Projective QMC — a new route to T=0

Karsten Held

MPI for solid state research, Stuttgart

Hamburg, May 19, 2005

- Motivation
- Projective quantum Monte Carlo (PQMC) method
- Results

  — One-band Hubbard model

  — Two-band Hubbard model

  — DCA (PQMC) study of the t-t' Hubbard model
- Conclusion

Thanks to...

M. Feldbacher, R. Arita — MPI Stuttgart

F. Assaad – Würzburg

Emmy Noether program of the DFG

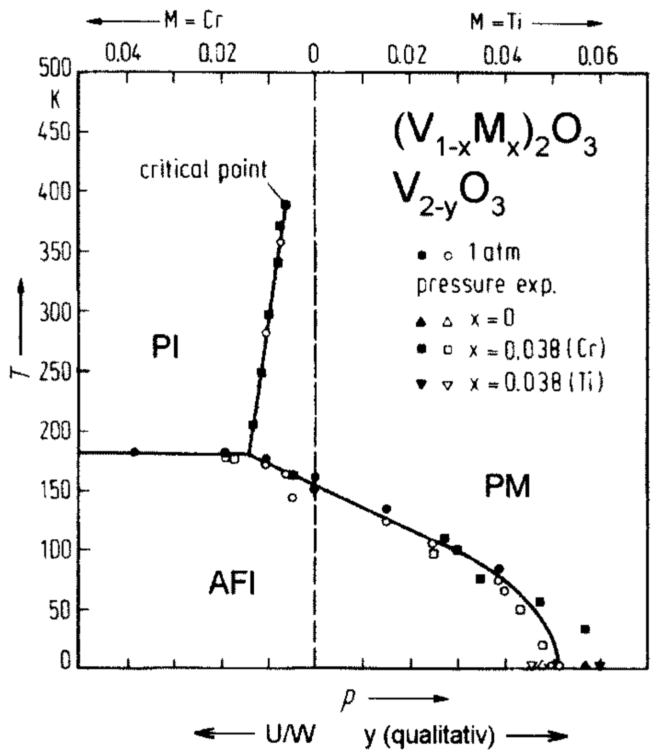
Please ask questions...

Motivation

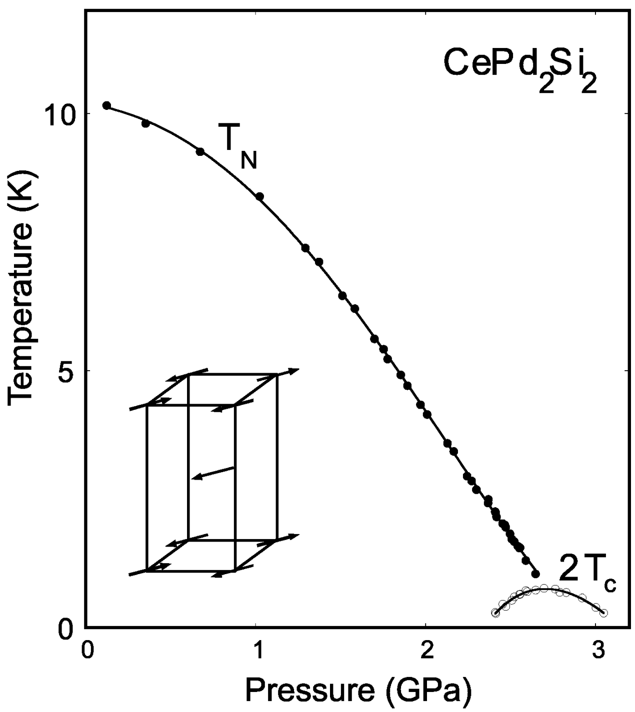
Realistic LDA+DMFT/quantum dot calculations

impurity problem • many orbitals

• often interesting physics at low T



not so low T



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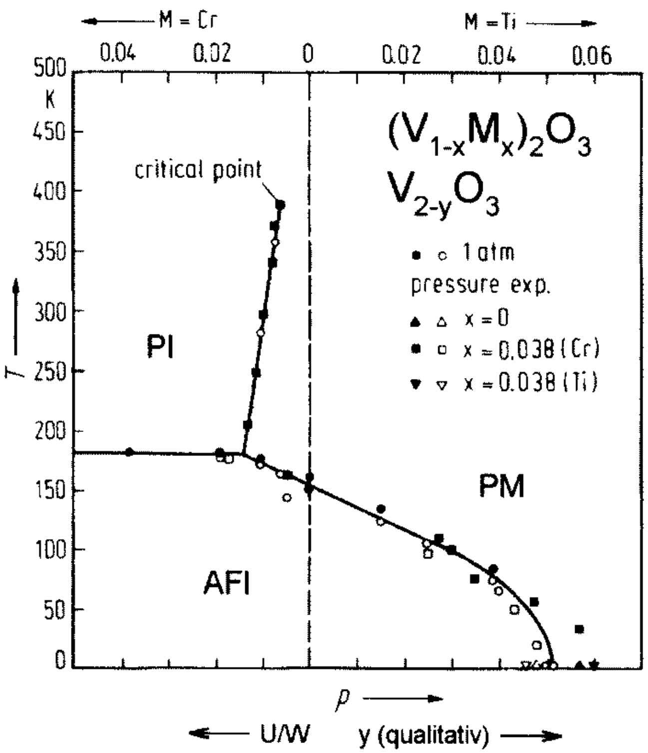

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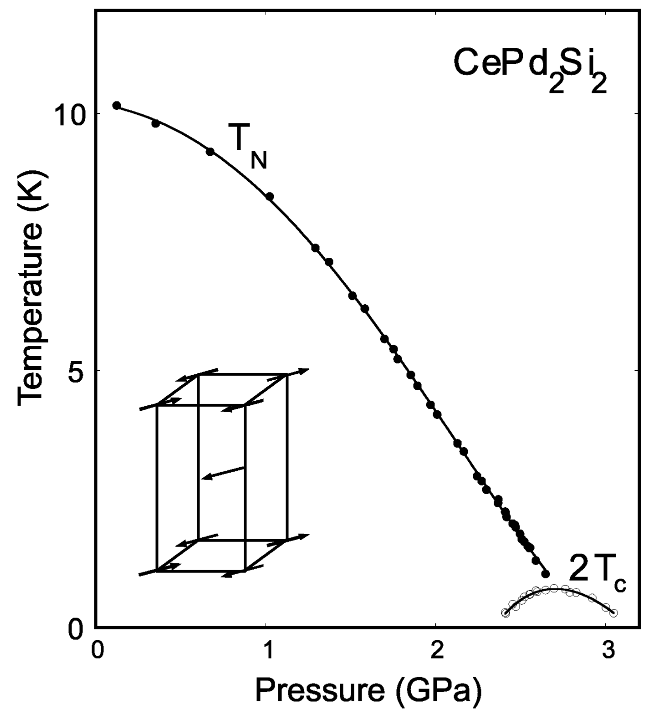

very low T

• Hirsch-Fye **QMC** $T \gtrsim 300\,\mathrm{K}$ scaling $\sim 1/T^3$

• Wilson's **NRG** ≤ 2 orbitals scaling exponential in #orbitals

Projective QMC for Anderson impurity model

Feldbacher, Held, Assaad PRL 93, 136405 (2004)

Finite-T Hirsch-Fye QMC (HF-QMC)

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\, \mathcal{O} e^{-\beta H}}{\mathrm{Tr} e^{-\beta H}}$$

- thermal fluctuations
- effort $\sim 1/T^3$

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Projective QMC (PQMC)

$$\langle \mathcal{O} \rangle_{T=0} = \frac{\langle \Psi_{\mathrm{GS}} | \mathcal{O} | \Psi_{\mathrm{GS}} \rangle}{\langle \Psi_{\mathrm{GS}} | \Psi_{\mathrm{GS}} \rangle}$$

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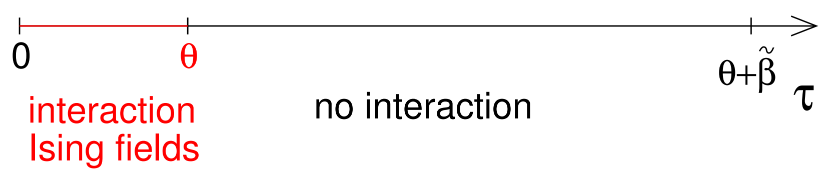

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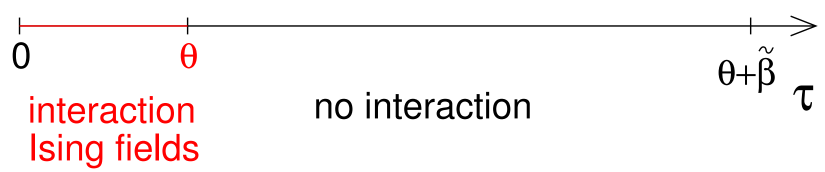

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but with $G_{T=0}(\tau)$ instead of $G_T(\tau)$

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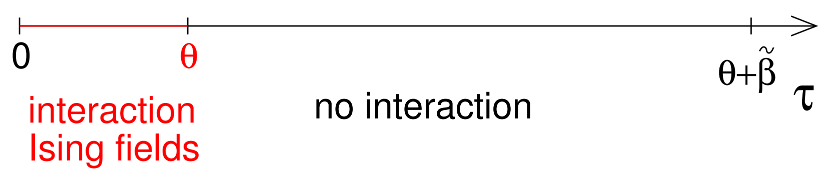

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extrapolation $\theta \to \infty$ at the end

In more detail...

