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Diagrammatic MC methods for quantum impurity models

Philipp Werner

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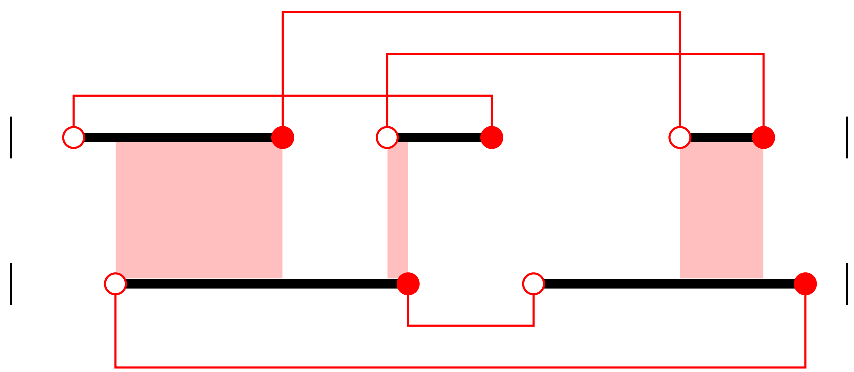


PRL 97, 076405 (2006)

PRB 74, 155107 (2006)

Outline

- Introduction
  - Dynamical mean field theory
  - Existing impurity solvers
- New approach
  - Diagrammatic expansion in the impurity-bath hybridization
  - Scaling with temperature and interaction strength
- Applications
  - Mott transition in the 1-band Hubbard model
  - Holstein-Hubbard model
  - Kondo lattice model
  - multi-orbital models with spin exchange

Collaborators

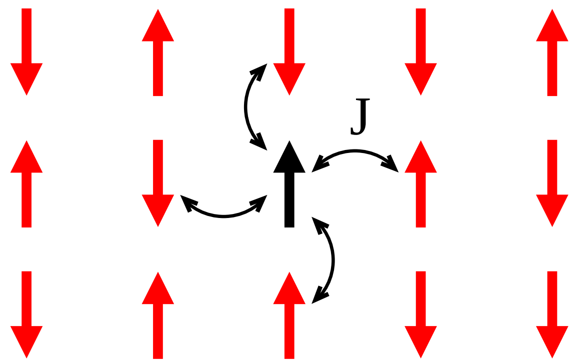
- A. J. Millis, M. Troyer, E. Gull

Introduction

Mean field theory for Ising model

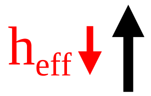
- Lattice model (nearest neighbor coupling J, coordination number z)

  $H_{\text{latt}} = -J \sum_{i,j} S_i S_j$



- Single site model ($m_i = \langle S_i \rangle$, $h_{\text{eff}} = J \sum_{0,i} m_i = zJm$)

  $H_0 = -h_{\text{eff}} S_0$



- Self-consistency condition

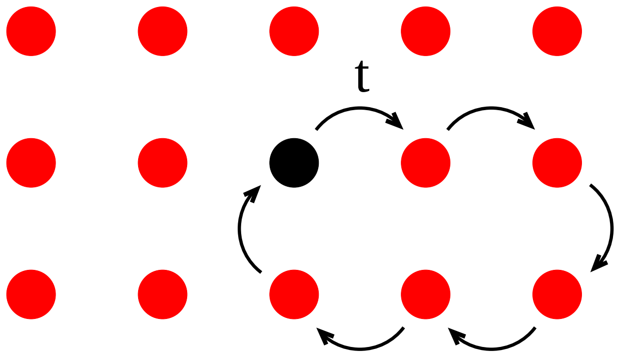
  $m = \langle m_0 \rangle_{H_0}$ ($= \tanh(\beta h_{\text{eff}}) = \tanh(\beta z J m)$)

Introduction

Dynamical mean field theory *Metzner & Vollhardt (1989), Georges & Kotliar (1992)*

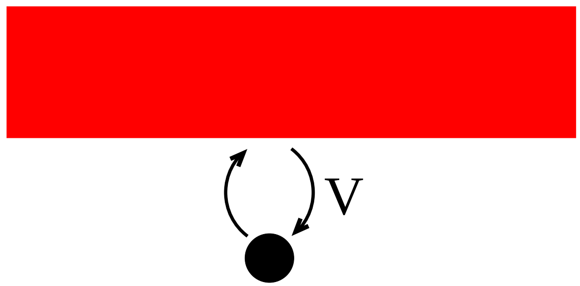
- Lattice model (Density of states $D(\epsilon)$, Self energy $\Sigma_{\text{latt}}(i\omega_n, k)$)

$$H_{\text{latt}} = -\mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma}$$



- Quantum impurity (Hybridization V_k, Self energy $\Sigma_{\text{imp}}(i\omega_n)$)

$$H_{\text{imp}} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \sum_k \epsilon^{\text{bath}}_{k,\sigma} n^{\text{bath}}_{k,\sigma} + \sum_{k,\sigma} (V_k c^\dagger_\sigma a^{\text{bath}}_{k,\sigma} + h.c.)$$



Introduction

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- Lattice model (Density of states $D(\epsilon)$, Self energy $\Sigma_{\text{latt}}(i\omega_n, k)$)

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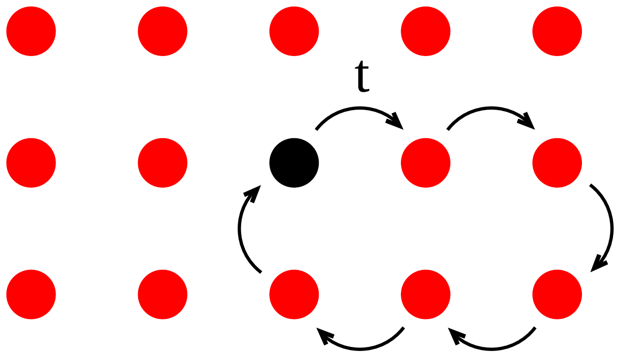
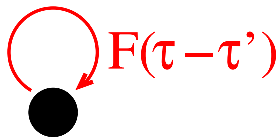


- Effective Action (Hybridization $F(\tau)$, Self energy $\Sigma_{\text{imp}}(i\omega)$)

$$S = \int d\tau (-\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow) - \sum_\sigma \int d\tau d\tau' c_\sigma(\tau) F_\sigma(\tau - \tau') c^\dagger_\sigma(\tau')$$



- Self-consistency condition

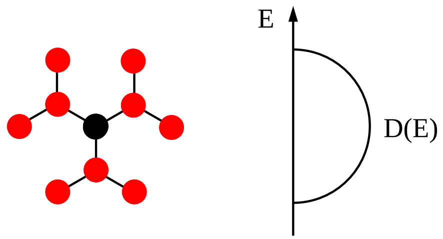
$$G^{\text{loc}}_{\text{latt}}(\tau) = G_{\text{imp}}(\tau)$$

Introduction

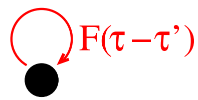
Dynamical mean field theory *Metzner & Vollhardt (1989), Georges & Kotliar (1992)*

- Self-consistency loop

Lattice model



Impurity model



$$G^{\text{loc}}_{\text{latt}}(i\omega_n) = G_{\text{imp}}(i\omega_n) \quad \Rightarrow \quad S_{\text{imp}}[F]$$

$$\Uparrow \qquad\qquad \Downarrow$$

$$G^{\text{loc}}_{\text{latt}}(i\omega_n) = \sum_k G_{\text{latt}}(k, i\omega_n) \qquad \text{impurity solver}$$

$$= \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\text{latt}}(i\omega_n, k)} \qquad \Downarrow$$

$$\approx \int d\epsilon \frac{D(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_{\text{imp}}(i\omega_n)} \qquad G_{\text{imp}}(i\omega_n)$$

$$\Uparrow \qquad\qquad \Downarrow$$

$$\Sigma_{\text{latt}}(i\omega_n, k) = \Sigma_{\text{imp}}(i\omega_n) \quad \Leftarrow \quad \Sigma_{\text{imp}}(i\omega_n)$$

Previous work

Hirsch-Fye solver *Hirsch & Fye (1986)*

- Hubbard model: $Z = TrT_\tau e^{-S}$ with action $S = S_0 + S_U$

$$S_0 = -\sum_\sigma \int_0^\beta d\tau d\tau' c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau') - \mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow)$$

$$S_U = U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

- Discretize imaginary time into N equal slices $\Delta\tau$
- Decouple $Un_\uparrow n_\downarrow$ using discrete Hubbard-Stratonovich transformation

$e^{-\Delta\tau U(n_\uparrow n_\downarrow + 1/2(n_\uparrow + n_\downarrow))} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda(U,\Delta\tau)s(n_\uparrow - n_\downarrow)}$, *Hirsch (1983)*

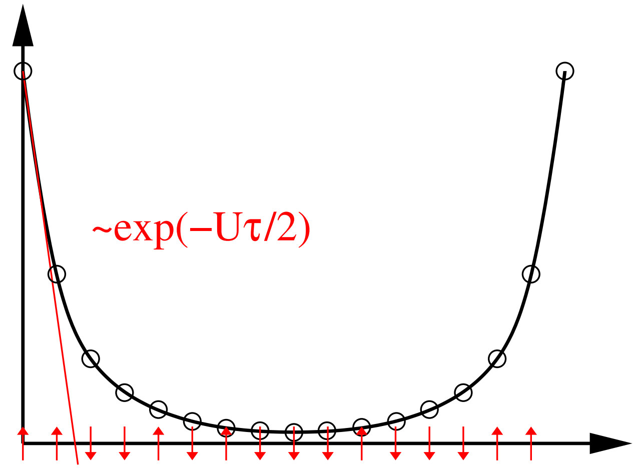
- Perform Gaussian integral

$Z = \sum_{s_i} \det G_{0,\uparrow}^{-1}(s_1, ..., s_N) G_{0,\downarrow}^{-1}(s_1, ..., s_N)$

- MC sampling of auxiliary Ising spins
- Initial drop of Green function $\sim e^{-U\tau/2}$

$\rightarrow$ Matrix size: $N \sim 5\beta U$

$\rightarrow$ Low temperatures not accessible



Previous work

Weak coupling expansion *Rubtsov et al. (2005)*

- Hubbard model: $Z = Tr T_\tau e^{-S}$ with action $S = S_0 + S_U$

  $$S_0 = -\sum_\sigma \int_0^\beta d\tau d\tau' c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau') - \mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow)$$

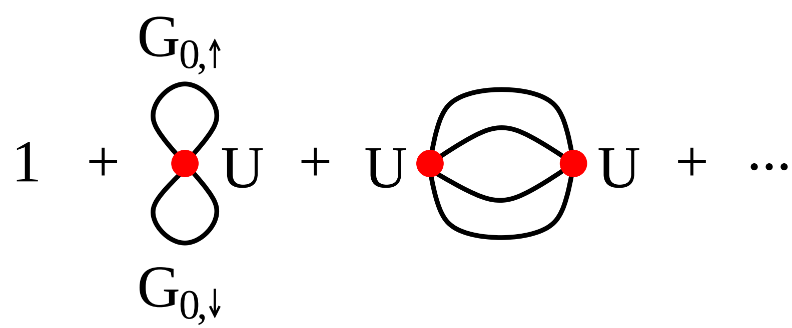
  $$S_U = U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

