A tale of two metals: How strong interactions can destroy an ordinary metal.

A.-M. Tremblay

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

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VERITATEM IN CHARITATE

Theory Canada 8, Bishop's, 2013

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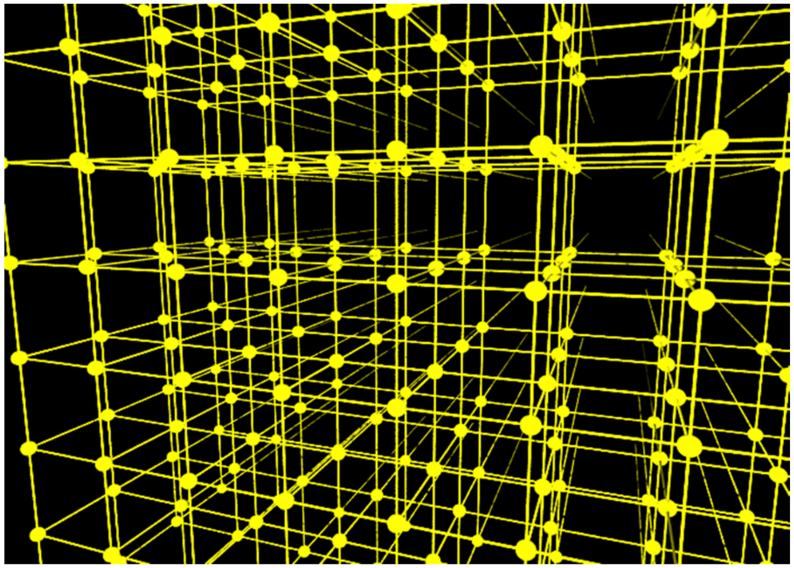
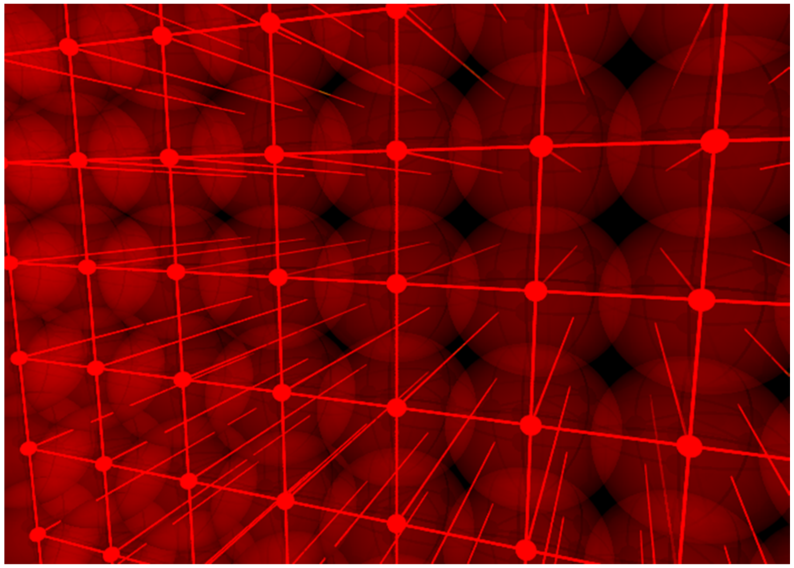
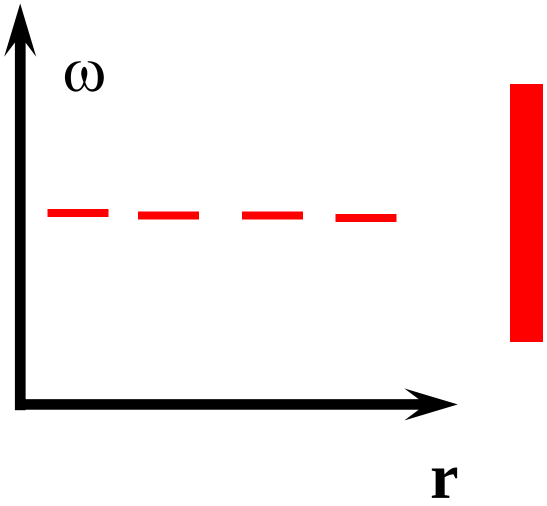
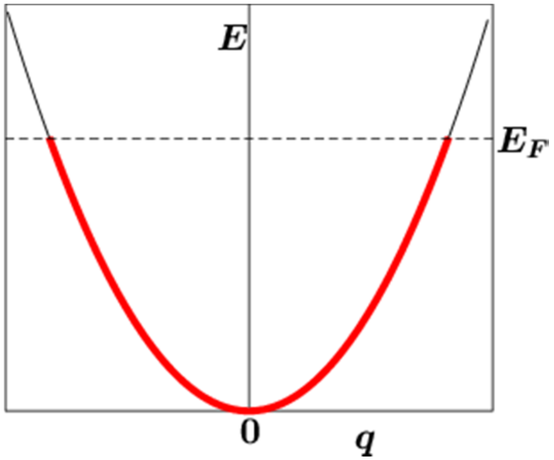
How to make a metal









Courtesy, S. Julian

Superconductivity

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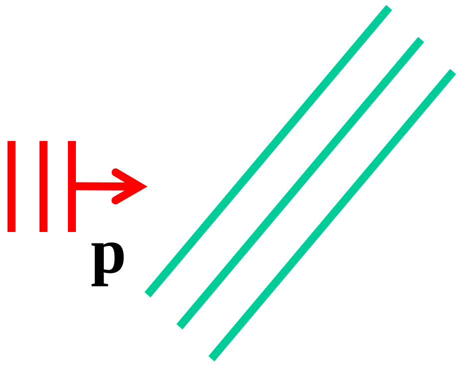
Attraction mechanism in the metallic state



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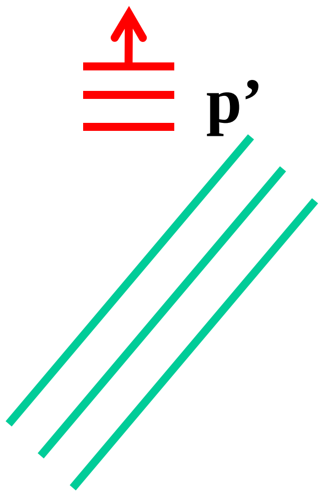
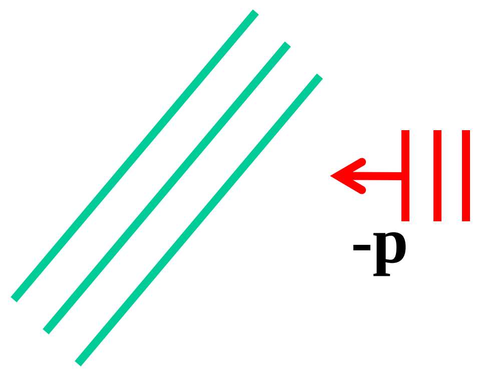
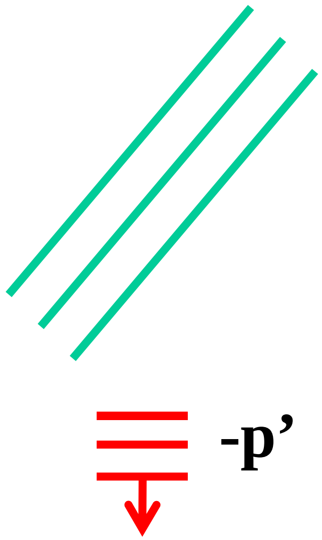
Attraction mechanism in the metallic state



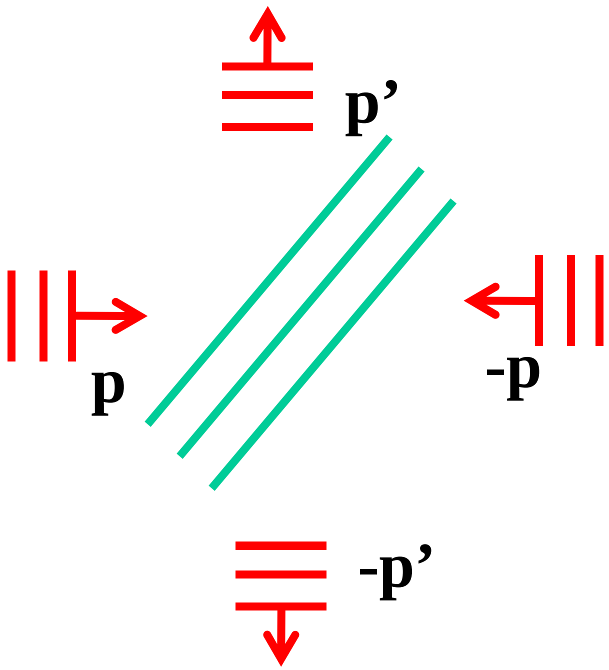
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

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

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

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

Half-filled band is metallic?

Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

« Conventional » Mott transition

T

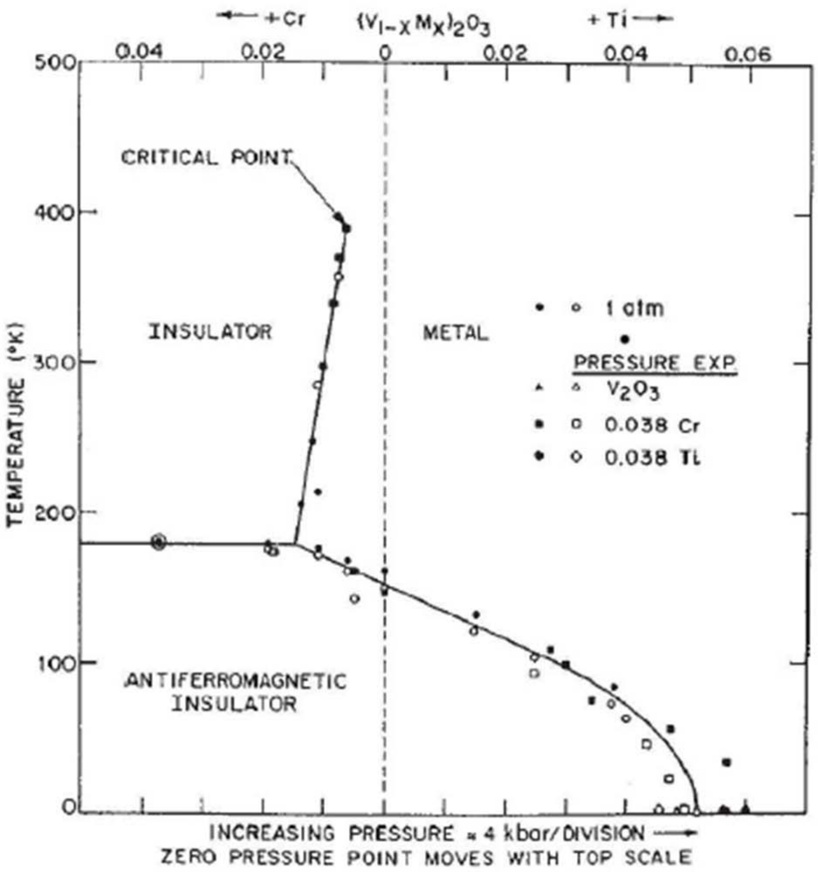


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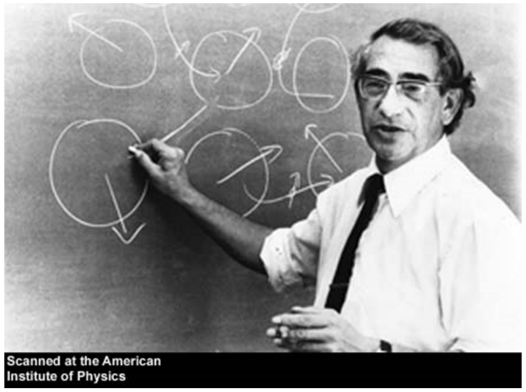
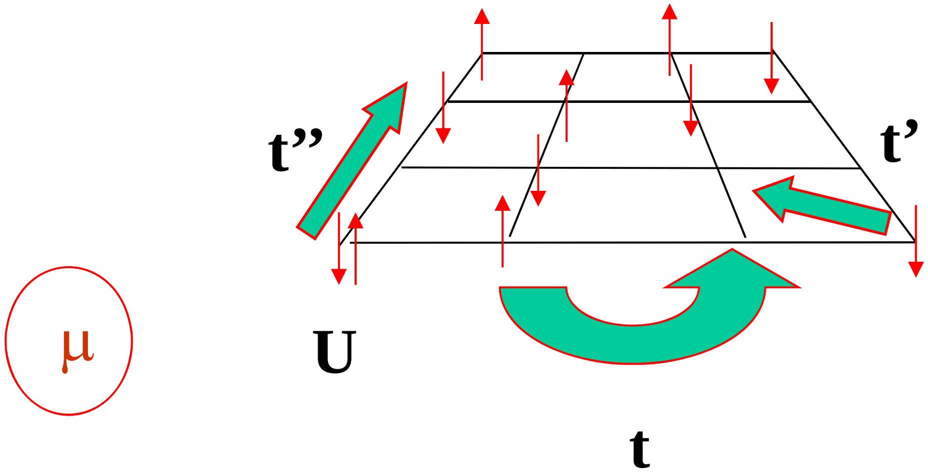
Figure: McWhan, PRB 1970; Limelette, Science 2003

