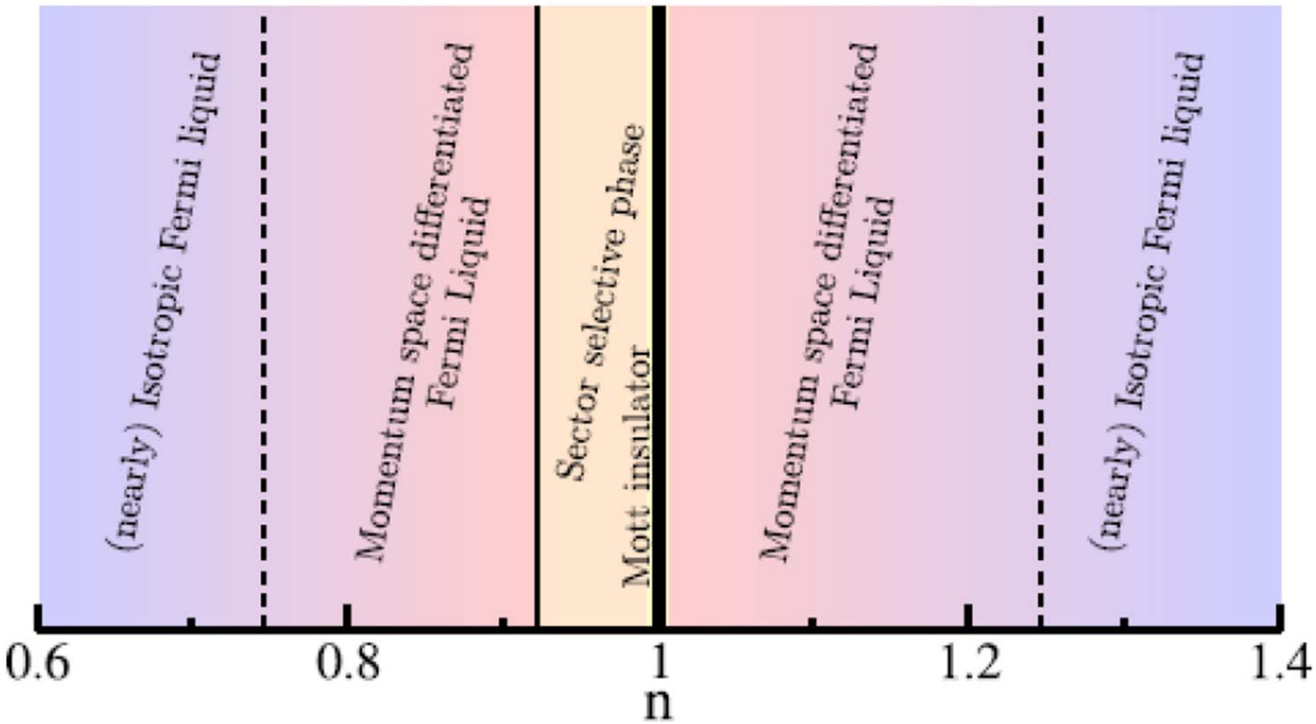


K. Haule, G. Kotliar, PRB (2008)



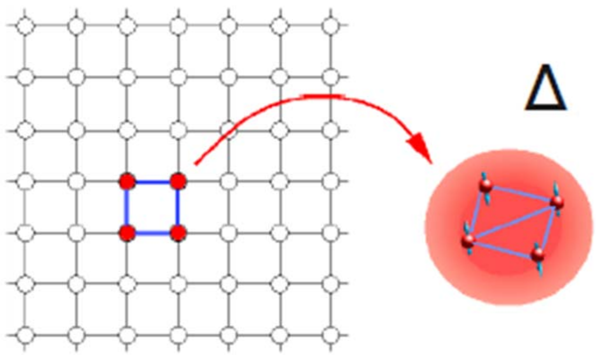
Vildhyadhiraja, PRL (2009)

Doping driven Mott transition



Gull, Werner, Millis, (2009)

C-DMFT



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

Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

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

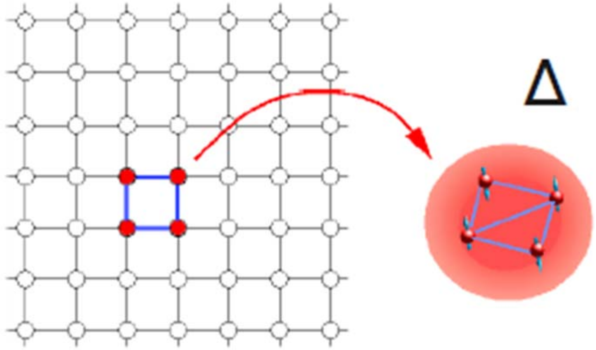
Here: continuous time QMC

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

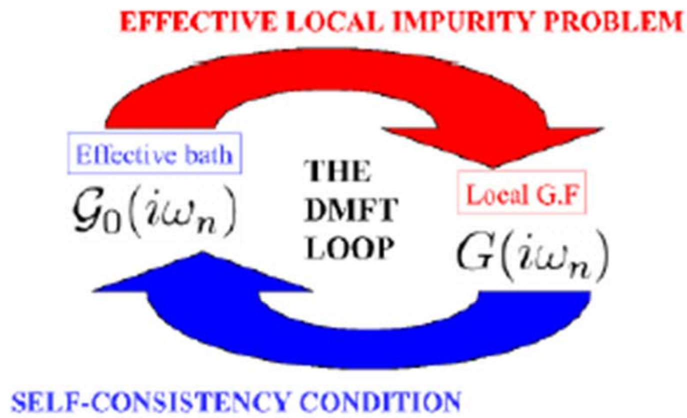
P. Werner, A. Comanac, L. de' Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

K. Haule, Phys. Rev. B **75**, 155113 (2007).

C-DMFT



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



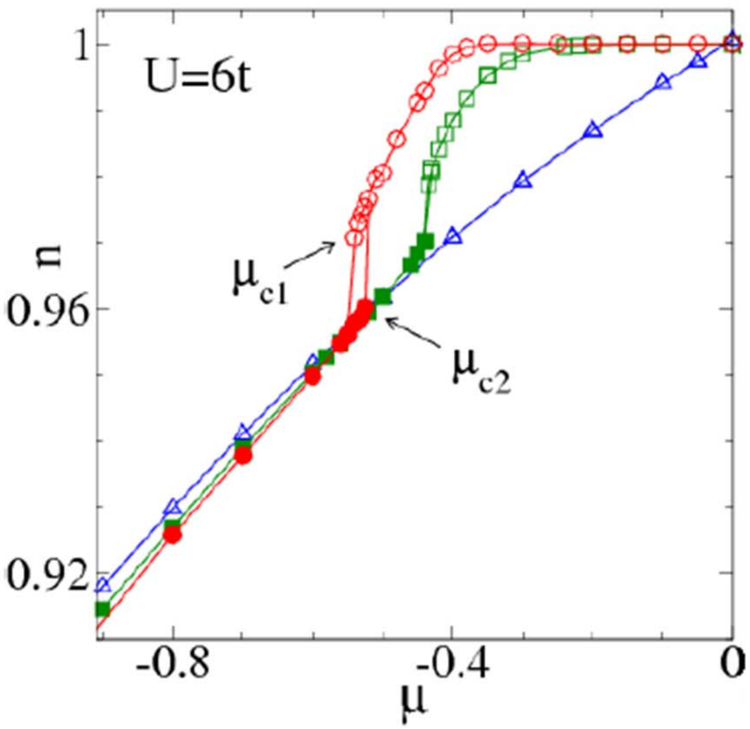
Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