- Continuous-time solver based on a diagrammatic expansion of Z
  Prokof'ev et al. (1996)
- Treat quadratic part S_0 as unperturbed action and expand $e^{-U \int d\tau n_\uparrow n_\downarrow}$

  $$Z = \sum_k \frac{(-U)^k}{k!} \int d\tau_1 ... d\tau_k \int \mathcal{D}[c, c^\dagger] e^{-S_0[c,c^\dagger]} n_\uparrow(\tau_1) n_\downarrow(\tau_1) ... n_\uparrow(\tau_k) n_\downarrow(\tau_k)$$

- Perform Gaussian integral

  $$Z = \sum_k \frac{(-U)^k}{k!} \int d\tau_1 ... d\tau_k$$
  $$\times \det G_{0,\uparrow}(\tau_1, ..., \tau_k) G_{0,\downarrow}(\tau_1, ..., \tau_k)$$

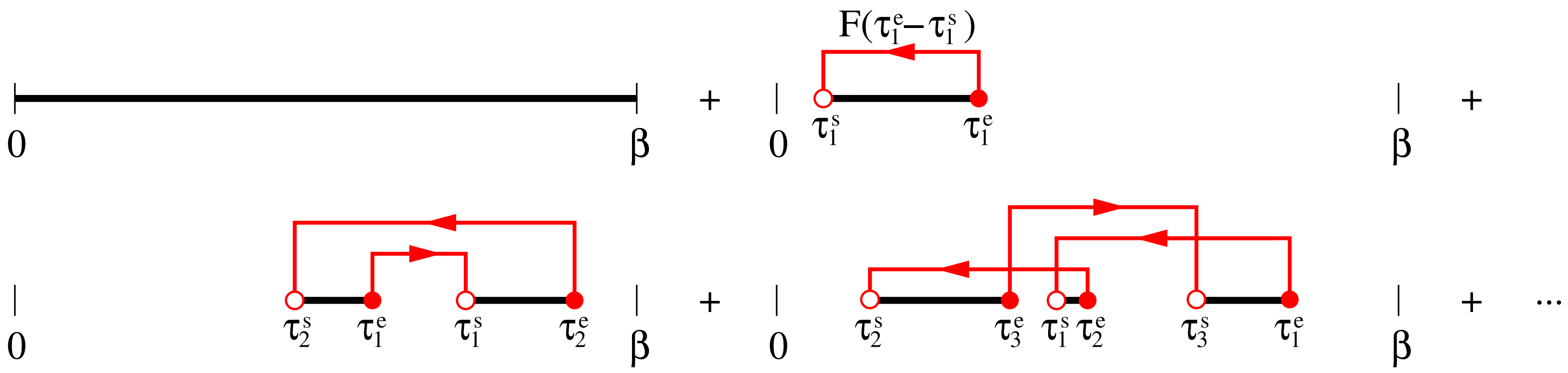


- MC sampling of configurations of interaction vertices $U n_\uparrow n_\downarrow(\tau)$
- Matrix size: $\langle k \rangle \sim 0.5 \beta U$

New impurity solver

Expansion in the impurity-bath hybridization F *PRL 97, 076405 (2006)*

- Non-interacting model: $Z = TrT_\tau \exp(\int_0^\beta d\tau d\tau' c(\tau)F(\tau-\tau')c^\dagger(\tau'))$
- Expand exponential, evaluate in the occupation number basis $\{|0\rangle, |1\rangle\}$
- $Z = \frac{1}{0!}Tr1$
  $+\frac{1}{1!}TrT_\tau \int d\tau_1^s d\tau_1^e \; c(\tau_1^e)F(\tau_1^e-\tau_1^s)c^\dagger(\tau_1^s)$
  $+\frac{1}{2!}TrT_\tau \int d\tau_1^s d\tau_1^e d\tau_2^s d\tau_2^e \; c(\tau_1^e)F(\tau_1^e-\tau_1^s)c^\dagger(\tau_1^s) \; c(\tau_2^e)F(\tau_2^e-\tau_2^s)c^\dagger(\tau_2^s)$
  $+\ldots$



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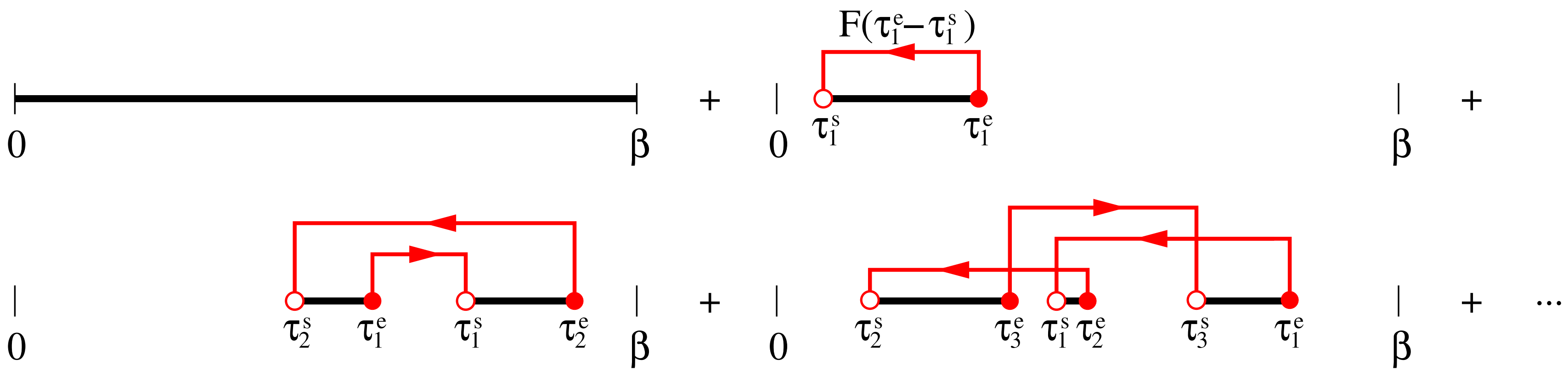
- Expand exponential, evaluate in the occupation number basis $\{|0\rangle, |1\rangle\}$
- $$Z = \frac{1}{0!} Tr 1 + \frac{1}{1!} TrT_\tau \int d\tau_1^s d\tau_1^e\, c(\tau_1^e) F(\tau_1^e - \tau_1^s) c^\dagger(\tau_1^s) + \frac{1}{2!} TrT_\tau \int d\tau_1^s d\tau_1^e d\tau_2^s d\tau_2^e\, c(\tau_1^e) F(\tau_1^e - \tau_1^s) c^\dagger(\tau_1^s)\, c(\tau_2^e) F(\tau_2^e - \tau_2^s) c^\dagger(\tau_2^s) + \ldots$$



- Some diagrams have negative weight

Segment picture

Expansion in the impurity-bath hybridization F *PRL 97, 076405 (2006)*

- Non-interacting model: $Z = TrT_\tau \exp(\int_0^\beta d\tau d\tau' c(\tau) F(\tau - \tau') c^\dagger(\tau'))$

- Collect the $k!$ diagrams with the same $\{c(\tau_i^s), c^\dagger(\tau_i^e)\}_{i=1\ldots k}$ into a determinant

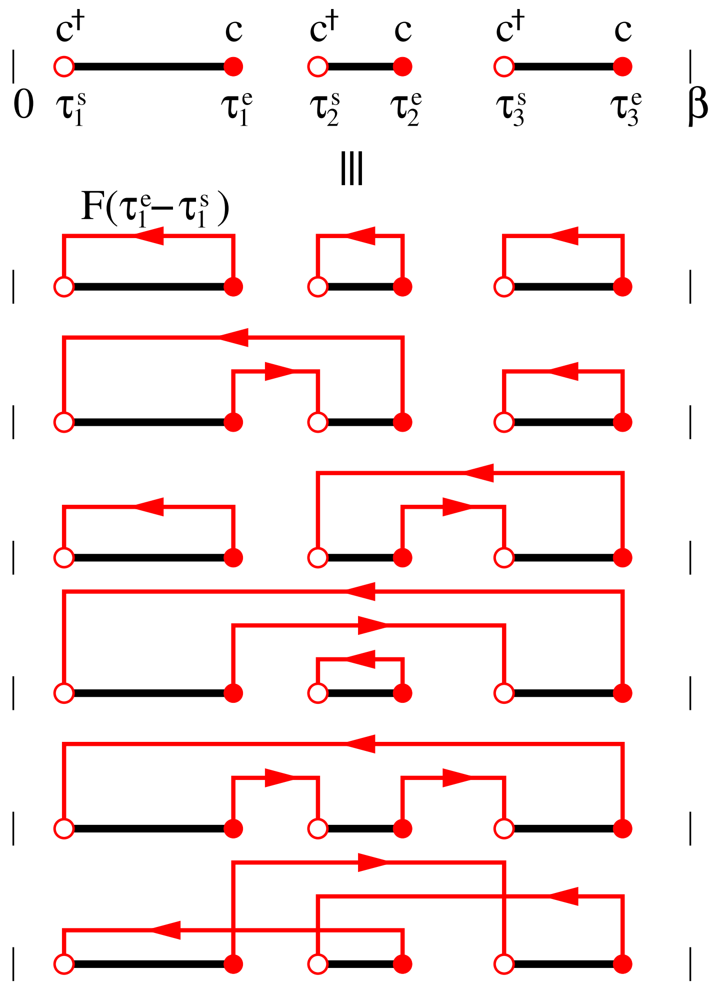
  $\det \mathcal{F}^{(k)}$

  $(\mathcal{F}^{(k)})_{m,n} = F(\tau_m^e - \tau_n^s)$

  $\rightarrow$ resums huge numbers of diagrams $(100! = 10^{158})$
  $\rightarrow$ eliminates the sign problem
  $\rightarrow$ leads to lower perturbation orders

- $\det \mathcal{F}^{(k)} \Leftrightarrow$ configuration of k segments

- $Z = 2 + \sum_{k=1}^\infty \int_0^\beta d\tau_1^s \ldots \int_{\tau_{k-1}^e}^\beta d\tau_k^s \int_{\tau_k^s}^{\circ\tau_1^s} d\tau_k^e \times \det \mathcal{F}^{(k)}$



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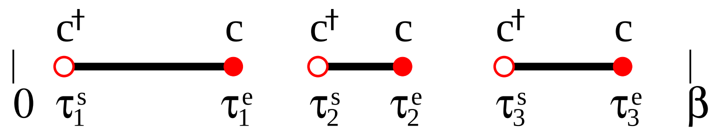

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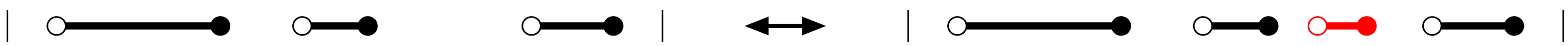
Monte Carlo sampling

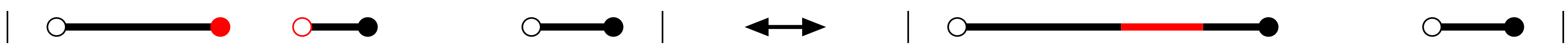
Expansion in the impurity-bath hybridization F *PRL 97, 076405 (2006)*

