Sucesses and limitations of dynamical mean field theory

A.-M. Tremblay

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S. Okamoto, B. Kyung, M. Civelli

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MIT, 20 October, 2011

VERITATEM IN CHARITATE

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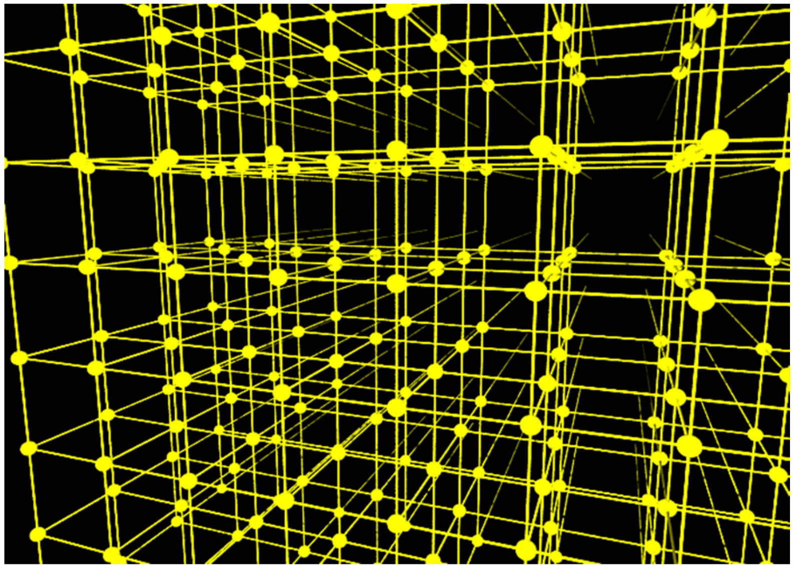
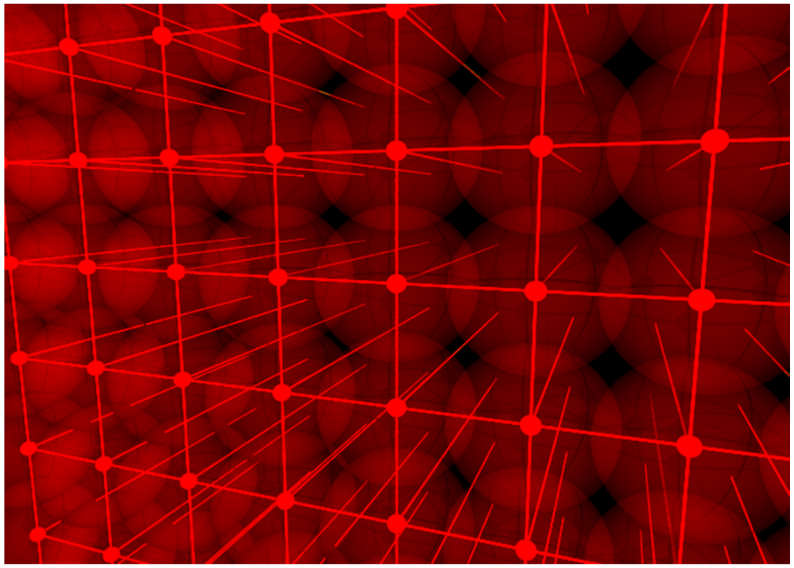
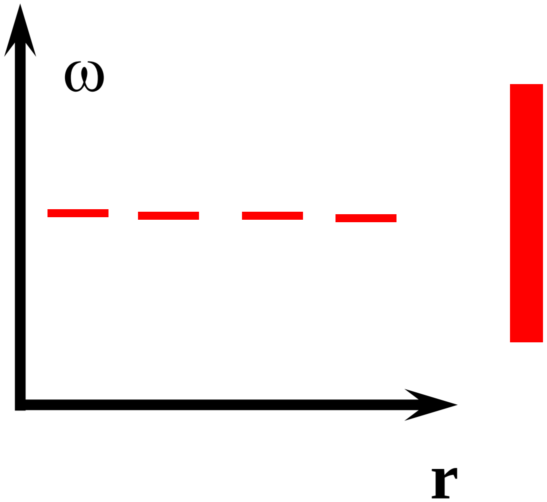
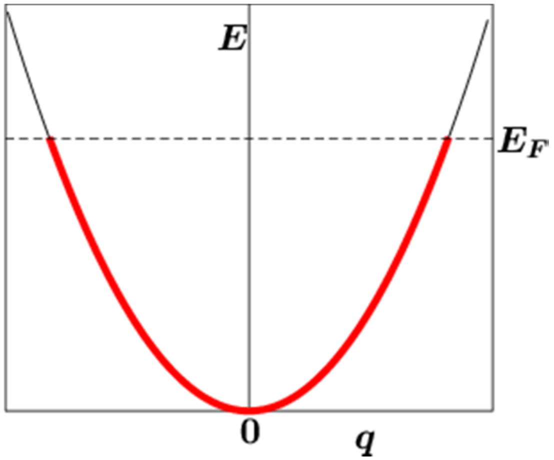
How to make a metal









Courtesy, S. Julian

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Not always

NiO, Boer and Verway

Peierls, 1937

Mott, 1949

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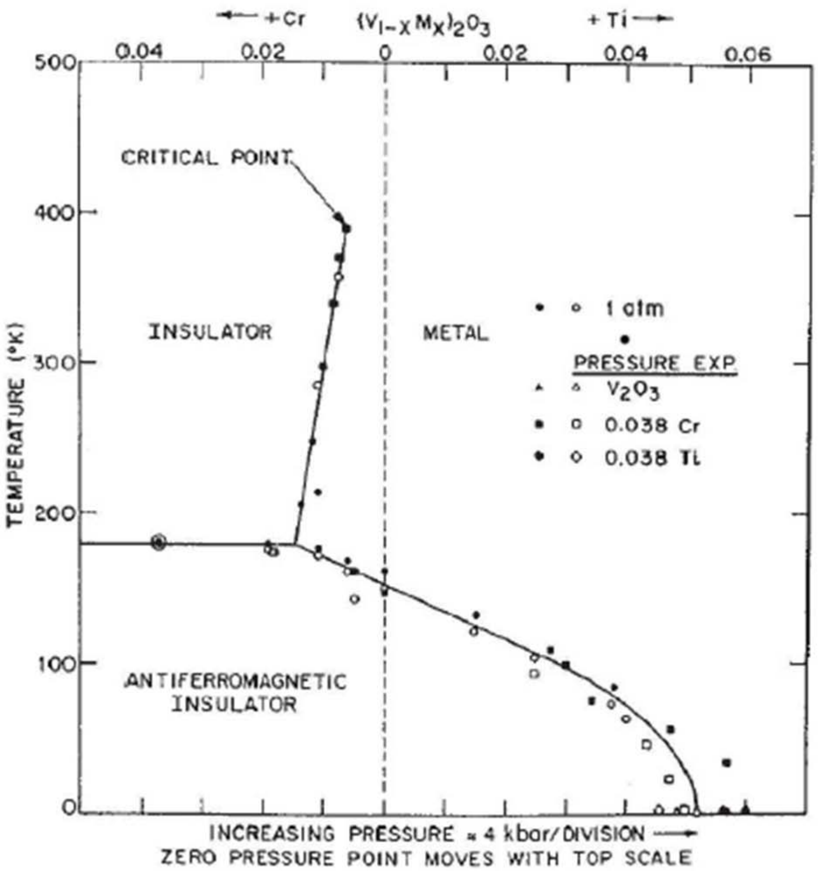
« Conventional » Mott transition

T



p

Understood from Hubbard model and dynamical mean field theory

Figure: McWhan, PRB 1970; Limelette, Science 2003

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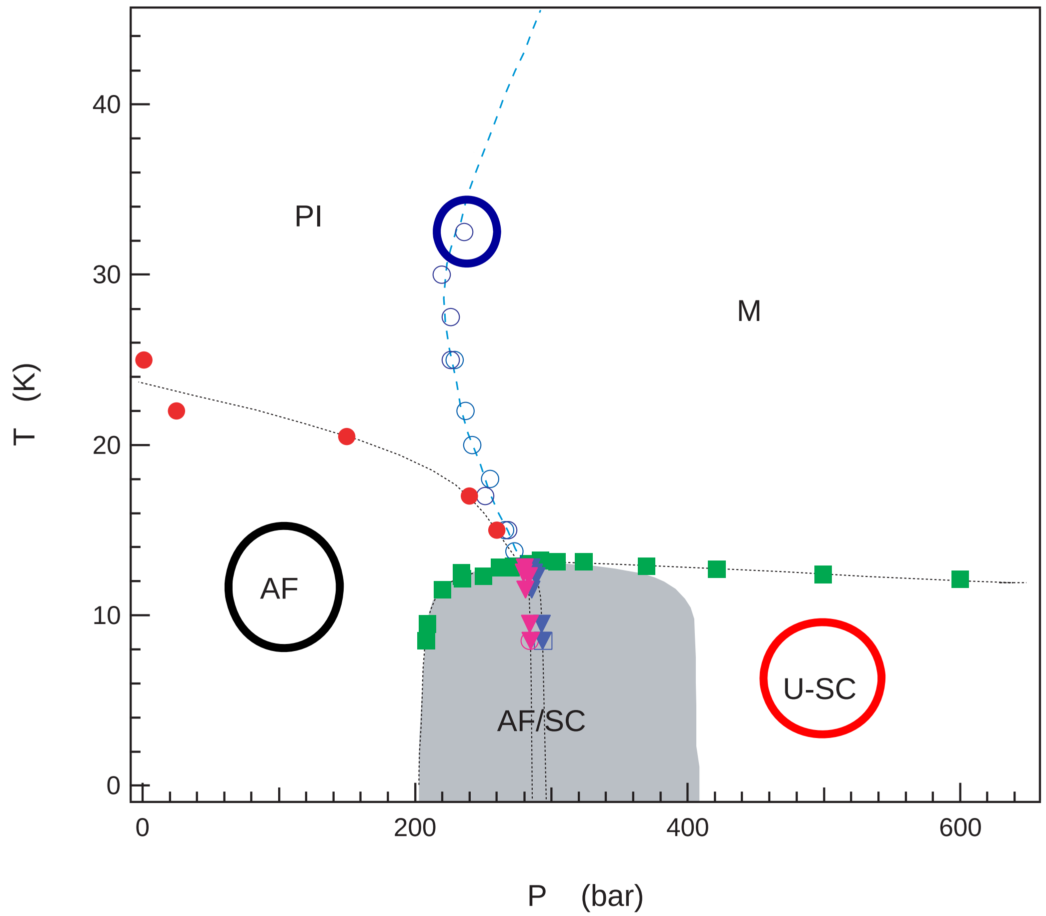
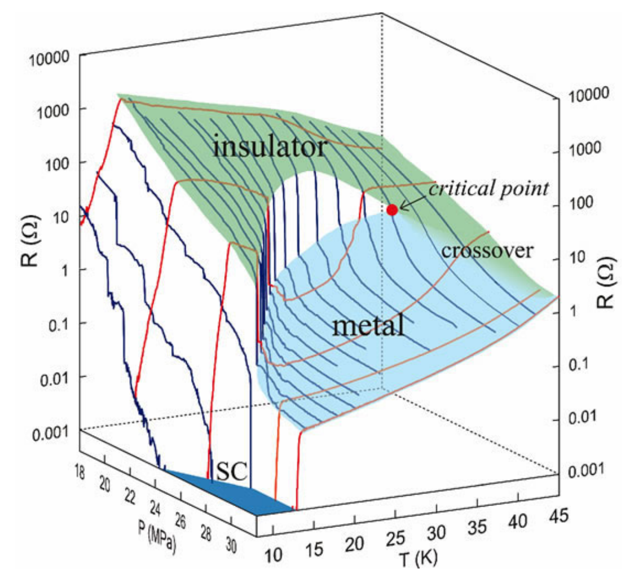
Bare Mott critical point in organics