We need Green function, i.e., $\mathcal{O} = -c(\tau_1)c^\dagger(\tau_2) = -e^{\tau_1/2\,H} c e^{-(\tau_1-\tau_2)/2\,H} c^\dagger e^{-\tau_2/2\,H}$

Green function matrix

$$G(\tau_1,\tau_2) = -\lim_{\tilde\beta\to\infty} \frac{\mathrm{Tr} e^{-\tilde\beta H_0} e^{-(\theta-\tau_1)/2\;H} c e^{-(\tau_1-\tau_2)/2\;H} c^\dagger e^{-(\theta+\tau_2)/2\;H}}{\mathrm{Tr} e^{-\tilde\beta H_0} e^{-\theta H}}$$

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$\tilde\beta = 0$ instead of $\lim_{\tilde\beta\to\infty}$

β instead of Θ physical meaning T

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- **Time discretization**

$$e^{\Theta\,H} \text{ or } e^{\int_0^\Theta \mathrm{d}\tau\,H} \longrightarrow e^{\Delta\tau \sum_{l=1}^{L} H}$$

- **Trotter decomposition**

$$e^{\Delta\tau H_0 + \Delta\tau H_U} = e^{\Delta\tau H_0} e^{\Delta\tau H_U} + \frac{1}{2}\Delta\tau^2 [H_0, H_U] + \mathcal{O}(\Delta\tau^3)$$

- **Hubbard-Stratonovich decoupling**

$$e^{\frac{\Delta\tau U}{2}(n_\uparrow - n_\downarrow)^2} = \frac{1}{2}\sum_{s_l=\pm1} e^{\lambda s_l (n_\uparrow - n_\downarrow)} \qquad \text{with } \cosh(\lambda) = \exp(\Delta\tau U/2)$$

$\Rightarrow$ sum of non-interacting problems (MC sampling)

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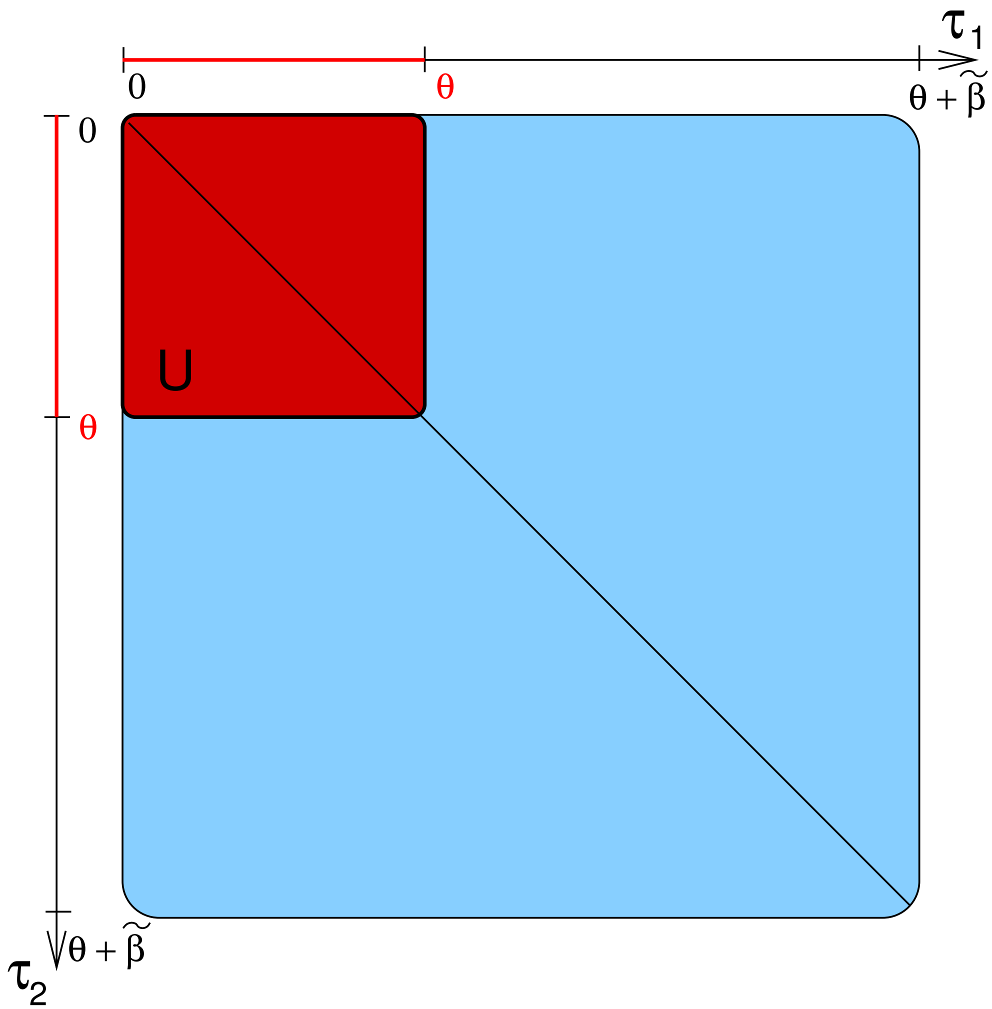

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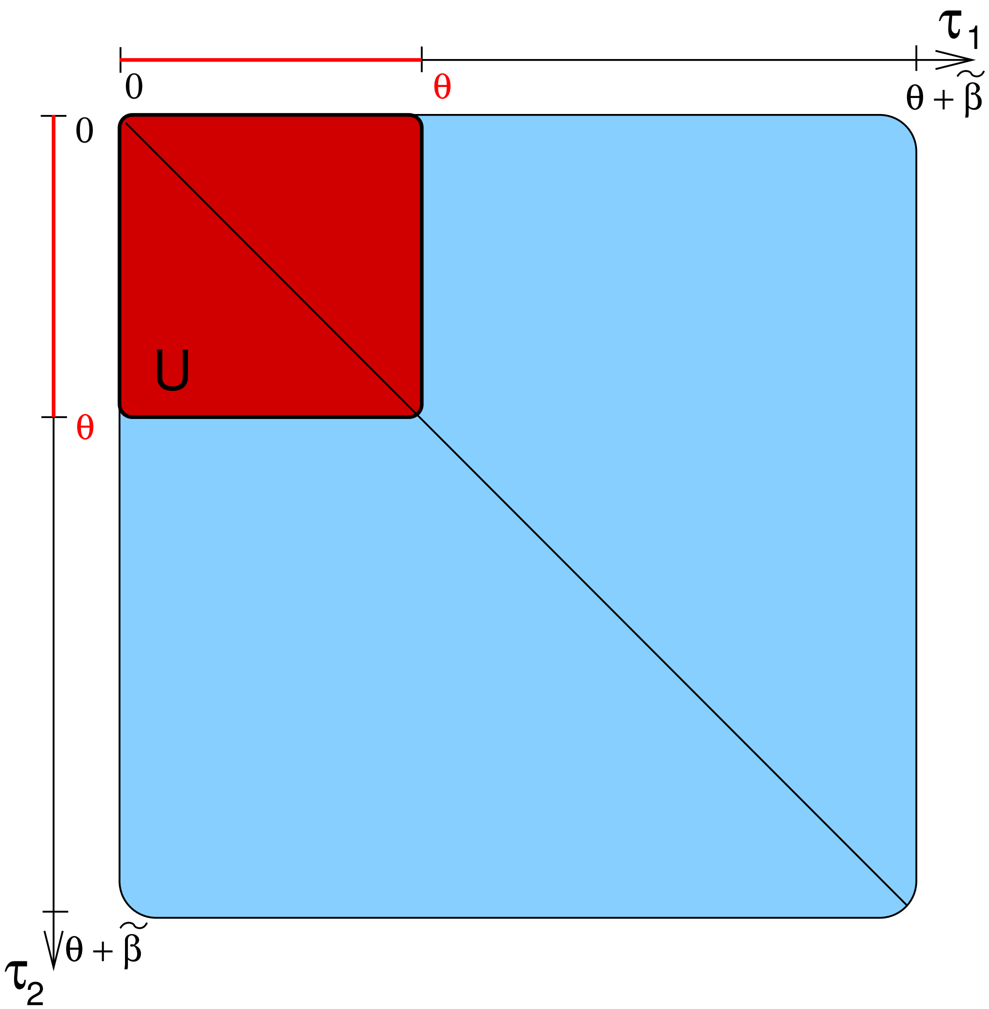

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Hubbard-Stratonovich transformation
⇒ only Ising fields in red part
Update of Ising field affects only red part

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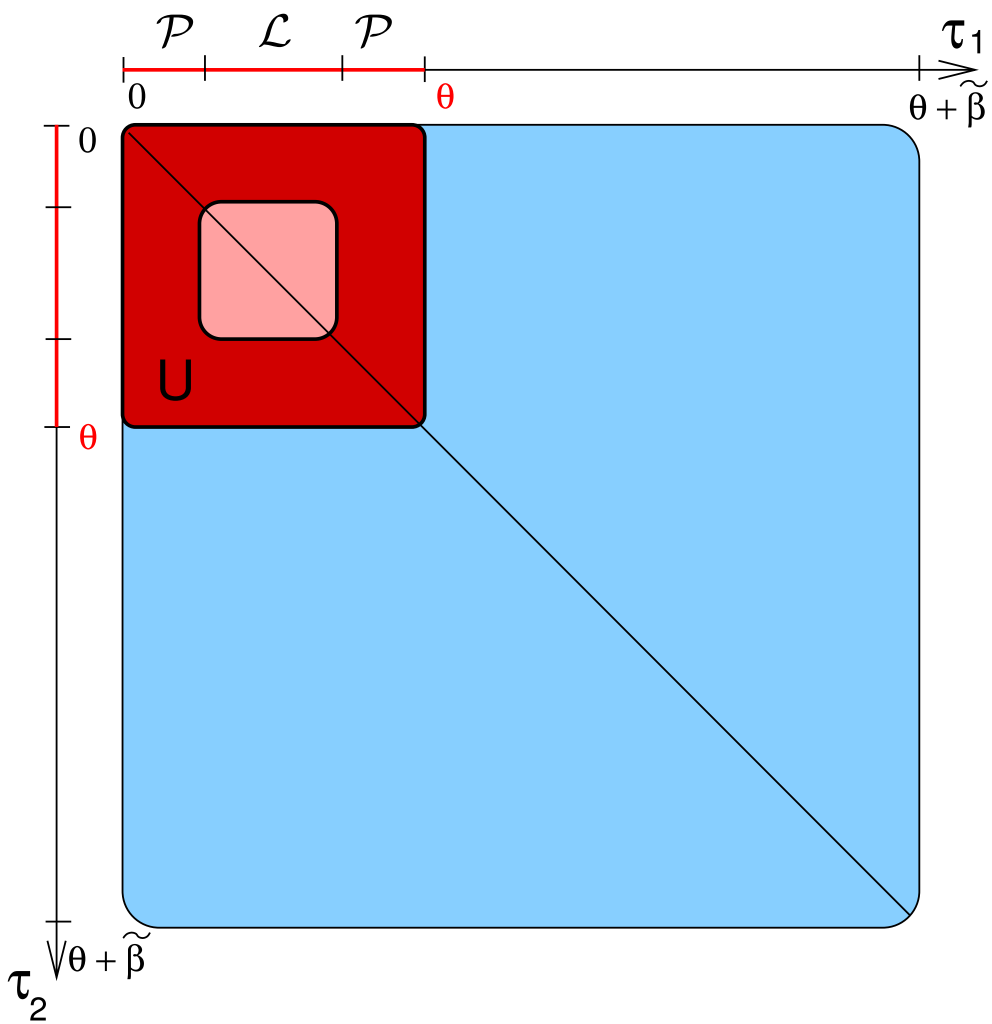

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Projection onto ground state needed
⇒ information only in light red part valid