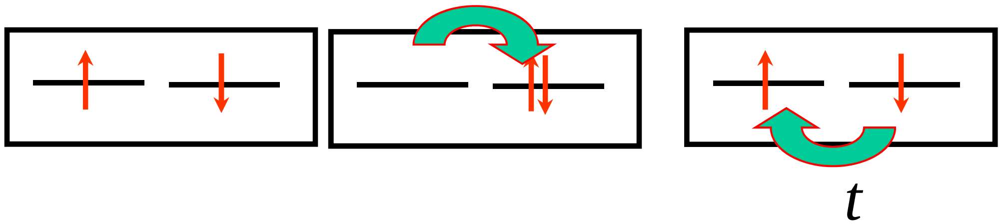
Hubbard model



1931-1980



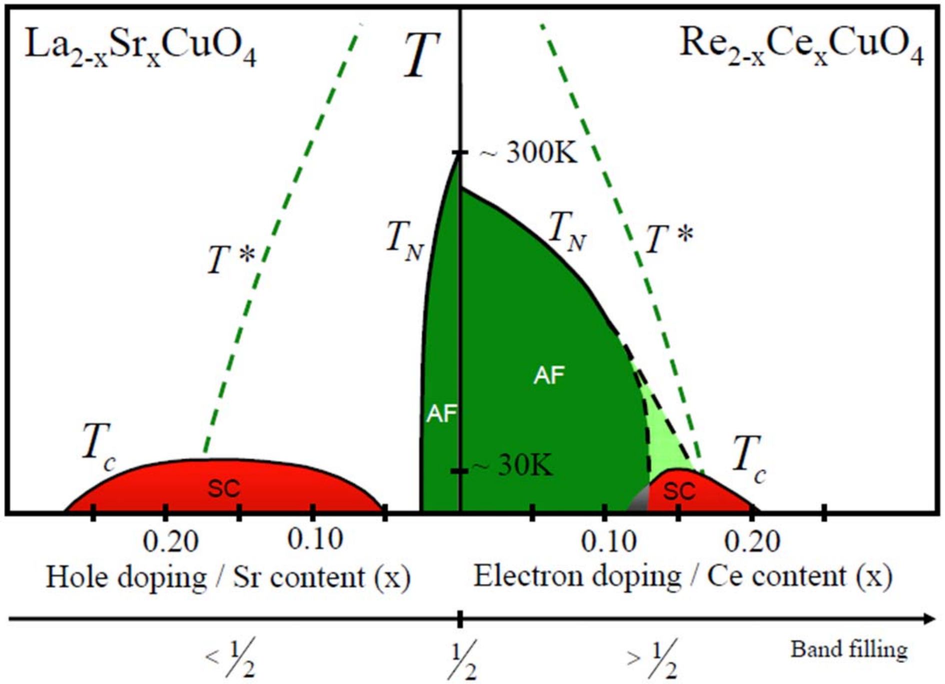
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



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

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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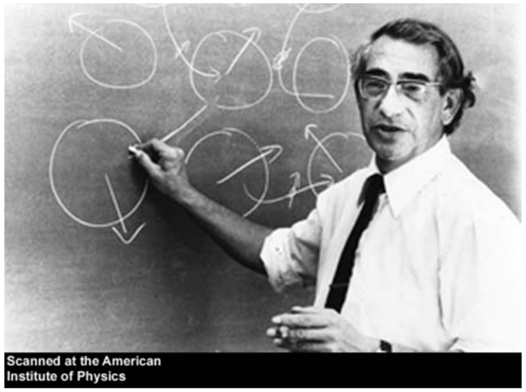
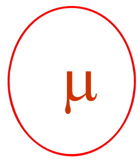
Outline

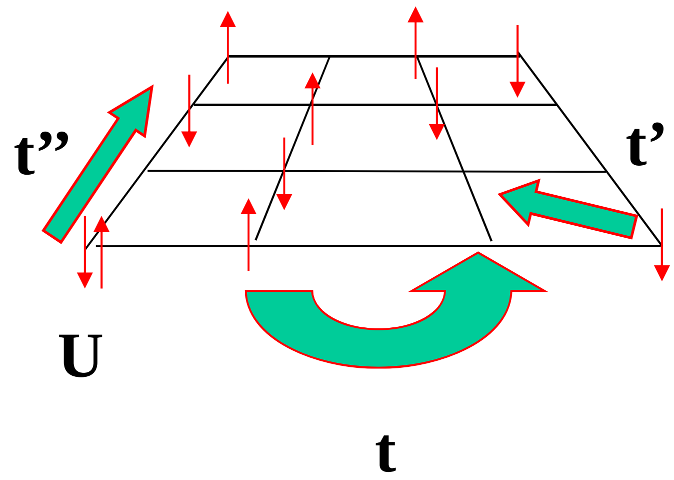
- Pseudogap
  - From AFM fluctuations
- **Weak vs strong coupling**
- Dynamical mean-field theory: crossover
- Phase diagram and pseudogap at strong coupling

Hubbard model

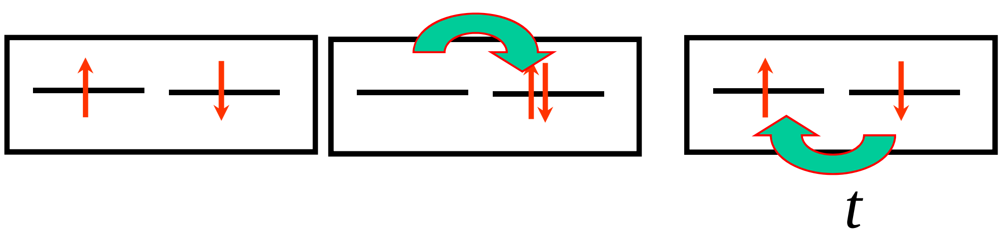


1931-1980





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



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

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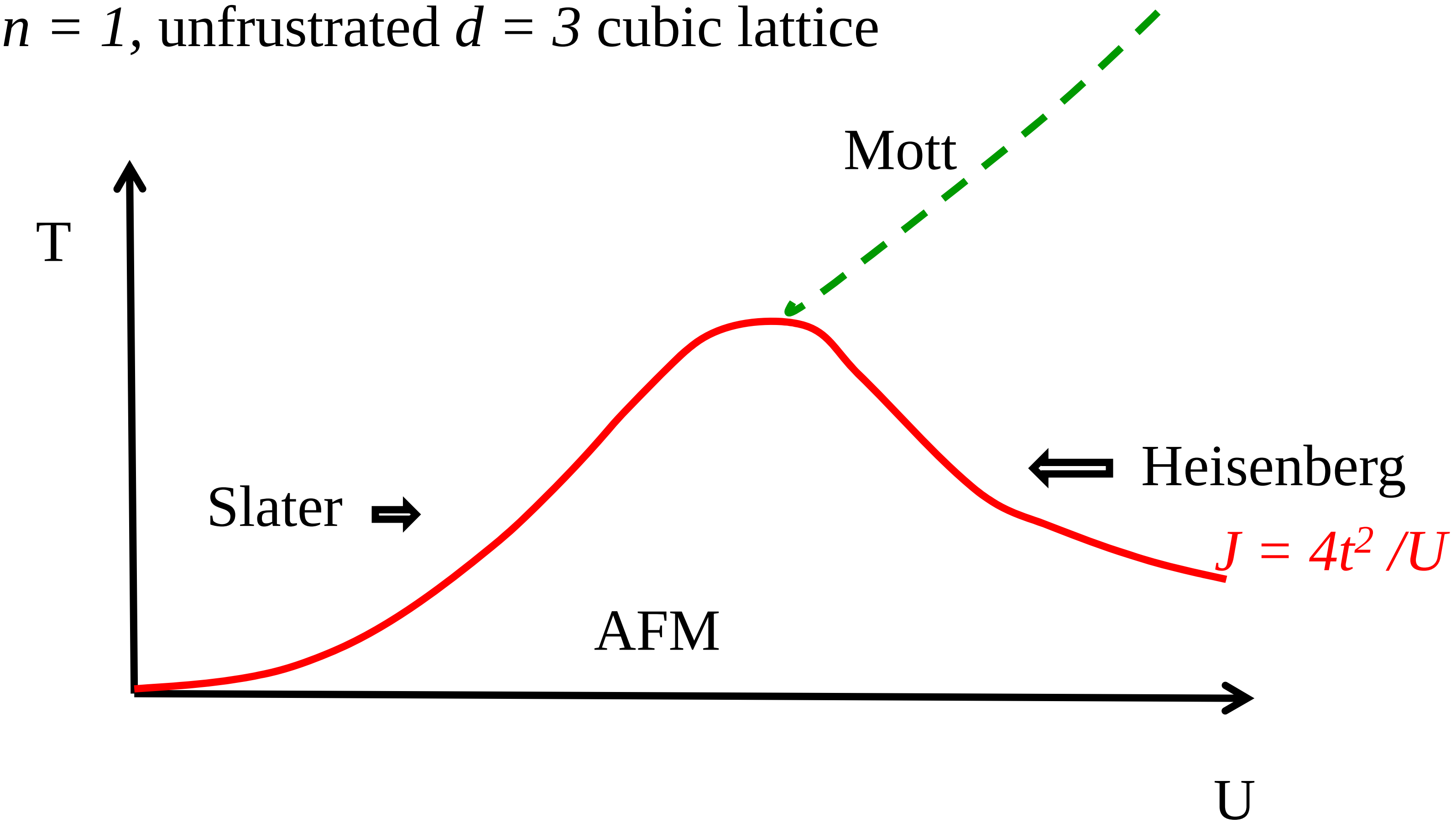
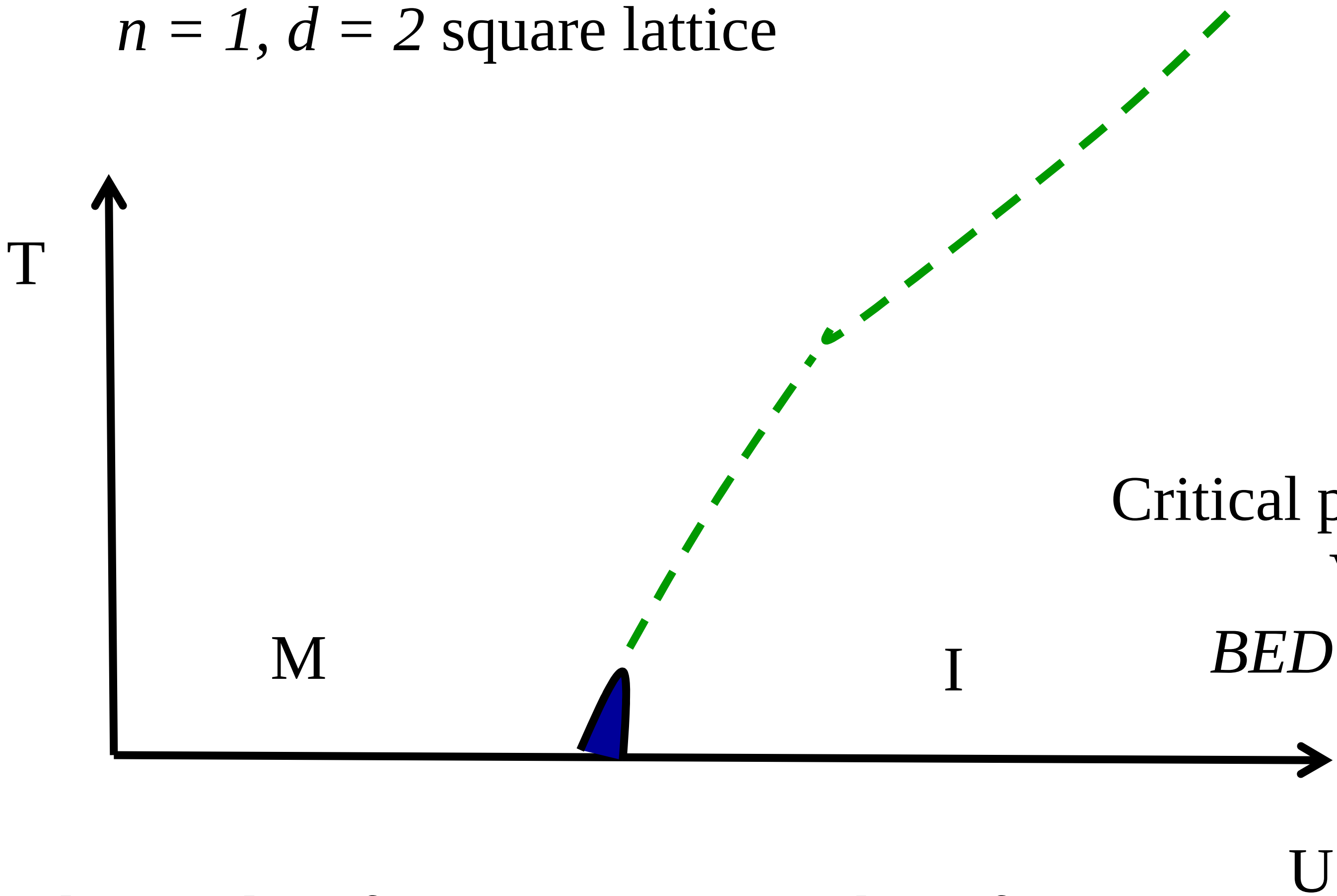
Weak-strong coupling, and Mott transition