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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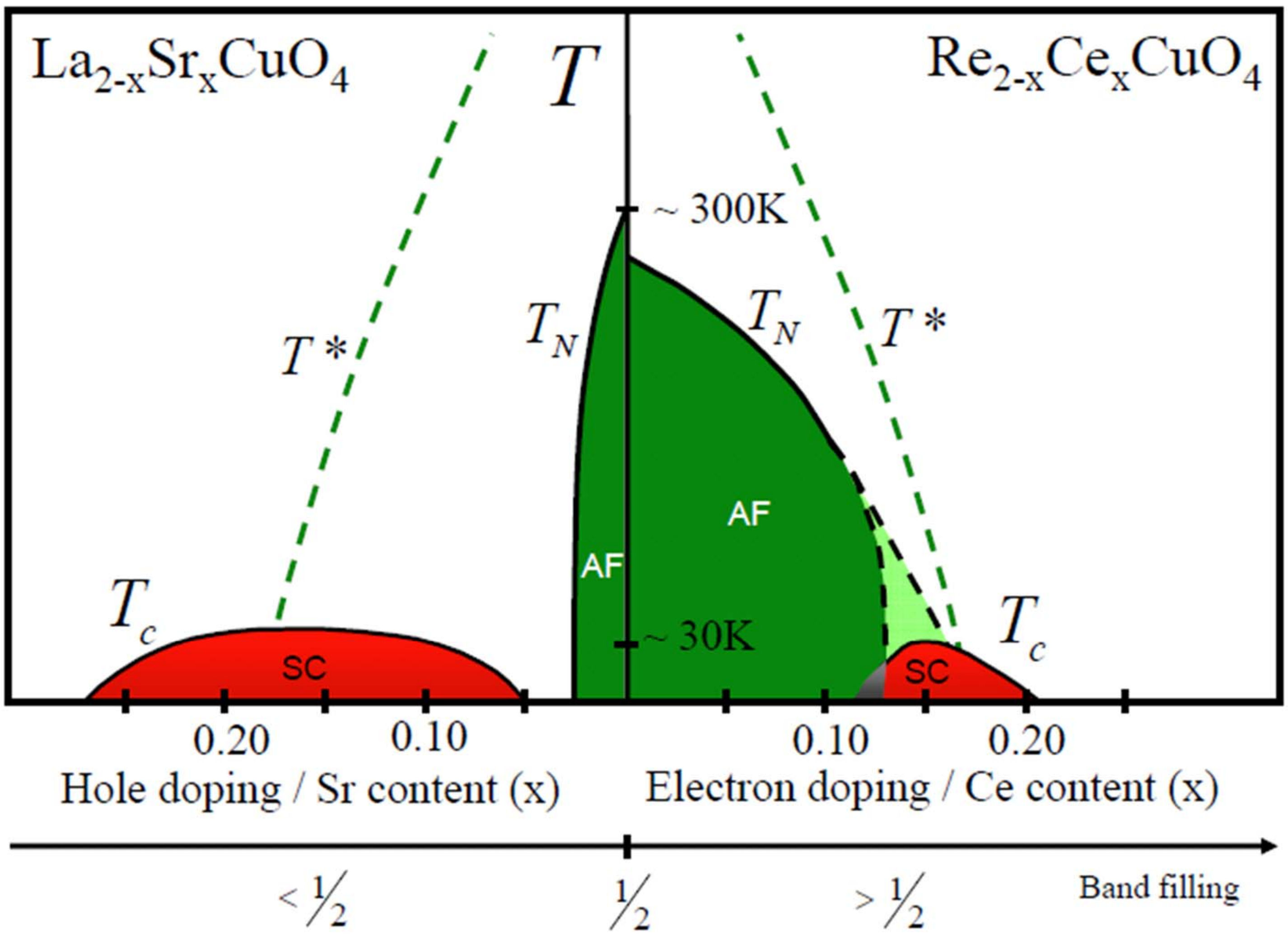
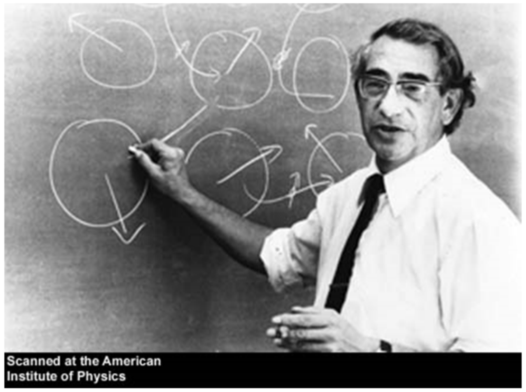
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

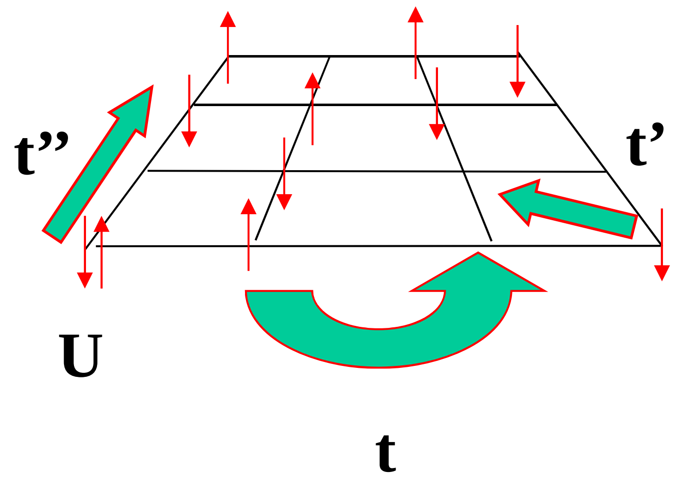


Hubbard model



1931-1980

μ



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

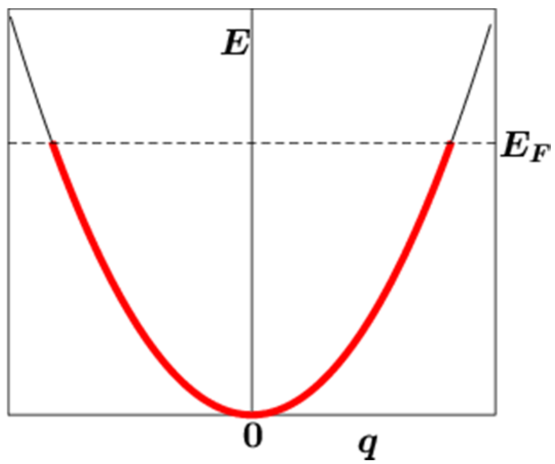
$U = 0$

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

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma}$$

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}$$

$$|\Psi\rangle = \prod_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma}^{\dagger} |0\rangle$$



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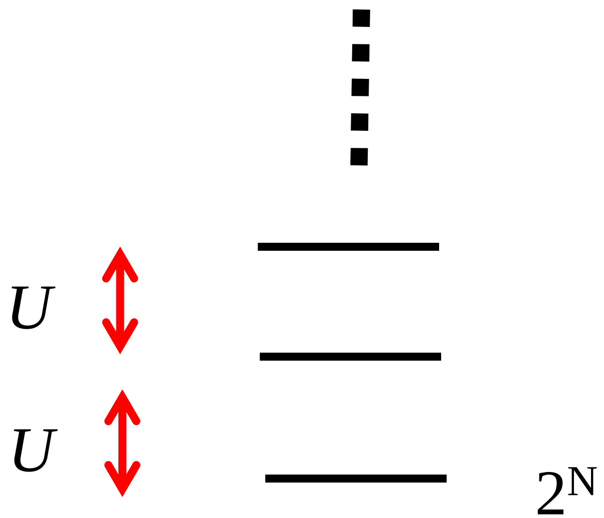
$t_{ij} = 0$

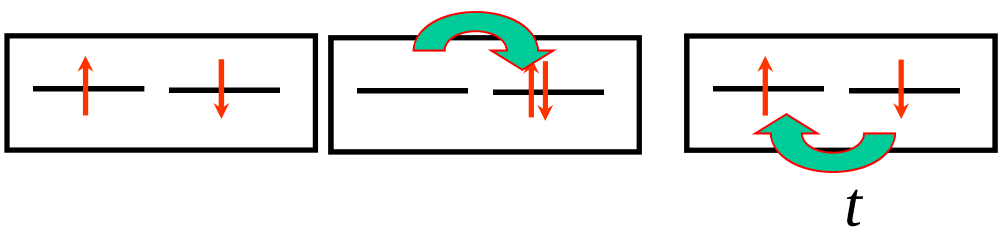
$$H = U\sum_i n_{i\uparrow}n_{i\downarrow}$$



$$|\Psi\rangle = \prod_{\mathbf{i}} c^{\dagger}_{\mathbf{i}\uparrow} \prod_{\mathbf{j}} c^{\dagger}_{\mathbf{j}\downarrow} |0\rangle$$

Antiferromagnetism in the Hubbard model

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



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

Measurable quantities : Green's functions

$$\langle \mathcal{O} \rangle \equiv \frac{Tr\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{Tr\left[e^{-\beta(H-\mu N)}\right]}$$

$$\begin{aligned}\mathcal{G}_{\mathbf{k}\sigma}(\tau) &= -\langle T_\tau[c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}\sigma}]\rangle \\ &= -\theta(\tau)\langle c_{\mathbf{k}\sigma}(\tau)c^\dagger_{\mathbf{k}\sigma}\rangle + \theta(-\tau)\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}(\tau)\rangle.\end{aligned}$$

$$c_{\mathbf{k}\sigma}(\tau) = e^{(H-\mu N)\tau}c_{\mathbf{k}\sigma}e^{-(H-\mu N)\tau}$$

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau}\mathcal{G}_{\mathbf{k}\sigma}(\tau)$$

$$\omega_n = (2n+1)\pi T$$

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Green's function: free electrons, atomic limit

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

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_{\mathbf{k}} - \mu)}$$

$$H = \qquad U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\langle n \rangle = 1 \qquad \mathcal{G}_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}$$

Self-energy and all that

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

$$\mathcal{G}_{\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_{\mathbf{k}} - \mu) - \Sigma_{\mathbf{k}\sigma}(i\omega_n)}$$

$$\mathcal{G}^{-1}_{\mathbf{k}\sigma}(i\omega_n) = \mathcal{G}^{0-1}_{\mathbf{k}\sigma}(i\omega_n) - \Sigma_{\mathbf{k}\sigma}(i\omega_n)$$

Self-energy in the atomic limit for $n = 1$

$$\mathcal{G}_\sigma(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}}$$

$$\mathcal{G}_\sigma(i\omega_n) = \frac{1}{i\omega_n + \frac{U}{2} - \Sigma(i\omega_n)} \qquad \Sigma(i\omega_n) = \frac{U}{2} + \frac{U^2}{i\omega_n}$$

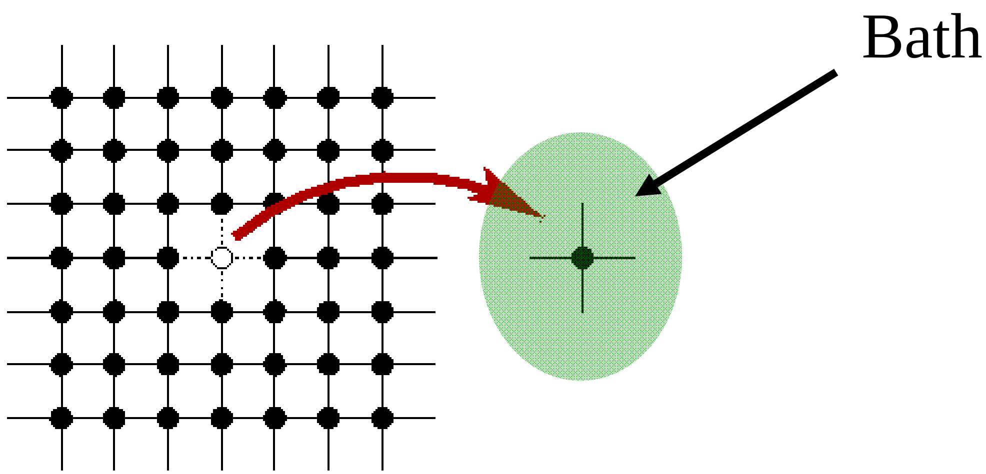
Outline

- Dynamical Mean-Field Theory (derivations)
- Example of « impurity solvers »
  - – Exact diagonalization
  - – Strong coupling continuous-time QMC
- Example of results
- Limitations, problems…

Dynamical Mean-Field Theory

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.

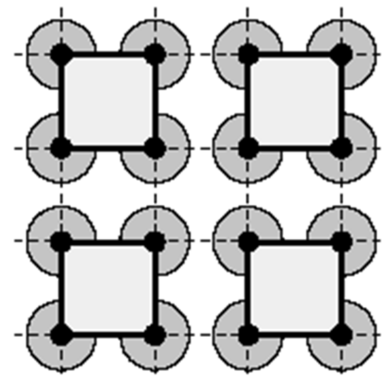


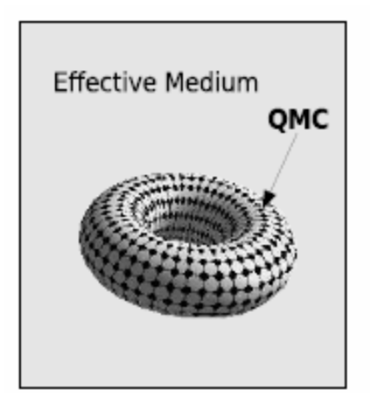
W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, (*d = 3)*

2d Hubbard: Quantum cluster method

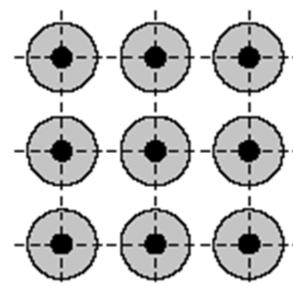
C-DMFT





DCA

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)

Self-consistency

$$\mathcal{G}_{\sigma}^{imp}(i\omega_n)^{-1} = \mathcal{G}_{\sigma}^{0-imp}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n)$$

$$N_c \int \frac{d^d\widetilde{\mathbf{k}}}{(2\pi)^d} \frac{1}{\mathcal{G}_{\widetilde{\mathbf{k}}\sigma}^{0}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n)} = \mathcal{G}_{\sigma}^{imp}(i\omega_n)$$

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Methods of derivation

- Cavity method
- Local nature of perturbation theory in infinite dimensions
- Expansion around the atomic limit
- Effective medium theory
- Potthoff self-energy functional

M. Potthoff, Eur. Phys. J. B **32**, 429 (2003).
A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).

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).