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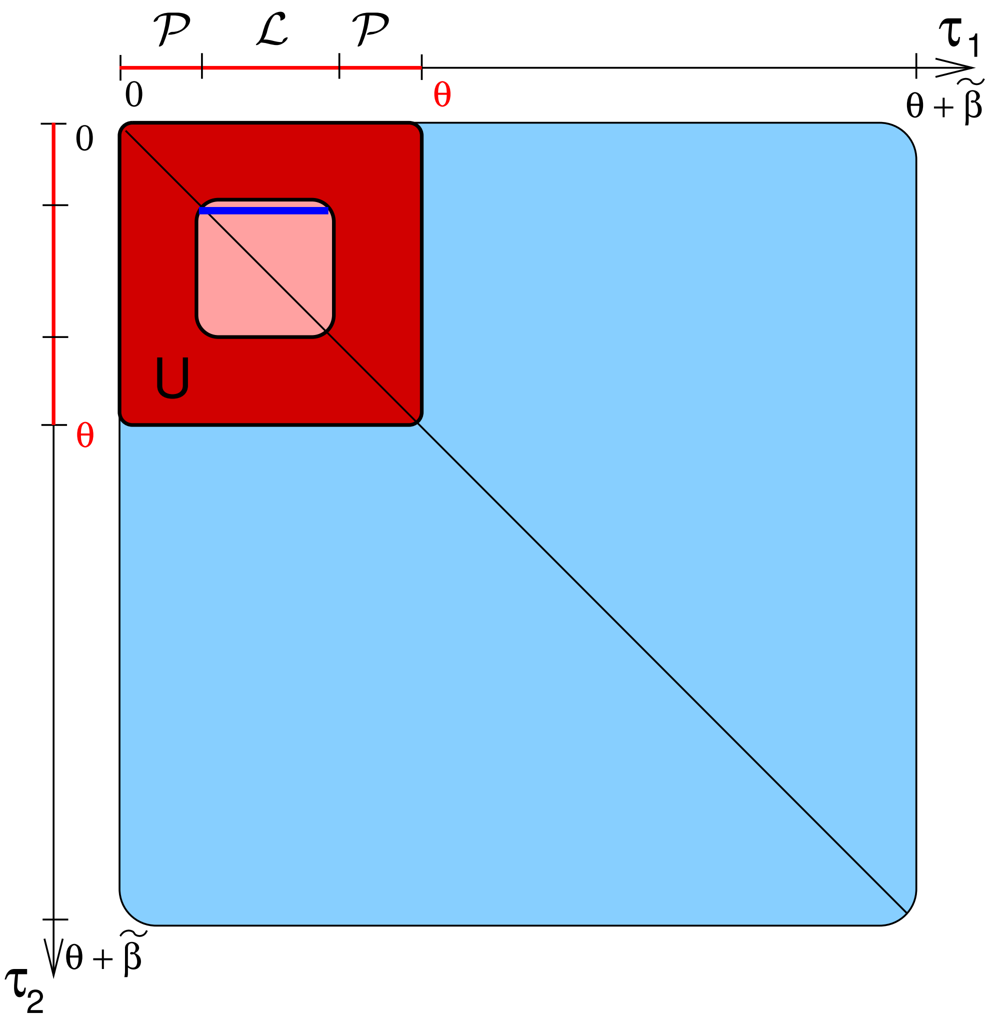

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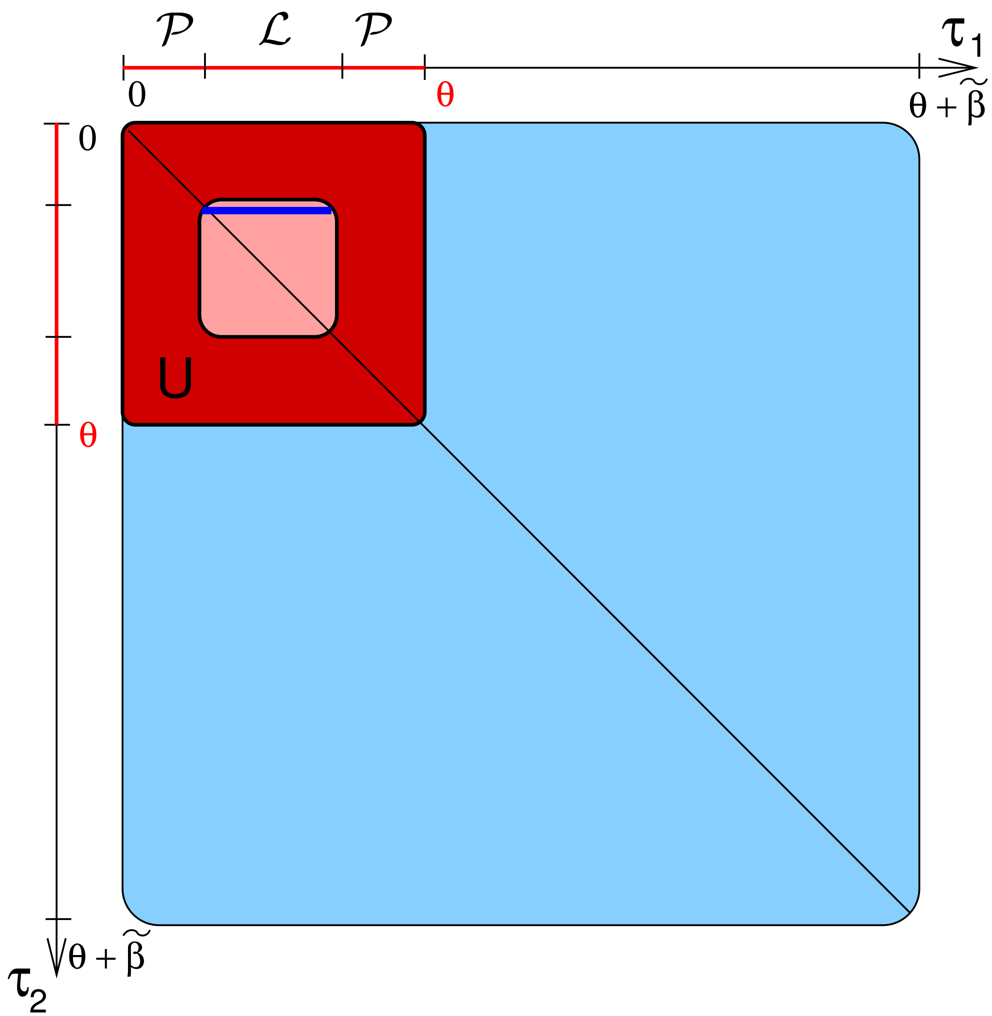

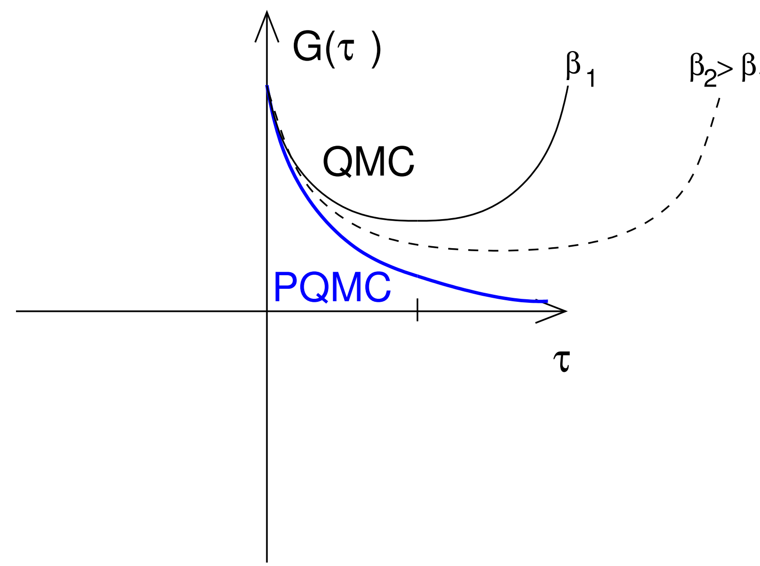

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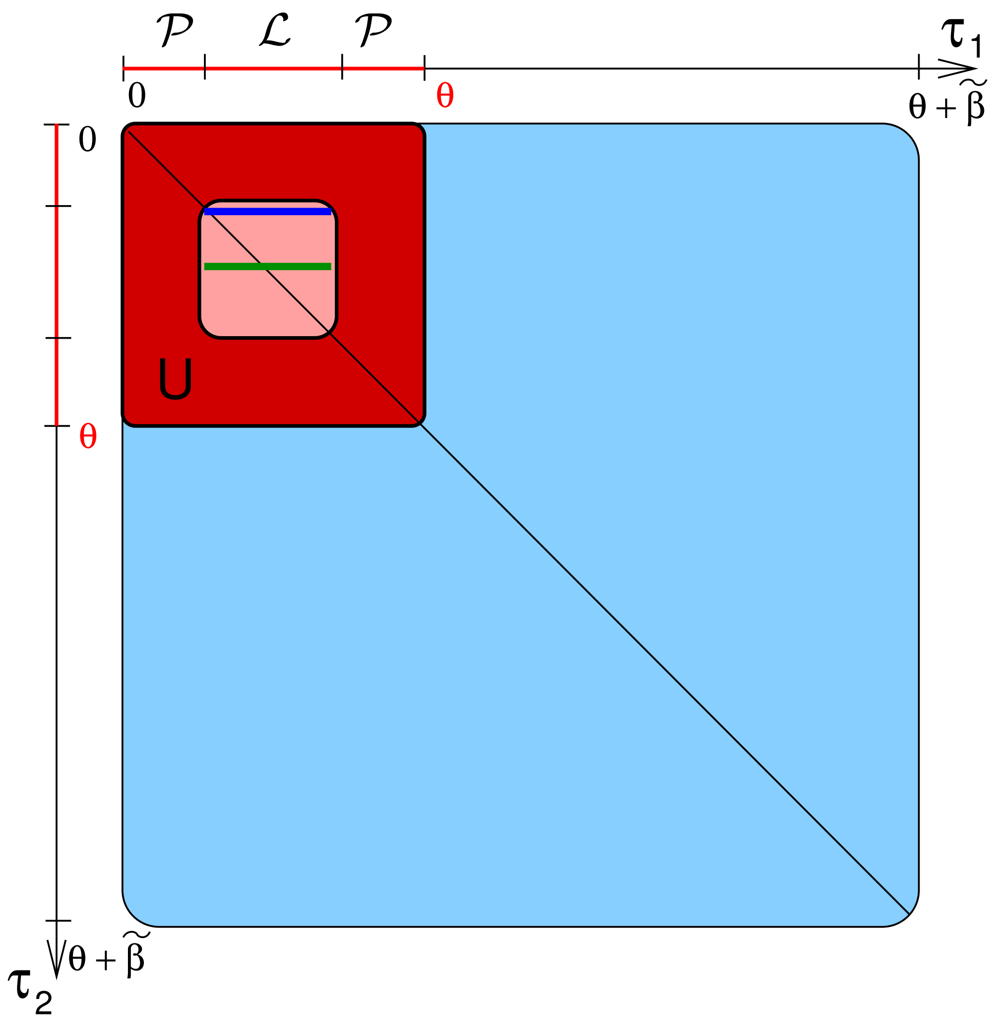