$n = 1$, 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 $T = 0$

Outline

- Pseudogap
  - From AFM fluctuations
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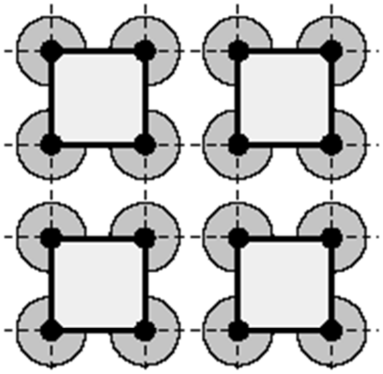
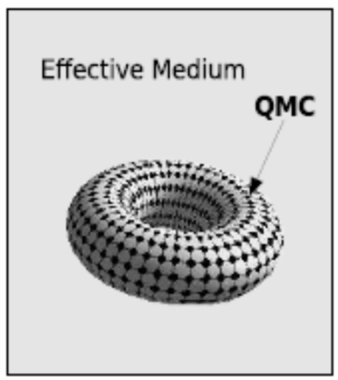
- **Dynamical mean-field theory: crossover**
- Phase diagram and pseudogap at strong coupling

The method

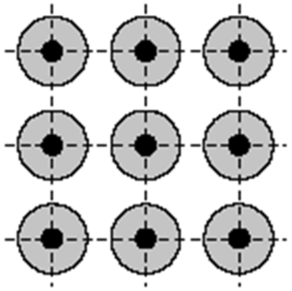
2d Hubbard: Quantum cluster method

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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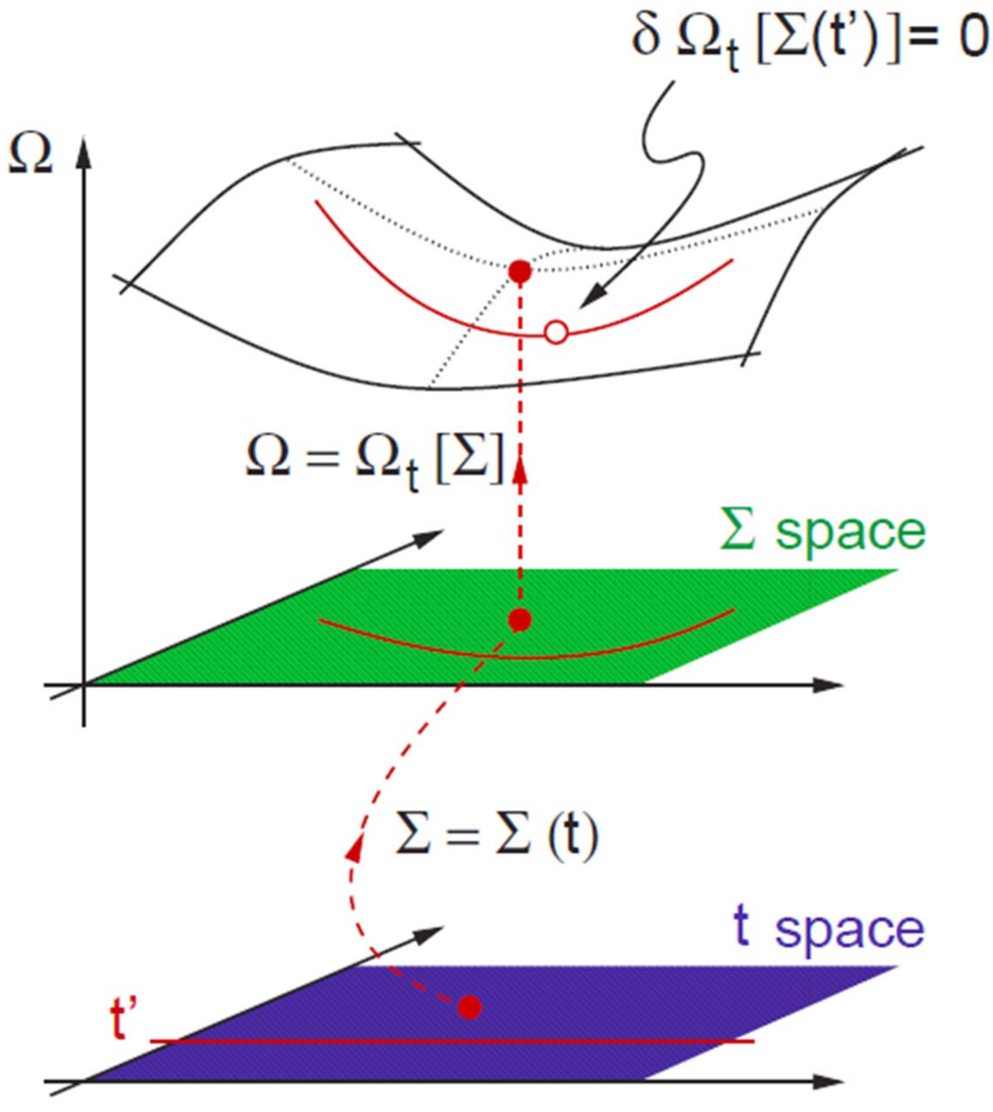
DMFT as a stationnary point



Another way to look at this (Potthoff)

$$\Omega_{\mathbf{t}}[G] = \Phi[G] - Tr[(G_{0\mathbf{t}}^{-1} - G^{-1})G] + Tr\ln(-G)$$

$$\frac{\delta\Phi[G]}{\delta G} = \Sigma$$

$$\Omega_{\mathbf{t}}[\Sigma] = \Phi[G] - Tr[\Sigma G] - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

Still stationary (chain rule)

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] - Tr\ln(-G_{0\mathbf{t}}^{-1} + \Sigma)$$

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

SFT : Self-energy Functional Theory

With $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to Σ and equal to grand potential there.

$$\Omega_{\mathbf{t}}[\Sigma] = \Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1}) + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in $H_0(\mathbf{t'})$

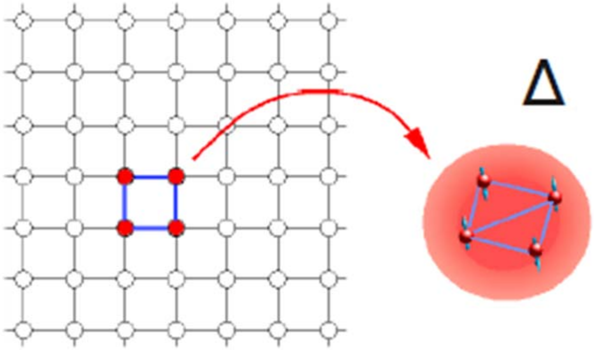
M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

+ and -

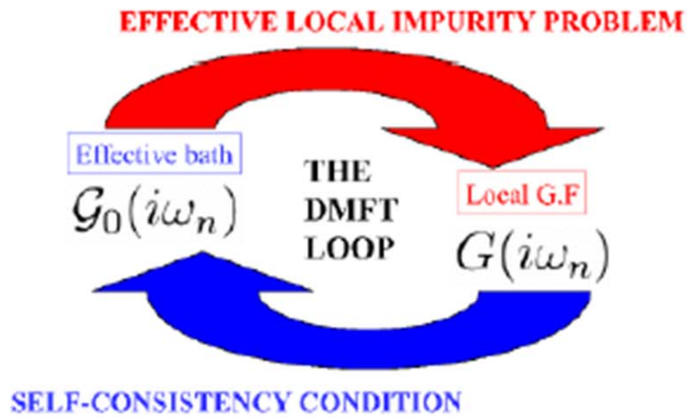
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations
- Missing:
  - Long wavelength p-h and p-p fluctuations

Solvers for the cluster-in-a-bath problem

C-DMFT



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



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

Here: continuous time QMC

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

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

At finite T, 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).

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Outline

- Pseudogap
  - From AFM fluctuations
- Weak vs strong coupling
- Dynamical mean-field theory: crossover
- **Phase diagram and pseudogap at strong coupling**

Giovanni Sordi

Finite T phase diagram

CTQMC as solver for cluster in a bath ($T=0$).