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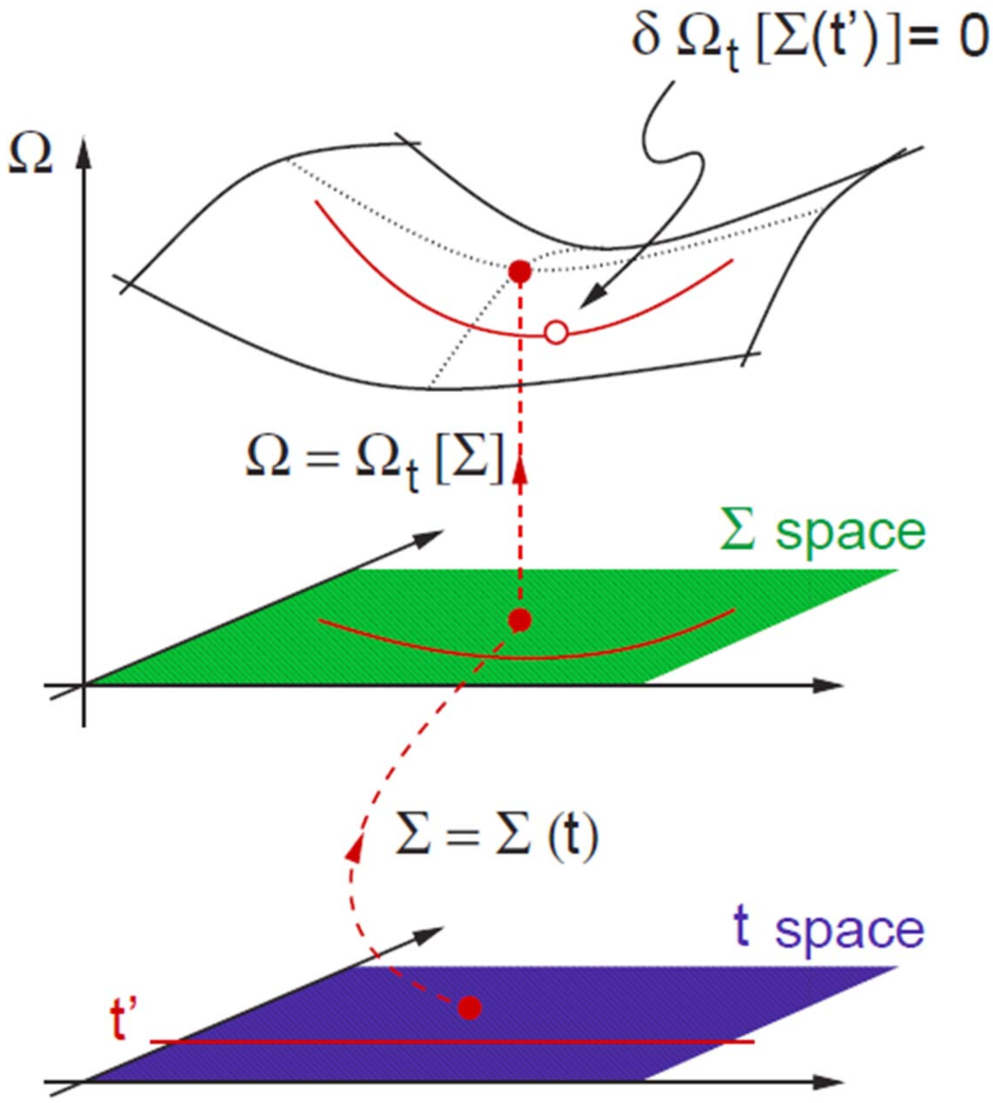
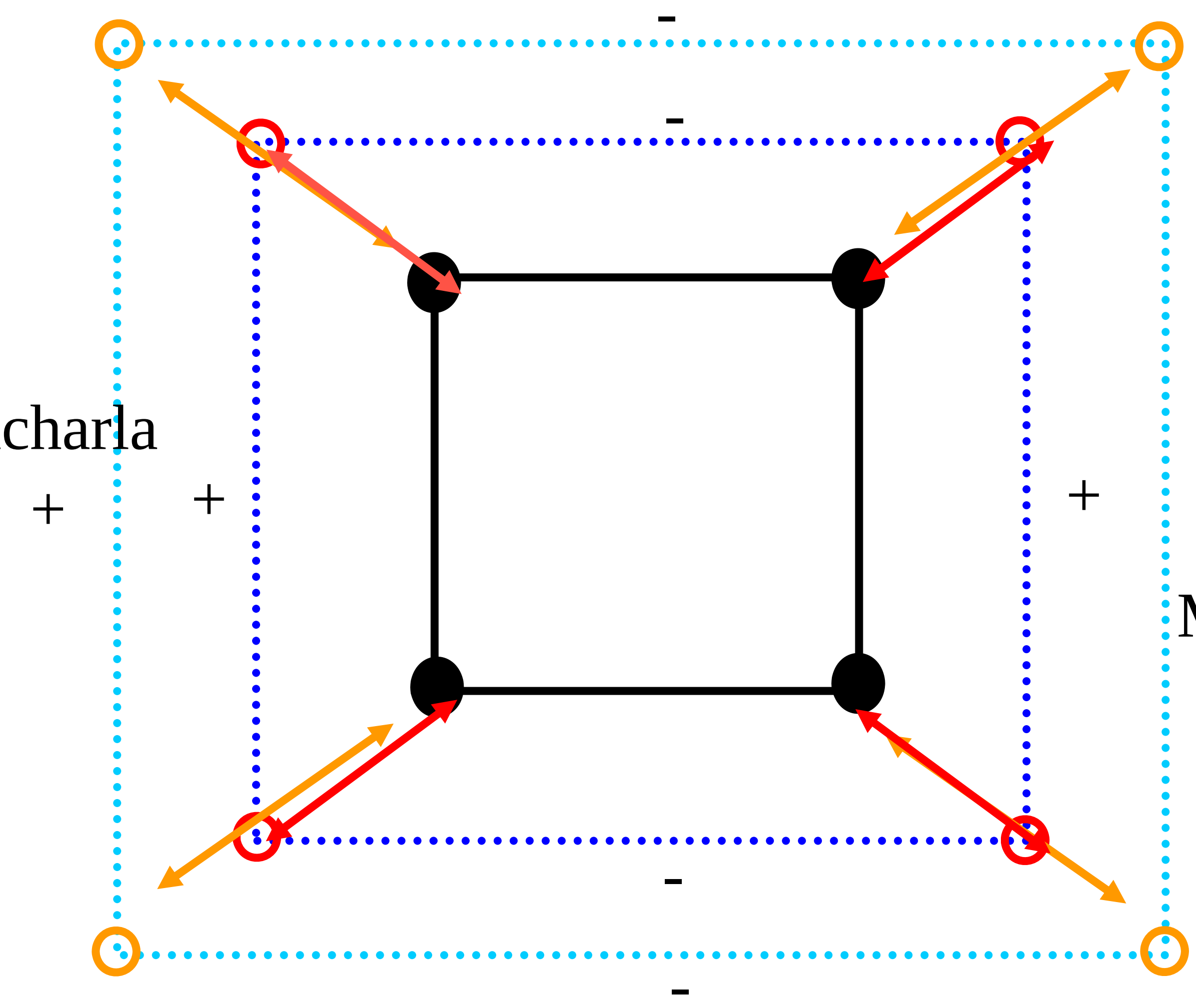
DMFT as a stationnary point



Impurity solvers

CDMFT + ED

Sarma Kancharla



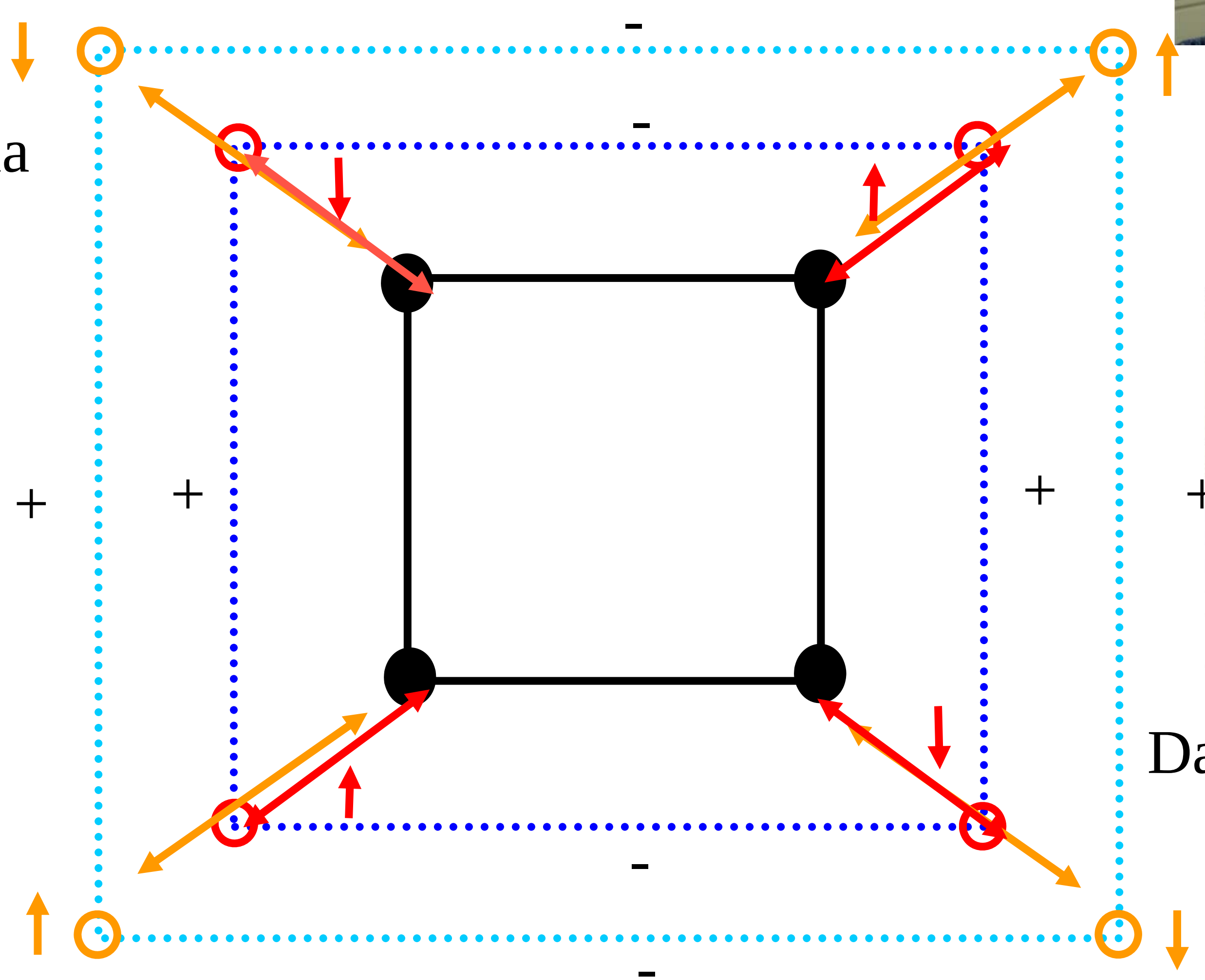
Marcello Civelli

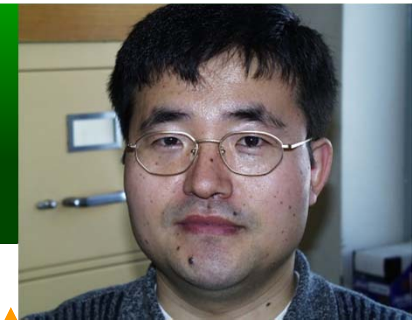
Caffarel and Krauth, PRL (1994)

No Weiss field on the cluster!