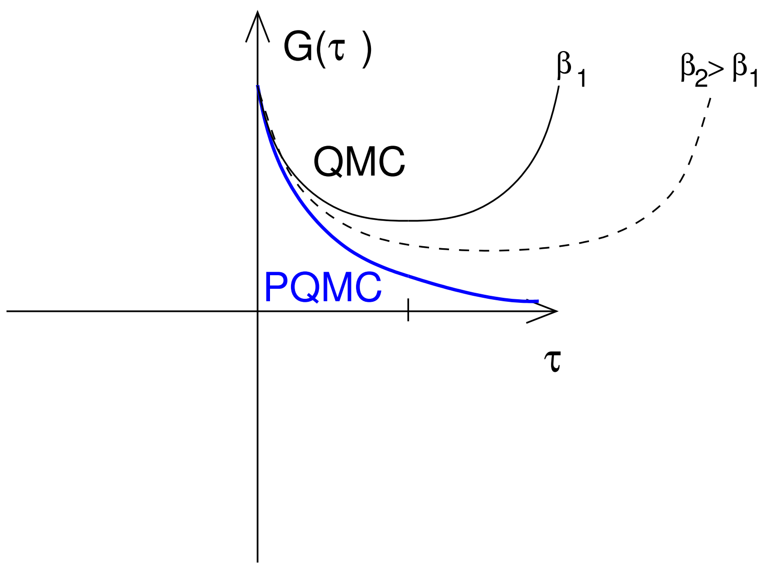

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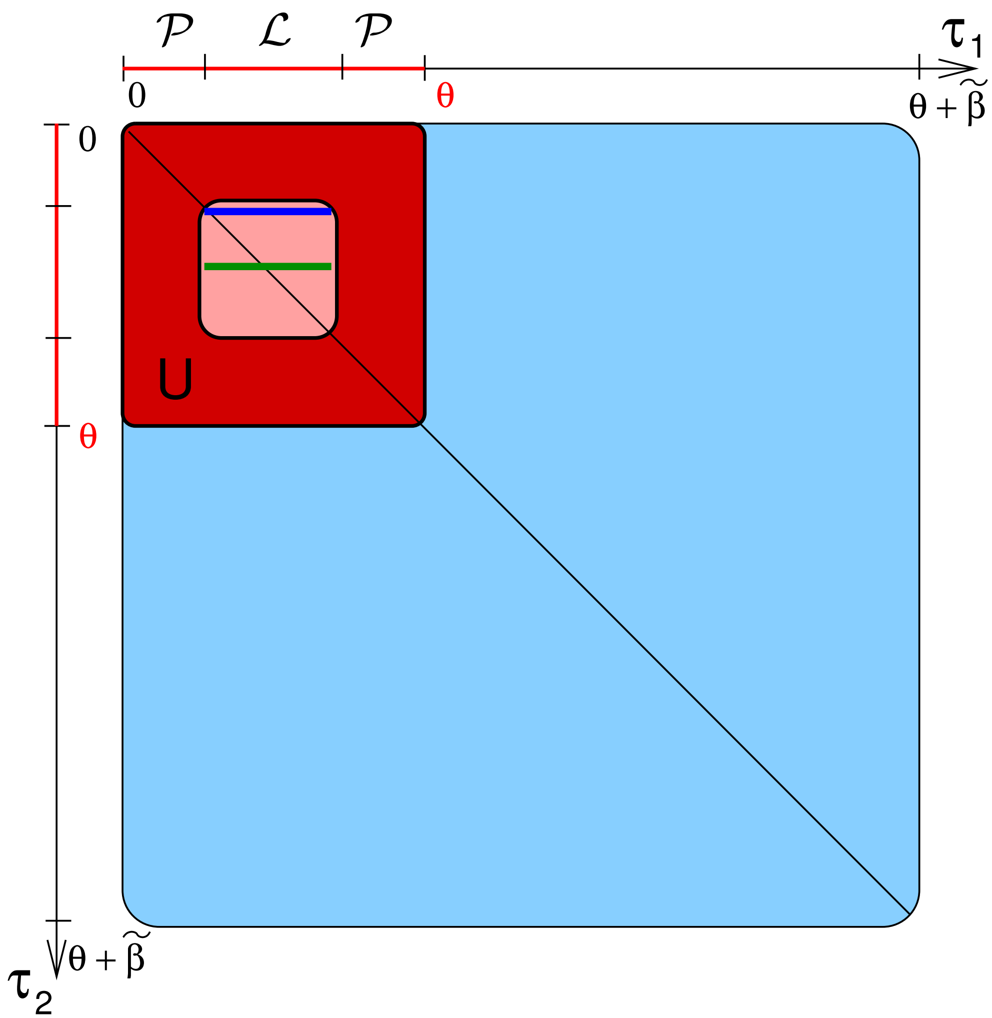
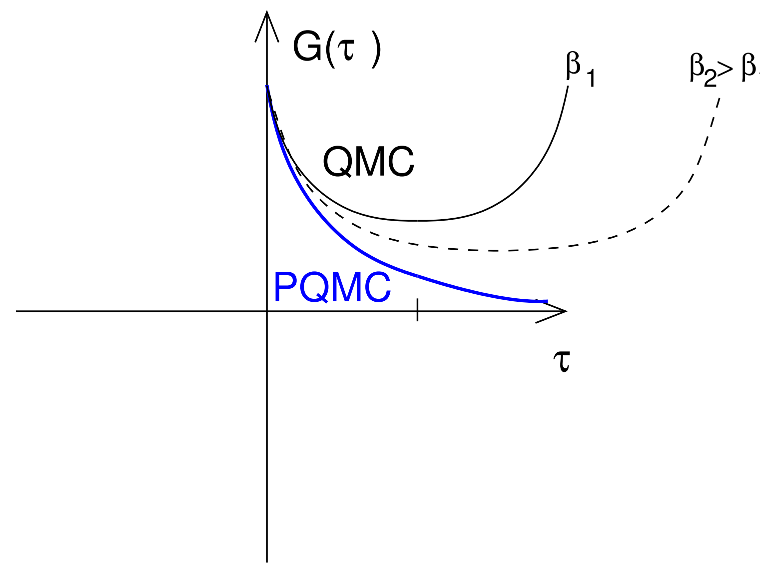
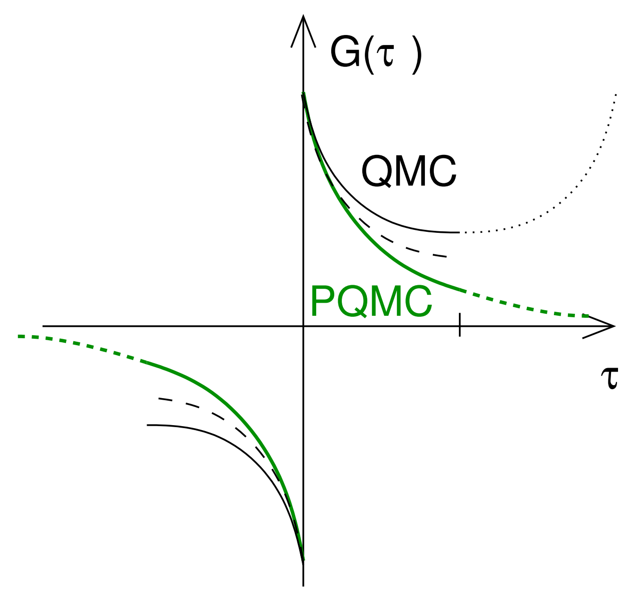






DMFT(PQMC)

Feldbacher, Held, Assaad PRL'04

Ground state (PQMC):

$\mathcal{G}_0(\tau,\tau') : \tau,\tau' < \theta$

$$\begin{array}{ccc} \Sigma(i\omega) \Rightarrow & \boxed{\text{Dyson}} & \Rightarrow G(i\omega) \\ \text{MaxEnt} \Uparrow & & \Downarrow \Sigma(i\omega) \\ G(\tau,\tau') \Leftarrow & \boxed{\text{PQMC}} & \Leftarrow \mathcal{G}_0(\tau,\tau') \end{array}$$

Maximum Entropy:

$$G(\tau) = \frac{1}{\pi}\int_0^\infty A(\omega) e^{-\omega\tau} d\omega$$

$$G(i\omega_n) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{A(\omega)}{i\omega_n - \omega} d\omega$$

finite-T (HF-QMC):

$\mathcal{G}_0^\sigma(\tau - \tau')$

$$G = \sum_k \frac{1}{\omega - \varepsilon_k - \Sigma}$$

$$\begin{array}{ccc} \Sigma(i\omega) \Rightarrow & \boxed{\text{Dyson}} & \Rightarrow G(i\omega) \\ \text{FT} \Uparrow & & \Downarrow \Sigma = \mathcal{G}_0^{-1} - G^{-1} \\ G(\tau) \Leftarrow & \boxed{\text{QMC}} & \Leftarrow \mathcal{G}_0(\tau) \end{array}$$

II Results

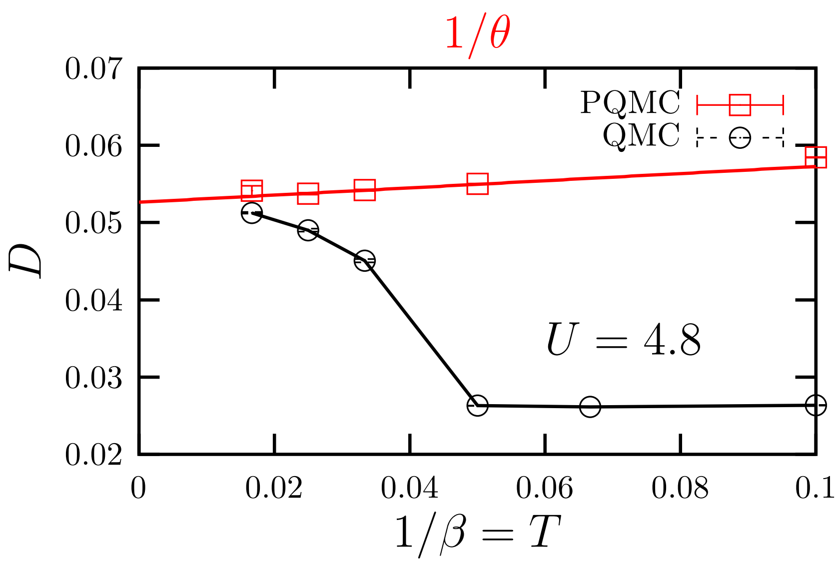
One-band Hubbard model (half-filling)

Hamiltonian:

$$H = -t \sum_{\langle i,j\rangle\,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{i\,\sigma} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Bethe-DOS; bandwidth $W = 4$

DMFT(QMC) vs. DMFT(PQMC)



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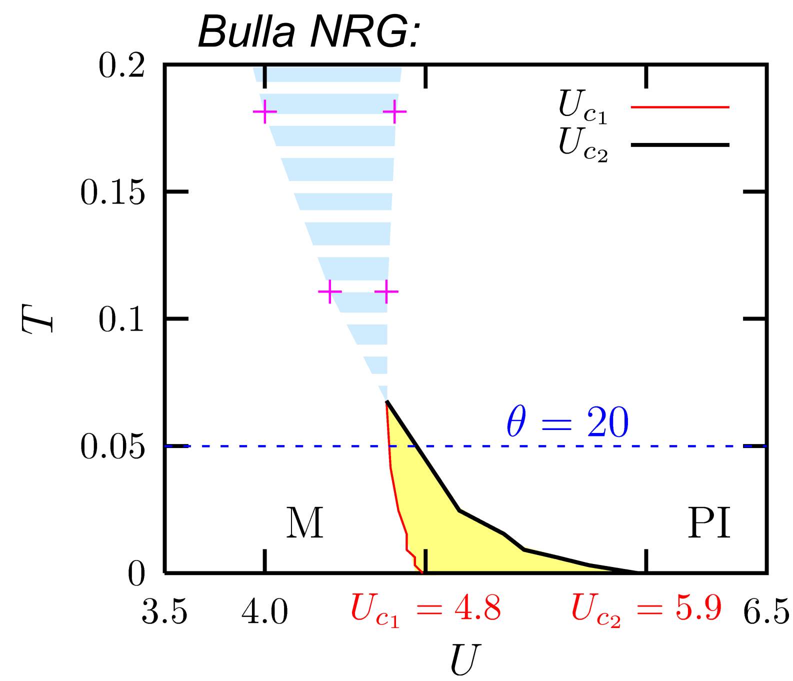