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

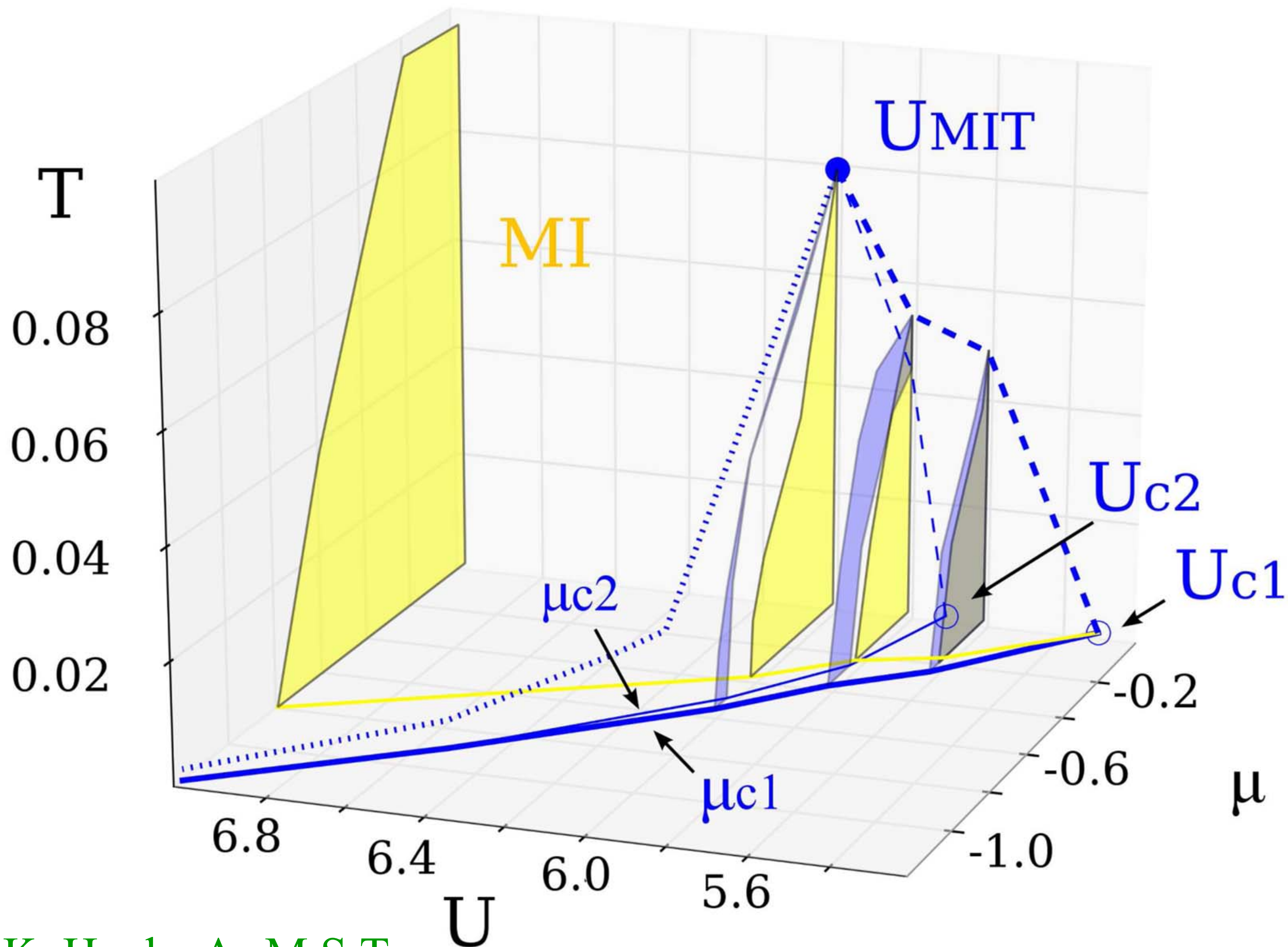
$$\Delta(i\omega_n) = i\omega_n + \mu - \Sigma_c(i\omega_n) - \left[\sum_{\tilde{k}} \frac{1}{i\omega_n + \mu - t_c(\tilde{k}) - \Sigma_c(i\omega_n)} \right]^{-1}$$

First order transition at finite doping



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

Normal state phase diagram

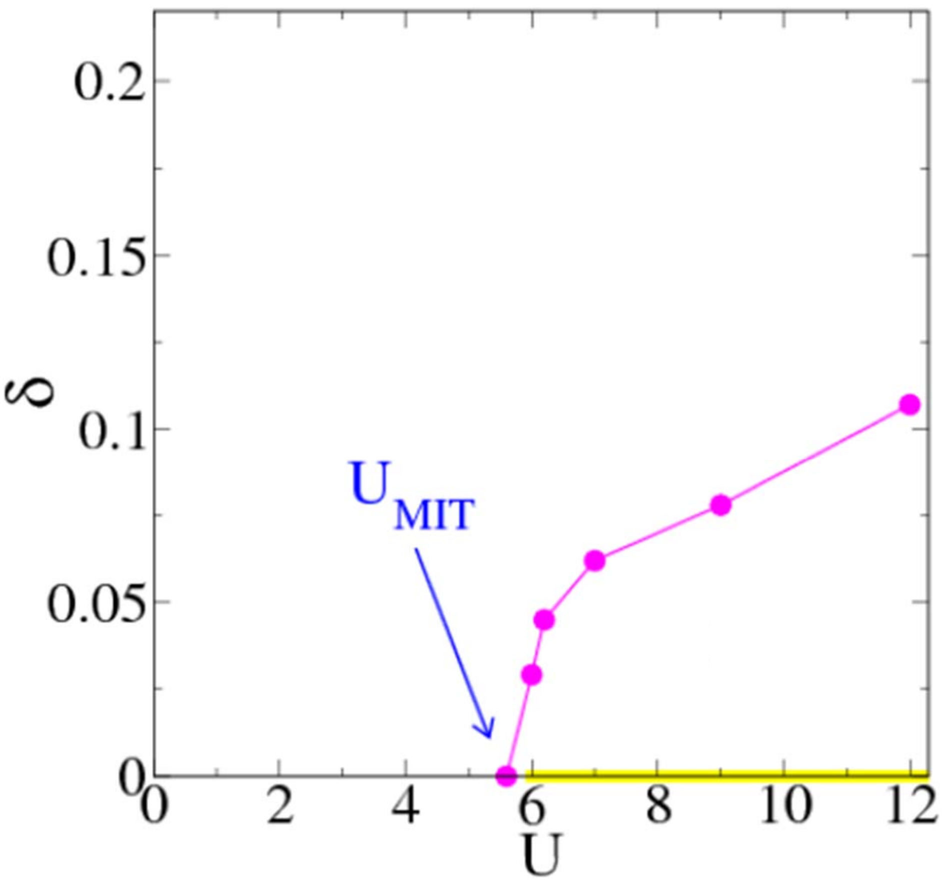


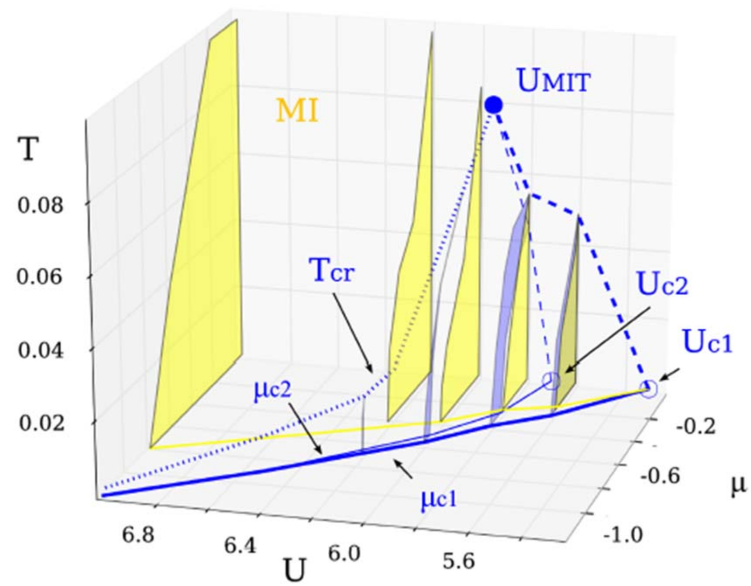
G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)

$\mu = 0$, H. Park, K. Haule, and G. Kotliar, Phys. Rev. Lett. 101, 186403 (2008)