- Sampling of Z through local updates of segment configurations

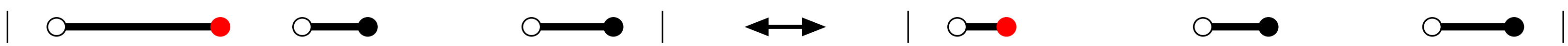
(i) insertion/removal of segments



(ii) insertion/removal of anti-segments



(iii) shifts of the segment end points



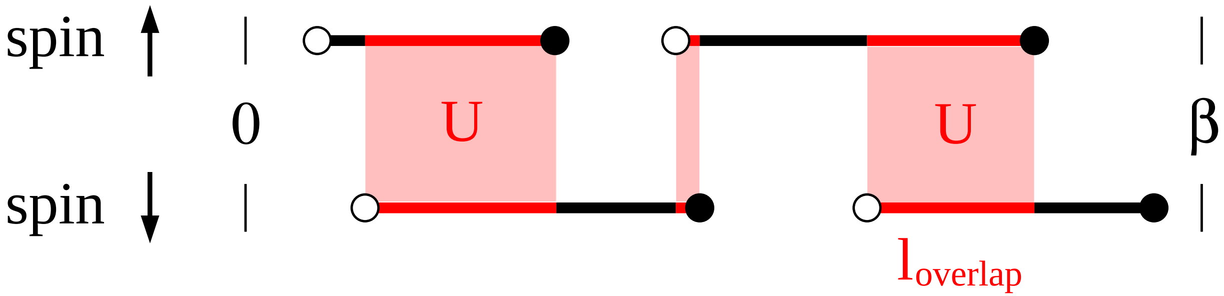
- Detailed balance

$$s_k \longrightarrow s_{k+1} = s_k + \tilde{s} \qquad \frac{p(s_k \longrightarrow s_{k+1})}{p(s_{k+1} \longrightarrow s_k)} = \frac{\det \mathcal{F}^{(k+1)}}{\det \mathcal{F}^{(k)}} \frac{\beta^2}{k+1} e^{\tilde{l}\mu}$$

Monte Carlo sampling

Expansion in the impurity-bath hybridization F *PRL 97, 076405 (2006)*

- Hubbard model ($U \neq 0$): Segment configurations for spin up/down



- Weight of MC configuration also depends on segment overlap

$$w = \det \mathcal{F}_\uparrow \det \mathcal{F}_\downarrow \exp[(l_\uparrow + l_\downarrow)\mu - U l_{\text{overlap}}]$$

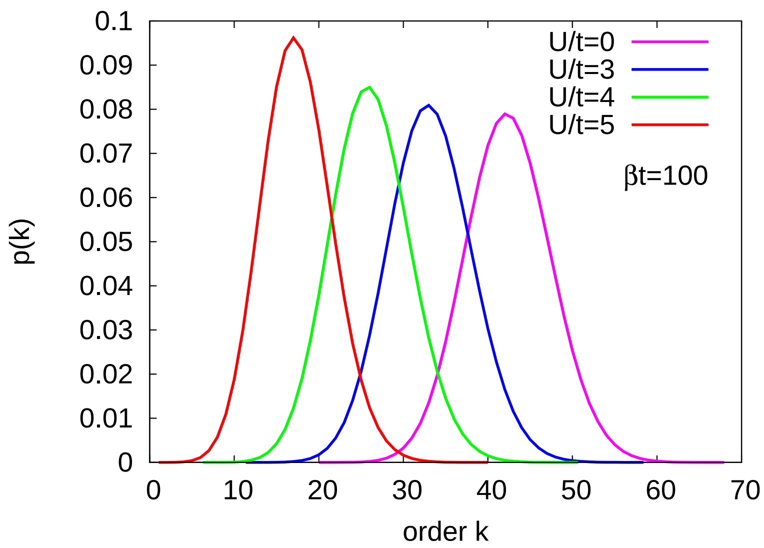
Efficiency

Expansion in the impurity-bath hybridization F *PRL 97, 076405 (2006)*

- Computational effort grows $O(k^3)$ with matrix size k
- $\langle k \rangle \sim \beta$
- $\langle k \rangle$ decreases with increasing U

  $\rightarrow$ ideal for strong correlations

  $\rightarrow$ works even at very low T
- Comparison: *cond-mat/0609438*

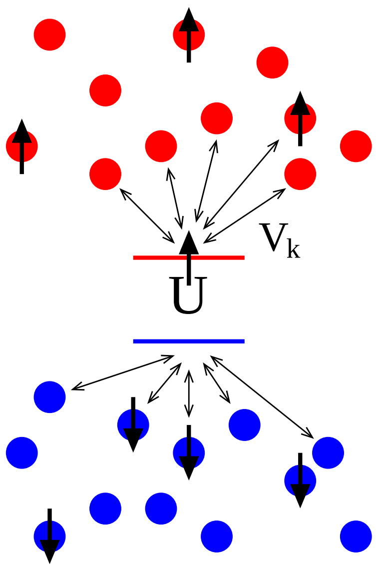


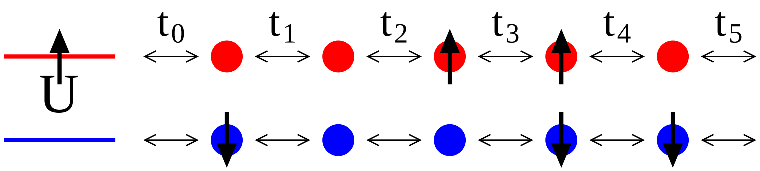
Method	Hirsch-Fye	Expansion in U	Expansion in F
Matrix size $\langle k \rangle$	$\sim \beta$	$\sim \beta$	$\sim \beta$
$\beta t = 100, U/t = 3$	1500	150	32
$\beta t = 100, U/t = 4$	2000	200	26
$\beta t = 100, U/t = 5$	2500	250	17

Sign problem

- Map "impurity+bath" to a "chain" *Kaul et al., J. Phys. A (2005)*

  $H_{\text{hyb}} = \sum_k V_k c^\dagger a_k^{\text{bath}}$ becomes hopping to first site: $t_0 c^\dagger a_0^{\text{chain}}$



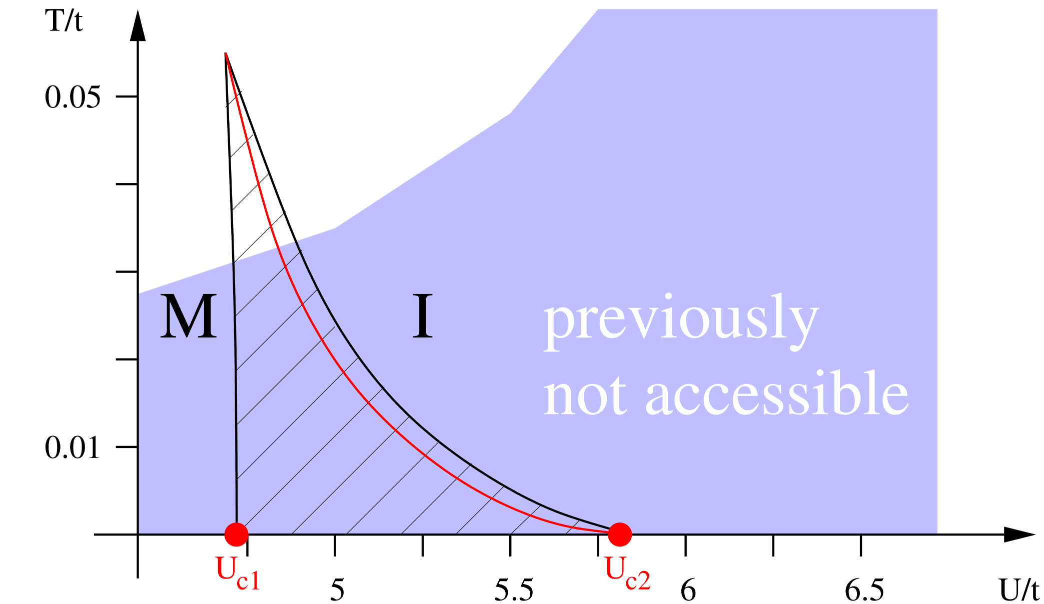


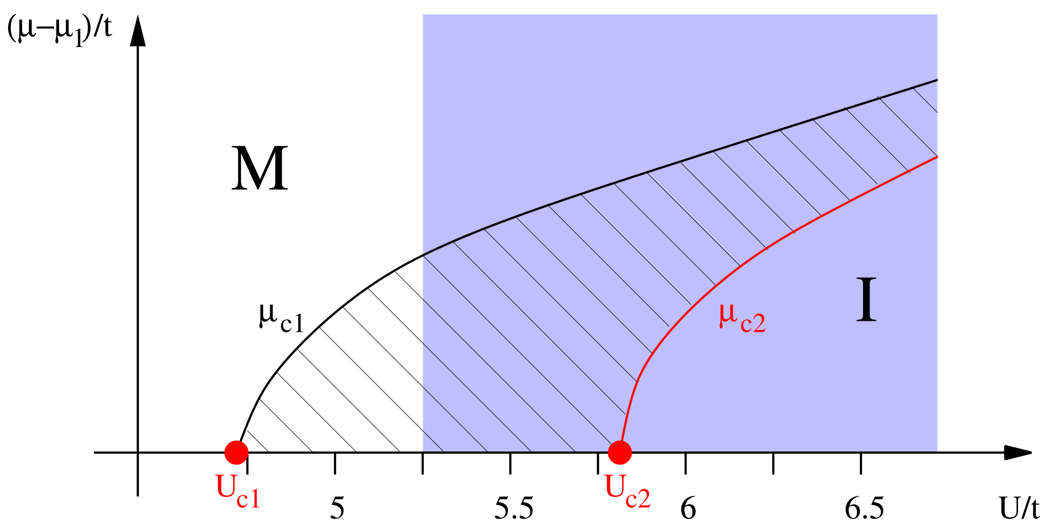
- In the chain representation, can choose basis $\{|\alpha\rangle\}$ such that H becomes tridiagonal with offdiagonal elements $t_i < 0$

- MC weight are of the form $Tr[e^{-\tau_1 H_{\text{loc}}}(-H_{\text{hyb}})e^{-(\tau_2-\tau_1)H_{\text{loc}}}(-H_{\text{hyb}})...]$
  - $\langle\alpha| - H_{\text{hyb}}|\beta\rangle = -t_0\delta_{\alpha,c}\delta_{\beta,0} \geq 0$
  - $\langle\alpha|e^{-\tau H_{\text{loc}}}|\beta\rangle = \langle\alpha|(1 - \frac{\tau}{N}H_{\text{loc}})^N|\beta\rangle \geq 0$