Patrick Sémon

Kristjan Haule

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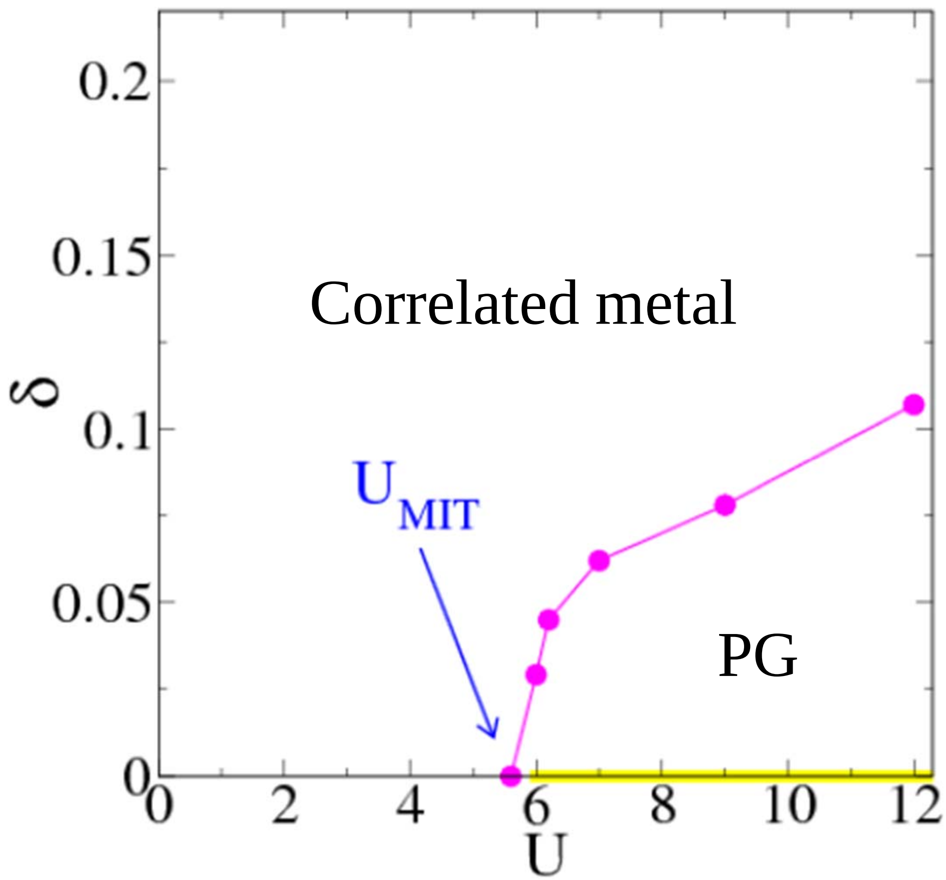
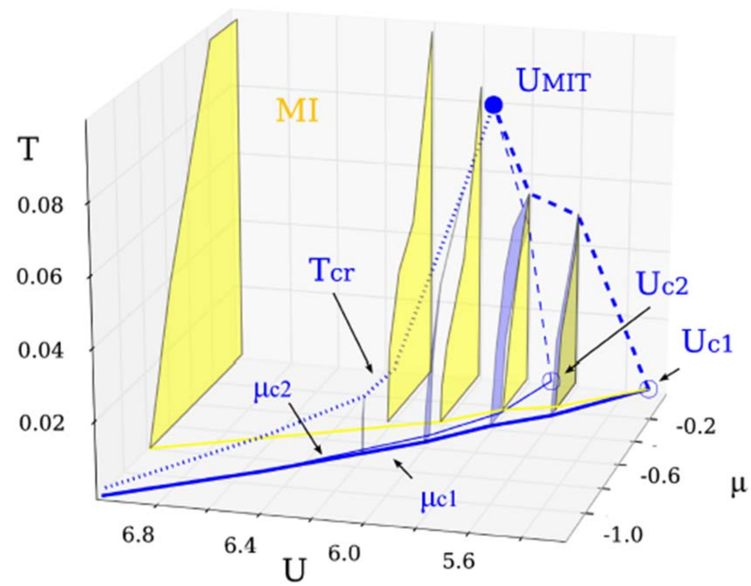
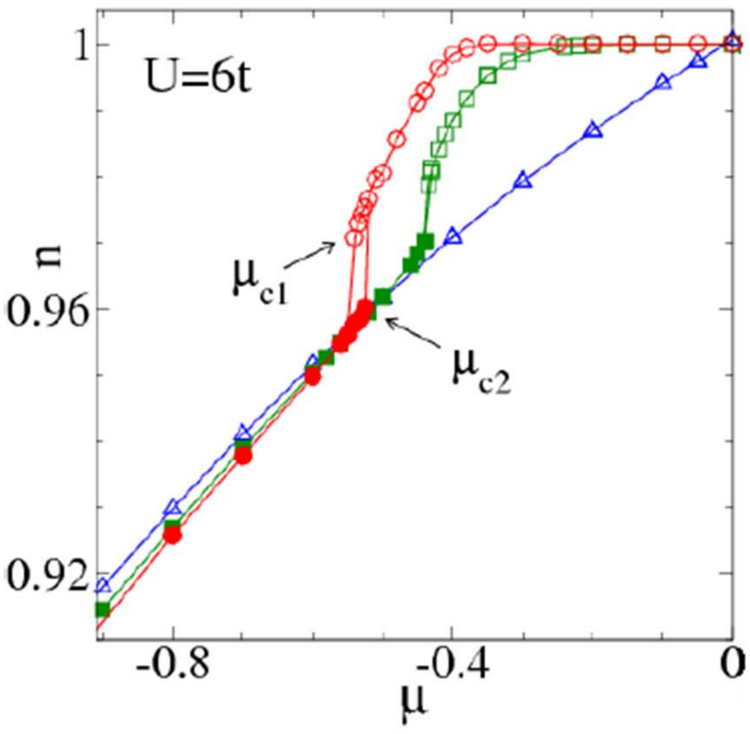
Link to Mott transition up to optimal doping

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





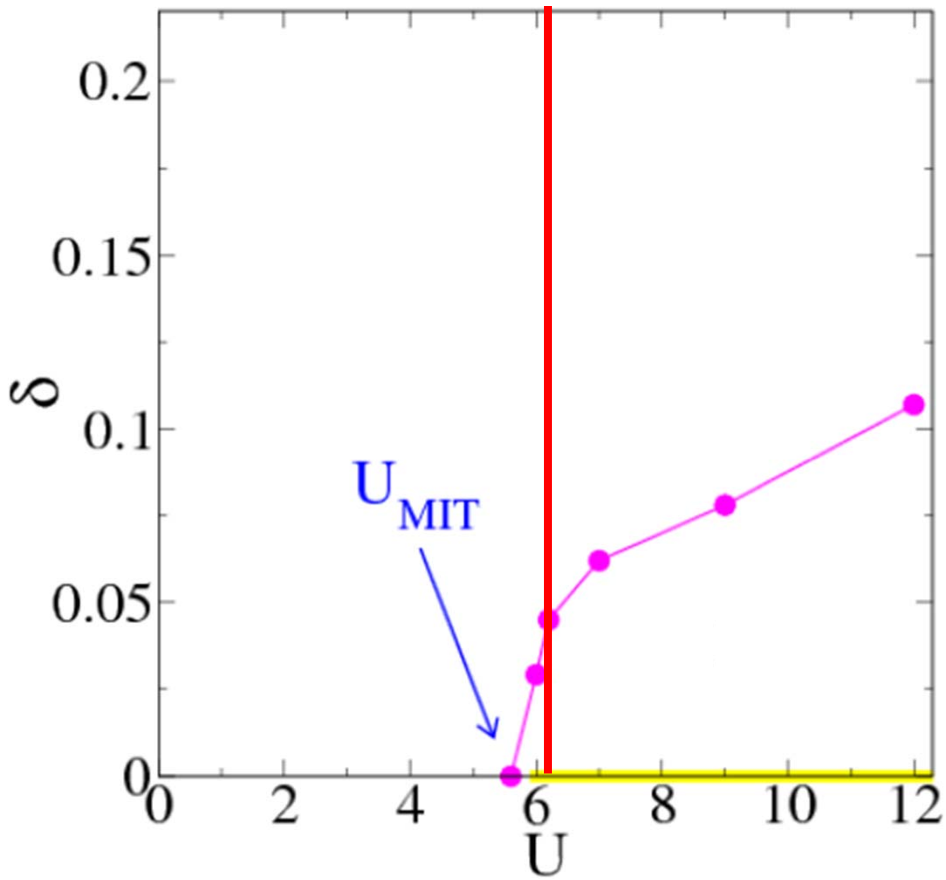
First order transition at finite doping

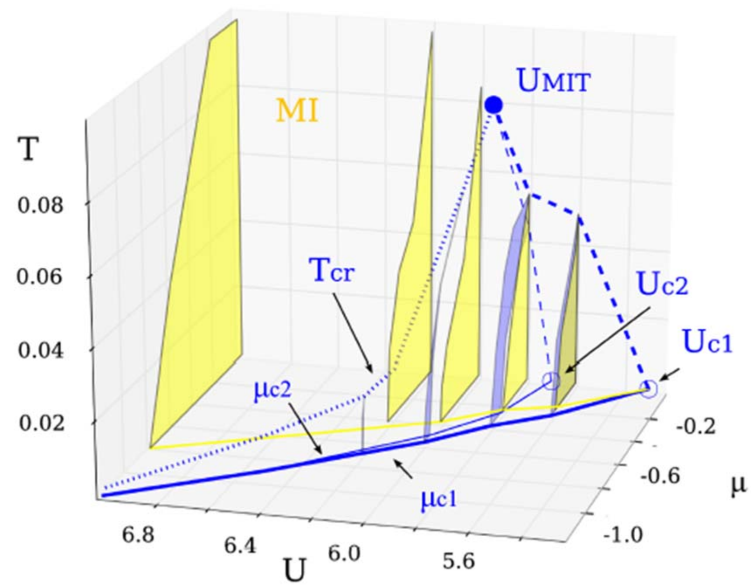


$n(\mu)$ for several temperatures:
$T/t = 1/10, 1/25, 1/50$

Link to Mott transition up to optimal doping

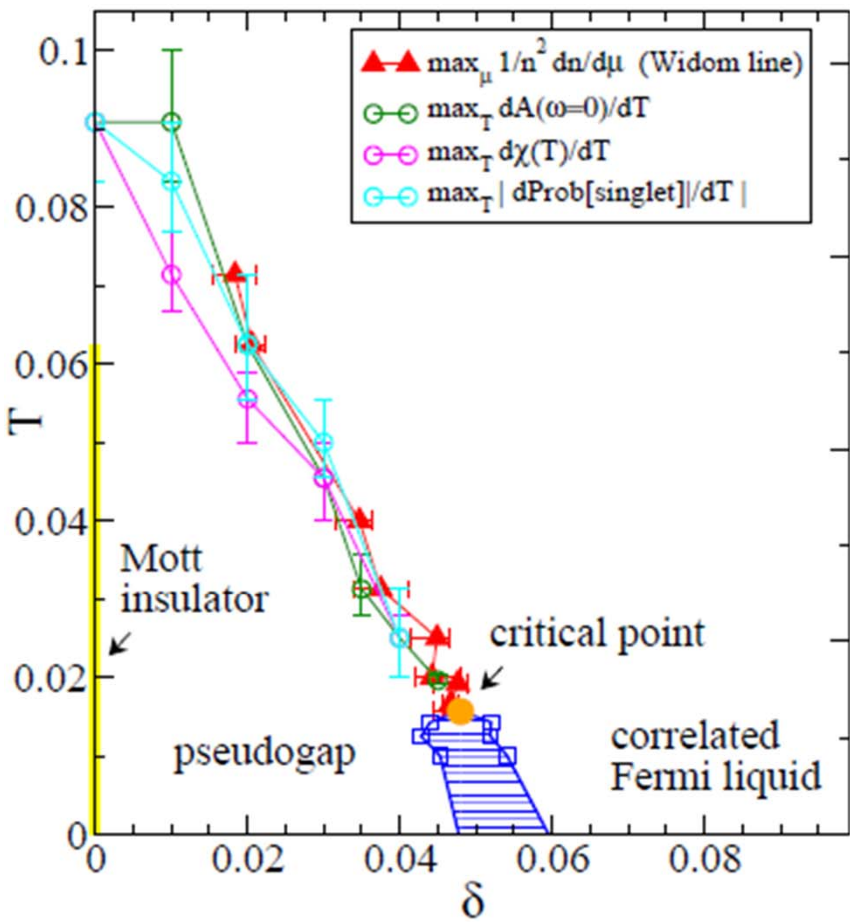
Doping dependence of critical point as a function of *U*