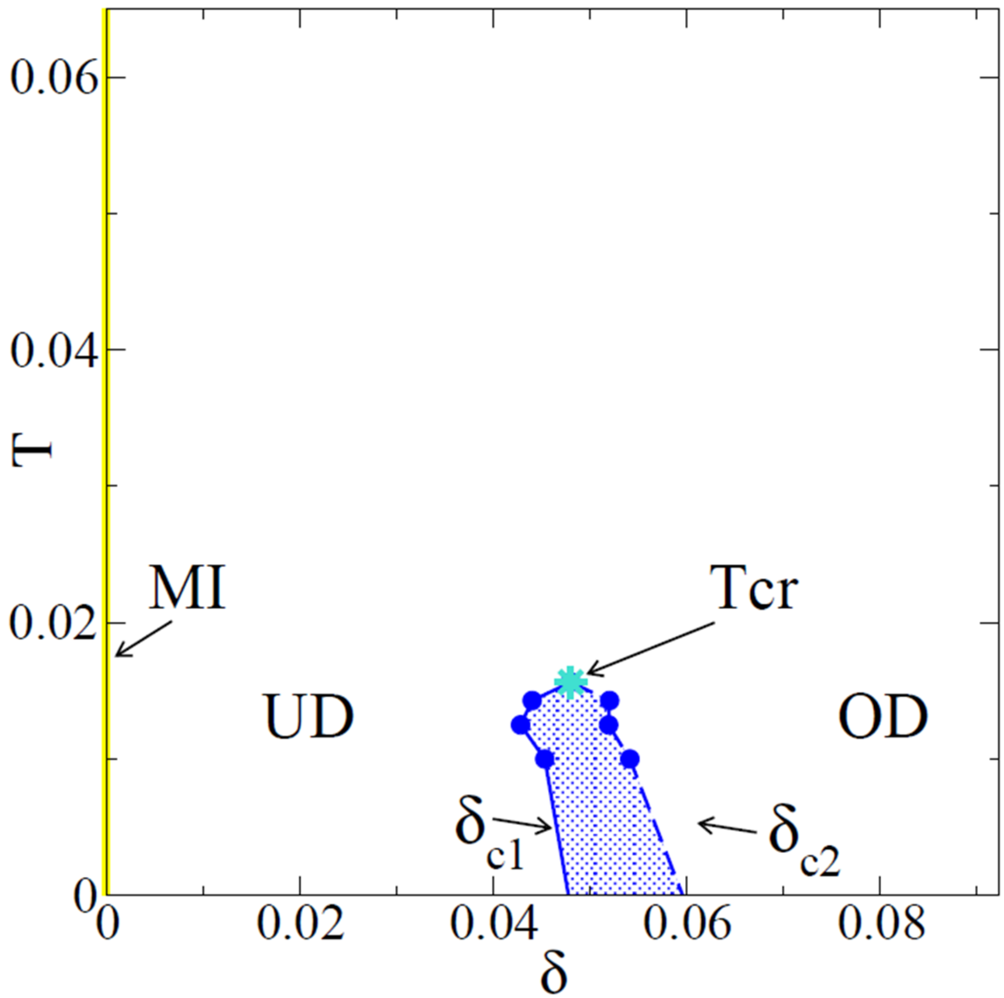
Link to Mott transition up to optimal doping

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





Characterisation of the phases (U=6.2t)



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

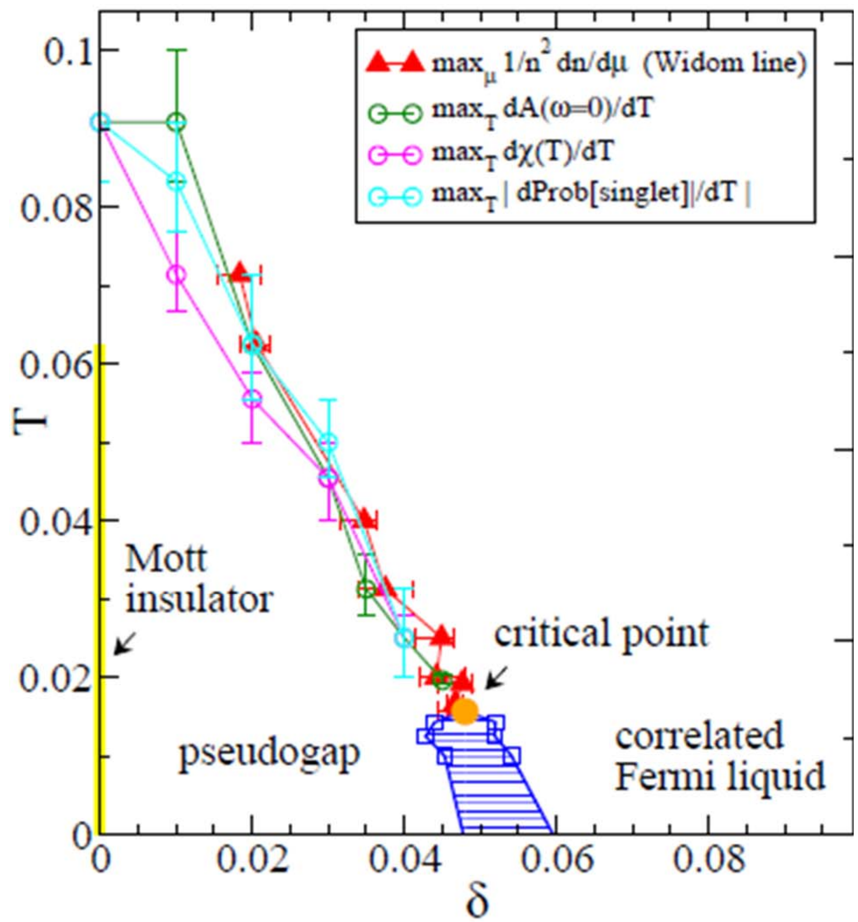
1. Mott insulator (MI)
2. Underdoped phase (UD): $\delta < \delta_c$
3. Overdoped phase (OD): $\delta > \delta_c$
4. Coexistence/forbidden region

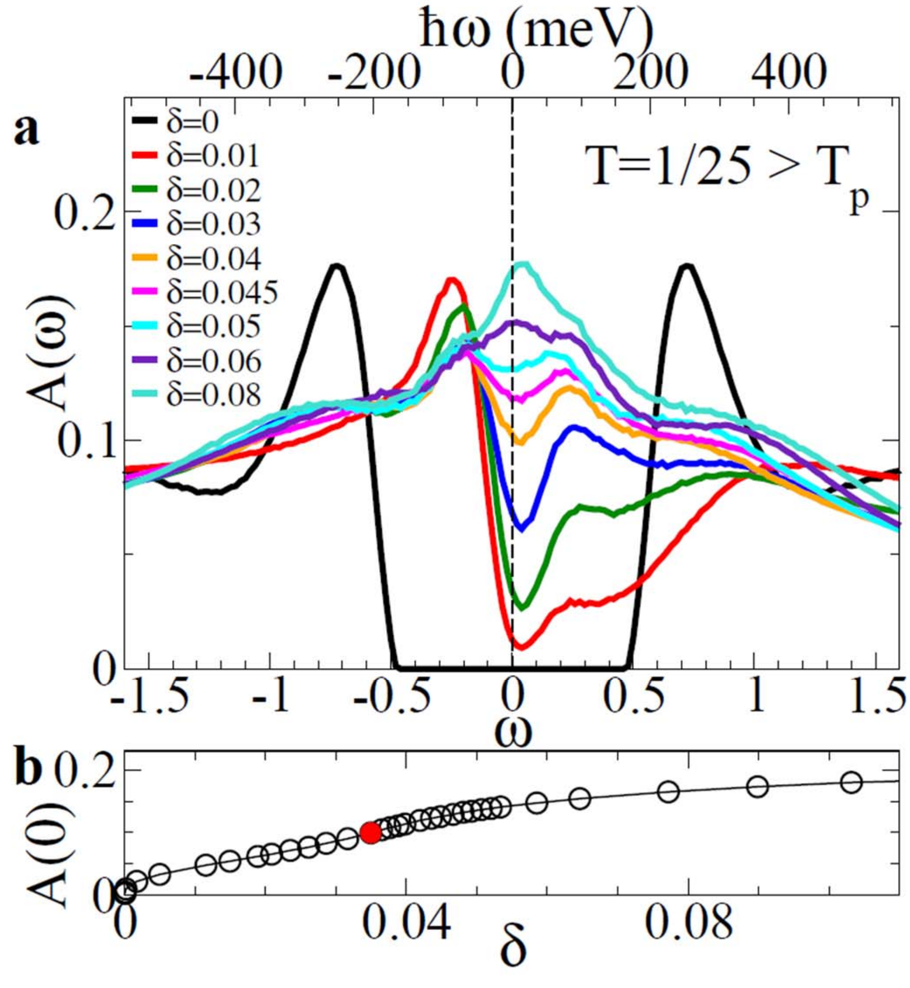
Here "optimal doping" δ_c = doping at which the 1st order transition occurs

How does the UD phase differ from the OD phase?