Hubbard model

Bethe lattice, paramagnetic phase

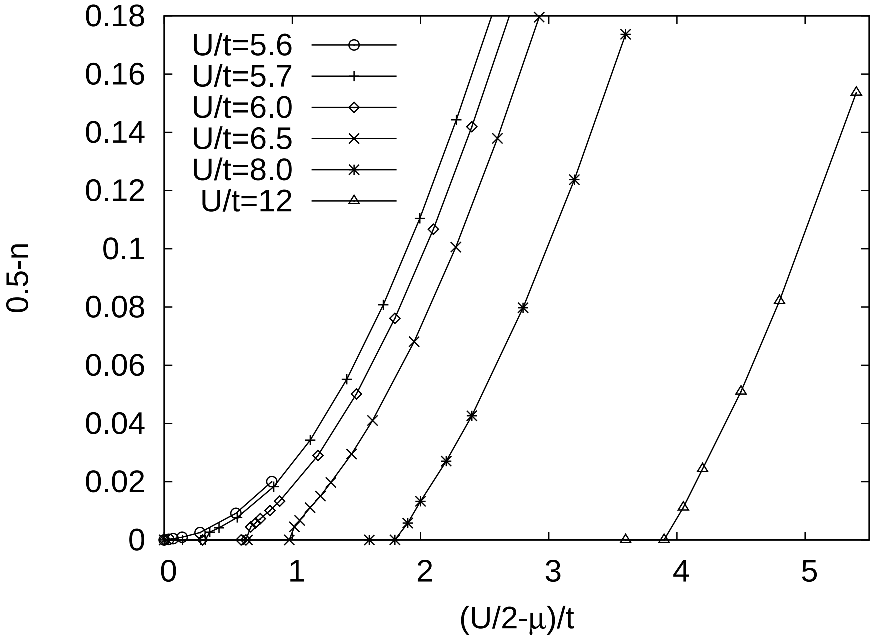


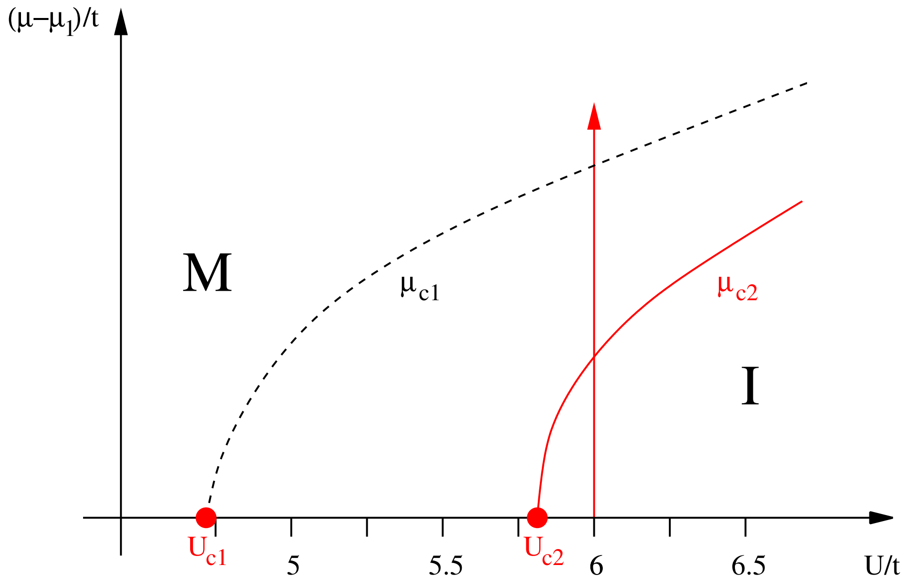


Hubbard model

Bethe lattice, paramagnetic phase *PRB 75, 085108 (2007)*

- Mott transition is first order for $T > 0$, but second order at $T = 0$
- Charge compressibility $\partial n/\partial\mu$ vanishes as $U \to U_{c2}^{+}$





Hubbard model

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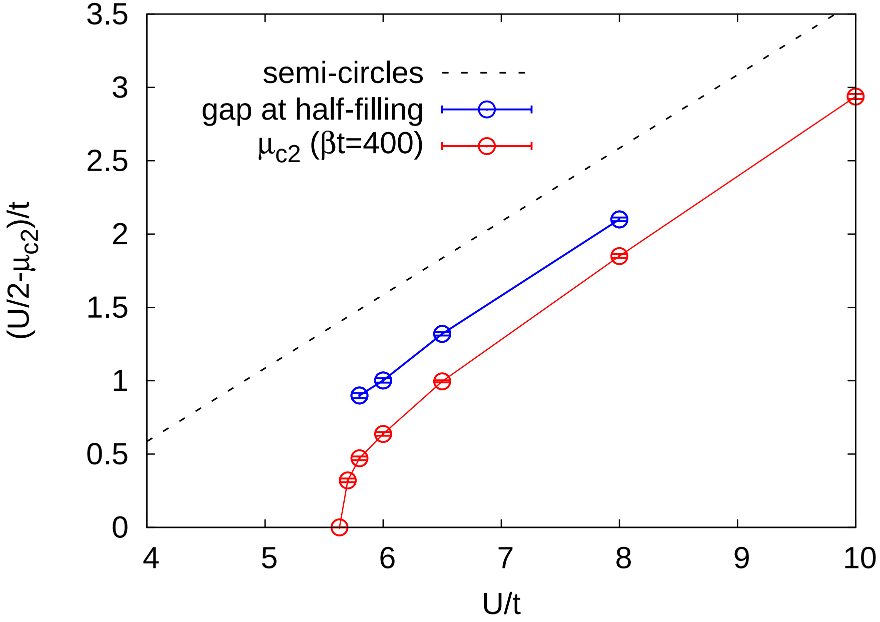
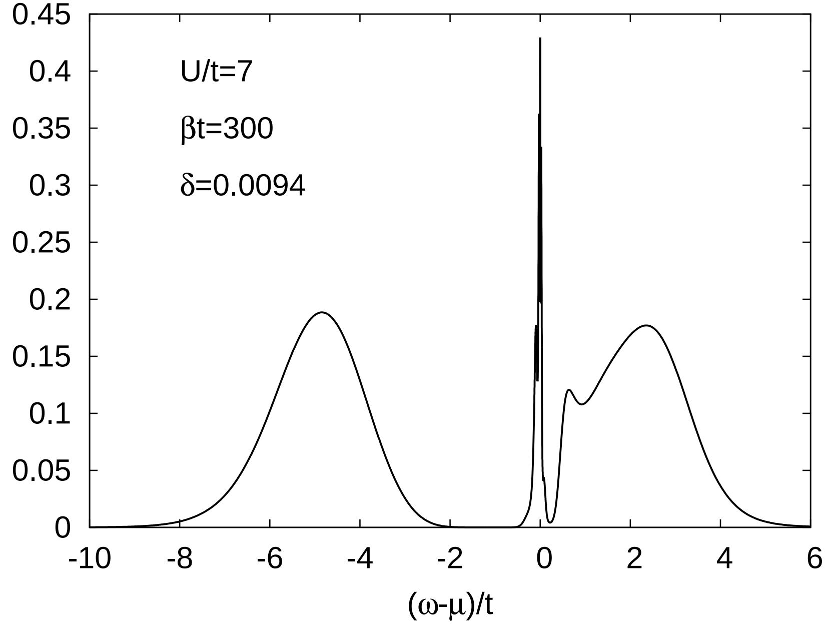
- Doping a Mott insulator induces states in the gap
  Fisher, Kotliar, Moeller (1995)
- In-gap nature of these states only relevant for dopings $\lesssim 2\%$





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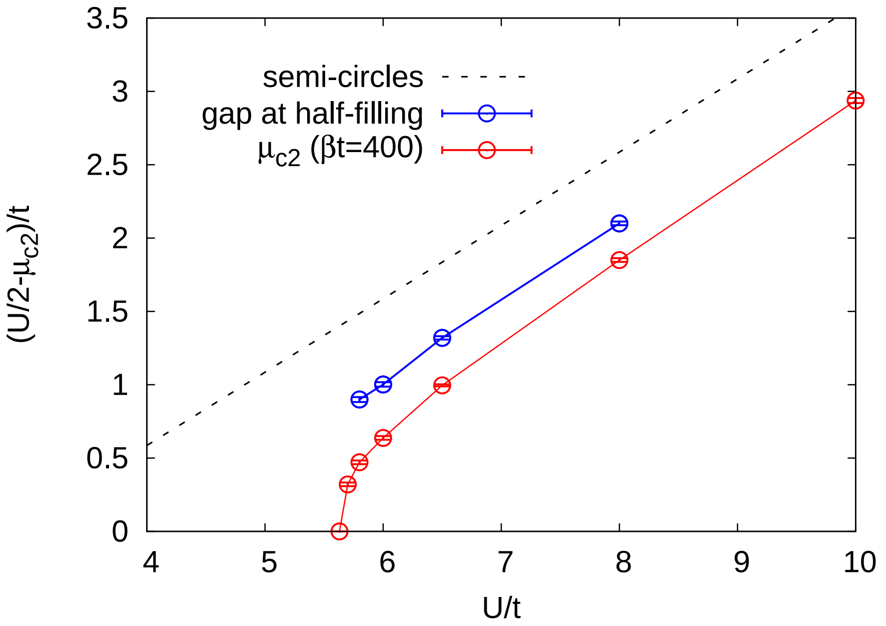