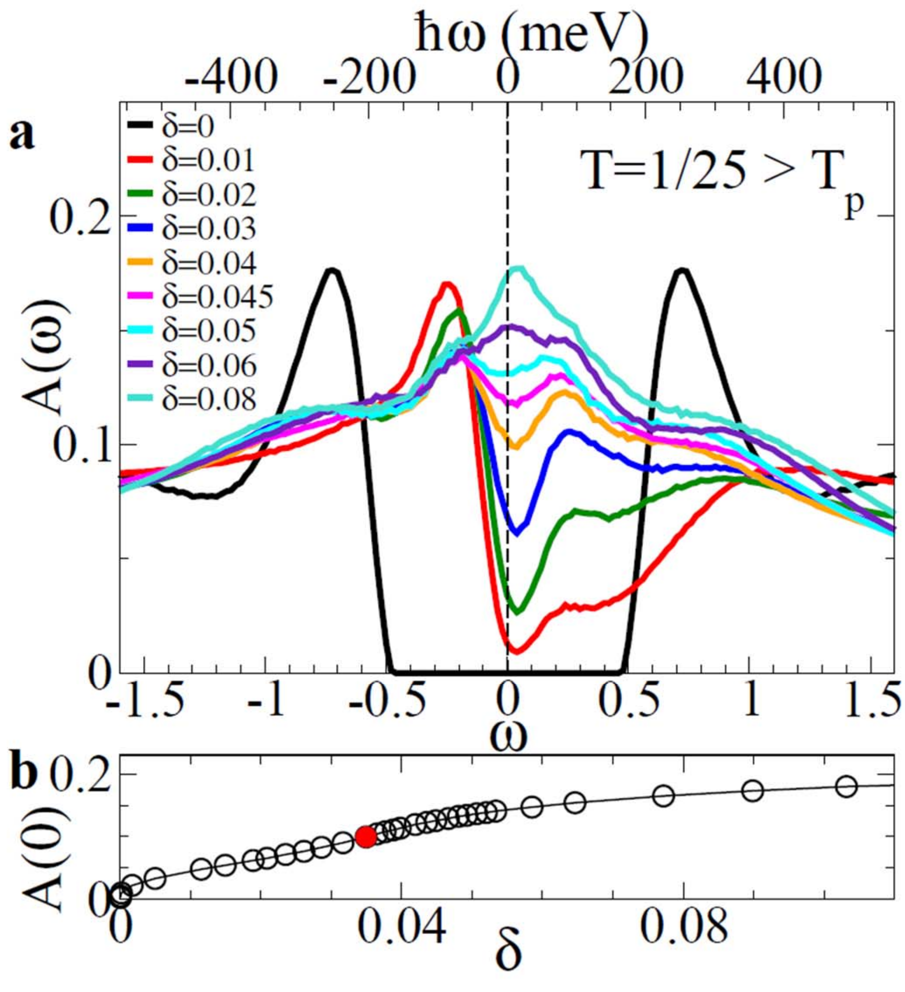




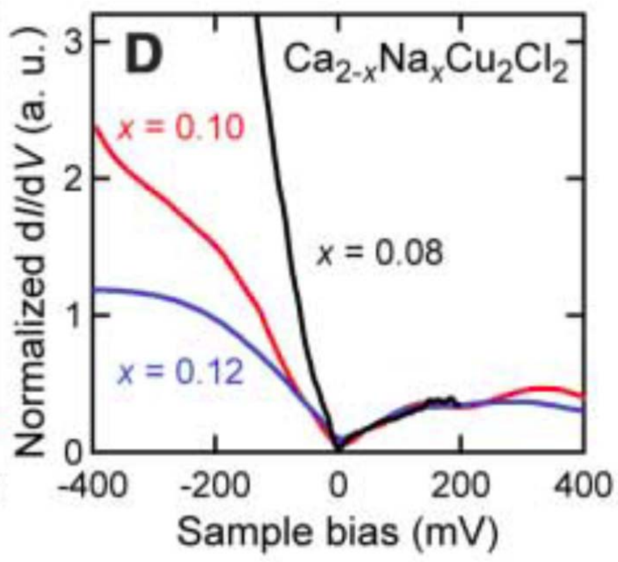
Smaller *D* and *S*

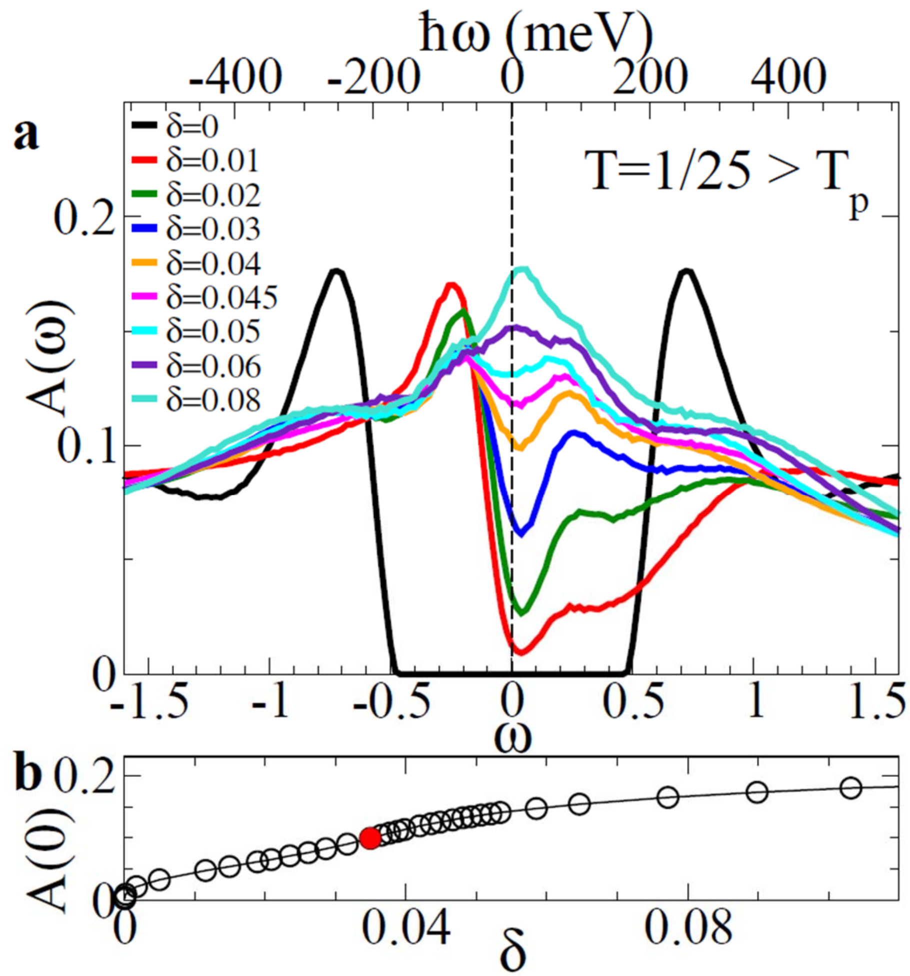
Density of states





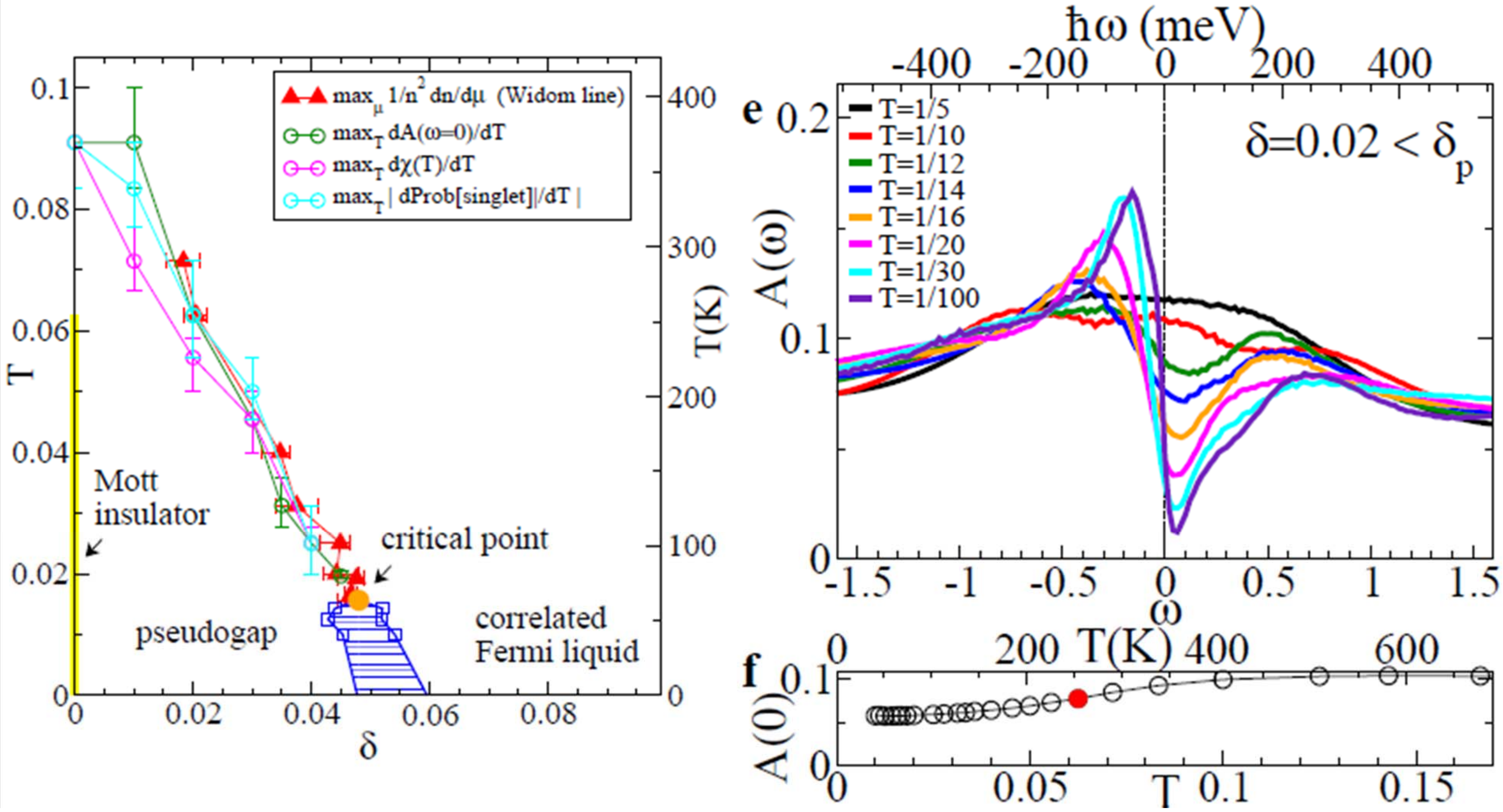
Density of states



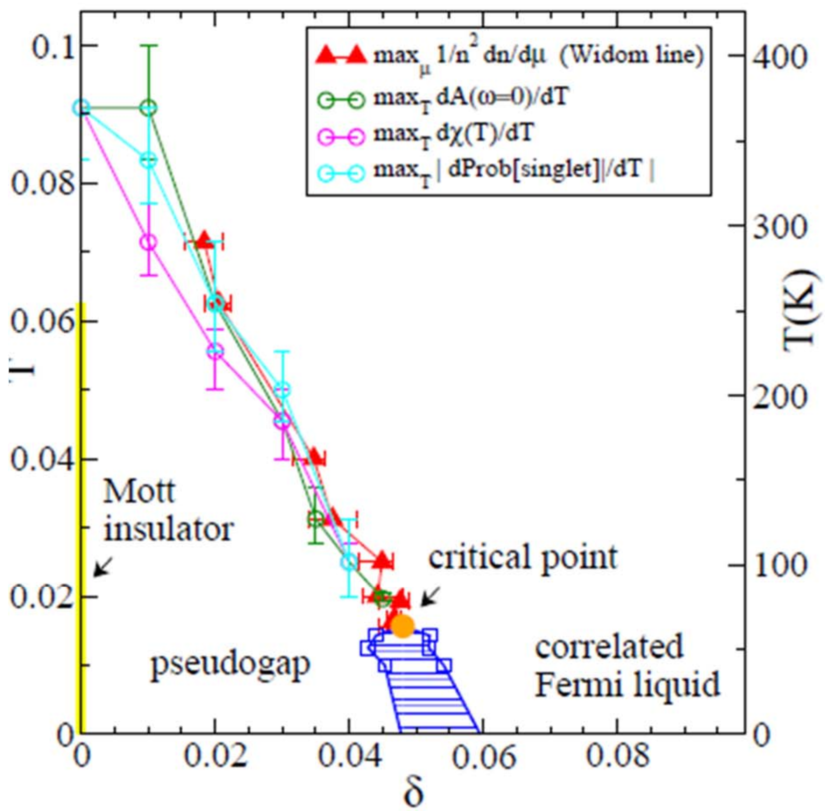


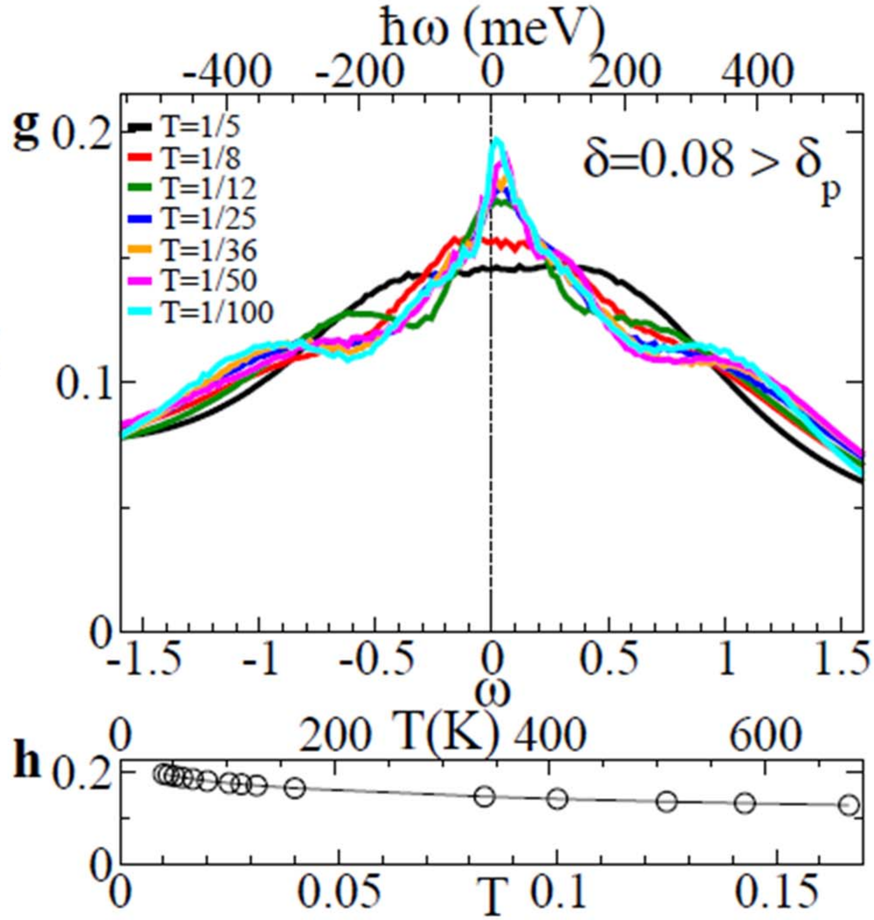
Khosaka et al. *Science* **315**, 1380 (2007);