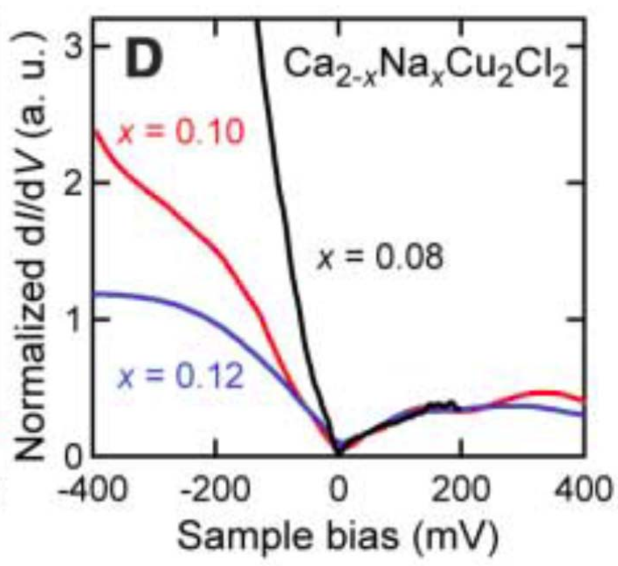
Smaller *D* and *S*

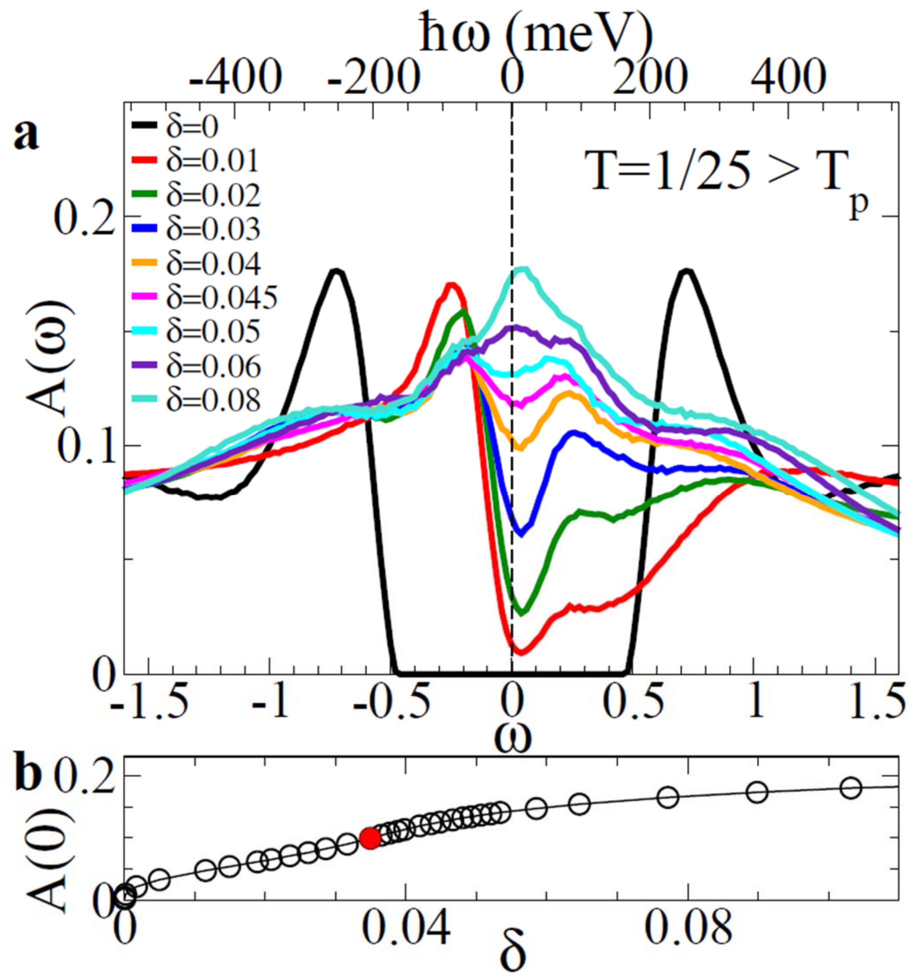
Density of states





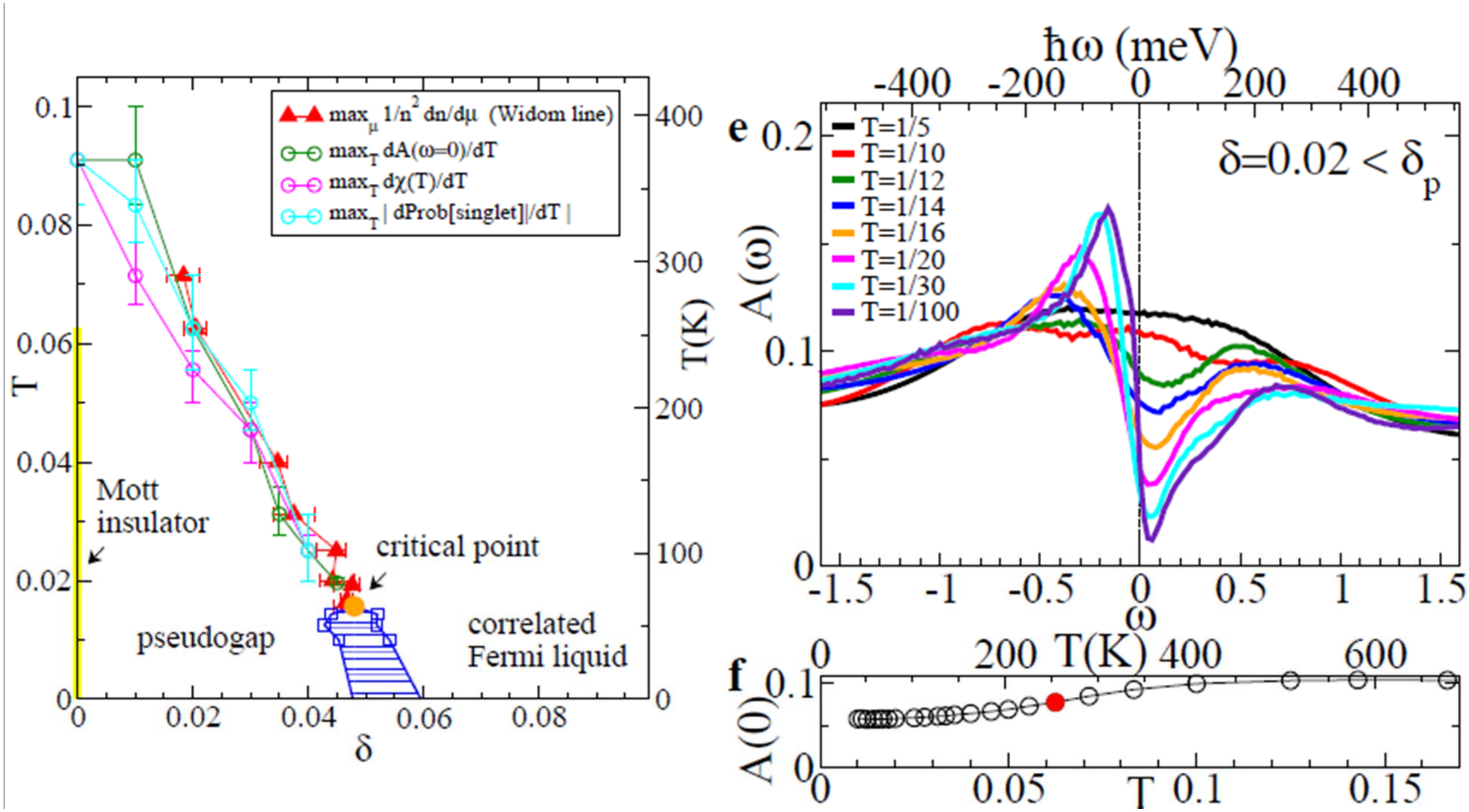
Density of states





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