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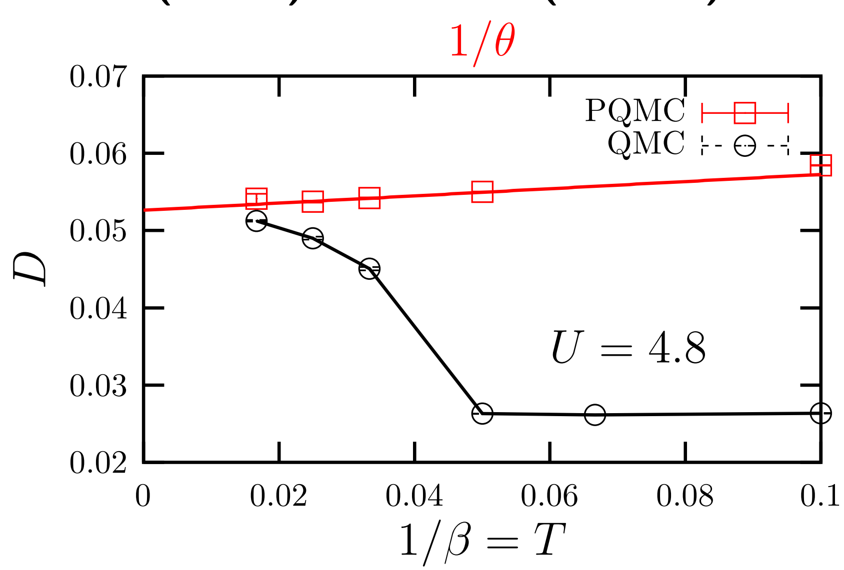

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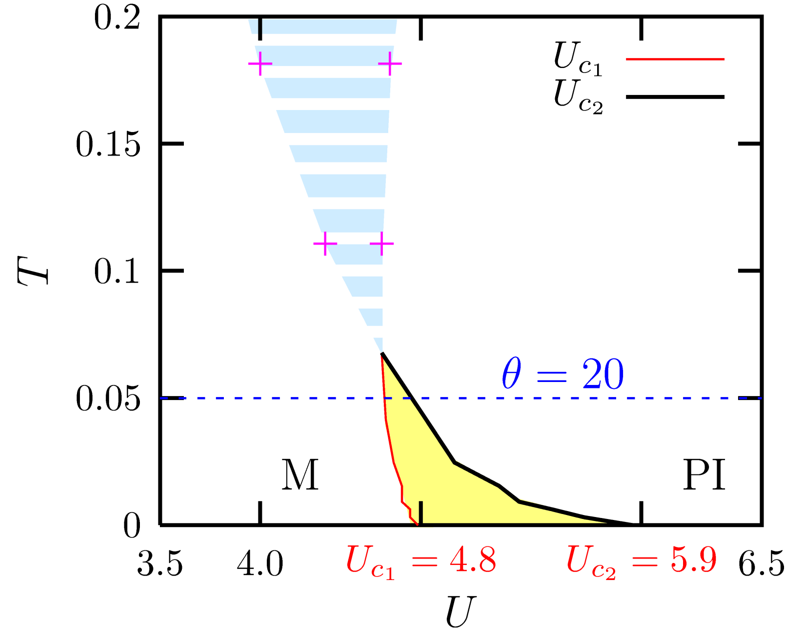

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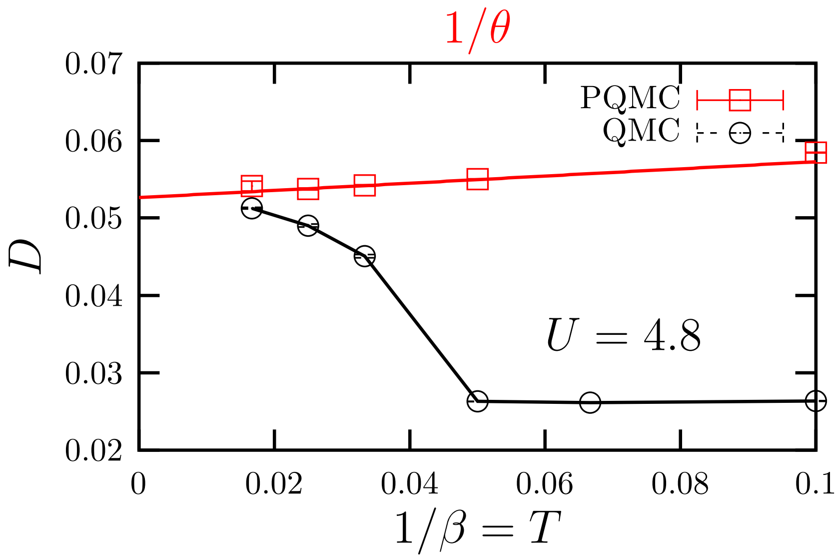
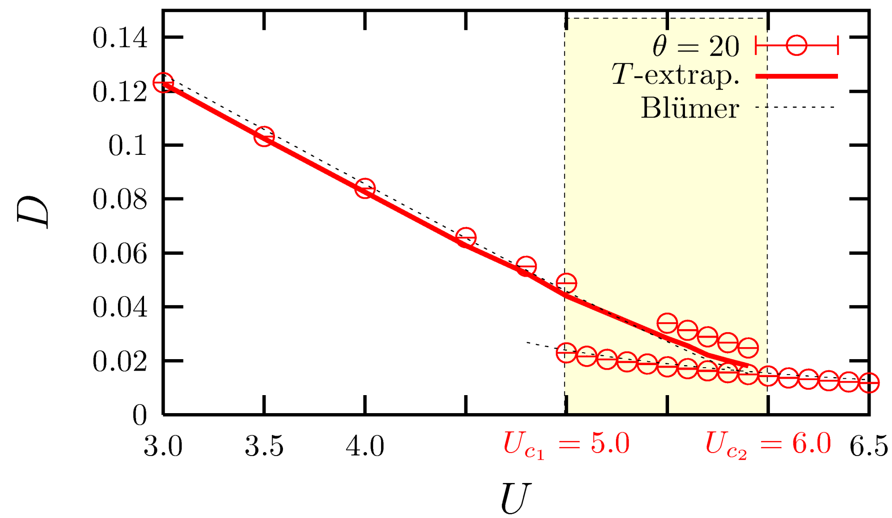
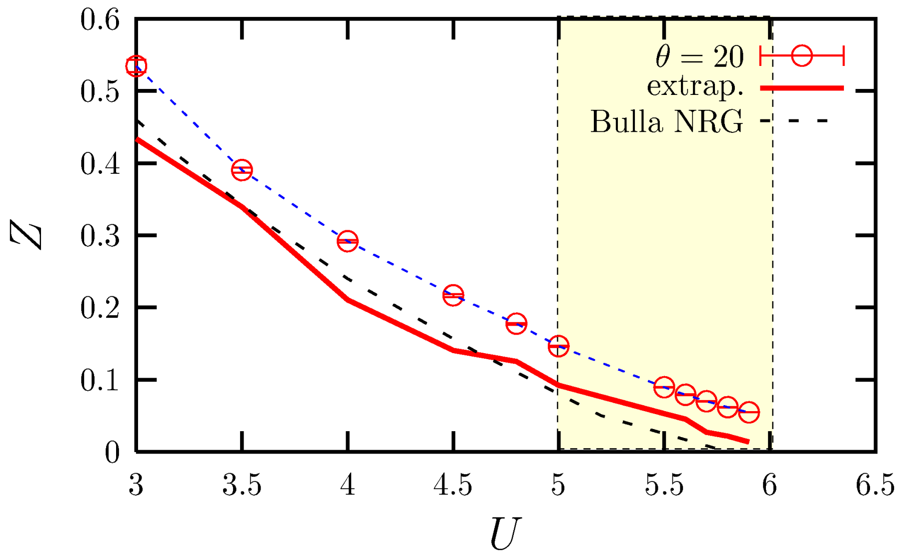


DMFT(PQMC) coexistence region

Feldbacher, Held, Assaad'04



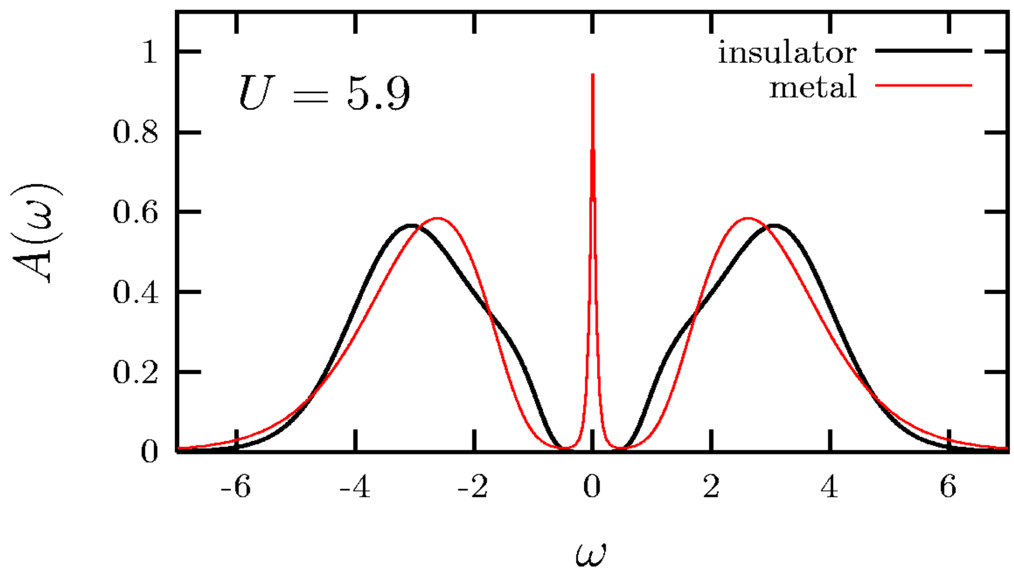
Quasiparticle weight Z



$$Z = \left(1 - \frac{\mathrm{Im}\,\Sigma(i\omega_{n=1})}{\omega_{n=1}} \right)^{-1}$$