Density of states

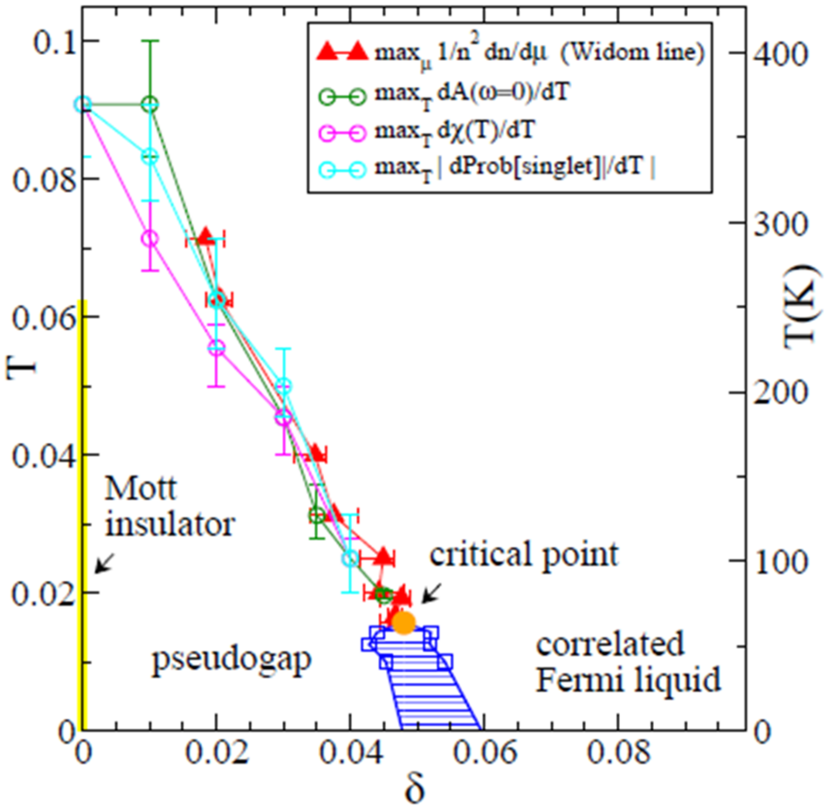


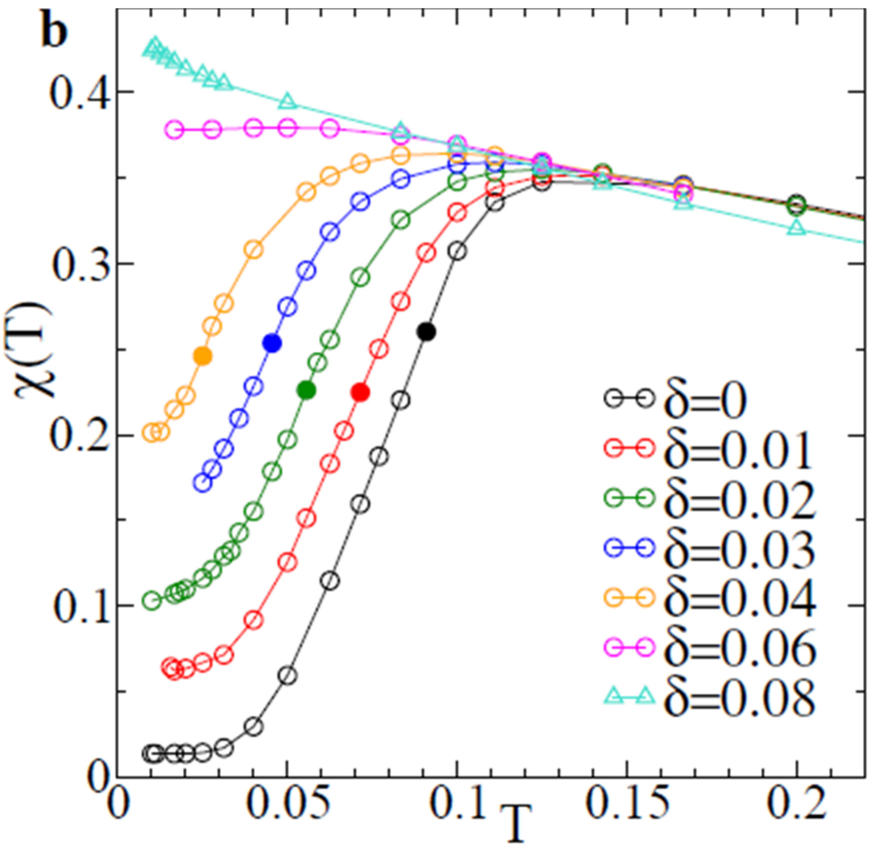
Density of states



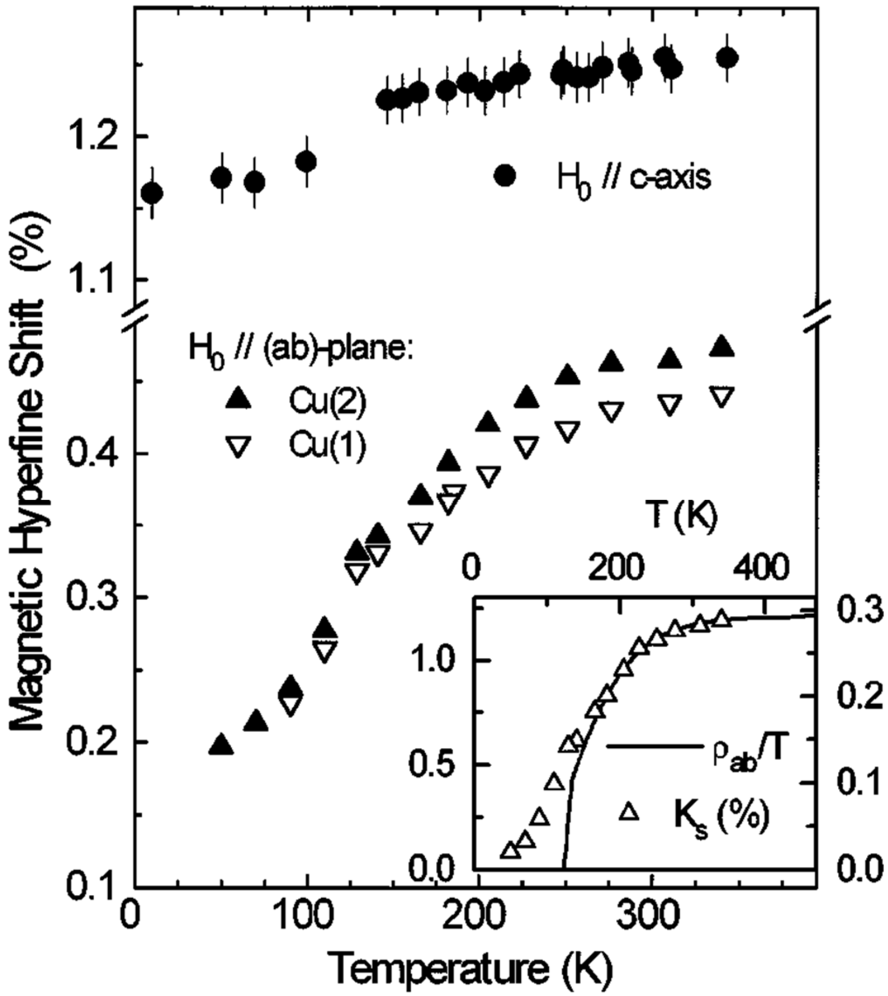


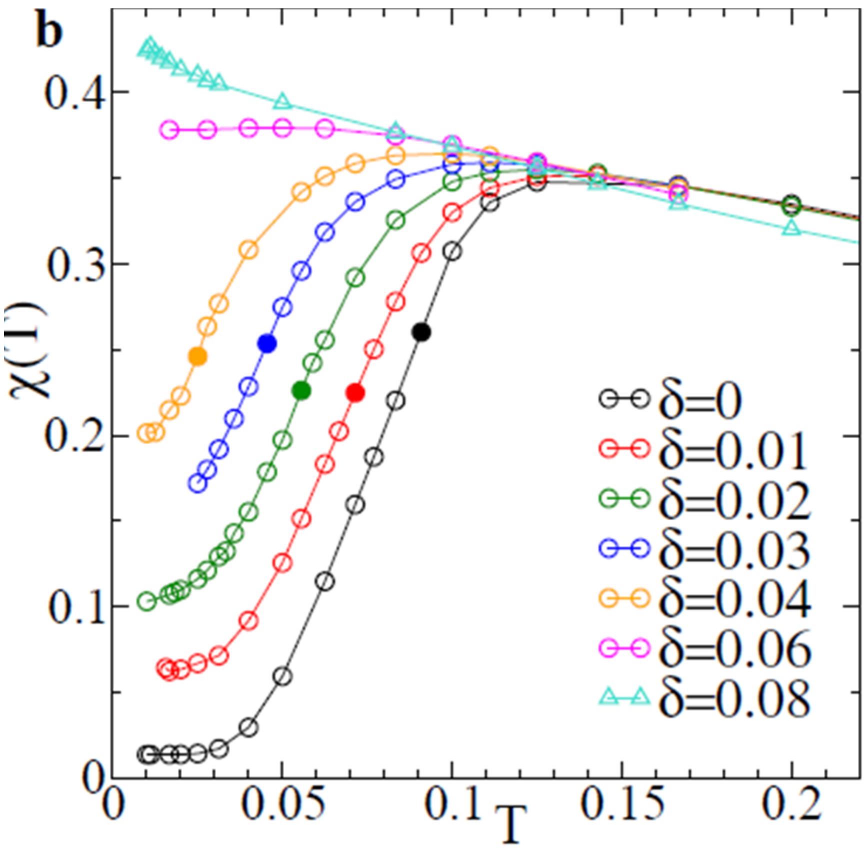
Spin susceptibility





Spin susceptibility

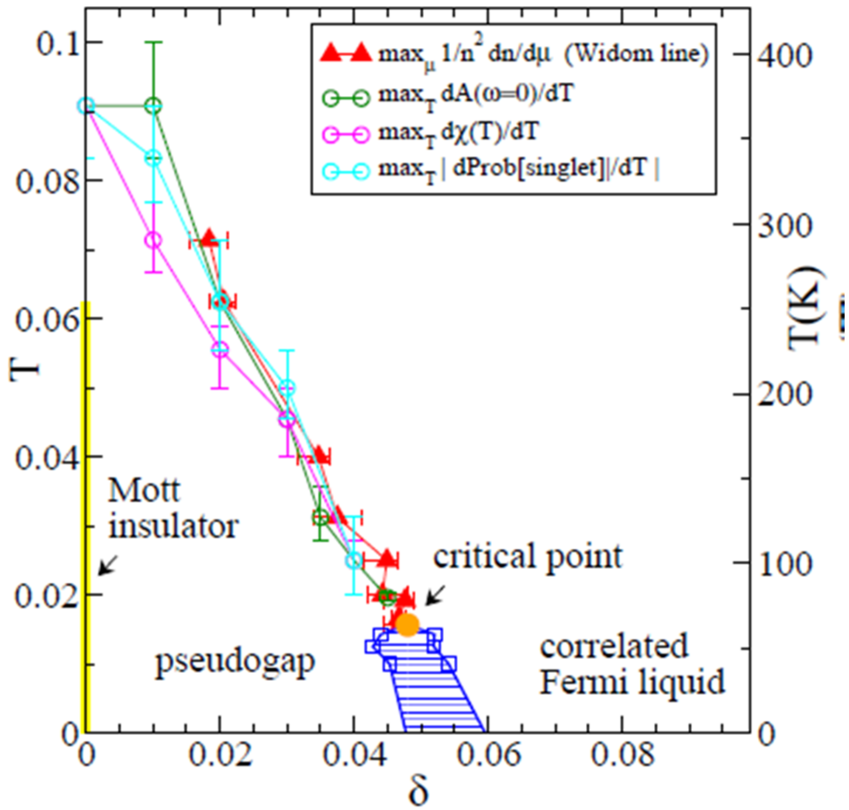


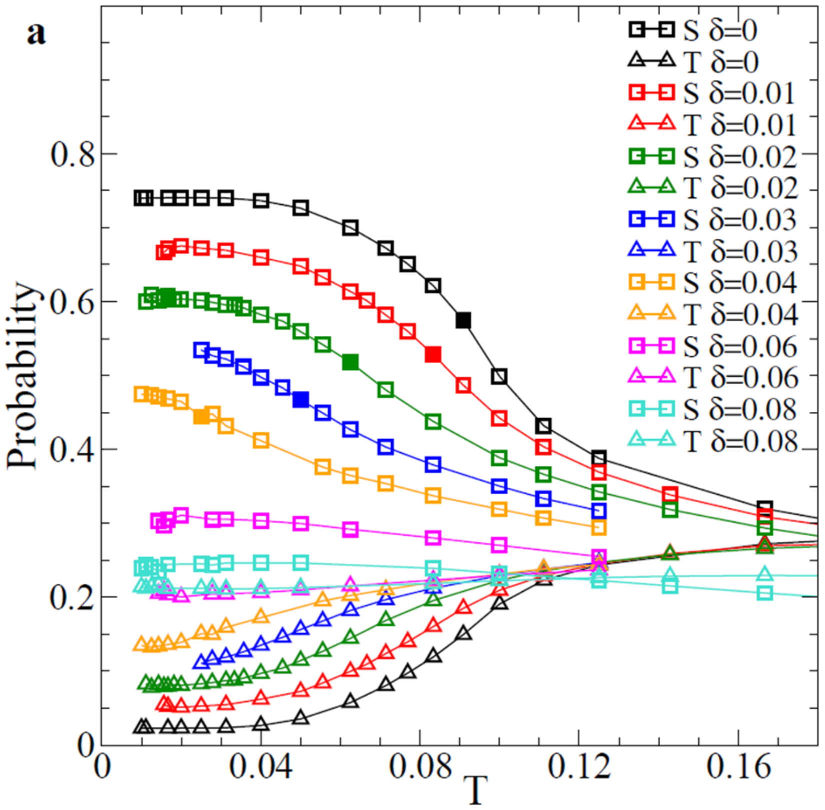


Underdoped Hg1223

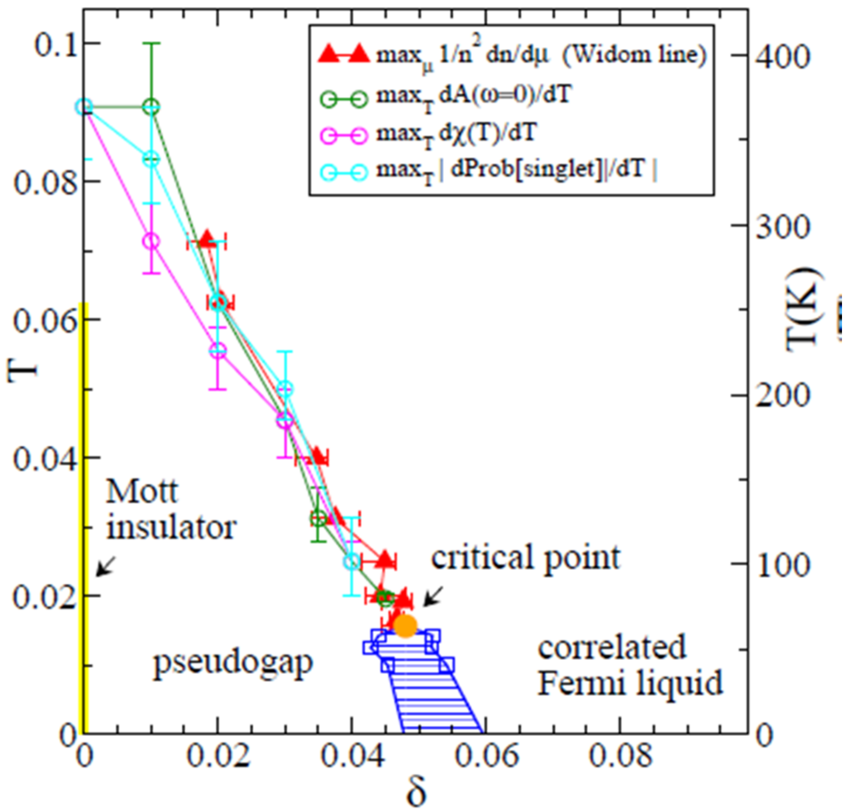
Julien et al. PRL **76,** 4238 (1996)

Plaquette eigenstates





Pseudogap *T** along the Widom line