Competition AFM-dSC

S. Kancharla





B. Kyung

David Sénéchal

See also, Capone and Kotliar, Phys. Rev. B 74, 054513 (2006),
Macridin, Maier, Jarrell, Sawatzky, Phys. Rev. B 71, 134527 (2005)

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Monte Carlo method

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner,
Rev.Mod.Phys. **83**, 349 (2011)

$$Z = \int_{\mathcal{C}} d\mathbf{x}\, p(\mathbf{x}).$$

$$\langle A \rangle_p = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}).$$

$$\langle A \rangle_p \approx \langle A \rangle_{\mathrm{MC}} \equiv \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(\mathbf{x}_i).$$

$$\langle A \rangle = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}) = \frac{\int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x})[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})}{\int_{\mathcal{C}} d\mathbf{x}[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})} \equiv \frac{\langle A(p/\rho) \rangle_\rho}{\langle p/\rho \rangle_\rho}.$$

Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

$$\frac{W_{\mathbf{xy}}}{W_{\mathbf{yx}}} = \frac{p(\mathbf{y})}{p(\mathbf{x})} \qquad W_{\mathbf{xy}} = W_{\mathbf{xy}}^{\text{prop}} W_{\mathbf{xy}}^{\text{acc}}$$

$$W_{\mathbf{xy}}^{\text{acc}} = \min[1, R_{\mathbf{xy}}] \qquad R_{\mathbf{xy}} = \frac{p(\mathbf{y}) W_{\mathbf{yx}}^{\text{prop}}}{p(\mathbf{x}) W_{\mathbf{xy}}^{\text{prop}}}$$

Reminder on perturbation theory

$$\exp(-\beta(H_a + H_b)) = \exp(-\beta H_a)U(\beta)$$

$$\frac{\partial U(\beta)}{\partial \beta} = -H_b(\beta)U(\beta)$$

$$U(\beta) = 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots$$

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Partition function as sum over configurations

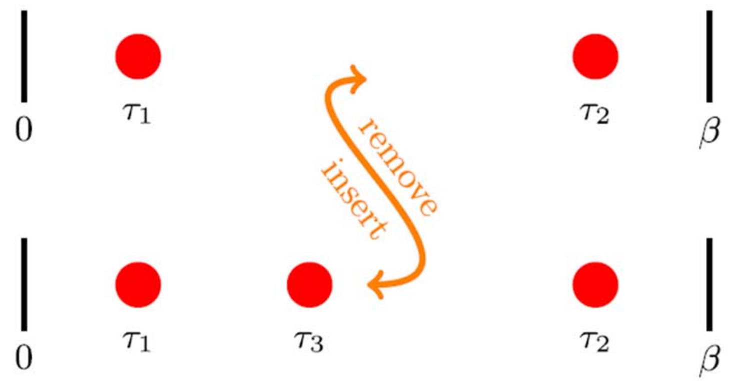
$$Z = \mathrm{Tr}[\exp(H_a + H_b)]$$

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \, \mathrm{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

$$Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k w(k, \gamma, \tau_1, \ldots, \tau_k)$$

$$\mathbf{x} = (k, \gamma, (\tau_1, \ldots, \tau_k)), \qquad p(\mathbf{x}) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k,$$

Updates



$$W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')} = \frac{d\tau}{\beta}$$

$$W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})} = \frac{1}{k+1}.$$

$$\begin{aligned} R_{(k,\vec{\tau}),(k+1,\vec{\tau}')} &= \frac{p((k+1,\vec{\tau}'))}{p((k,\vec{\tau}))} \frac{W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})}}{W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')}} \\ &= \frac{w(k+1)d\tau'_1 \cdots d\tau'_{k+1}}{w(k)d\tau_1 \cdots d\tau_k} \frac{1/(k+1)}{d\tau/\beta} \\ &= \frac{w(k+1)}{w(k)} \frac{\beta}{k+1}. \end{aligned}$$

Beard, B. B., and U.-J. Wiese, 1996, Phys. Rev. Lett. **77**, 5130.

Prokof'ev, N. V., B. V. Svistunov, and I. S. Tupitsyn, 1996, JETP Lett. **64**, 911.

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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).

Expansion in powers of the hybridization

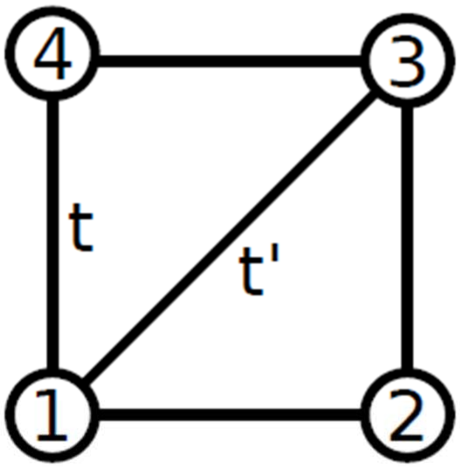
$$H_{\text{hyb}} = \sum_{pj}(V_p^j c_p^\dagger d_j + V_p^{j*} d_j^\dagger c_p) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^\dagger$$

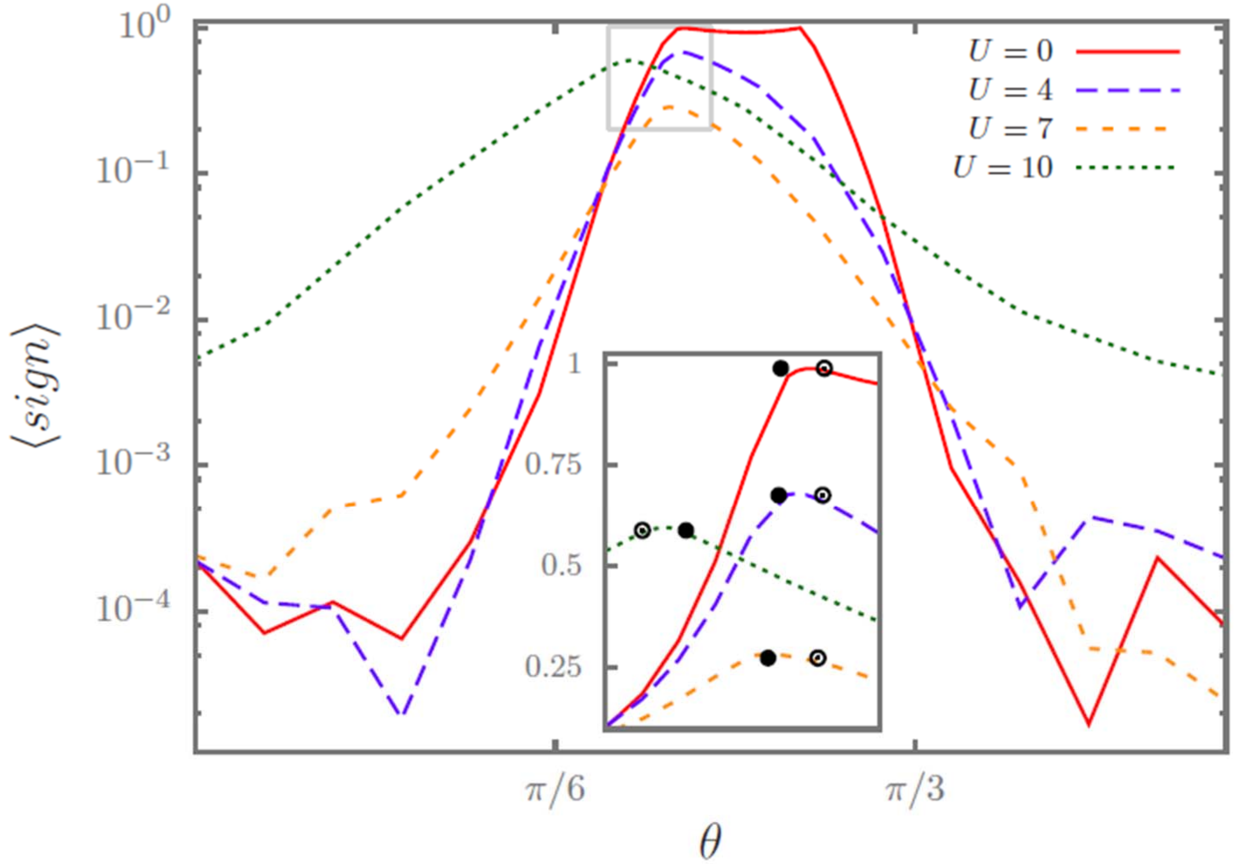
$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau_1' \cdots \int_{\tau_{k-1}'}^\beta d\tau_k'$$
$$\times \sum_{\substack{j_1,\ldots,j_k \\ j_1',\ldots,j_k'}} \sum_{\substack{p_1,\ldots,p_k \\ p_1',\ldots,p_k'}} V_{p_1}^{j_1} V_{p_1'}^{j_1'*} \cdots V_{p_k}^{j_k} V_{p_k'}^{j_k'*}$$
$$\times \mathrm{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j_k'}^\dagger(\tau_k') \cdots d_{j_1}(\tau_1) d_{j_1'}^\dagger(\tau_1')]$$
$$\times \mathrm{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p_{k'}}(\tau_k') \cdots c_{p_1}^\dagger(\tau_1) c_{p_1'}(\tau_1')].$$

$$P_m = \frac{\langle m | e^{-\beta H_{loc}} d_{j_k}(\tau_k) d_{j_k'}^\dagger(\tau_k') \ldots d_{j_1}(\tau_1) d_{j_1'}^\dagger(\tau_1') | m \rangle}{\sum_n \langle n | e^{-\beta H_{loc}} d_{j_k}(\tau_k) d_{j_k'}^\dagger(\tau_k') \ldots d_{j_1}(\tau_1) d_{j_1'}^\dagger(\tau_1') | n \rangle}$$

Sign problem

$$S = S_{\rm cl}(\boldsymbol{c}^\dagger, \boldsymbol{c}) + \int_0^\beta d\tau d\tau' \boldsymbol{c}^\dagger(\tau')\boldsymbol{\Delta}(\tau'-\tau)\boldsymbol{c}(\tau)$$





P. Sémon, A.-M.S. Tremblay, (unpub.)

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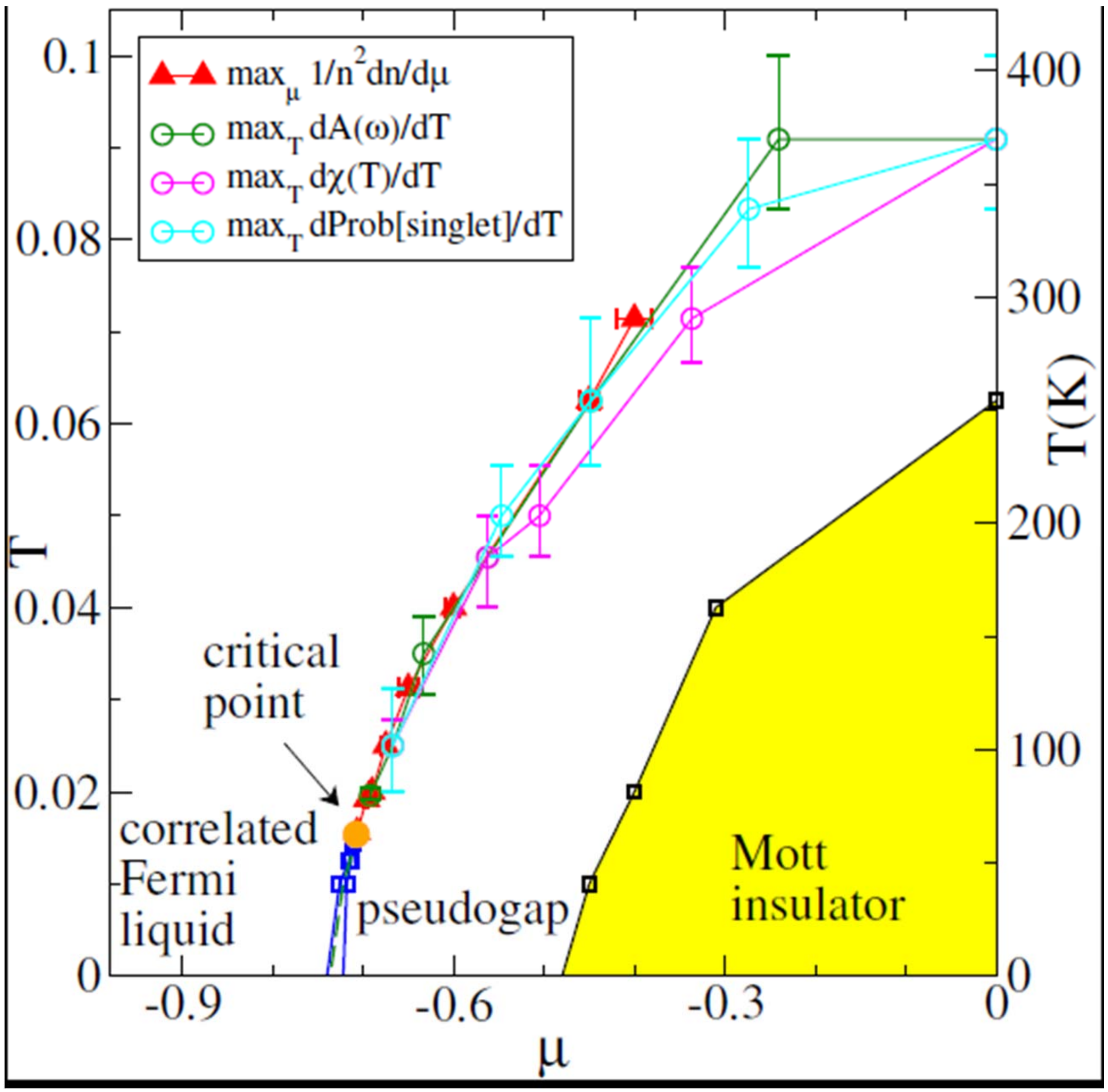
Example of results