Spectra

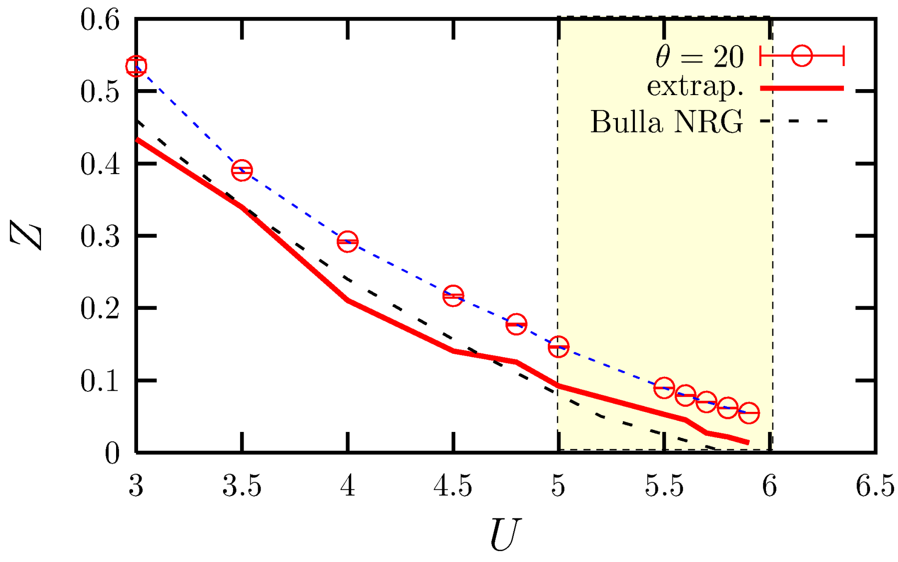
Feldbacher, Held, Assaad PRL'04;



Maximum Entropy:

$$G(\tau) = \frac{1}{\pi} \int_0^\infty A(\omega) e^{-\omega\tau} d\omega$$

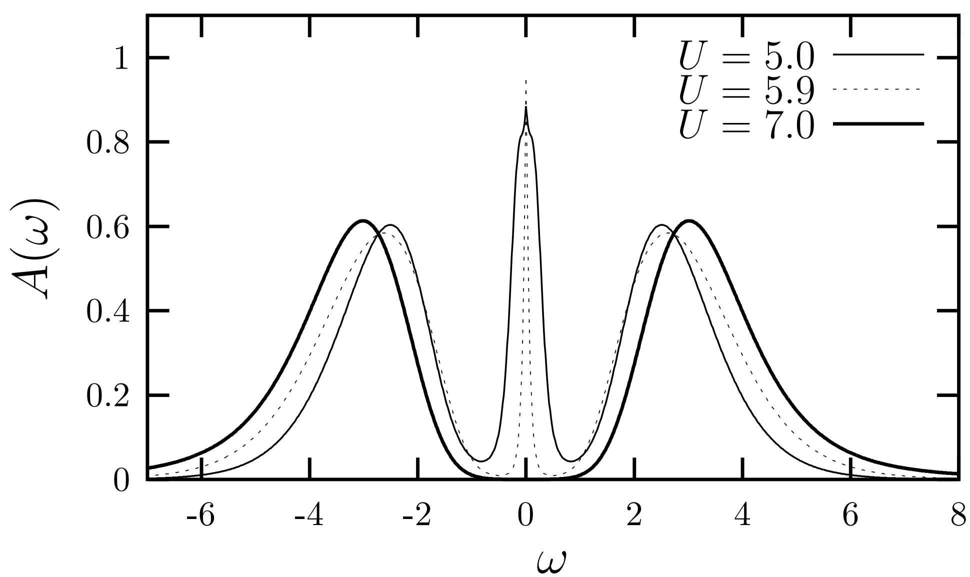
Quasiparticle weight Z



$$Z = \left(1 - \frac{\text{Im}\Sigma(i\omega_{n=1})}{\omega_{n=1}}\right)^{-1}$$

Spectra

Feldbacher, Held, Assaad PRL'04; PHYSICA B'05



Maximum Entropy:

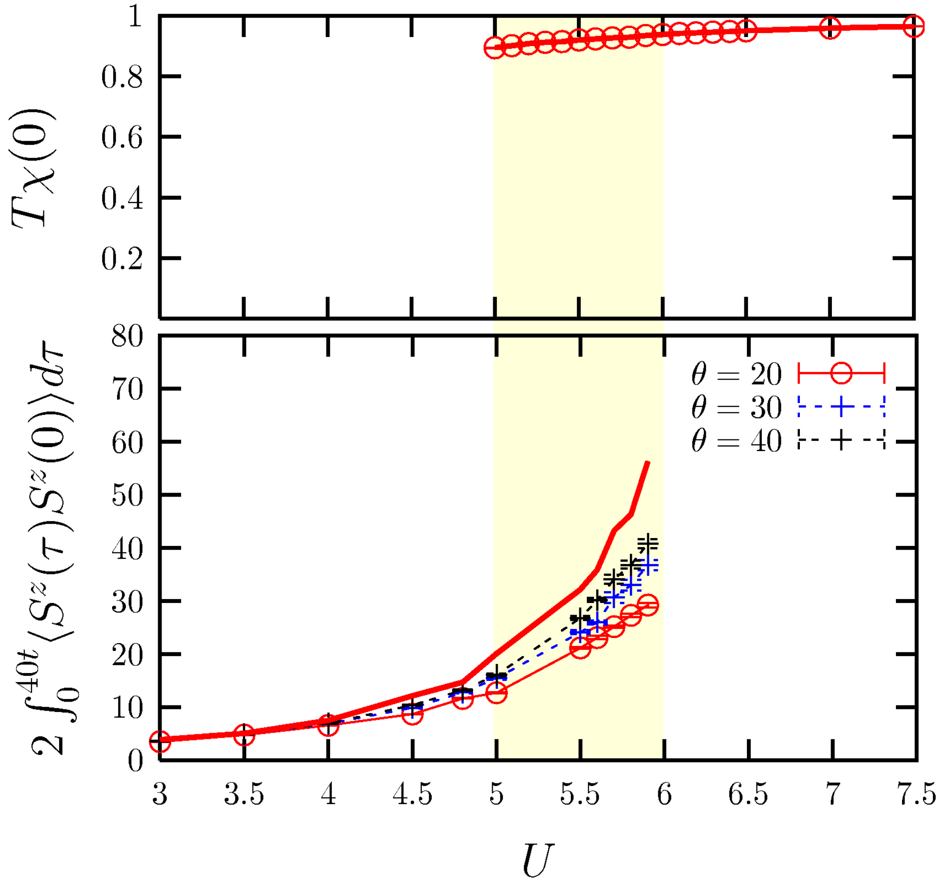
$$G(\tau) = \frac{1}{\pi}\int_0^\infty A(\omega)e^{-\omega\tau}d\omega$$

Local spin susceptibility

Feldbacher, Held, Assaad PRL'04

Insulator:

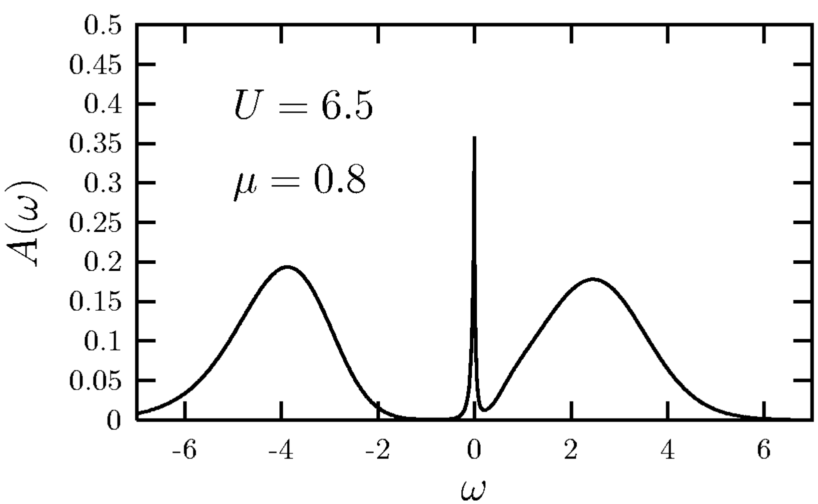
Metal:

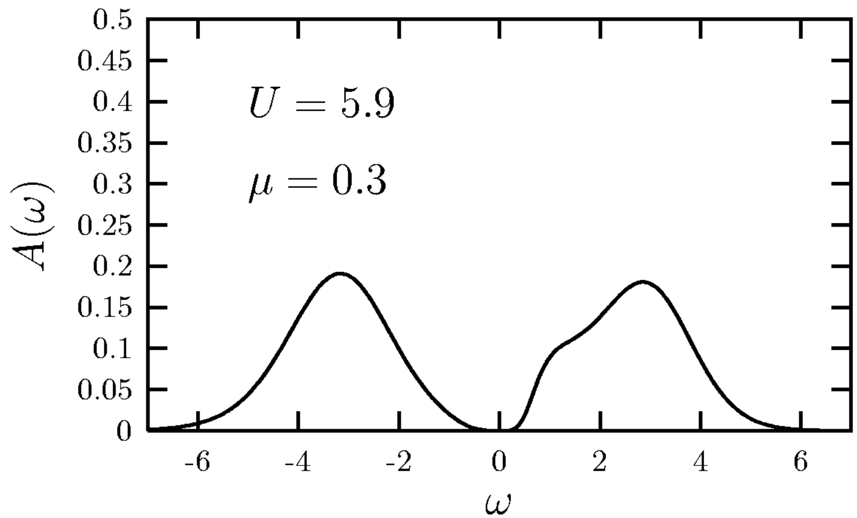


$$\int_0^{\tau_c} \left\langle S^z(\tau) S^z(0) \right\rangle d\tau$$

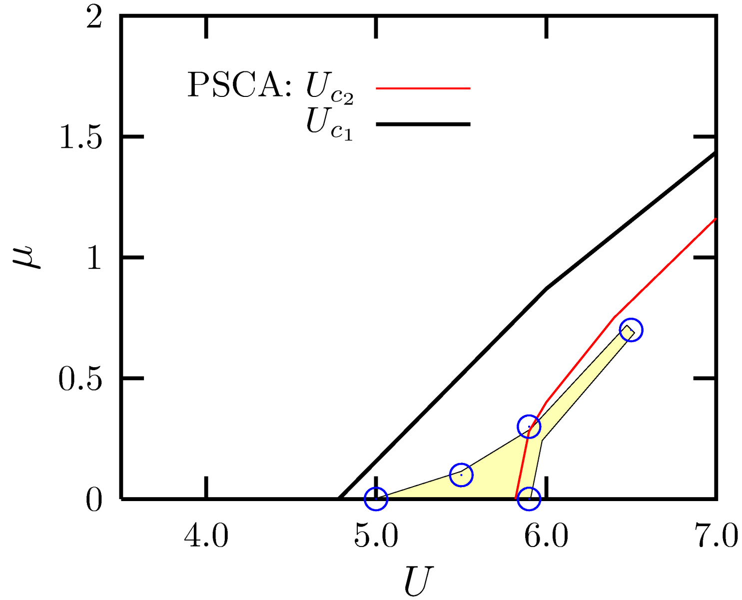
Away from half-filling ...