Giovanni Sordi

Patrick Sémon

Kristjan Haule

The Widom line

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

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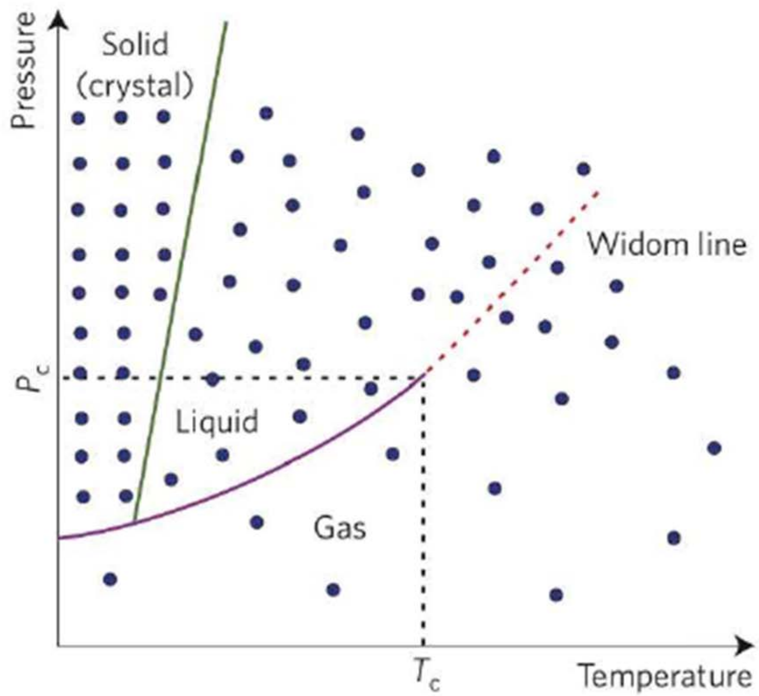
What is the Widom line?

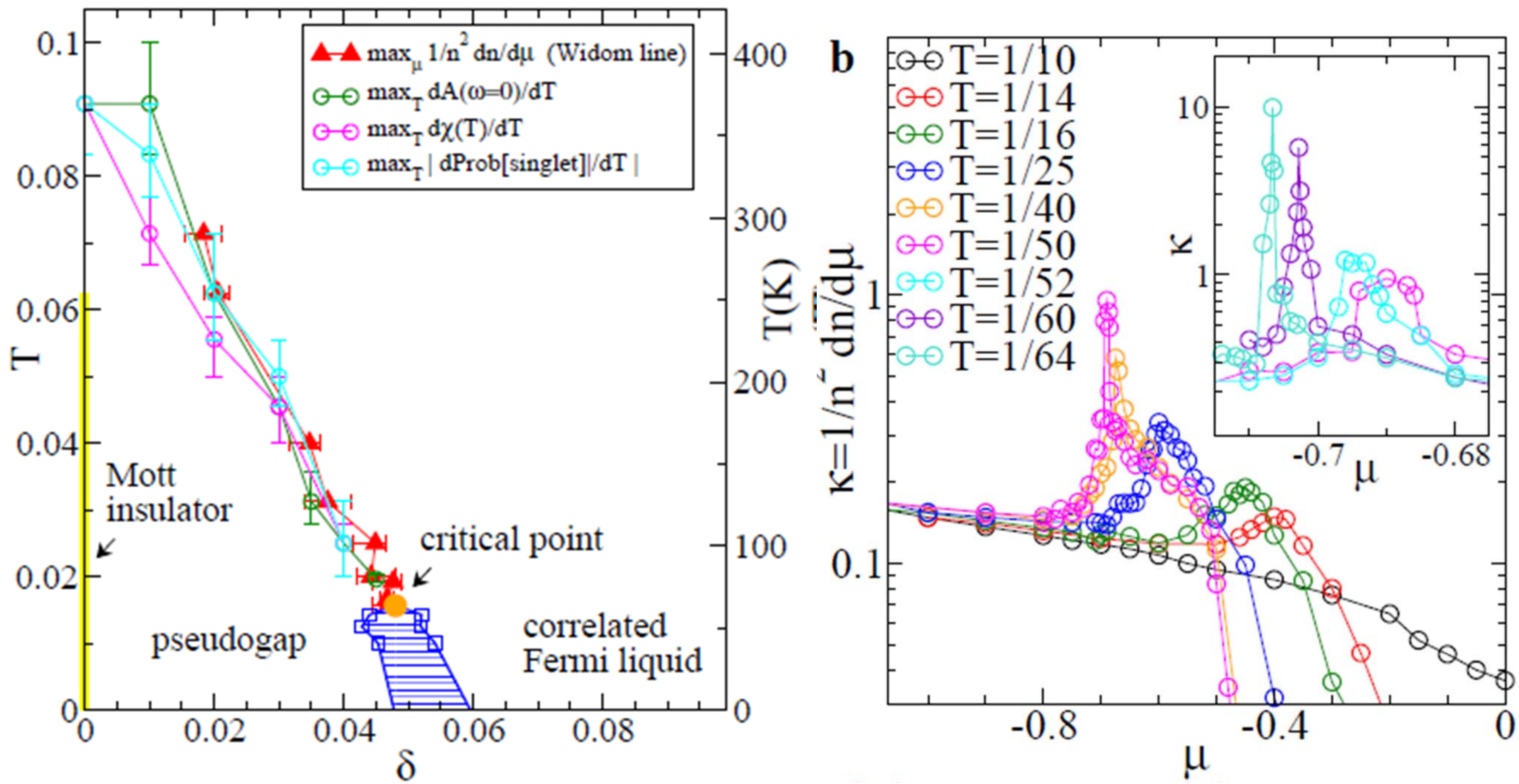


McMillan and Stanley, Nat Phys 2010

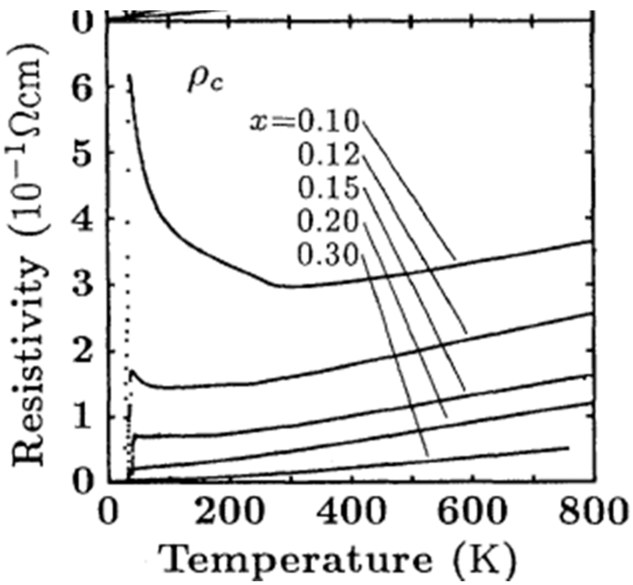
- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity C_p, isothermal compressibility, isobaric heat expansion, etc