« Normal » state

Rapid change also in dynamical quantities



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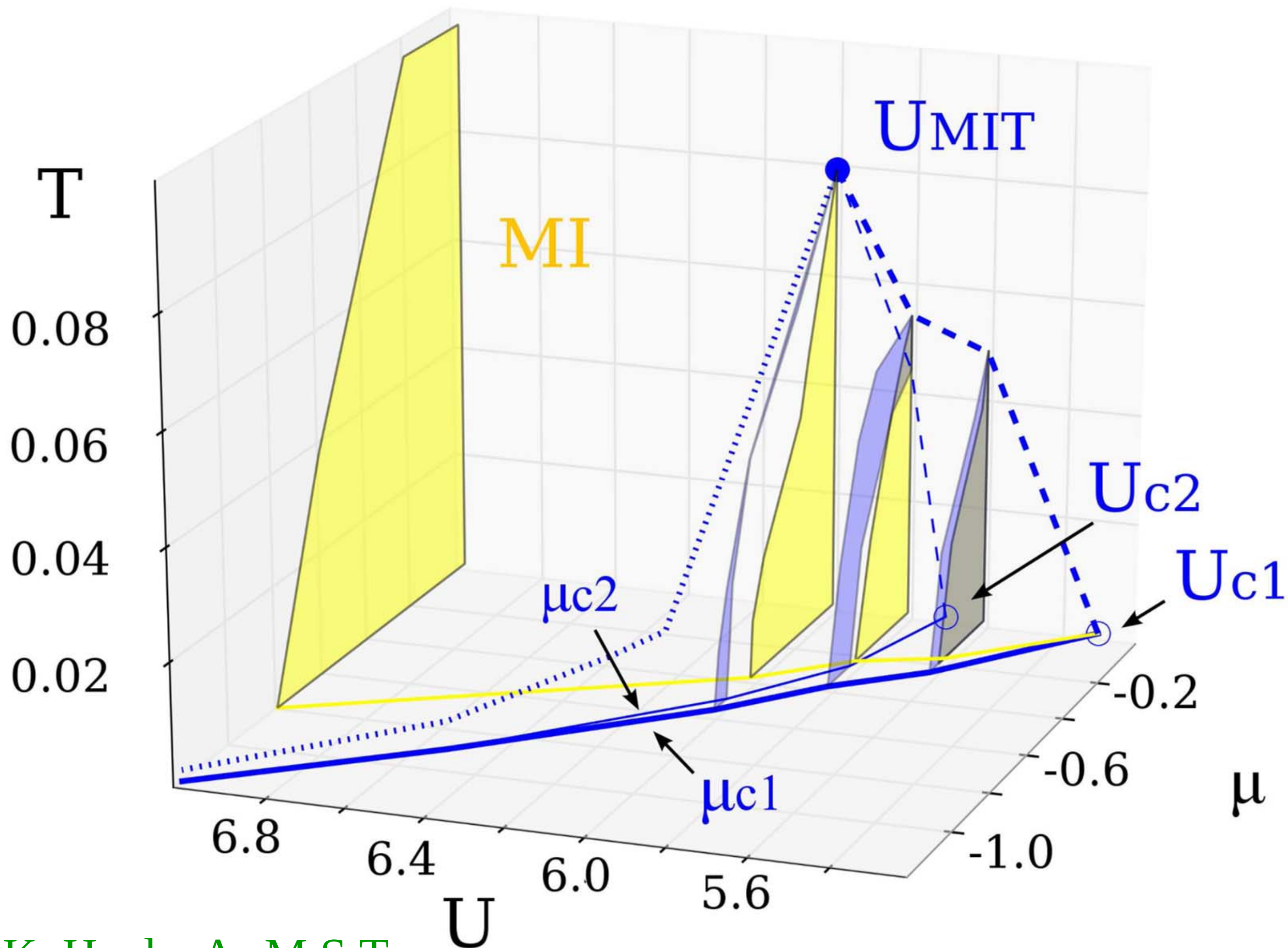
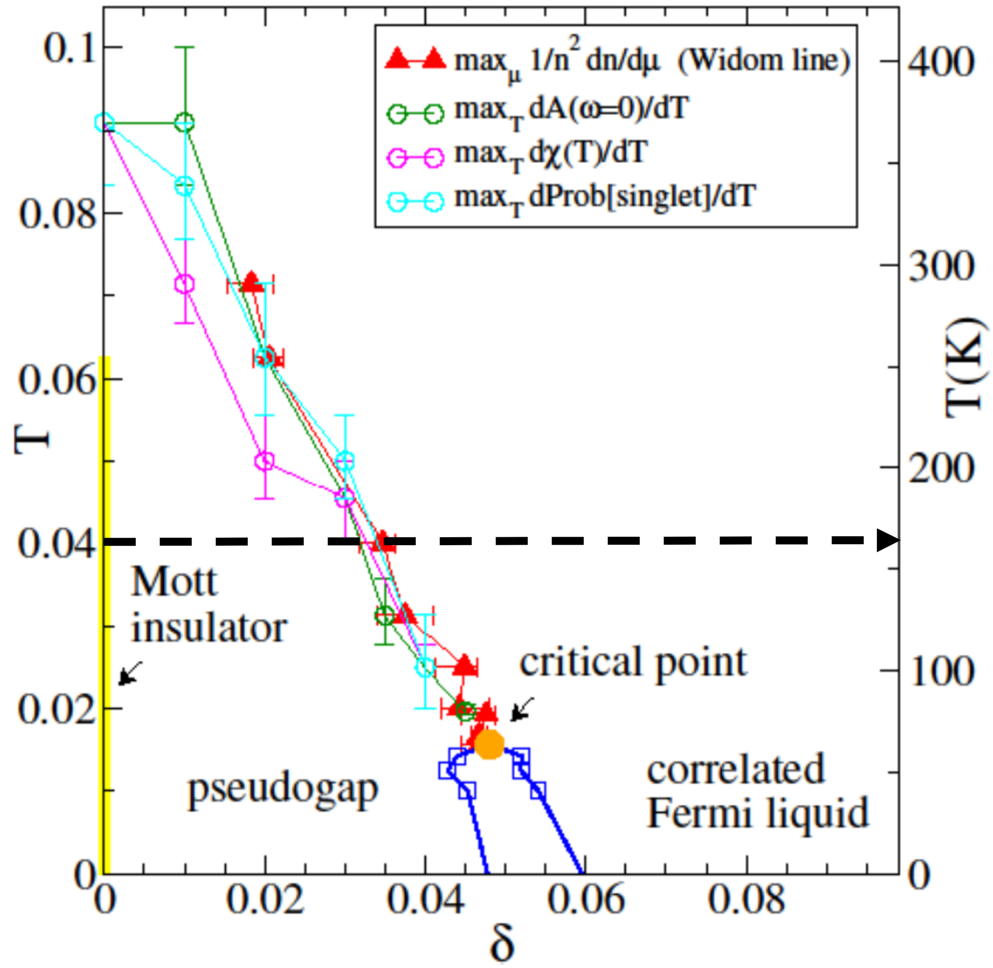
Normal state phase diagram

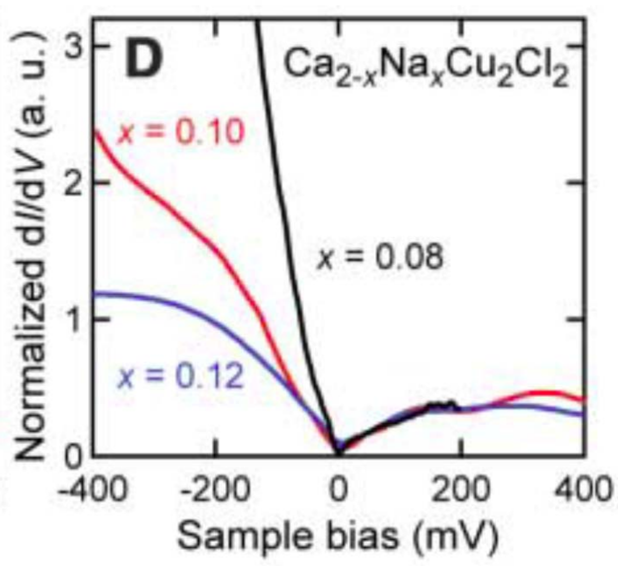


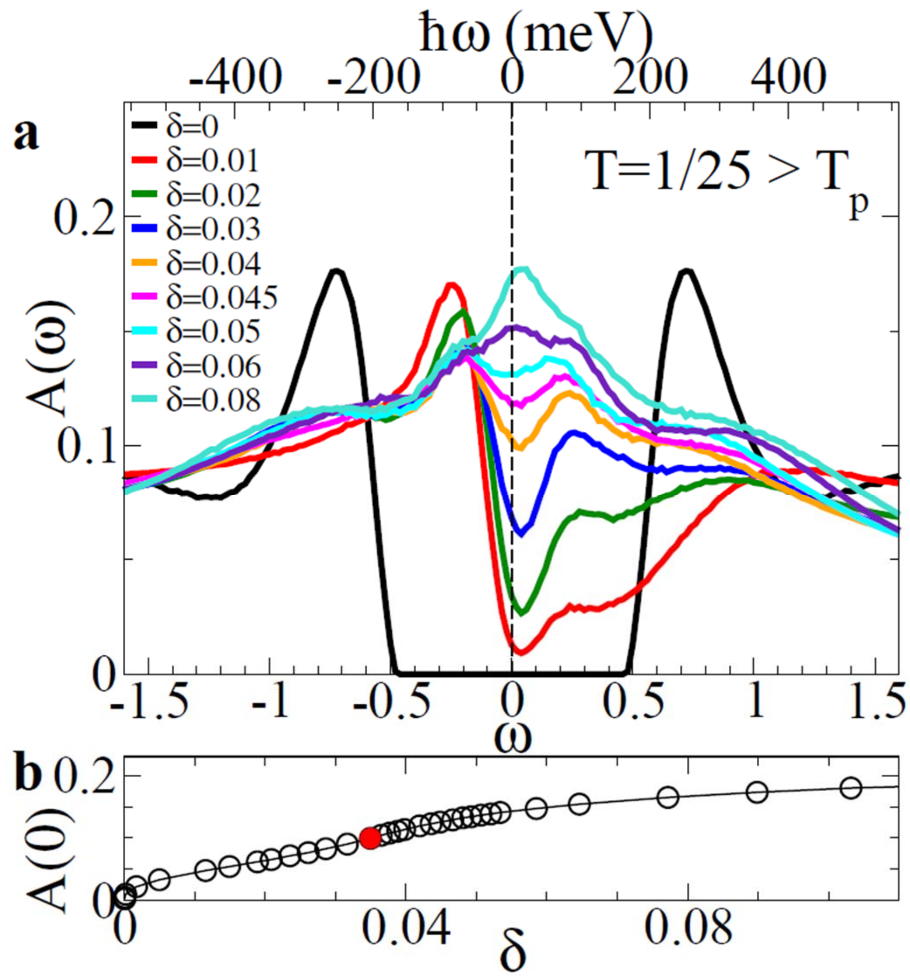
G. Sordi, K. Haule, A.-M.S.T
PRL, **104**, 226402 (2010)