Density of states



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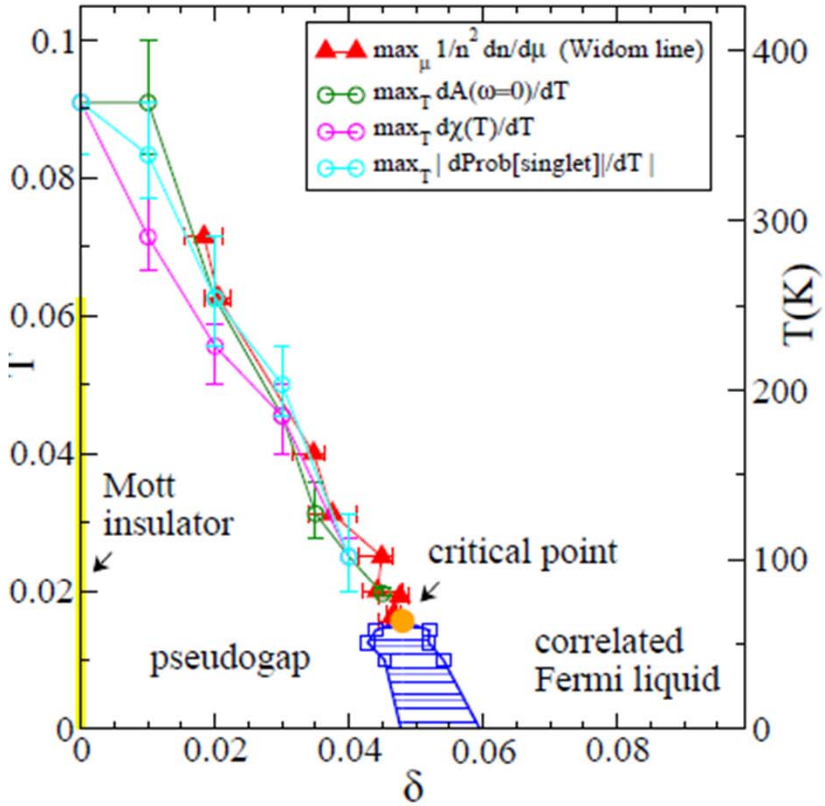
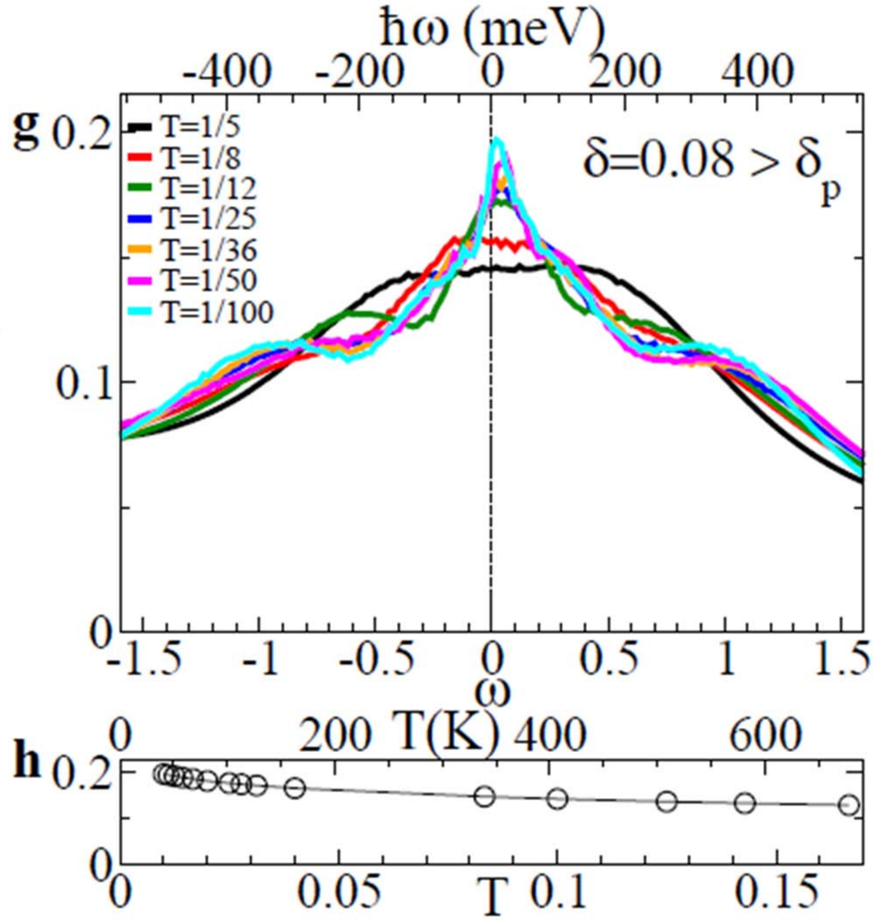
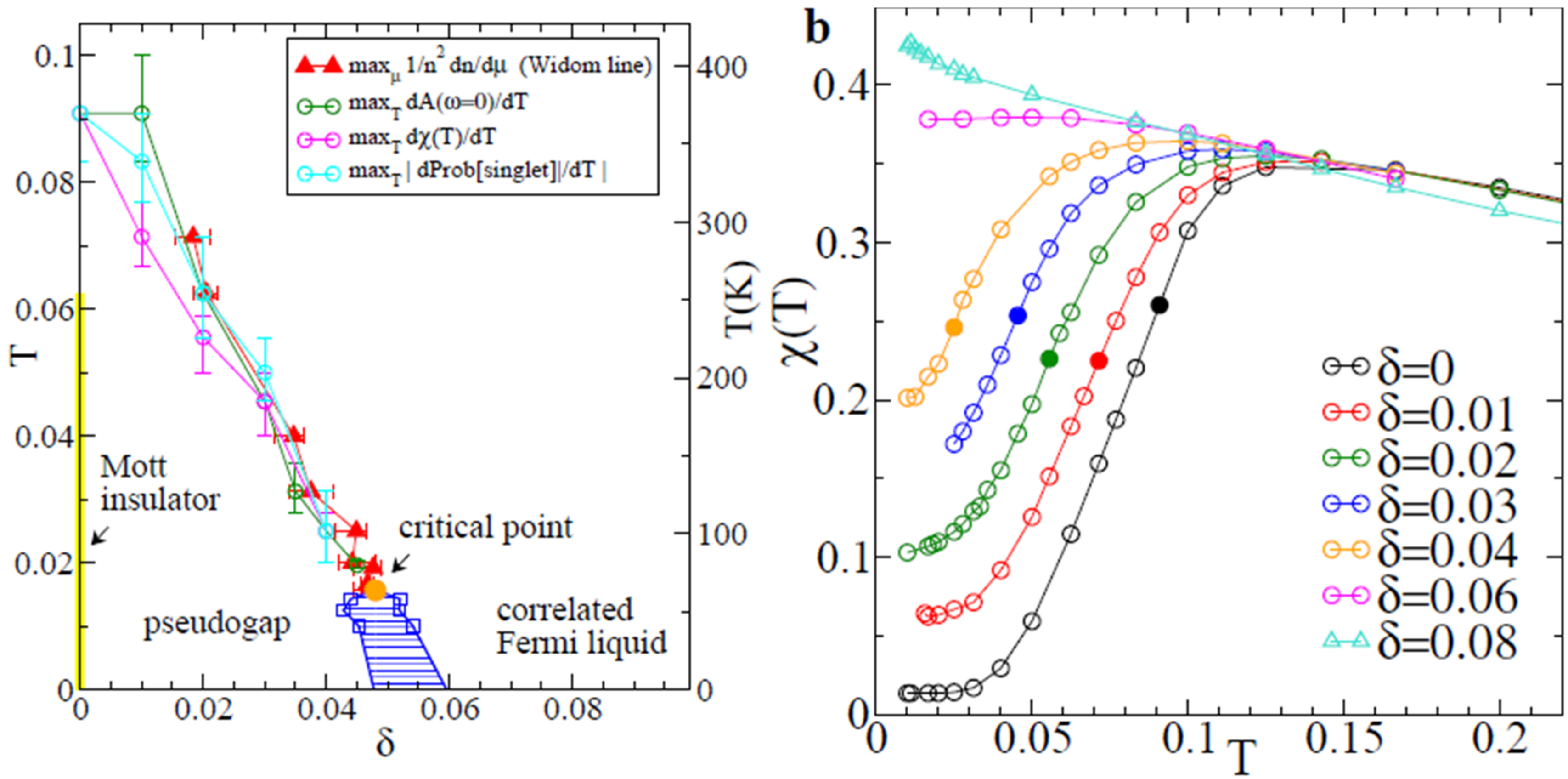
Density of states