- DYNAMIC crossover arises from crossing the Widom line!
  water: Xu et al, PNAS 2005, Simeoni et al Nat Phys 2010

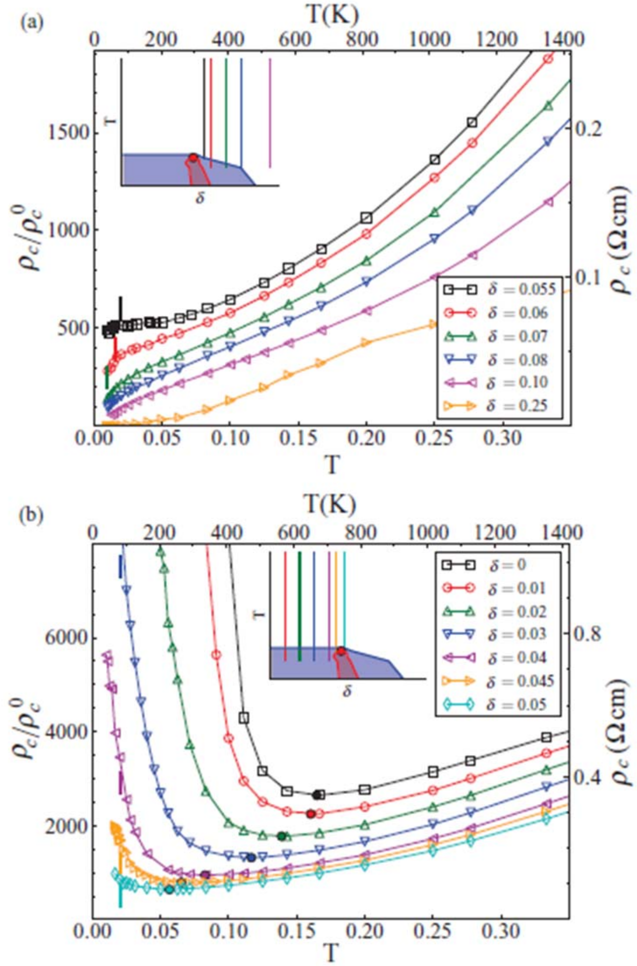
Phase diagram



C-axis resistivity

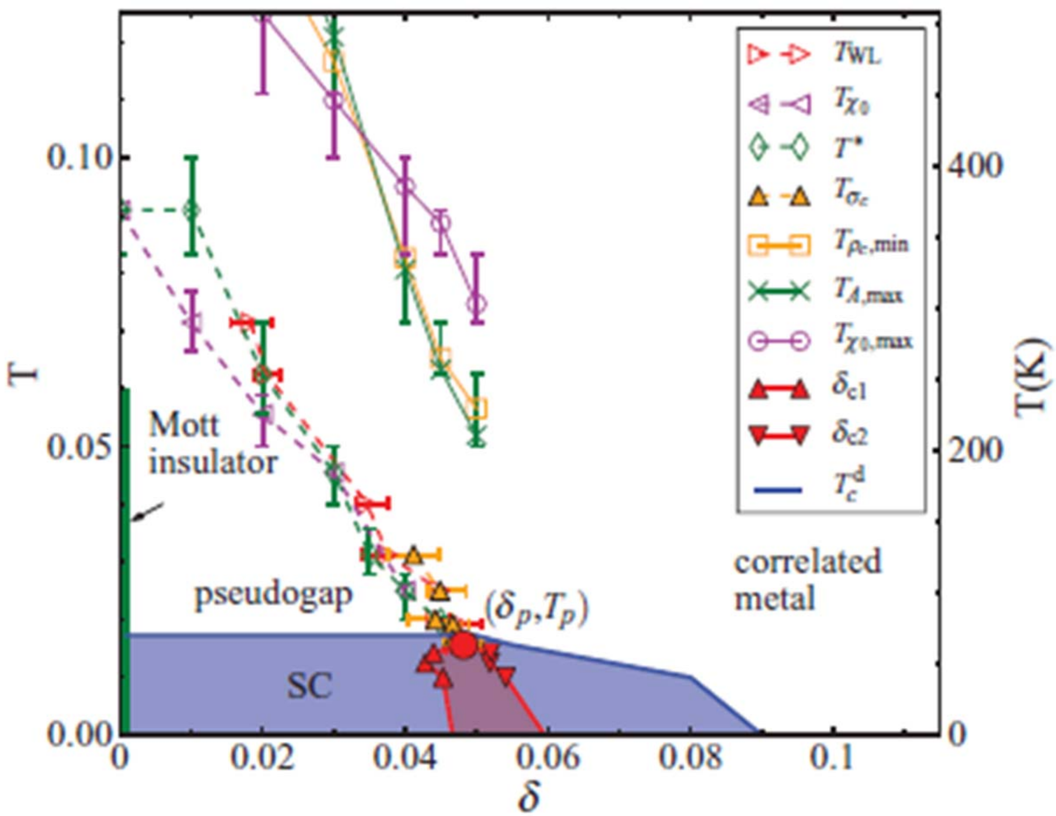


Y. Nakamura, S. Uchida, PRB **47**, 8369 (1993)



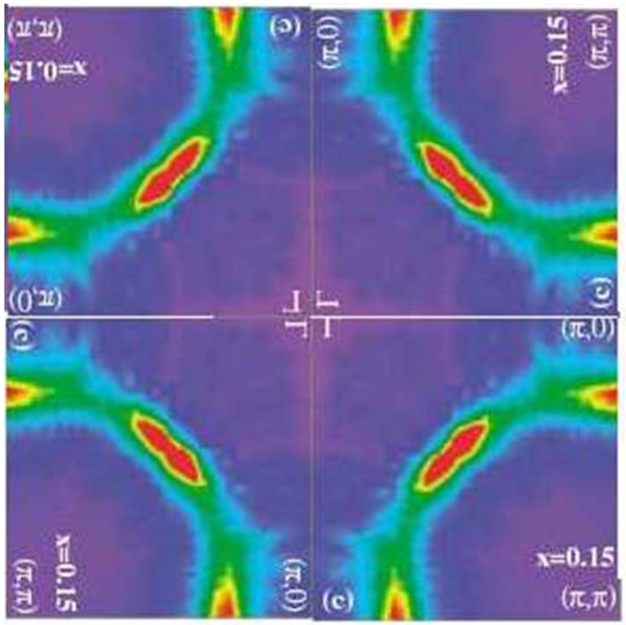
G. Sordi, P. Sémon, K. Haule, A.-M.S.T
PRB, **87**, 041101(R) (2013)

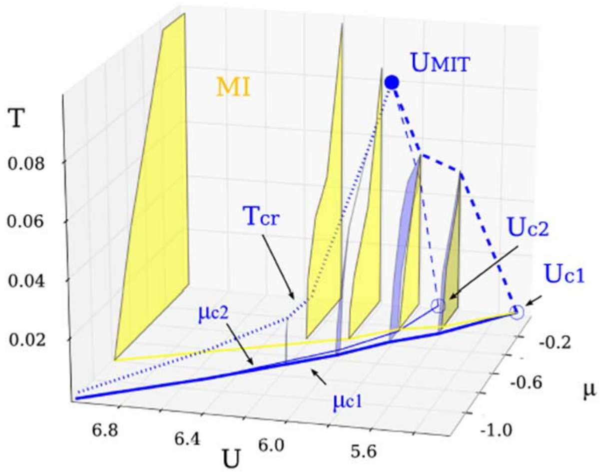
Two crossover lines



G. Sordi, P. Sémon, K. Haule, A.-M.S.T
PRB, **87**, 041101(R) (2013)

Summary


x=0.15
(π,π)
(π,0)
Γ
(c)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MI
U_MIT
T_cr
U_c2
U_c1
μ_c2
μ_c1
U
μ
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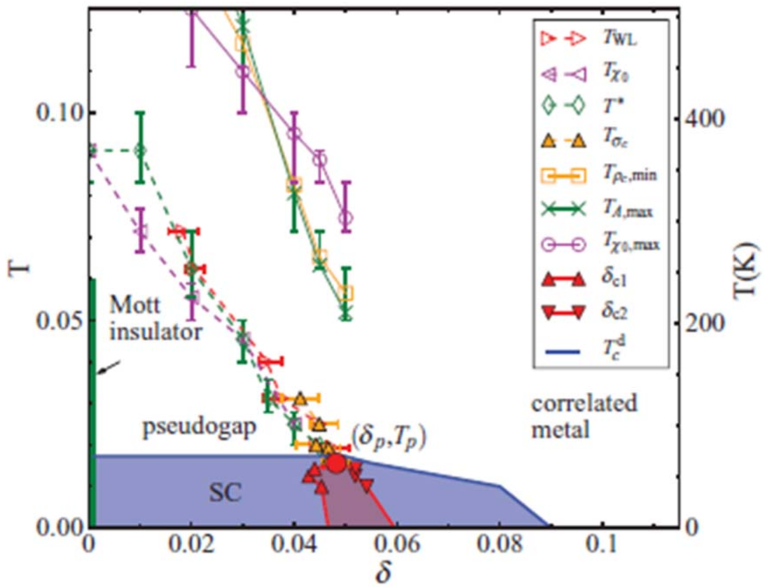
0.02
6.8
6.4
6.0
5.6
-0.2
-0.6
-1.0


Mott insulator
pseudogap
SC
correlated metal
(δ_p,T_p)
T
T(K)
δ
0.10
0.05
0.00
400
200
0
0.02
0.04
0.06
0.08
0.1

Main collaborators

Giovanni Sordi

Kristjan Haule

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David Sénéchal

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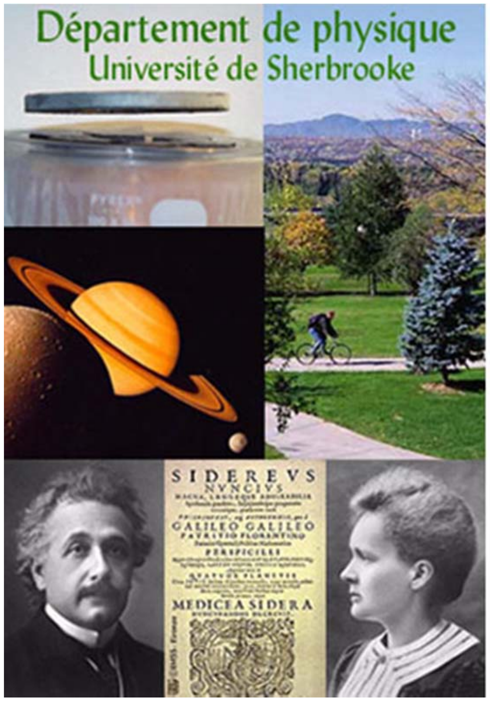
André-Marie Tremblay



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Merci

Thank you