Phase diagram



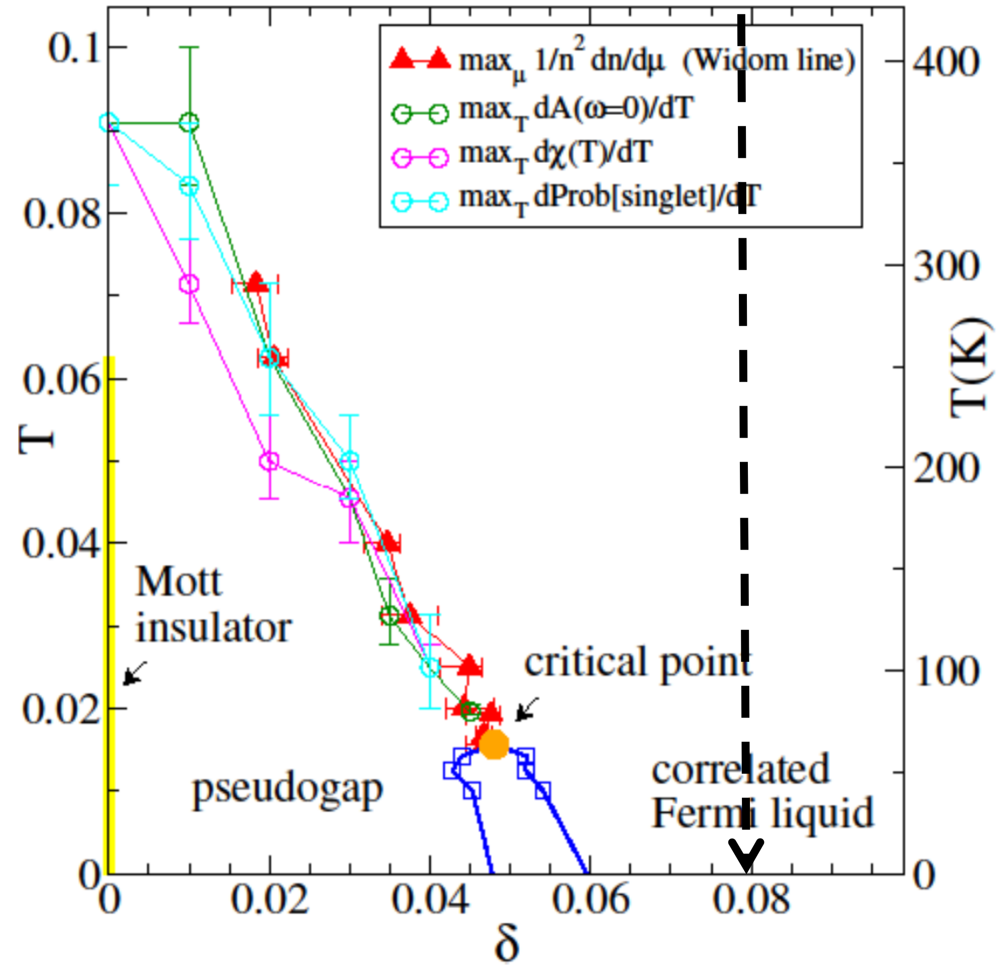
Tunneling DOS

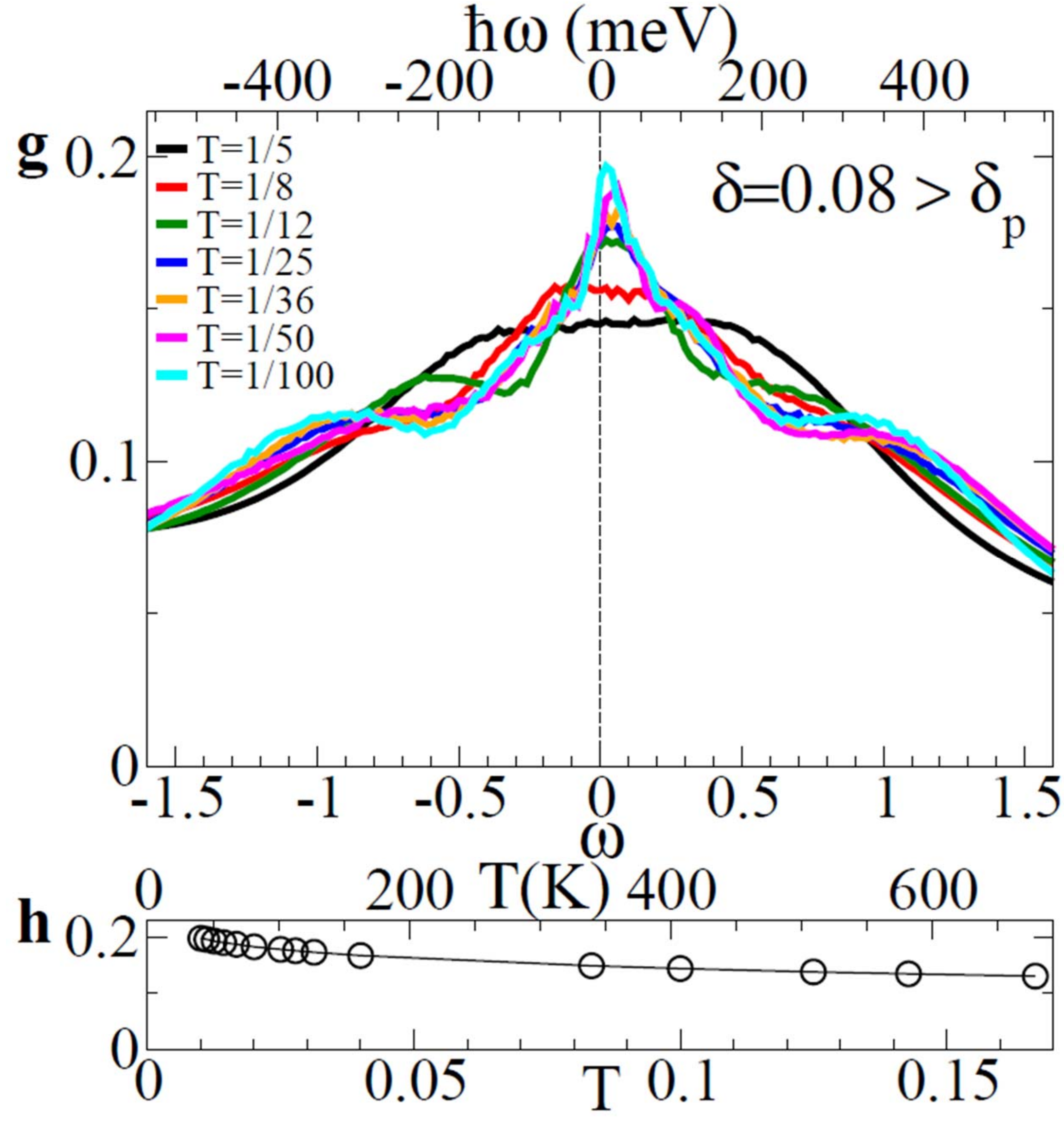




Khosaka et al. *Science* **315**, 1380 (2007);

Phase diagram





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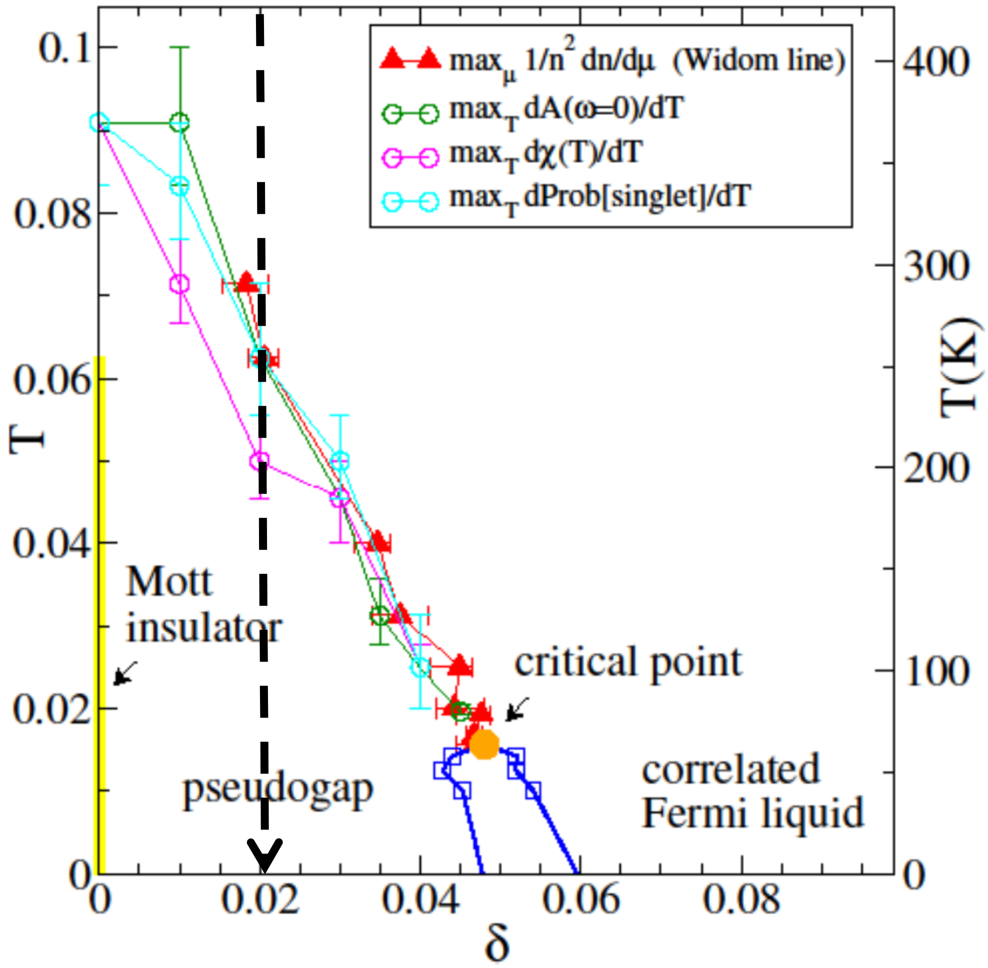
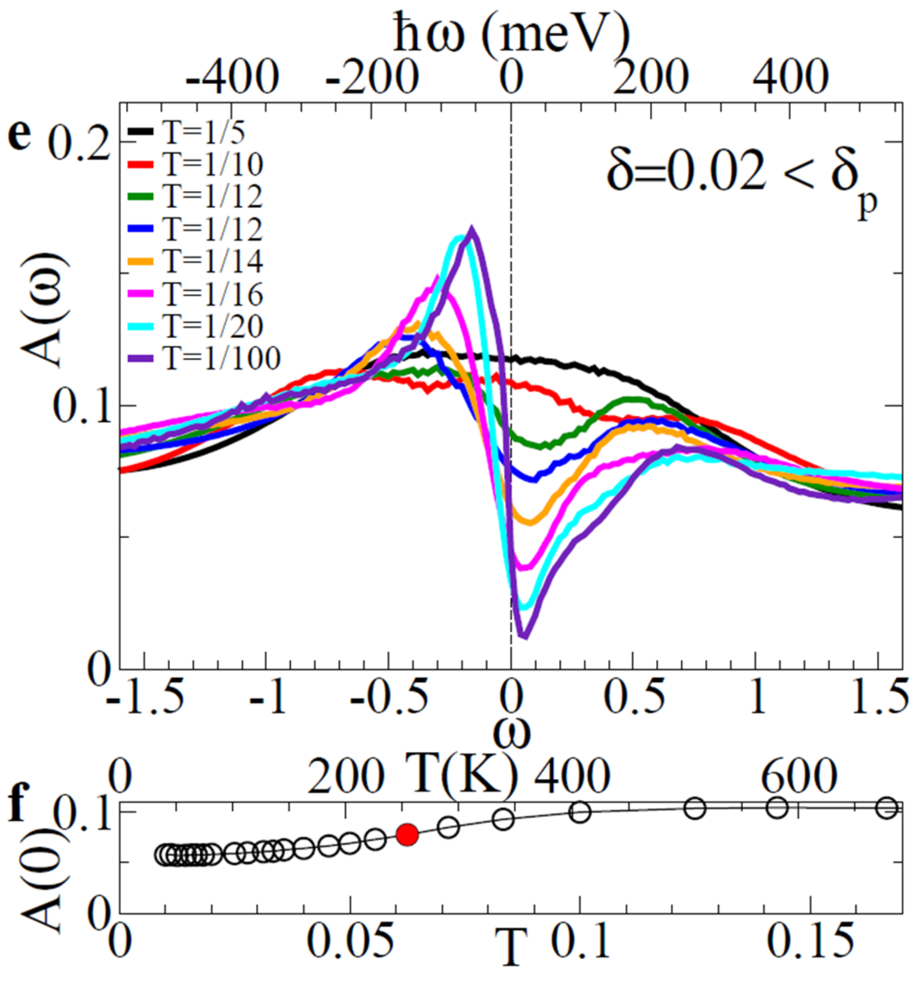
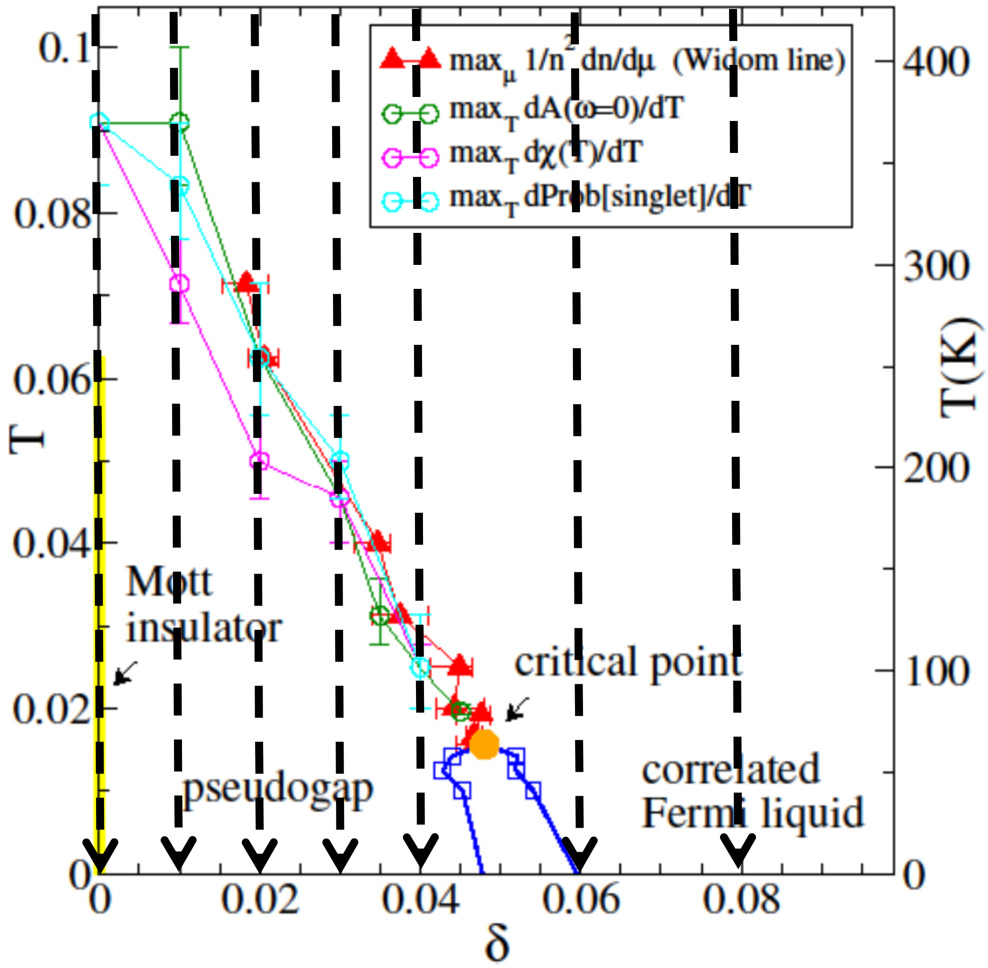
Phase diagram