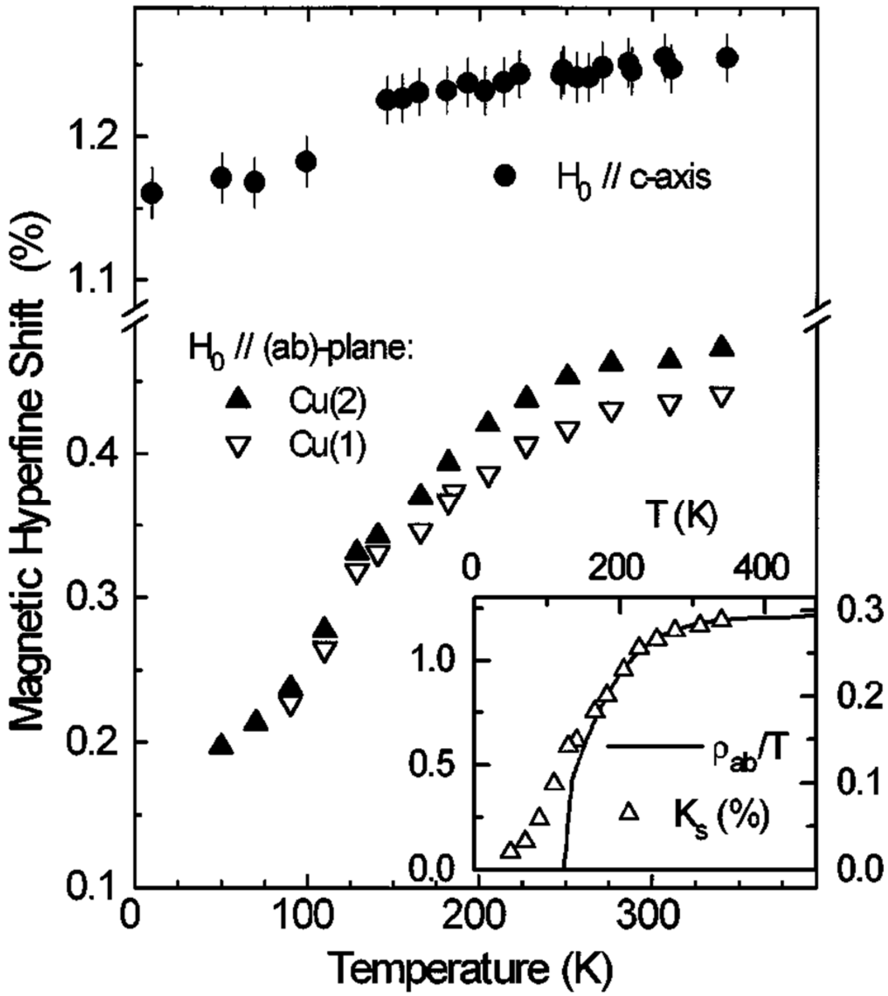




Spin susceptibility

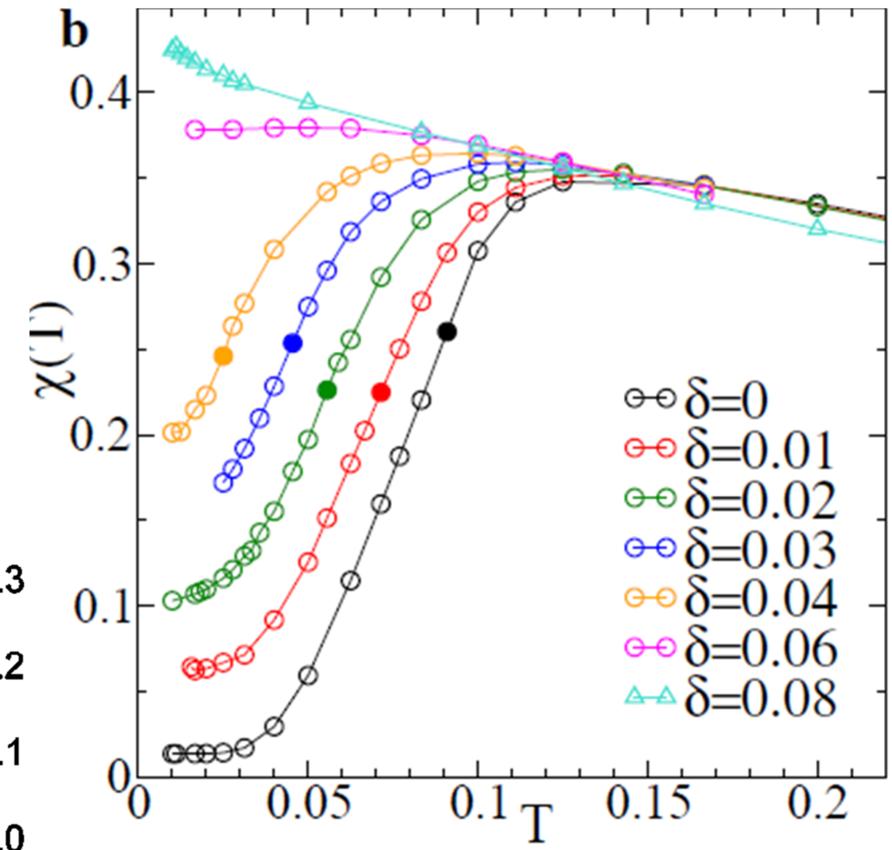


Spin susceptibility

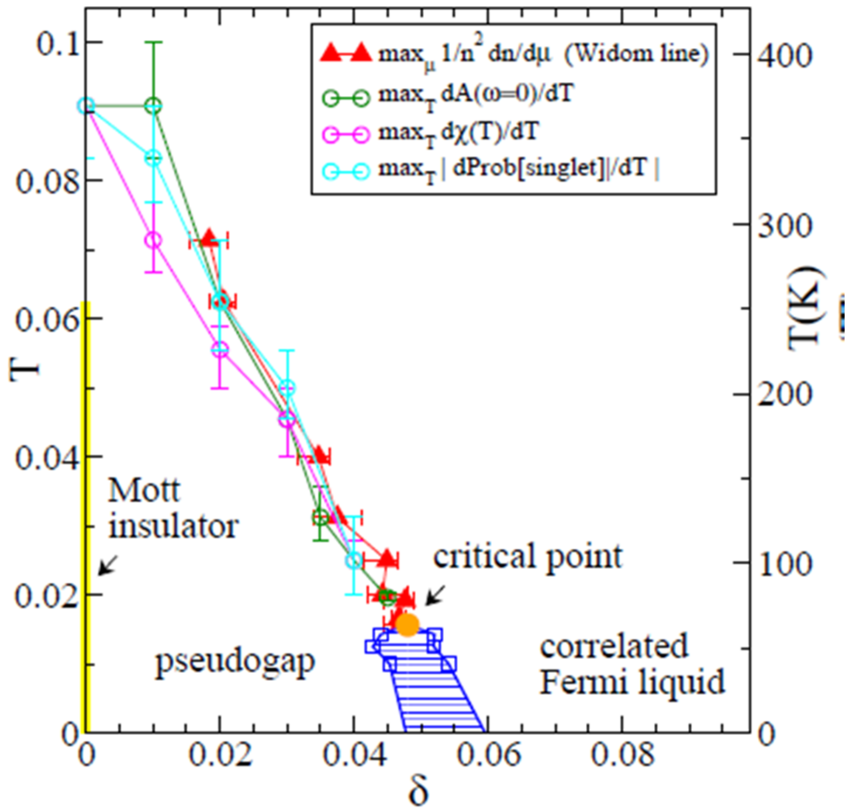


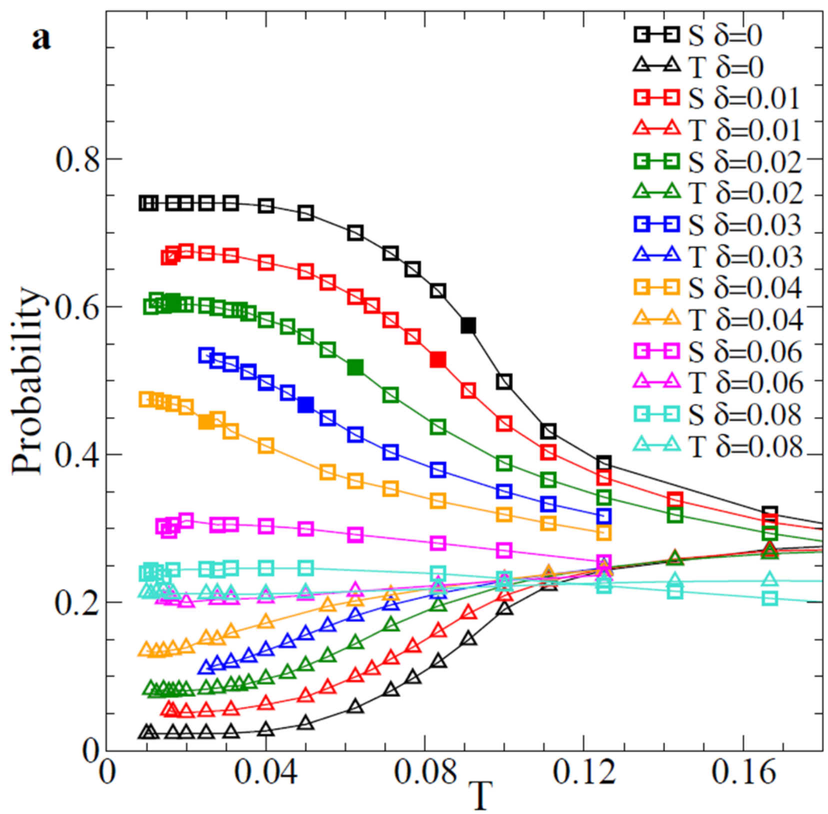
Underdoped Hg1223

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

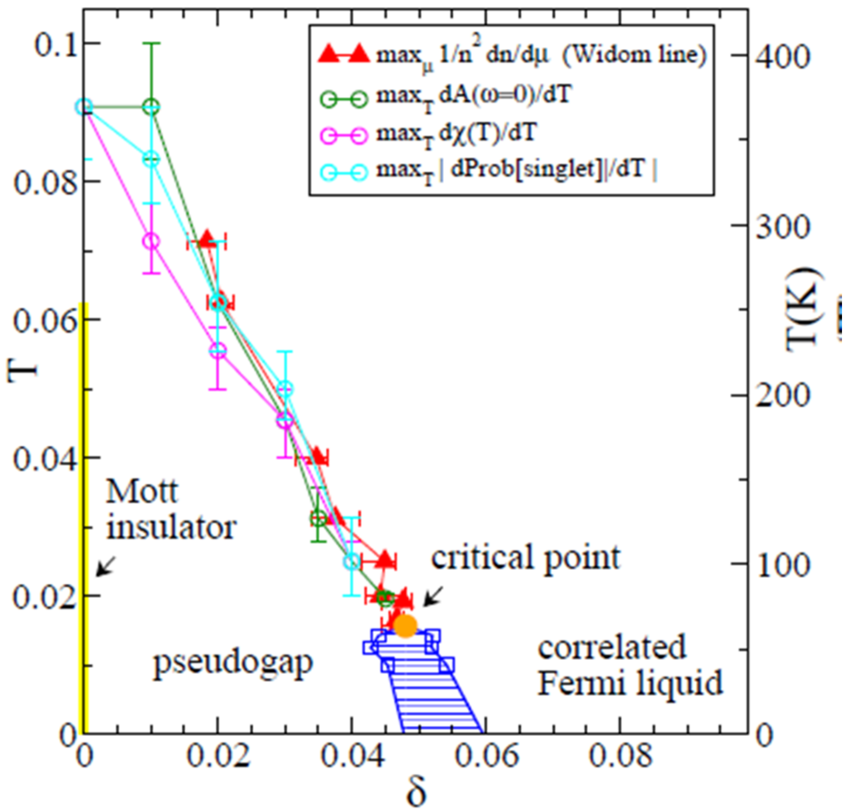


Plaquette eigenstates





Pseudogap *T** along the Widom line



Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