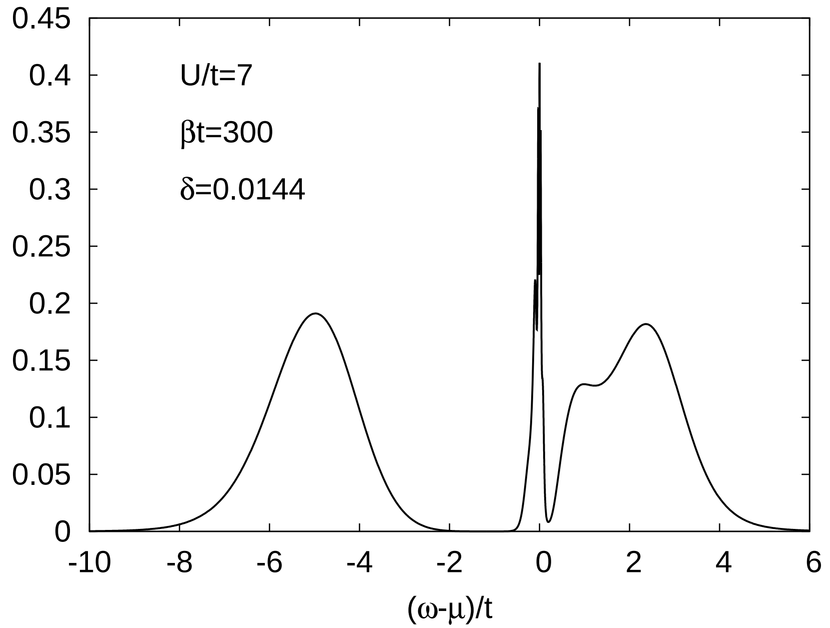

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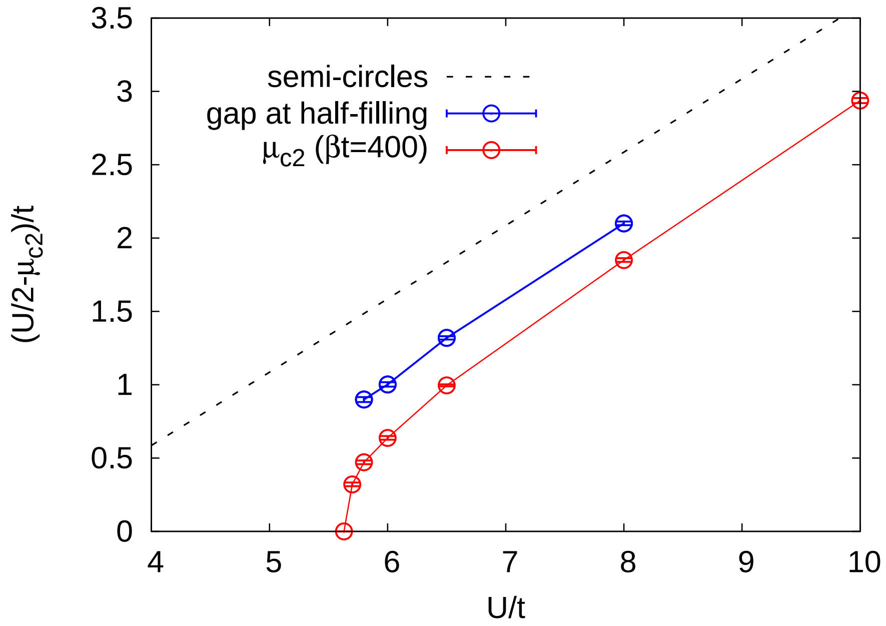
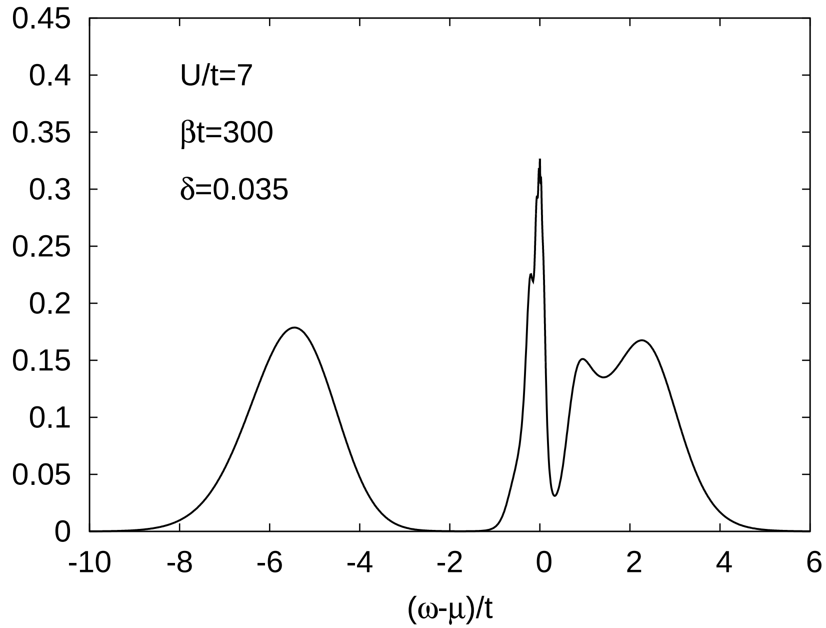
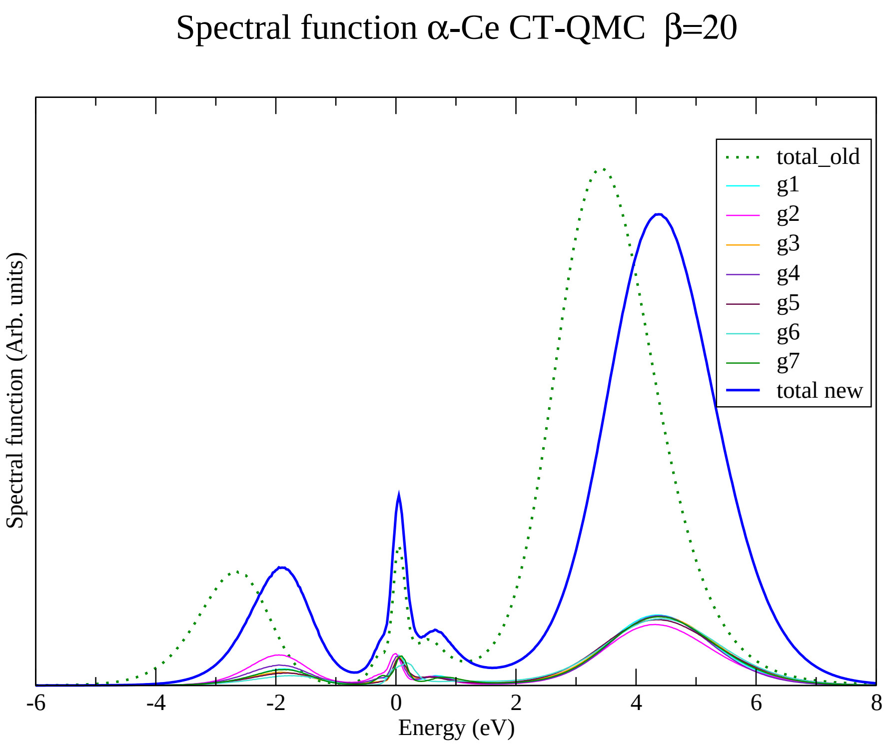


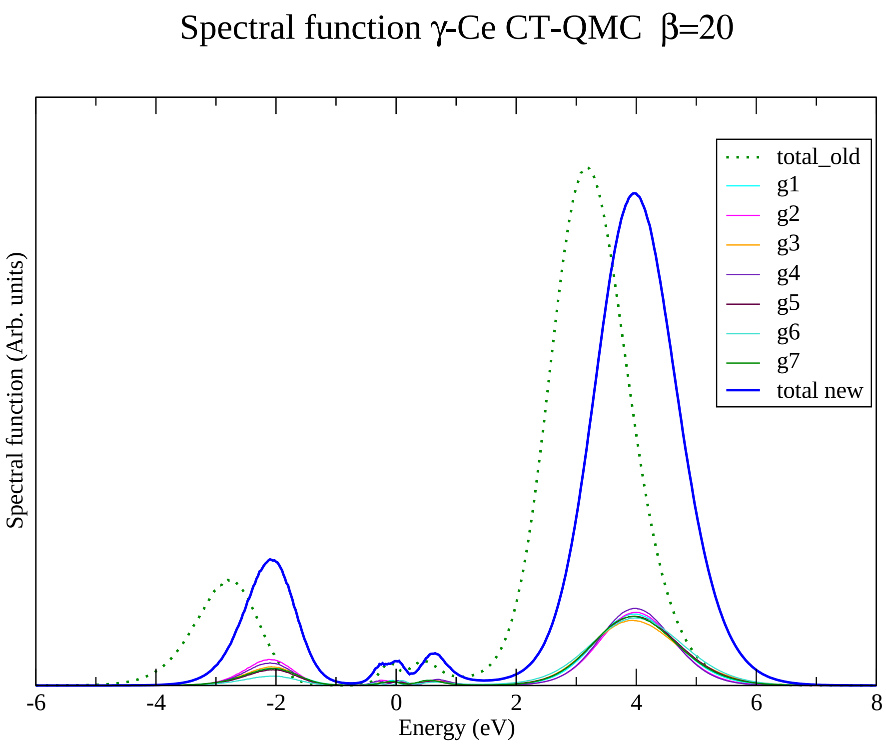


LDA+DMFT

Cerium (7-band model, density-density interactions)

in collaboration with A. Lukoyanov, A. Shorikov & V. Anisimov



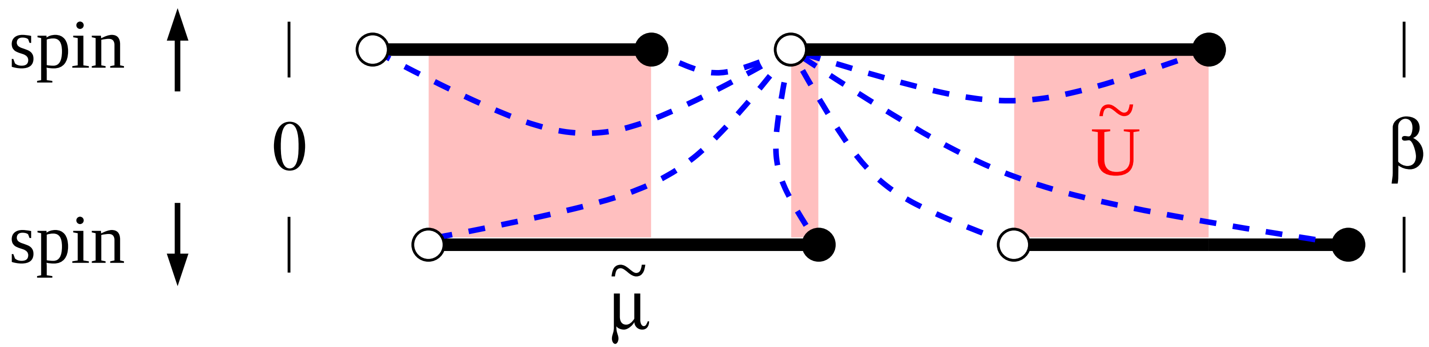


Holstein-Hubbard model

- On-site repulsion and coupling to Einstein phonons *PRL 99, 146404 (07)*

$$H_{\text{loc}} = H_{\text{loc}}^{\text{Hubbard}} + \lambda(n_\uparrow + n_\downarrow - 1)(b^\dagger + b) + \omega_0 b^\dagger b$$

- Evaluate $Tr_b[\cdots]$ analytically using Lang-Firsov transformation
  $\Rightarrow$ additional interaction between segment start/end points
- No truncation of phonons; negligible extra computational cost



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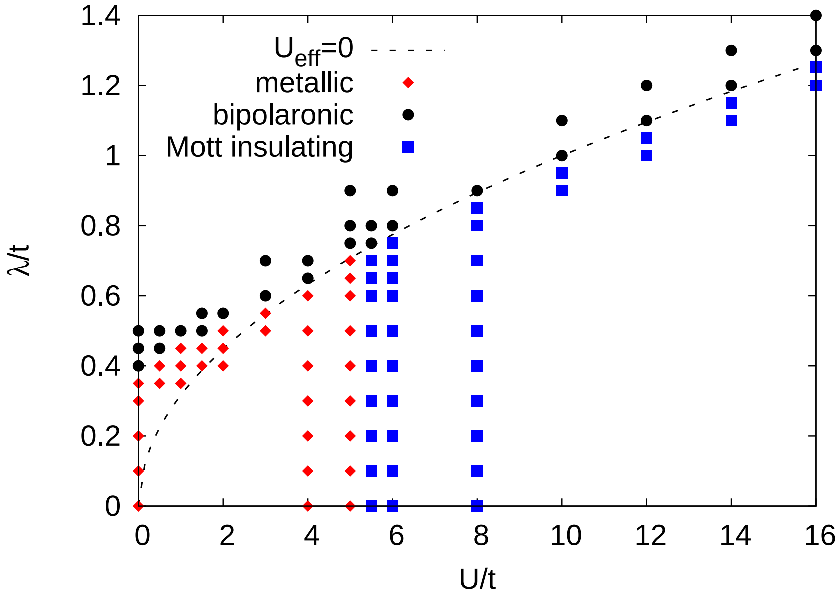
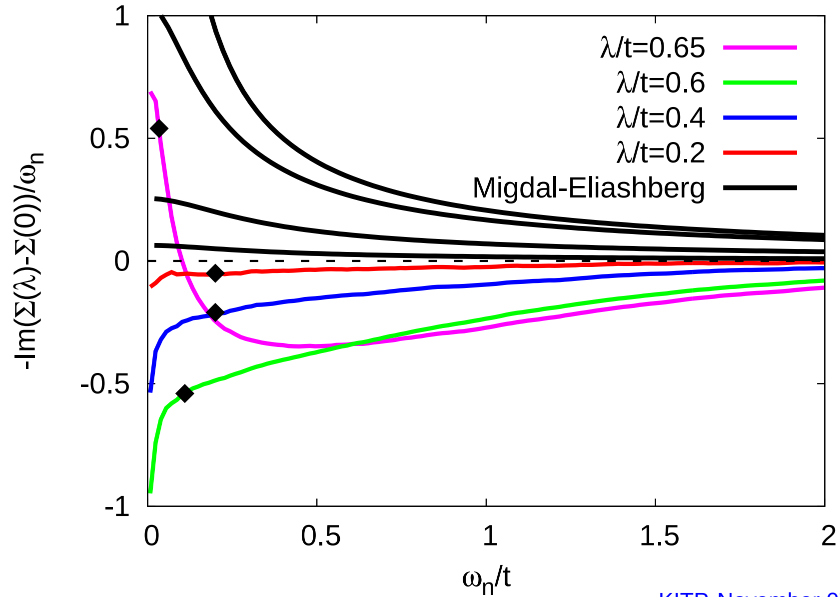
- On-site repulsion and coupling to Einstein phonons *PRL 99, 146404 (07)*

$$H_{\text{loc}} = H_{\text{loc}}^{\text{Hubbard}} + \lambda(n_\uparrow + n_\downarrow - 1)(b^\dagger + b) + \omega_0 b^\dagger b$$