T dependence of the DOS



Phase diagram



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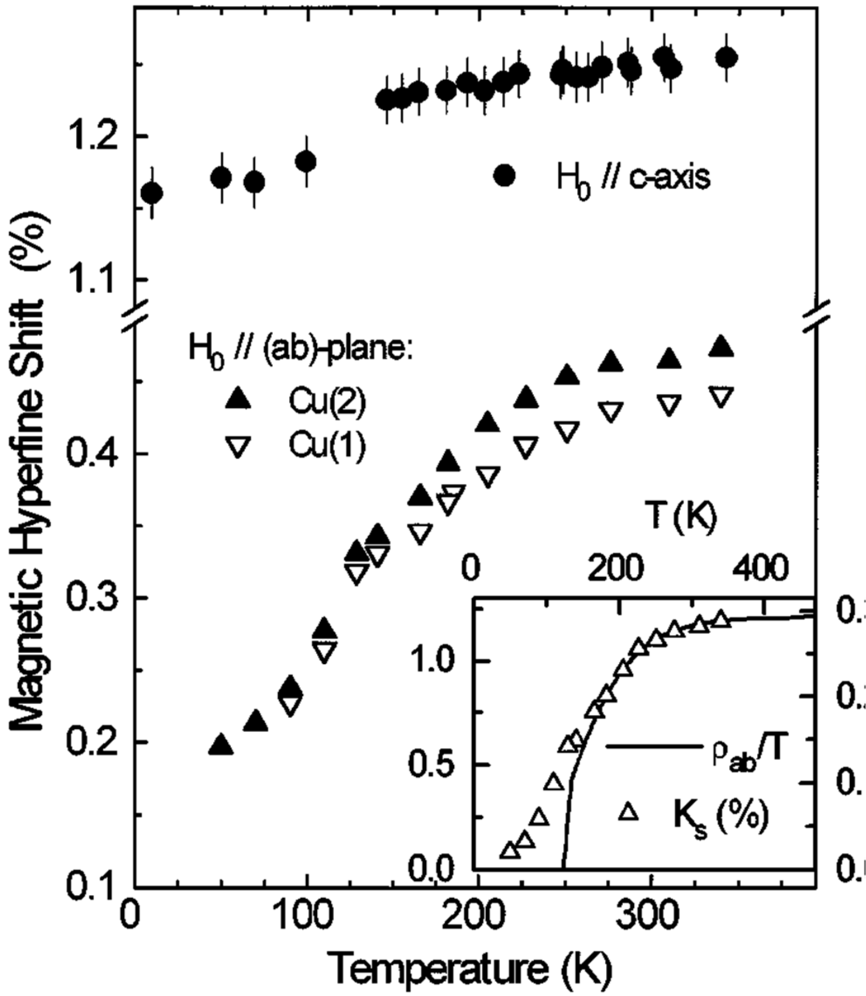
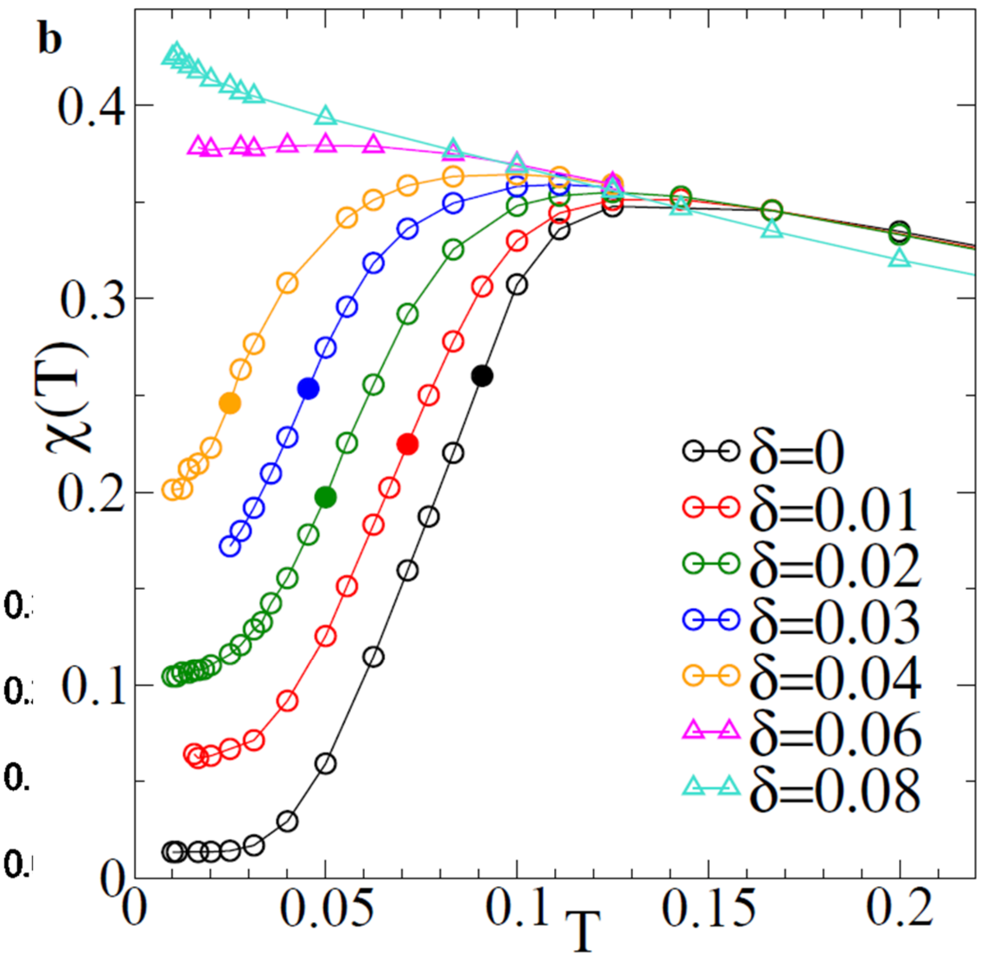
Spin susceptibility