Feldbacher, Held'04/05





Coexistence:



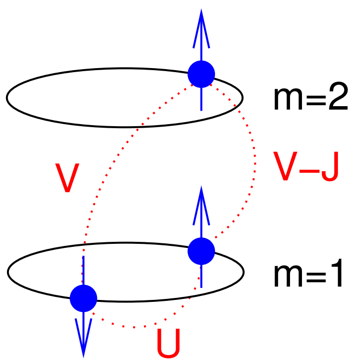
○ DMFT(PQMC)

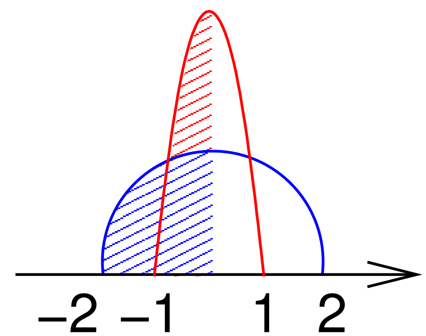
Fischer, Kotliar, Moeller'95

Two-band Hubbard model (half-filling)

Arita, Held cond-mat/0504040

$$H = -\sum_{\langle i,j\rangle\, m\sigma} t_m\, \hat{c}^\dagger_{im\sigma}\hat{c}_{jm\sigma} + U\sum_{i\,m\sigma}\hat{n}_{im\uparrow}\hat{n}_{im\downarrow} + \sum_{i;(m,\sigma)<(m',\sigma')}(V-\delta_{\sigma\sigma'}J)\hat{n}_{im\sigma}\hat{n}_{im'\sigma'}$$
$$-\frac{1}{2}J\sum_{i\sigma;l\neq m}\hat{c}^\dagger_{il\sigma}\hat{c}_{il\bar\sigma}\hat{c}^\dagger_{im\bar\sigma}\hat{c}_{im\sigma} - \frac{1}{2}J\sum_{i\sigma;l\neq m}\hat{c}^\dagger_{il\sigma}\hat{c}^\dagger_{il\bar\sigma}\hat{c}_{im\sigma}\hat{c}_{im\bar\sigma}$$



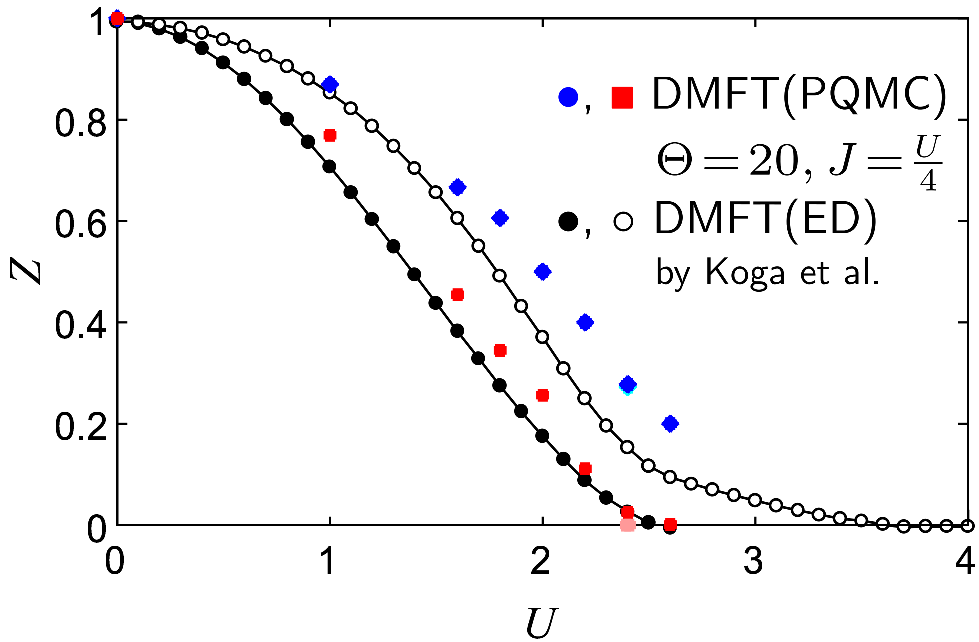


Controversy:
One first-order Mott-Hubbard transition
[Liebsch'03'04; DMFT(QMC) only **first line** of H]
or **two** [Koga, Kawakami, Rice, Anisimov'04; DMFT(ED)]?

We:
DMFT(PQMC)
Correct multiplet structure via
Hubbard-Stratonovich decoupling of Sakai, Arita, Aoki'04

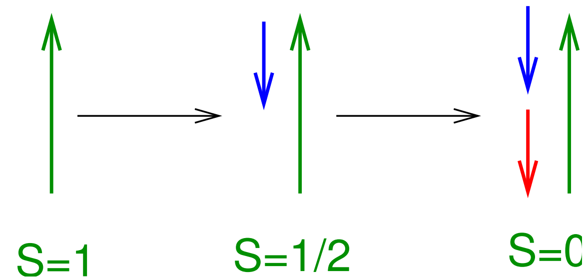
DMFT(PQMC) results

Arita, Held cond-mat/0504040



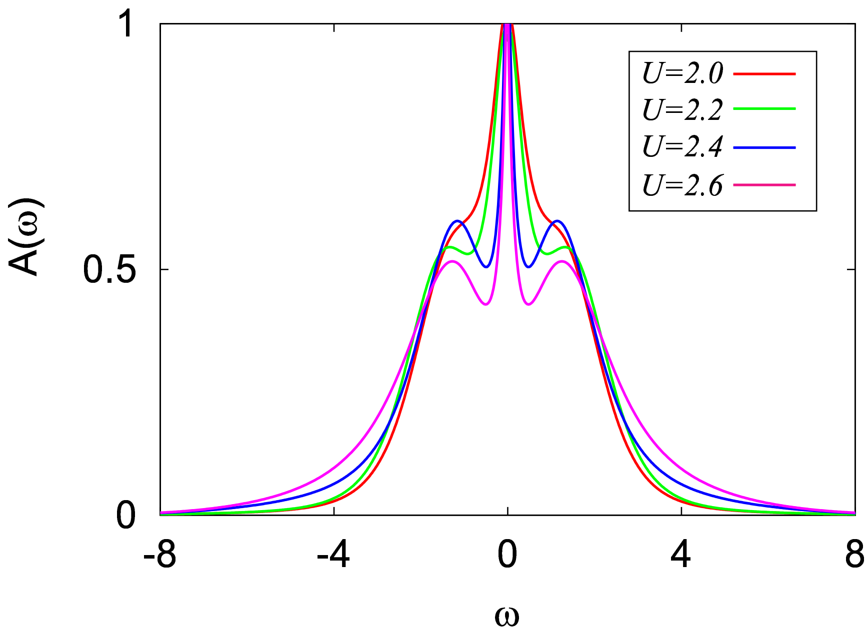
two consecutive 1. order transitions!

$J >$ effective T_K:

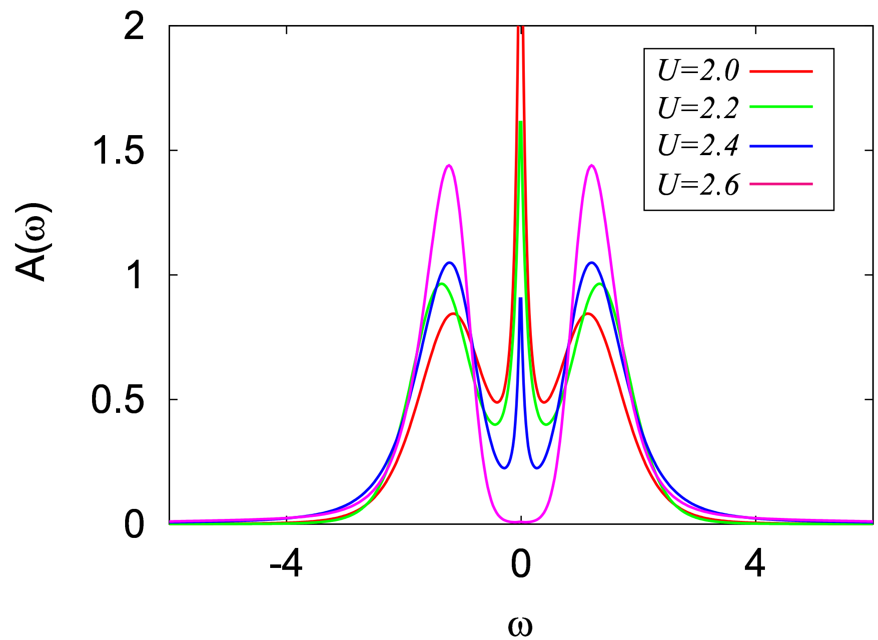


two stage screening

wide band



narrow band



DCA(PQMC) study of the t-t' Hubbard model

Arita, Held'05

$$H = -t \sum_{\langle i,j \rangle_{\mathrm{NN}}\, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + t' \sum_{\langle i,j \rangle_{\mathrm{NNN}}\, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i\,\sigma} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Does the Hubbard model describe **d-/p-wave** superconductivity??

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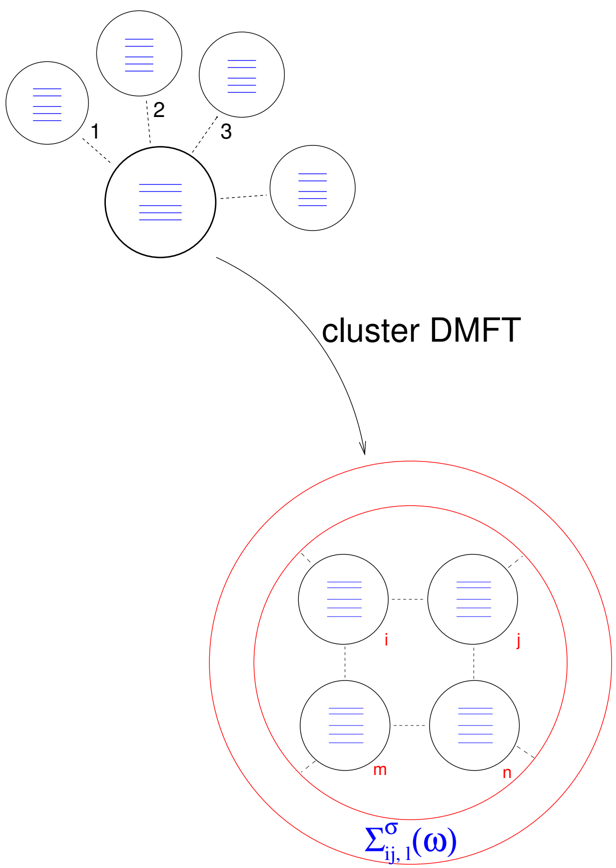
Does the Hubbard model describe **d-/p-wave** superconductivity??

$\mathbf{k}$-dependence essential $\longrightarrow$ DCA



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Does the Hubbard model describe **d-/p-wave** superconductivity??