- Evaluate $Tr_b[\cdots]$ analytically using Lang-Firsov transformation
  $\Rightarrow$ additional interaction between segment start/end points
- No truncation of phonons; negligible extra computational cost
- Phase diagram and phonon contribution to the self-energy





General formalism

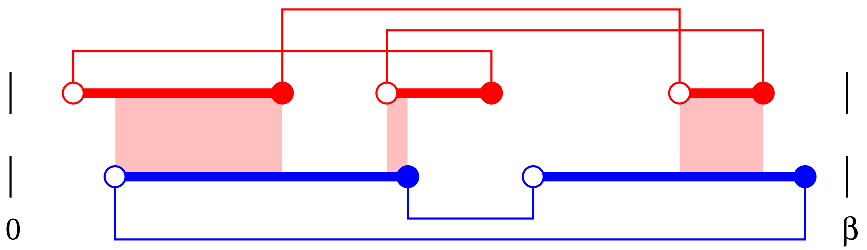
Matrix method *PRB 74, 155107 (2006)*

General impurity model: $Z = TrT_\tau e^{-S}$ with action $S = S_F + S_{\text{loc}}$

$$S_F = -\sum_a \int_0^\beta d\tau d\tau' \psi_a(\tau) F_a(\tau - \tau') \psi_a^\dagger(\tau')$$

$$S_{\text{loc}} = \int_0^\beta d\tau \underbrace{(\psi^\dagger Q \psi + U^{abcd} \psi_a^\dagger \psi_b^\dagger \psi_c \psi_d)}_{H_{\text{loc}}}$$

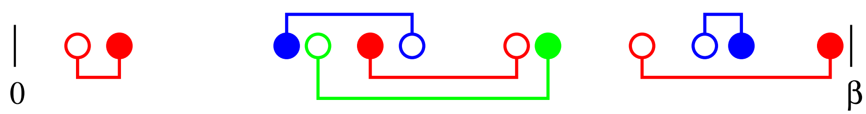
segment formulation ($U^{ab} n_a n_b$)



$$w = \prod_a \det \mathcal{F}_a$$

$$\times\ e^{\mu \sum l_a - U \sum l^{ab}_{\text{overlap}}}$$

matrix formulation ($U^{abcd} \psi_a^\dagger \psi_b^\dagger \psi_c \psi_d$)



$$w = \prod_a \det \mathcal{F}_a$$

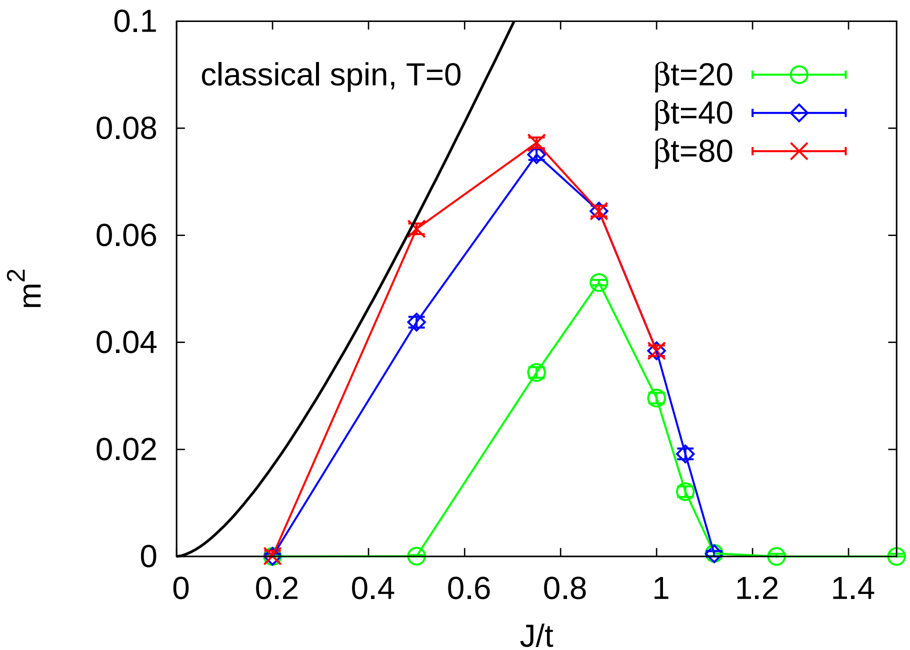
$$\times\ Tr[e^{-H_{\text{loc}}(\tau_1)} O_1 e^{-H_{\text{loc}}(\tau_2 - \tau_1)} O_2 \ldots]$$

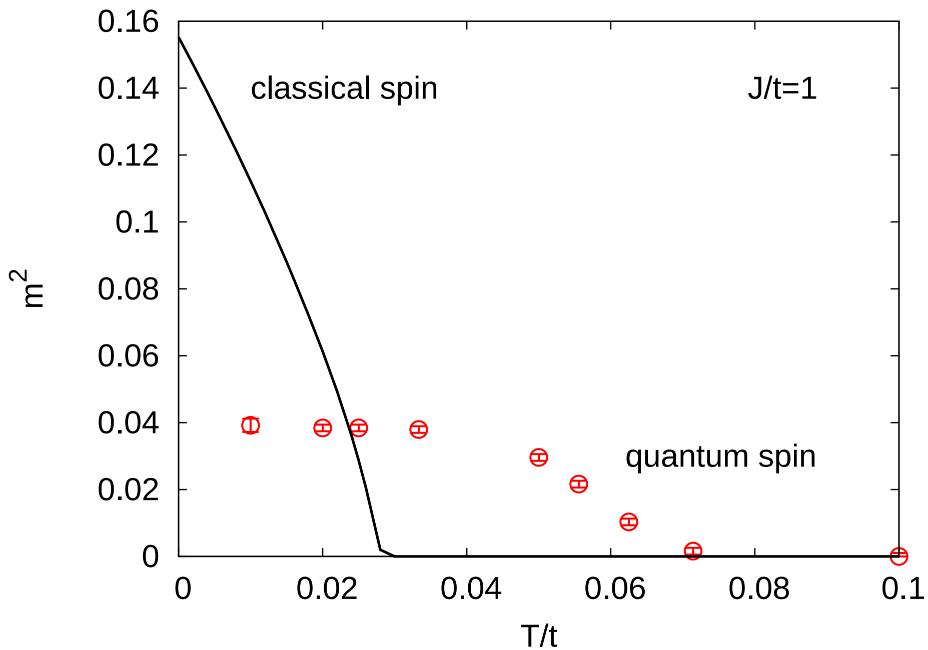
Kondo lattice model

Antiferromagnetic self-consistency loop, $J > 0$ *PRB 74, 155107 (2006)*

$$H_{\text{loc}} = -\mu \sum_a \psi_a^\dagger \psi_a + J\vec{S} \cdot \frac{1}{2} \psi_a^\dagger \vec{\sigma}_{a,b} \psi_b$$

- Quantum phase transition: antiferromagnet $\Leftrightarrow$ paramagnet
- Classical spins would yield $m^2 > 0$ for all J