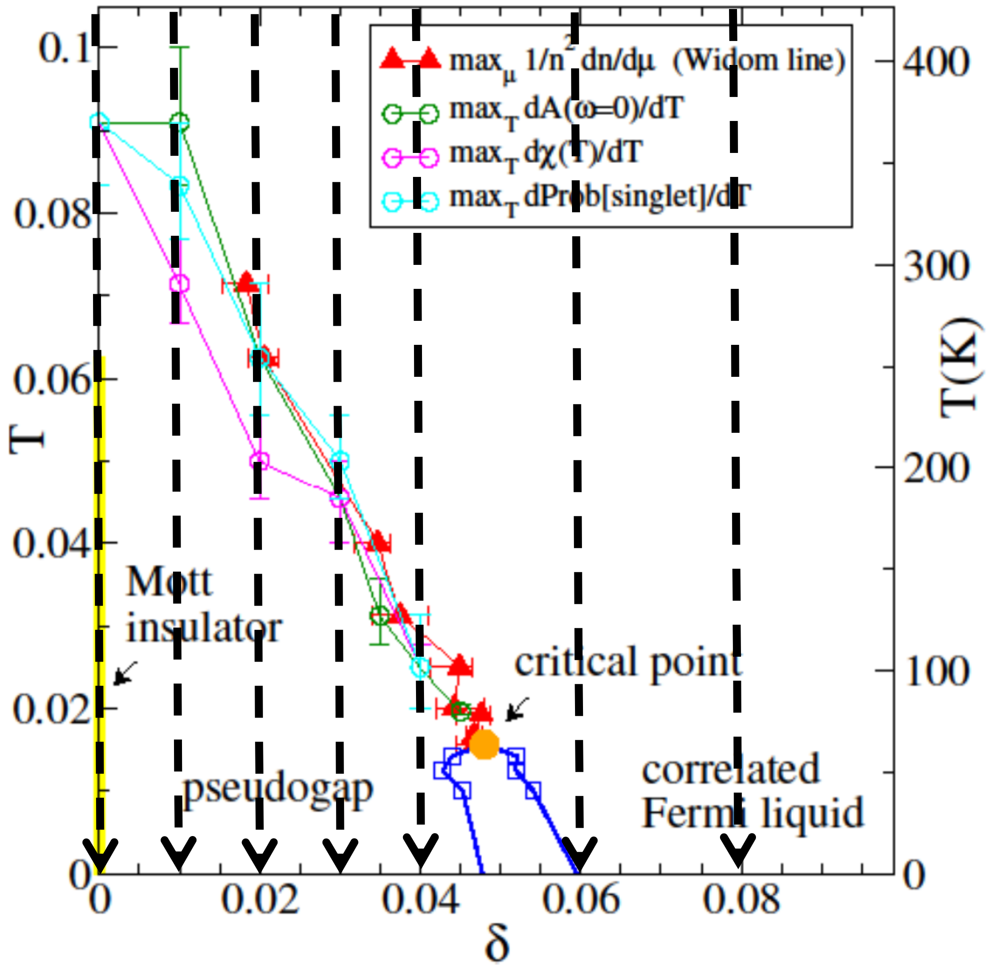




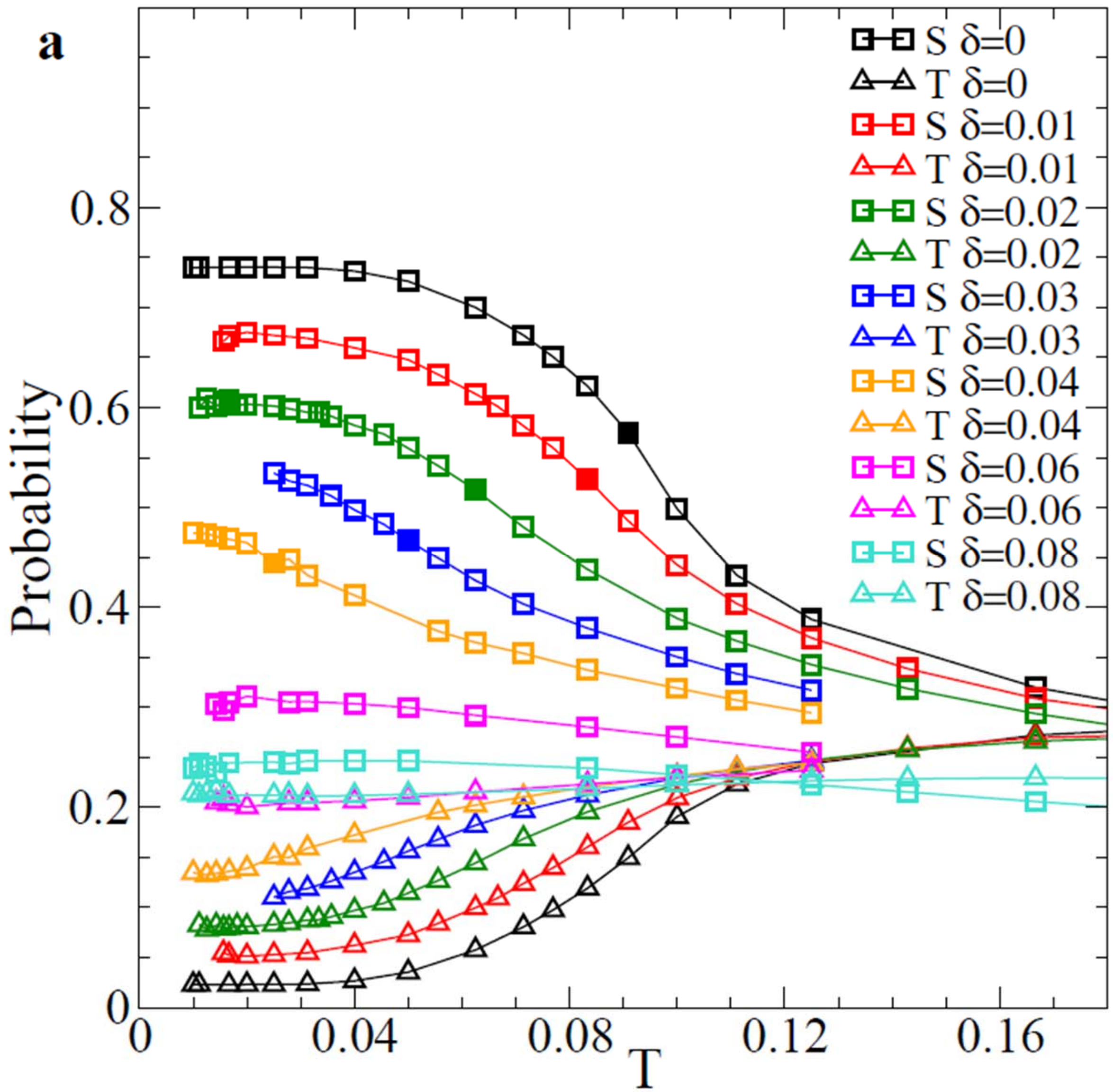
Underdoped Hg1223

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

Phase diagram



Plaquette eigenstates



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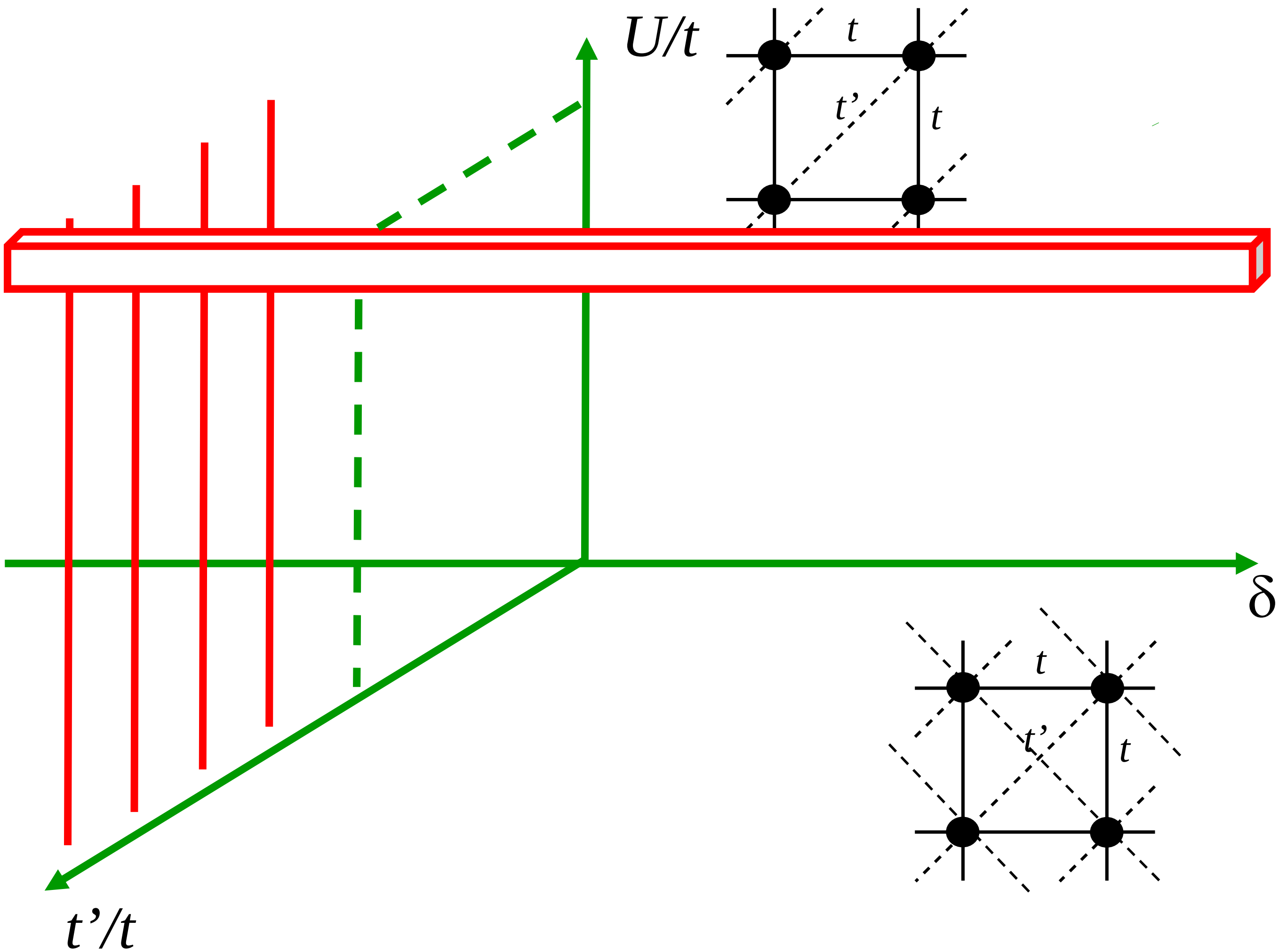
Superconductivity

Phase diagram

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

Perspective



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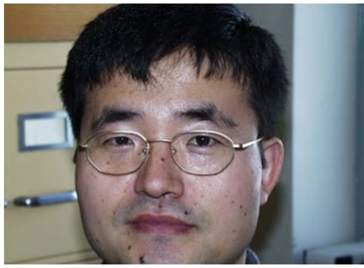
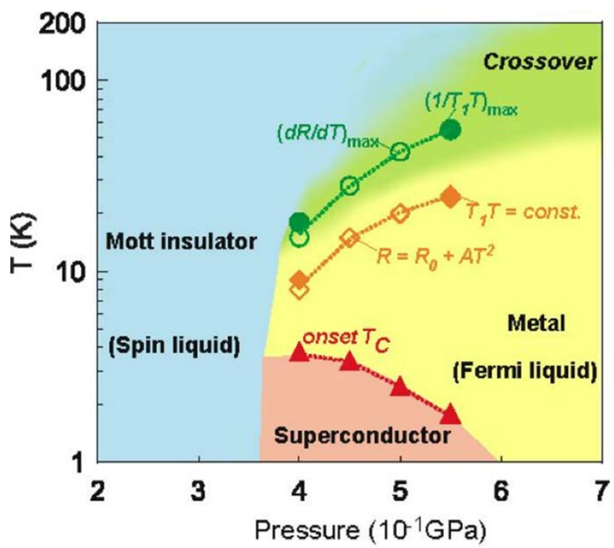


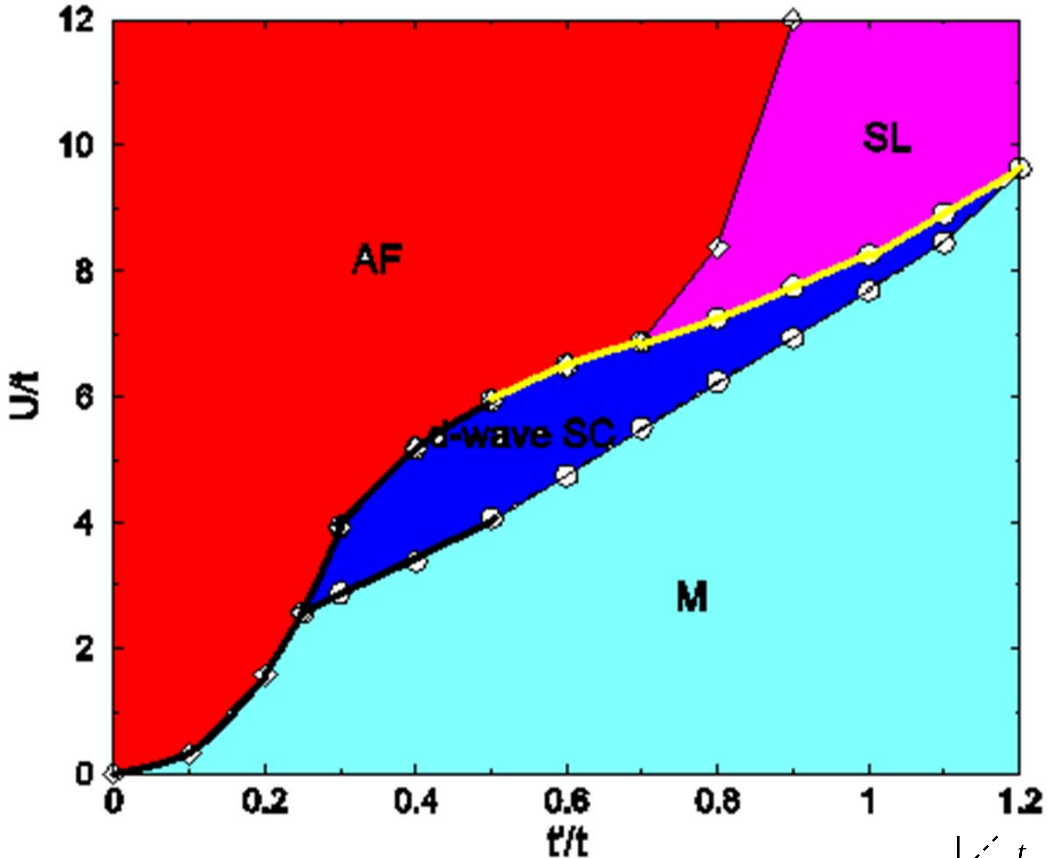
Theoretical phase diagram BEDT

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

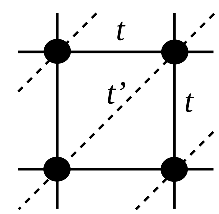


Y. Kurisaki, et al.

Phys. Rev. Lett. **95**, 177001(2005)

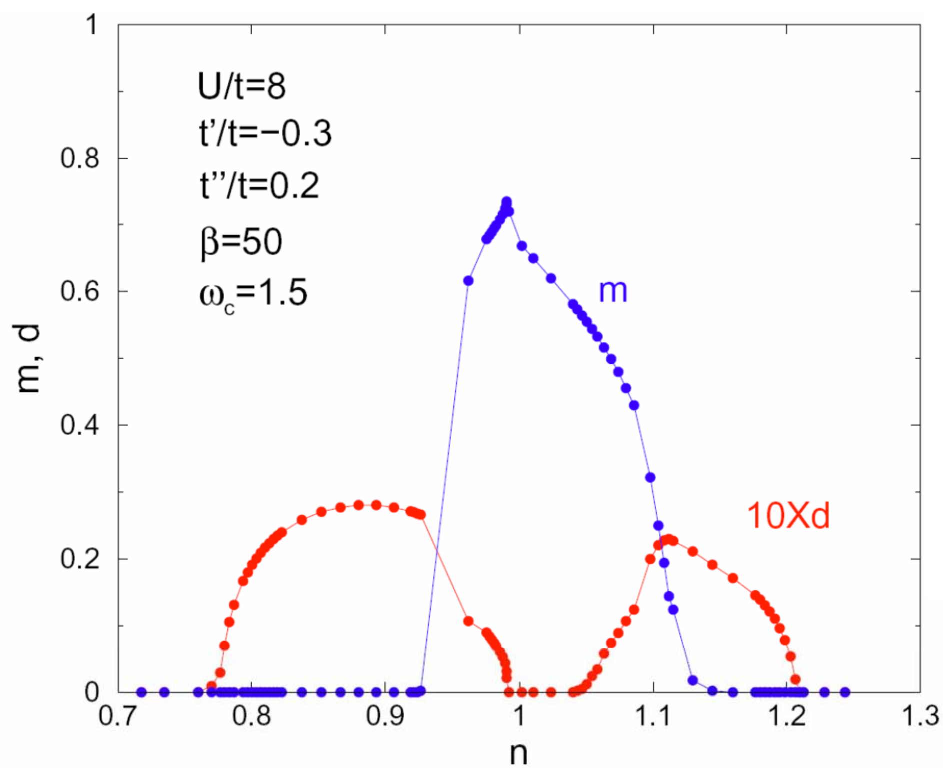


Kyung, A.-M.S.T. PRL 97, 046402 (2006)

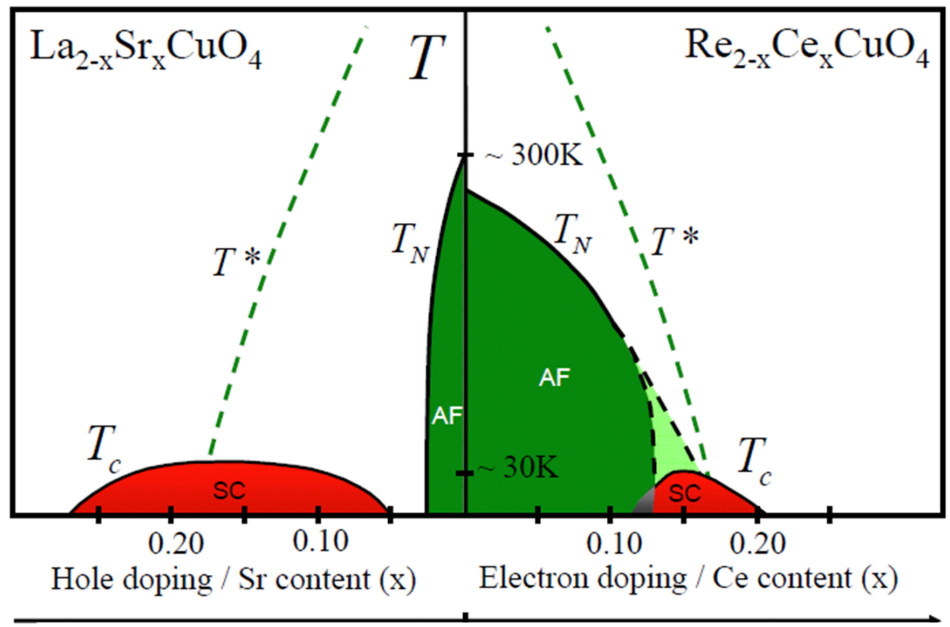


Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

CDMFT global phase diagram



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



Armitage, Fournier, Greene, RMP (2009)

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Bumsoo Kyung

Marcello Civelli

Satoshi Okamoto

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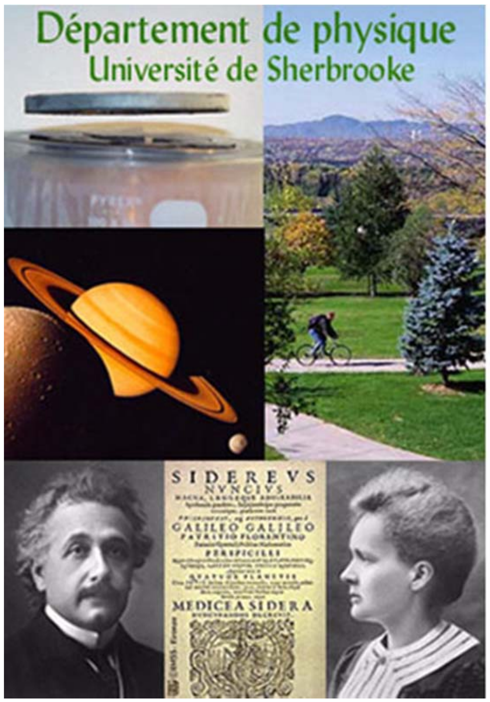

André-Marie Tremblay

CANADA RESEARCH CHAIRS
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Strenghts and weaknesses

- Strenghts
  - « One particle properties » of phases
  - Phase diagrams
- Weaknesses
  - Order parameters not coupled to observables quadratic in creation-annihilation operators
  - Transport (four point correlation functions)
  - Analytic continuation for QMC solvers
- Challenge: Optimum environment

Merci

Thank you