Some Indications for superconductivity:

fRG Honerkamp, Salmhofer'01; Katanin, Kampf'03

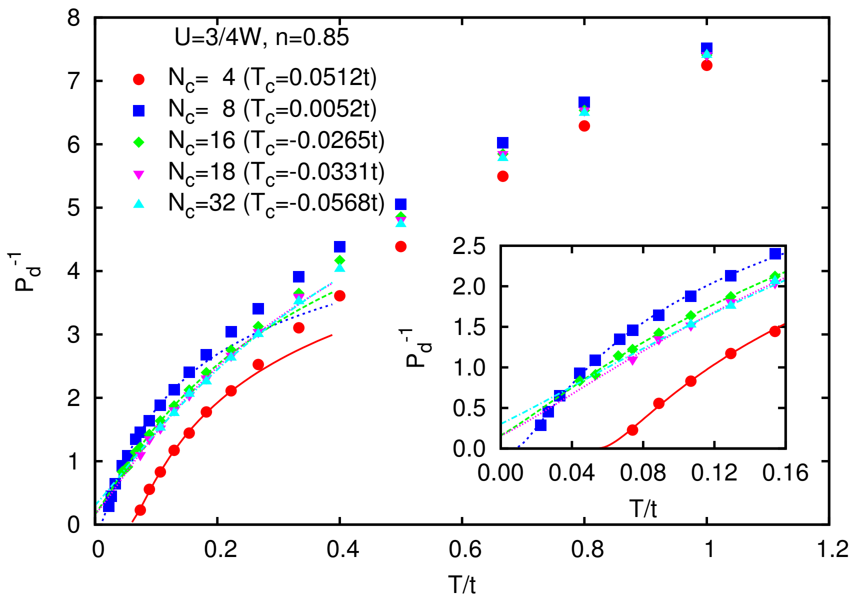
$\longrightarrow$ weak coupling

DCA(QMC) Hettler *et al.*'98; Lichtenstein, Katsnelson'01; Maier *et al.* '04, '05...

$\longrightarrow$ definite answer difficult

$T \longrightarrow 0$ extrapolation

$N_c \longrightarrow \infty$ extrapolation

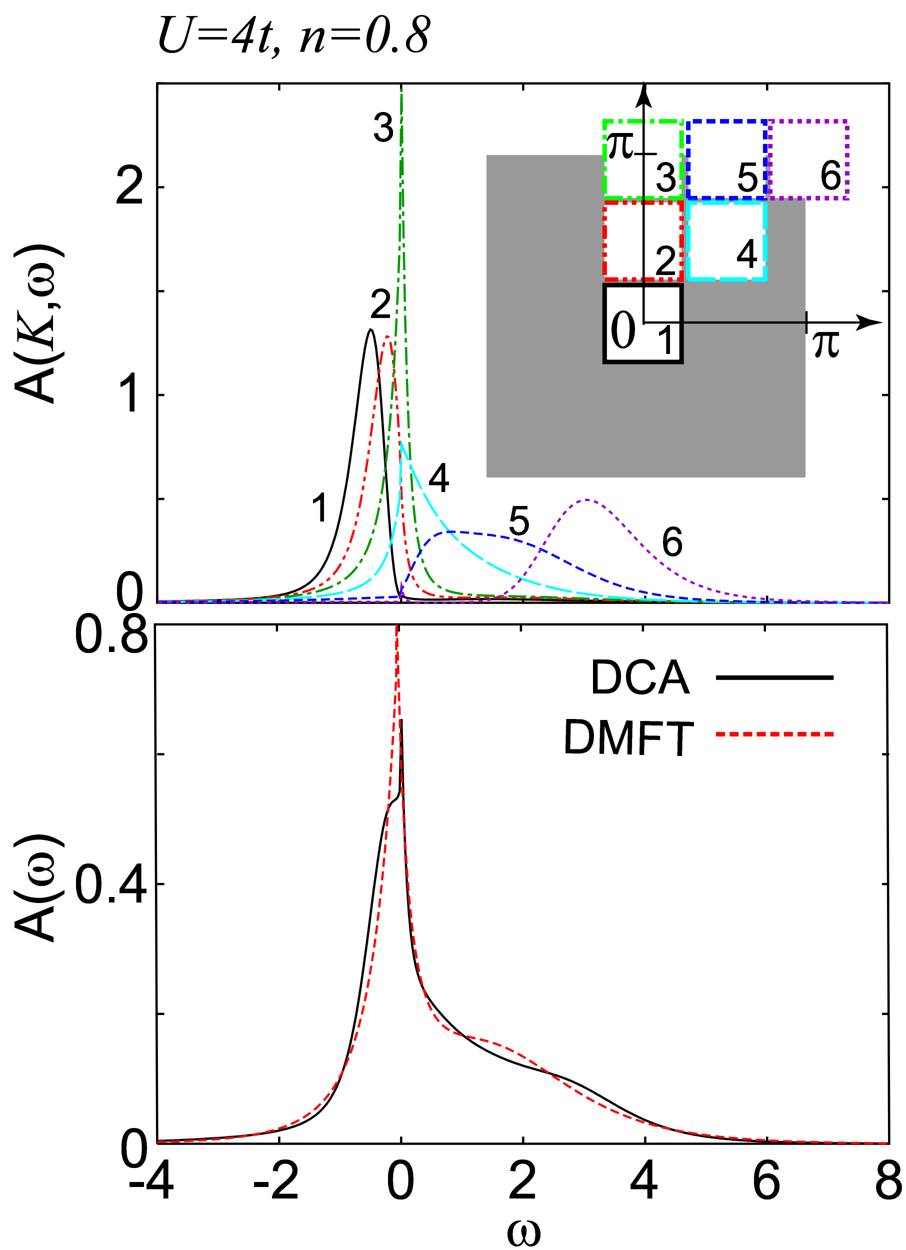


Maier et al. cond-mat/0409669

We: **DCA(PQMC)** $\longrightarrow$ fast, direct route to $T = 0$

Spectral function within PM phase

Arita, Held'05

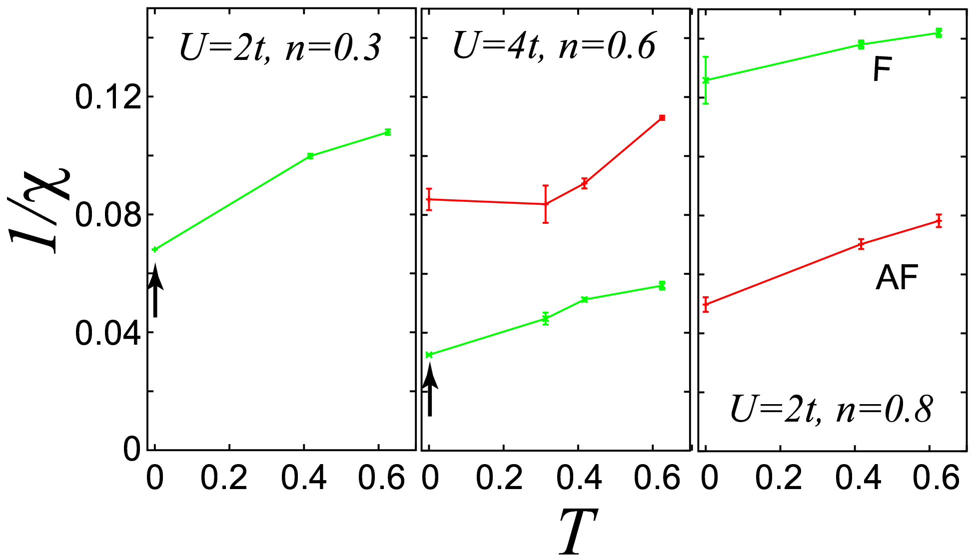


Here and in the following: $t' = 0.4t$, $N_c = 4 \times 4 = 16$

Cluster susceptibilities

Arita, Held'05

Magnetic susceptibility:



Pair susceptibility:

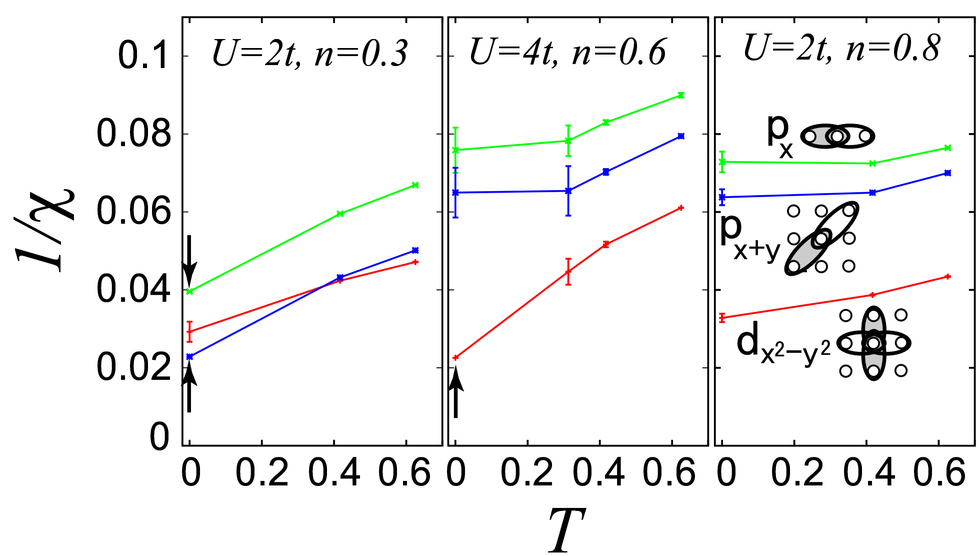
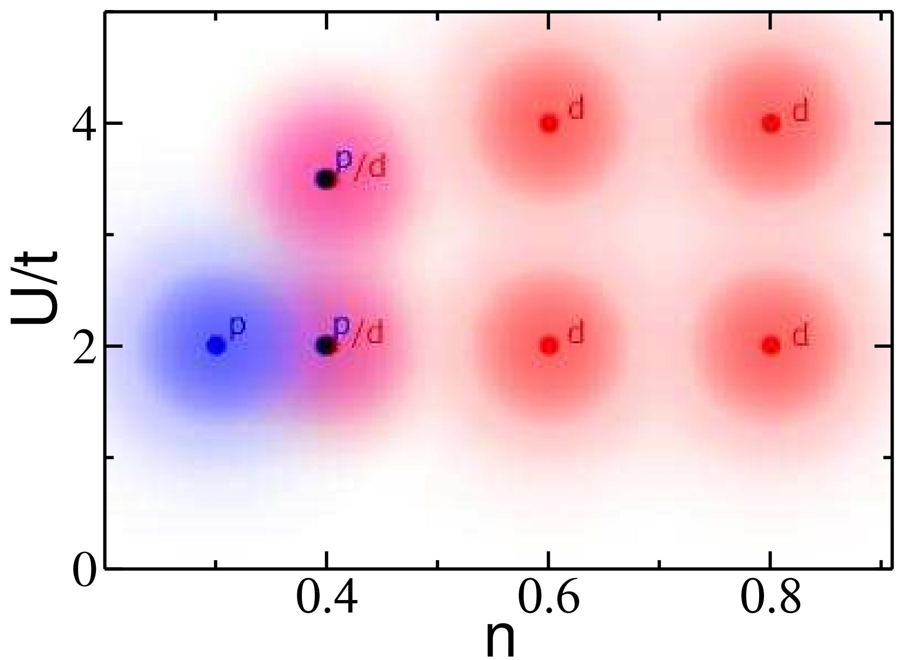


Diagram of dominant pairing symmetry

Arita, Held'05



Conclusion

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- Applications so far:
  - One-band Hubbard model at and away from half-filling
  - Two-band Hubbard model — two consecutive Mott-Hubbard transitions
  - DCA(PQMC) — pair susceptibility in the t-t' Hubbard model

- Outlook:

  PQMC for LDA+DMFT and LDA+DCA