arXiv:1110.1392

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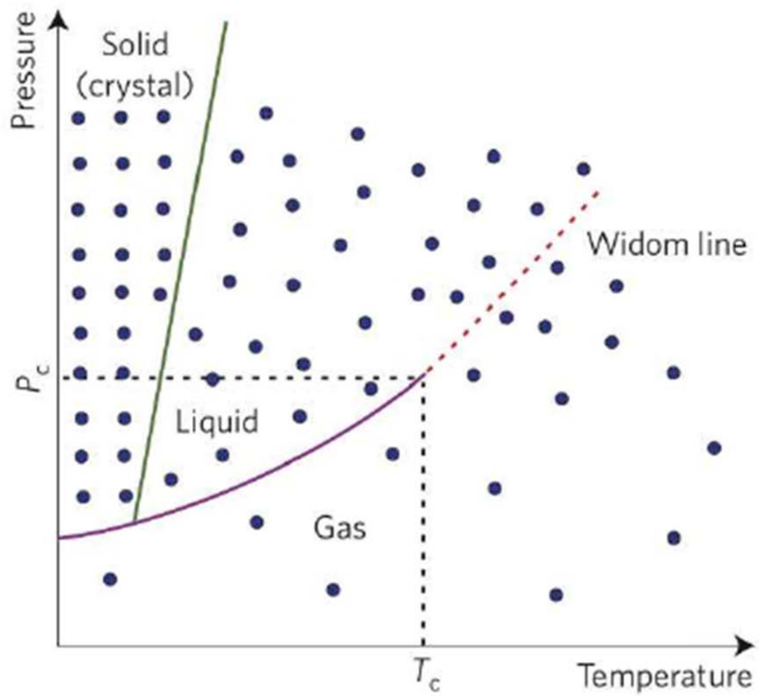
What is the Widom line?



McMillan and Stanley, Nat Phys 2010

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc
- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

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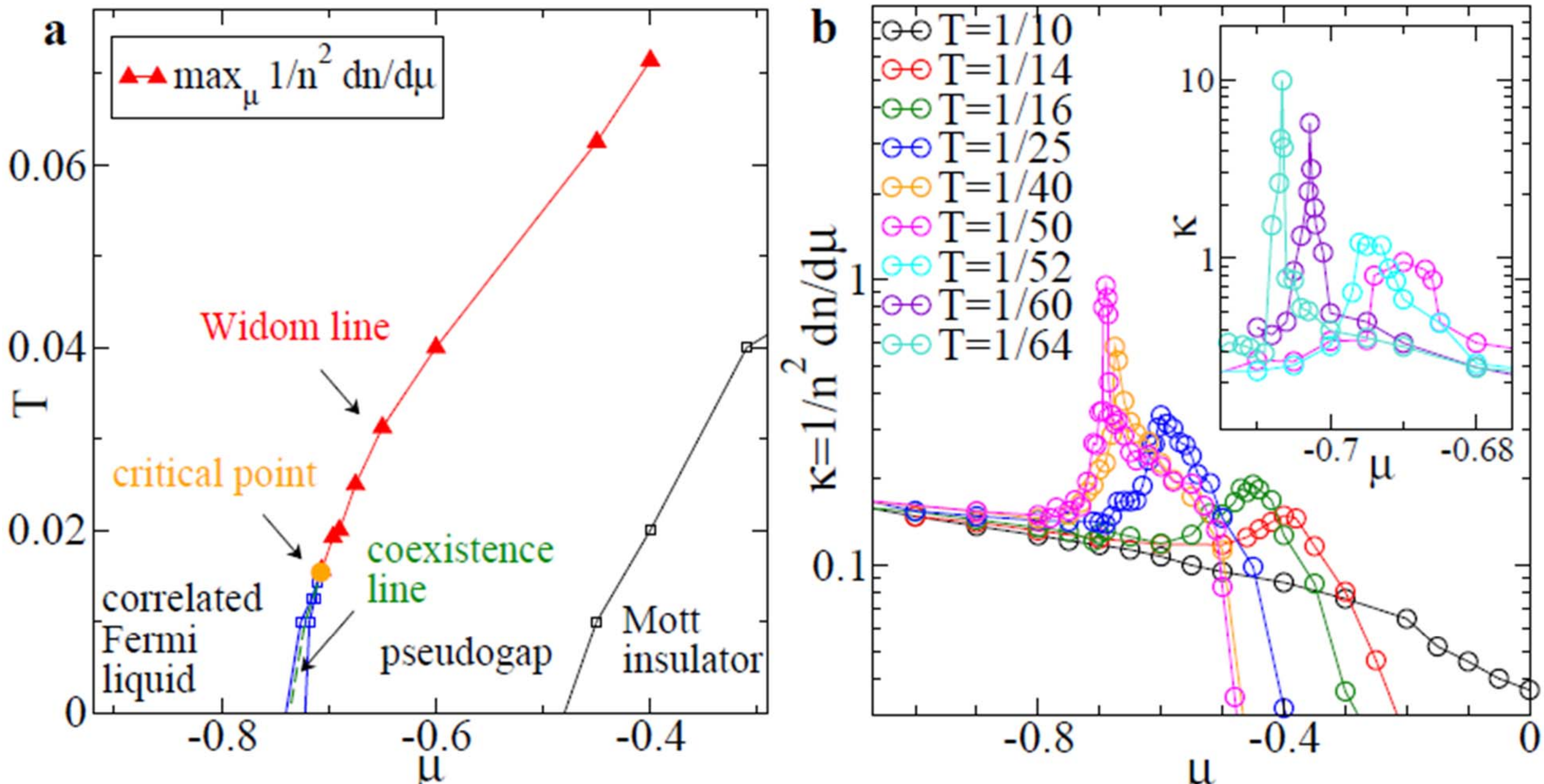
Pseudogap *T** along the Widom line