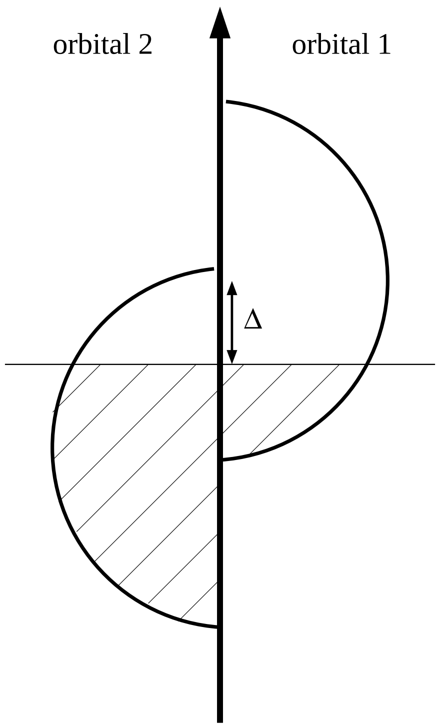


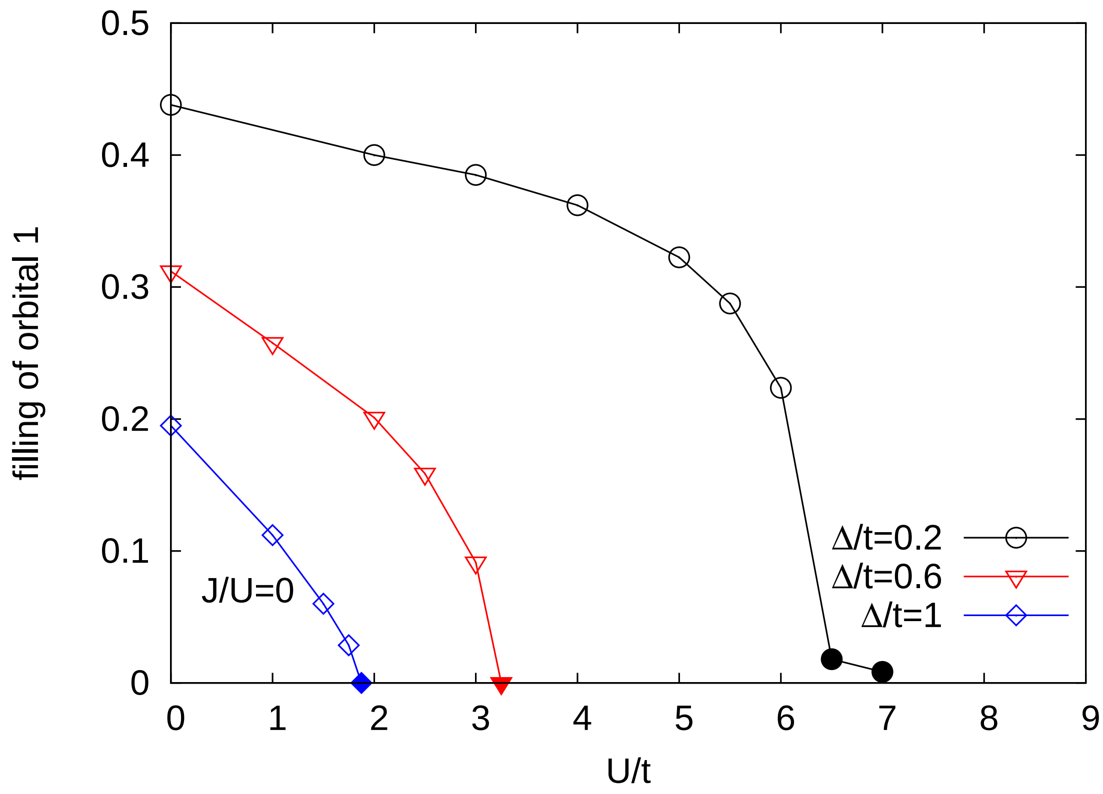
2-orbital model

Effect of Hund coupling J and crystal field splitting Δ, *PRL 99, 126405 (2007)*

$$H_{\text{loc}} = \sum_\alpha U n_{\alpha,\uparrow} n_{\alpha,\downarrow} + \sum_\sigma U' n_{1,\sigma} n_{2,-\sigma} + \sum_\sigma (U' - J) n_{1,\sigma} n_{2,\sigma}$$
$$- J(\psi^\dagger_{1,\downarrow}\psi^\dagger_{2,\uparrow}\psi_{2,\downarrow}\psi_{1,\uparrow} + \psi^\dagger_{2,\uparrow}\psi^\dagger_{2,\downarrow}\psi_{1,\uparrow}\psi_{1,\downarrow} + h.c.) - (\mu - \Delta) n_1 - (\mu + \Delta) n_2$$

- Results for half-filling, $\beta t = 50$, $U' = U - 2J$, $\Delta/t = 0.2$, 0.6, 1





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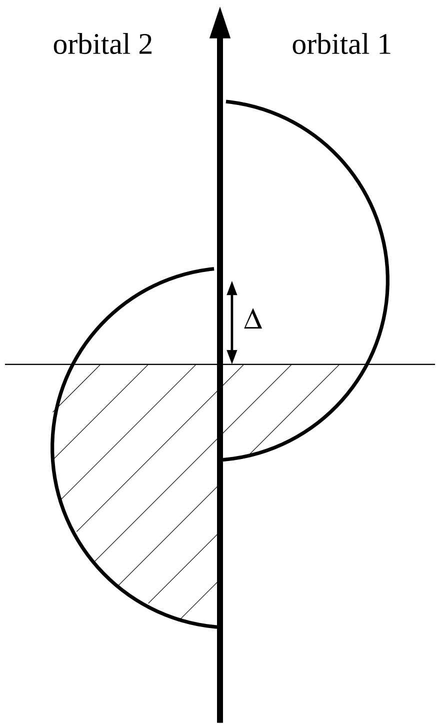

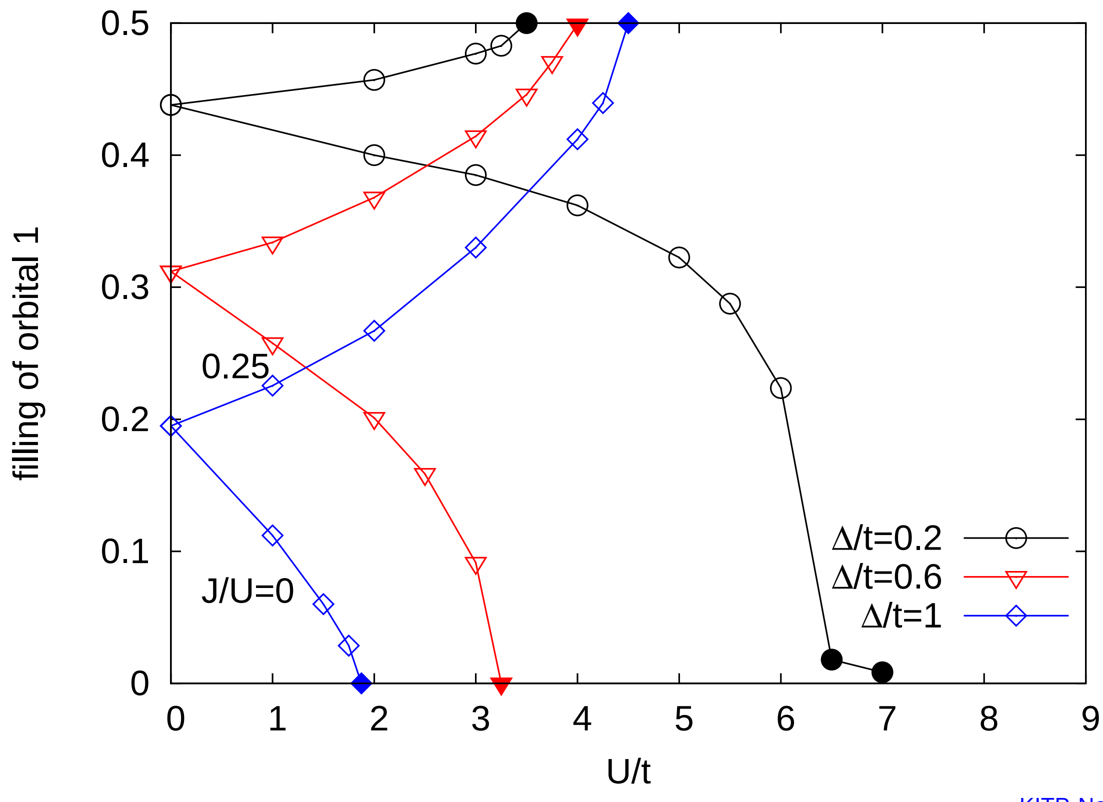

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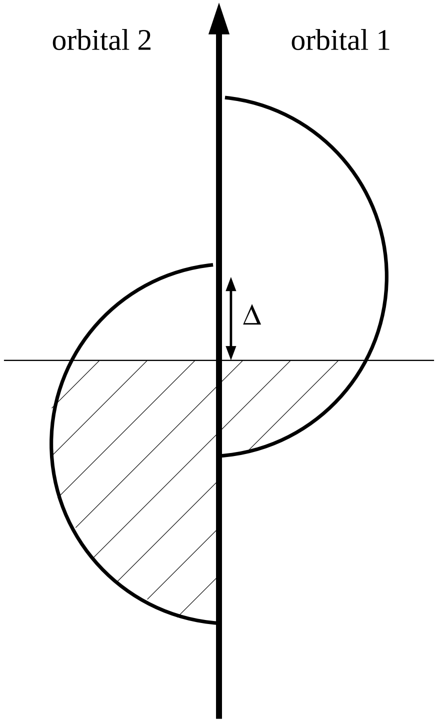
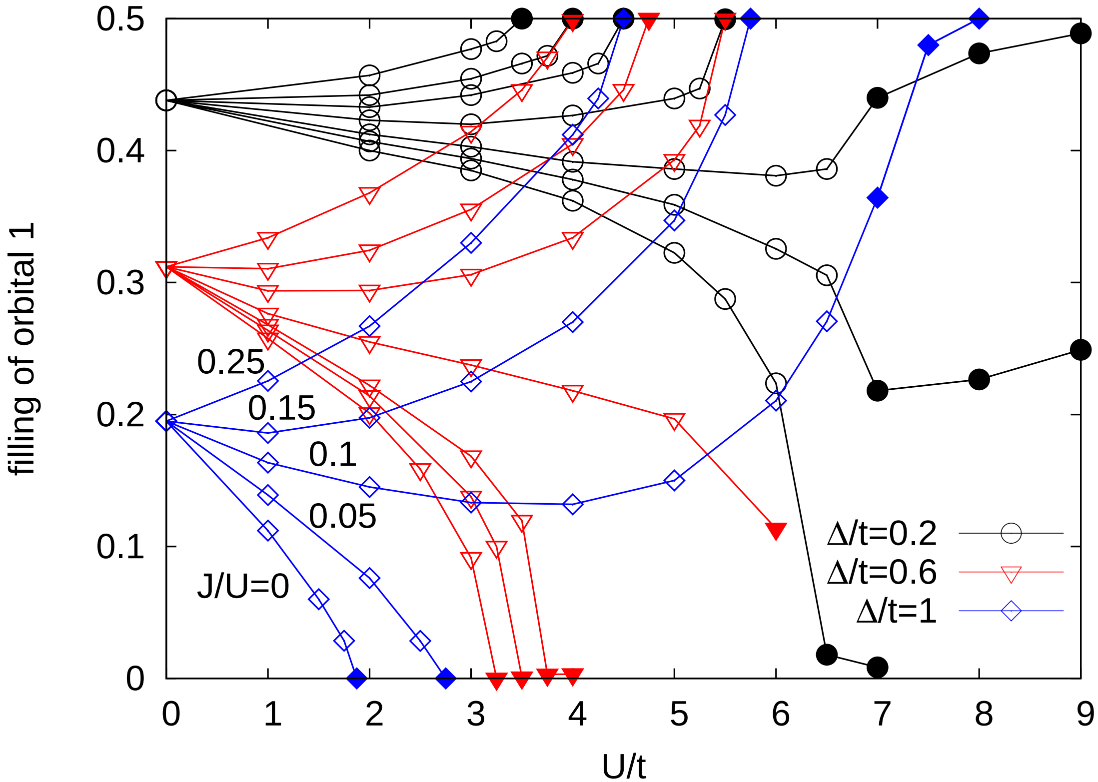




2-orbital model

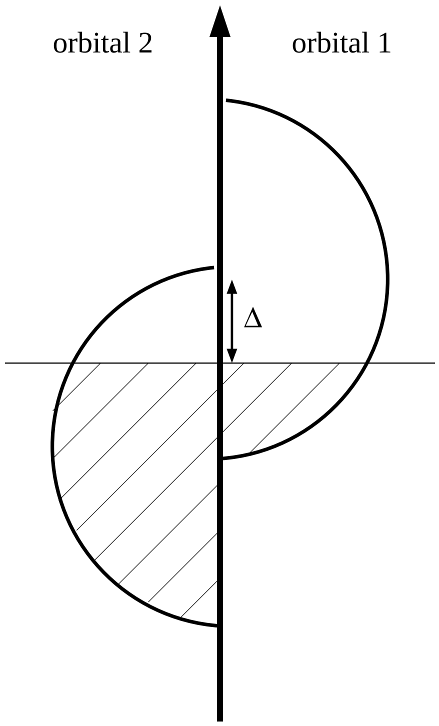
Effect of Hund coupling J and crystal field splitting Δ, *PRL 99, 126405 (2007)*