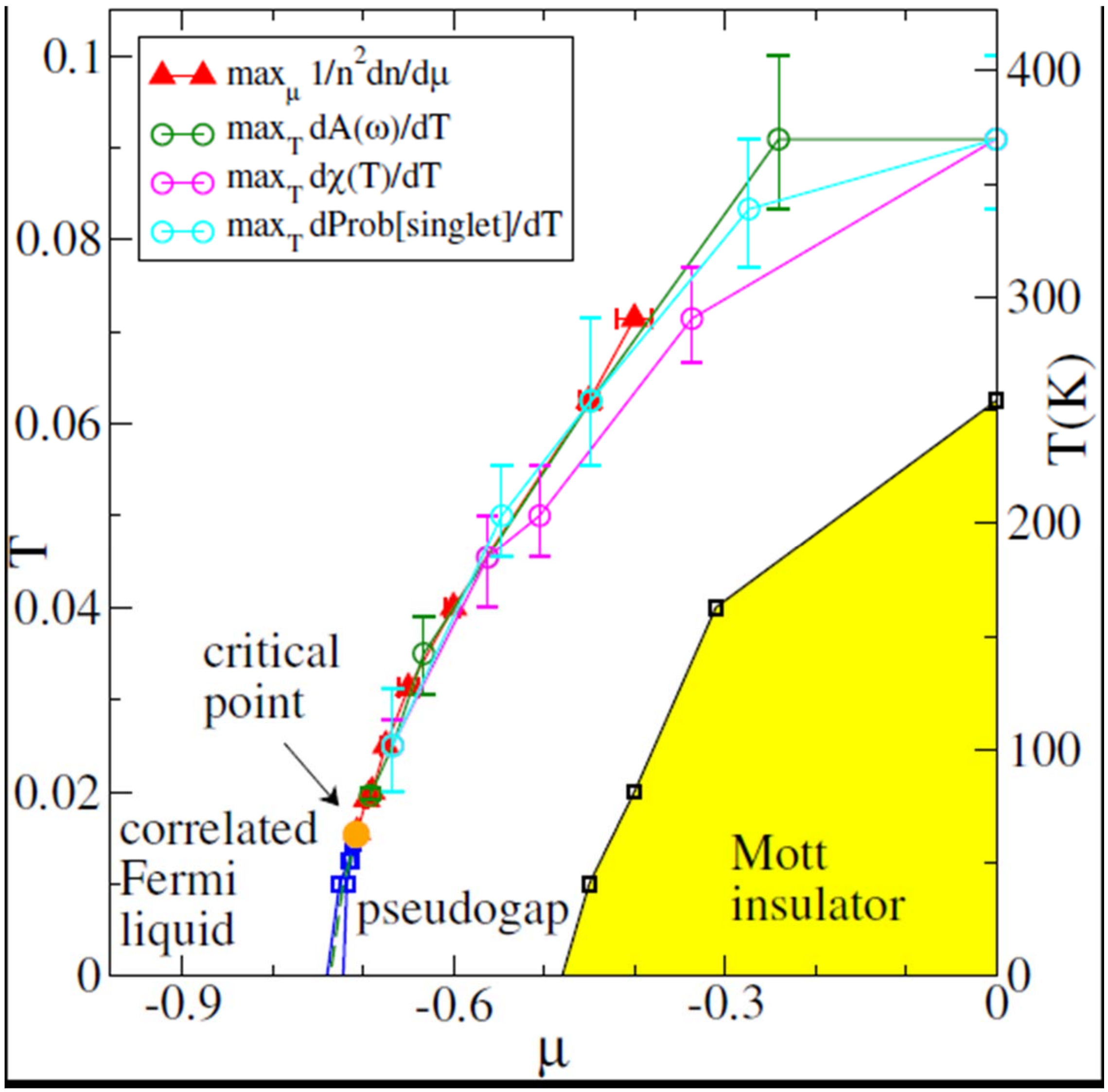


Widom line: defined from maxima of charge compressibility

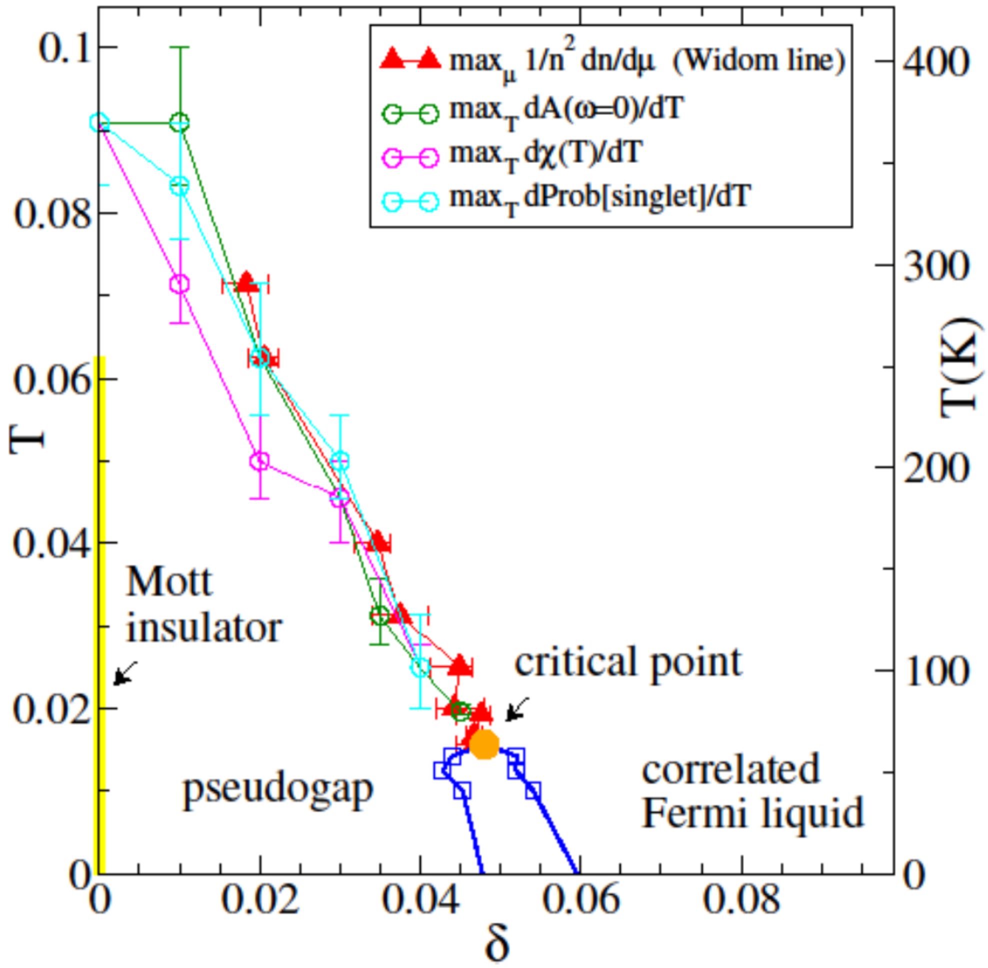
$\kappa = 1/n^2(dn/d\mu)_T$

divergence of κ at the (classical) critical point!

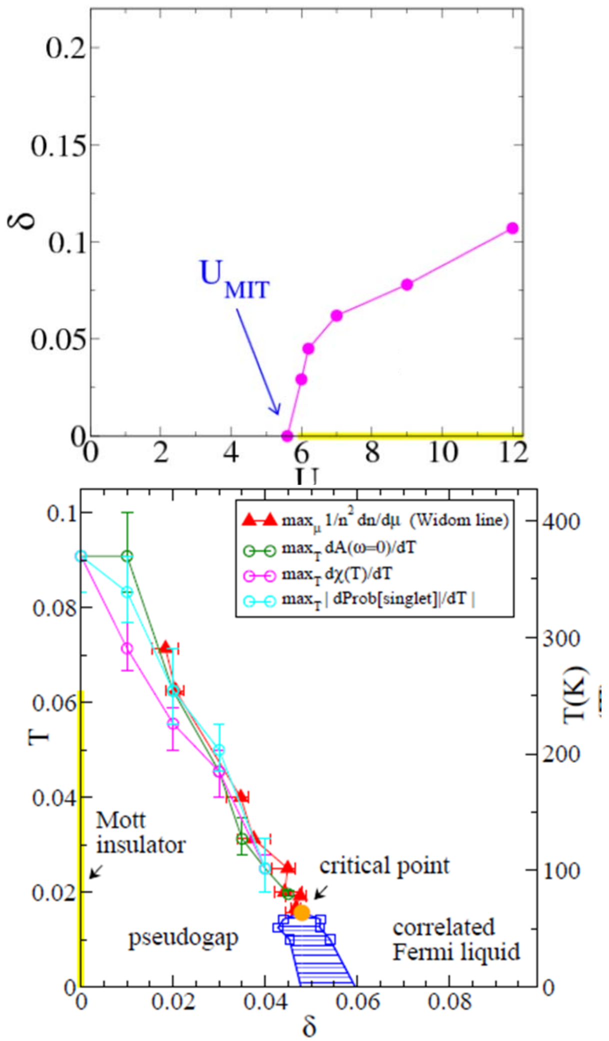
Rapid change also in dynamical quantities



Phase diagram



Summary



- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap *T** is a Widom line
- High compressibility (stripes?)

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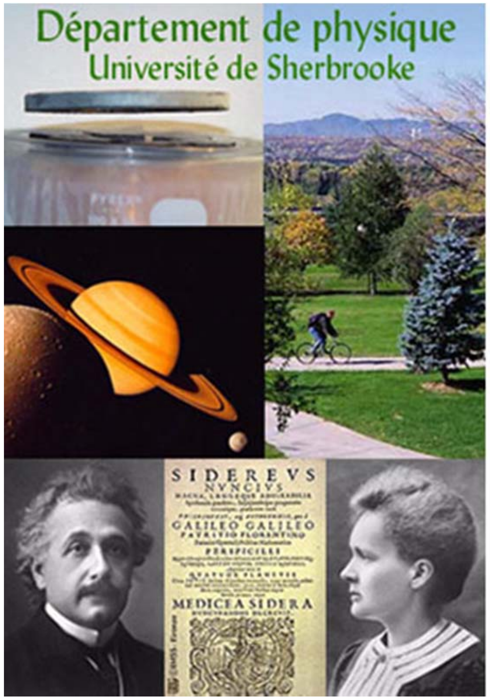

André-Marie Tremblay

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Merci

Thank you