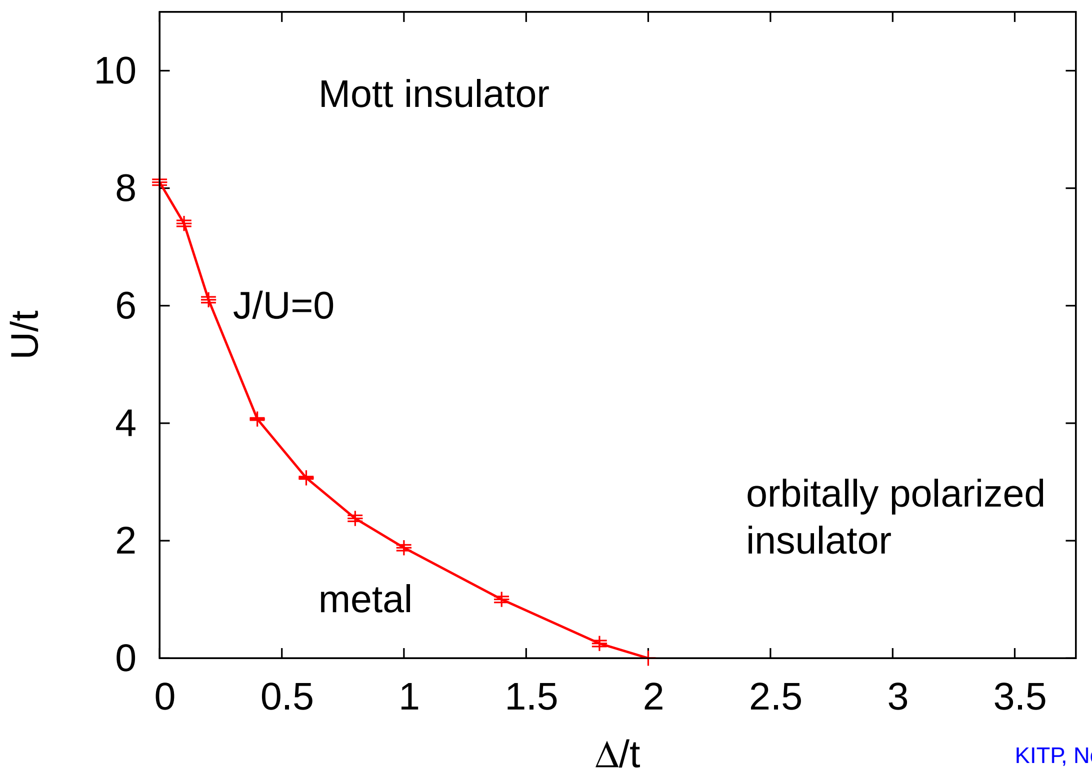
- Lowest energy eigenstates of H_{loc}

$$|6\rangle = |T_1\rangle,\ |7\rangle = |T_0\rangle,\ |8\rangle = |T_{-1}\rangle \qquad S=1 \qquad E = U - 3J - 2\mu$$

$$|10\rangle = \cos\theta|\uparrow\downarrow,0\rangle + \sin\theta|0,\uparrow\downarrow\rangle \qquad S=0 \qquad E = U - \sqrt{J^2+4\Delta^2} - 2\mu$$

- Energy levels cross at $\Delta = \sqrt{2}J \Rightarrow$ insulator-insulator transition





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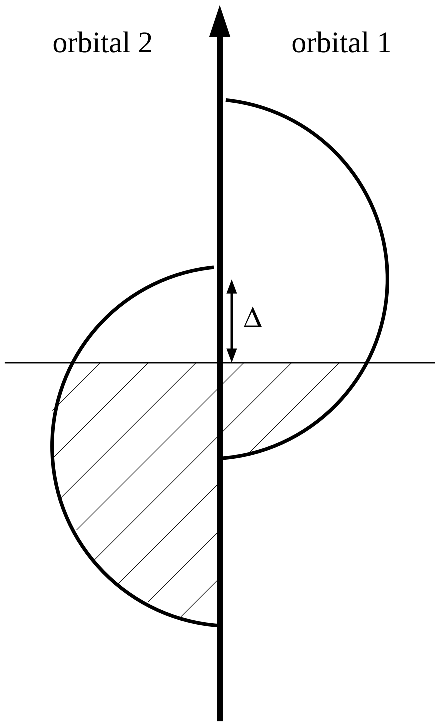

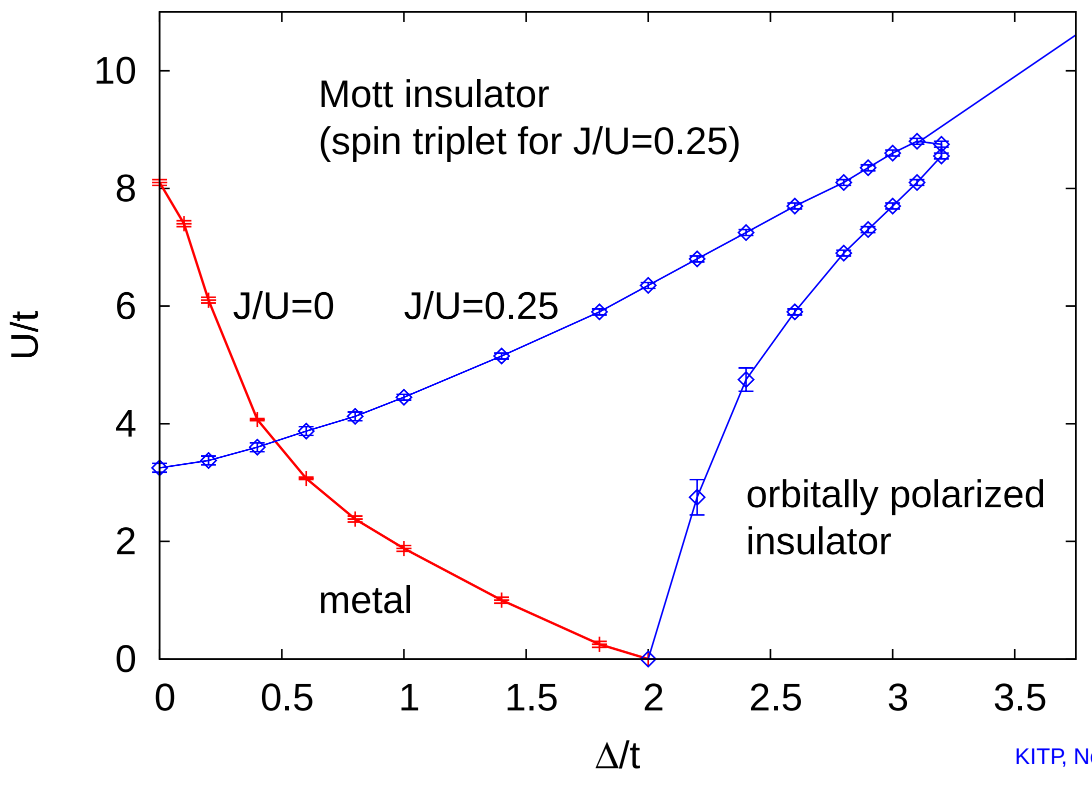

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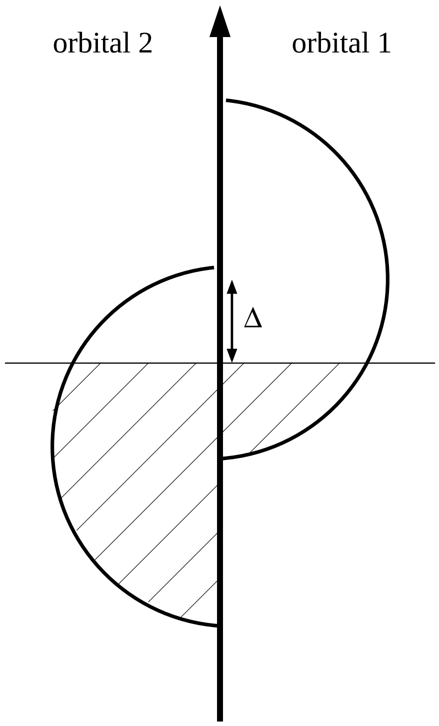
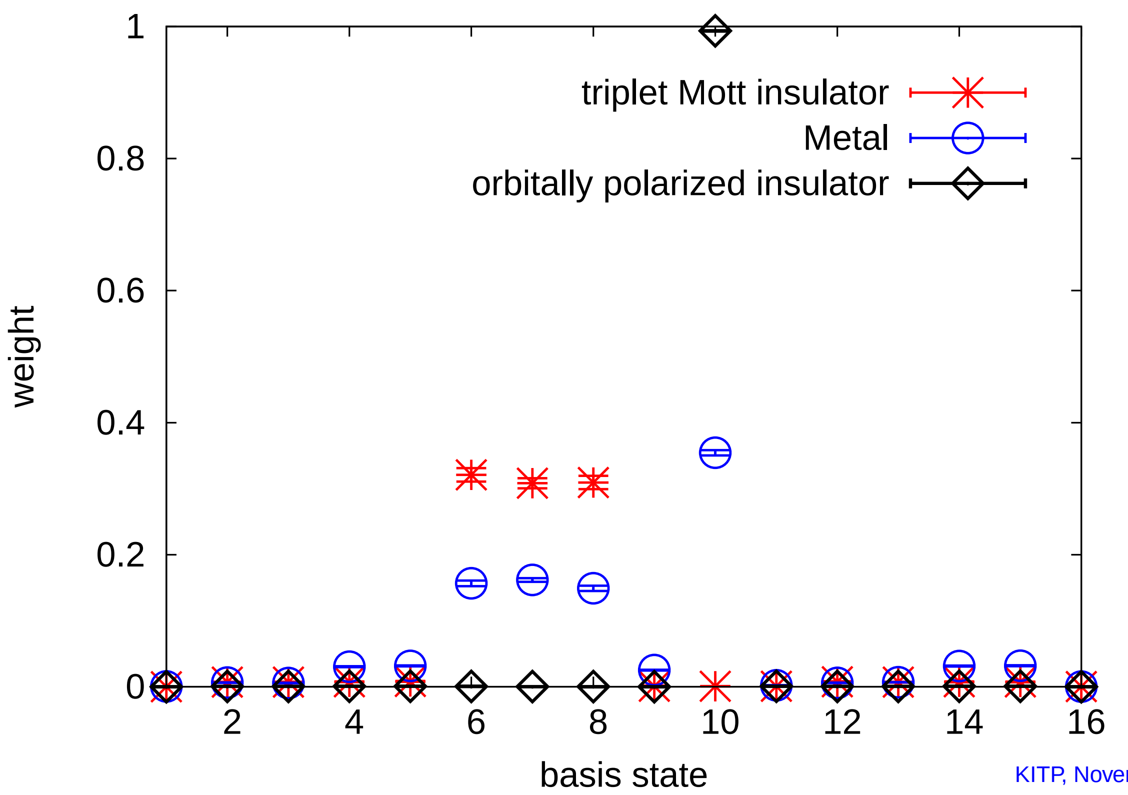
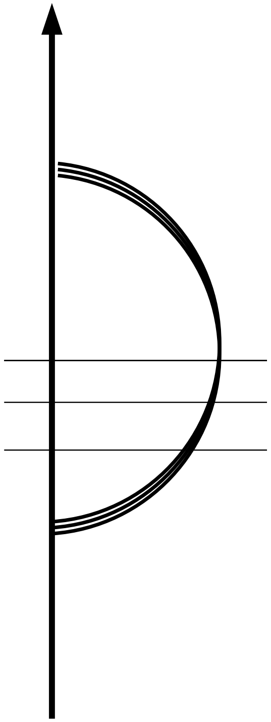
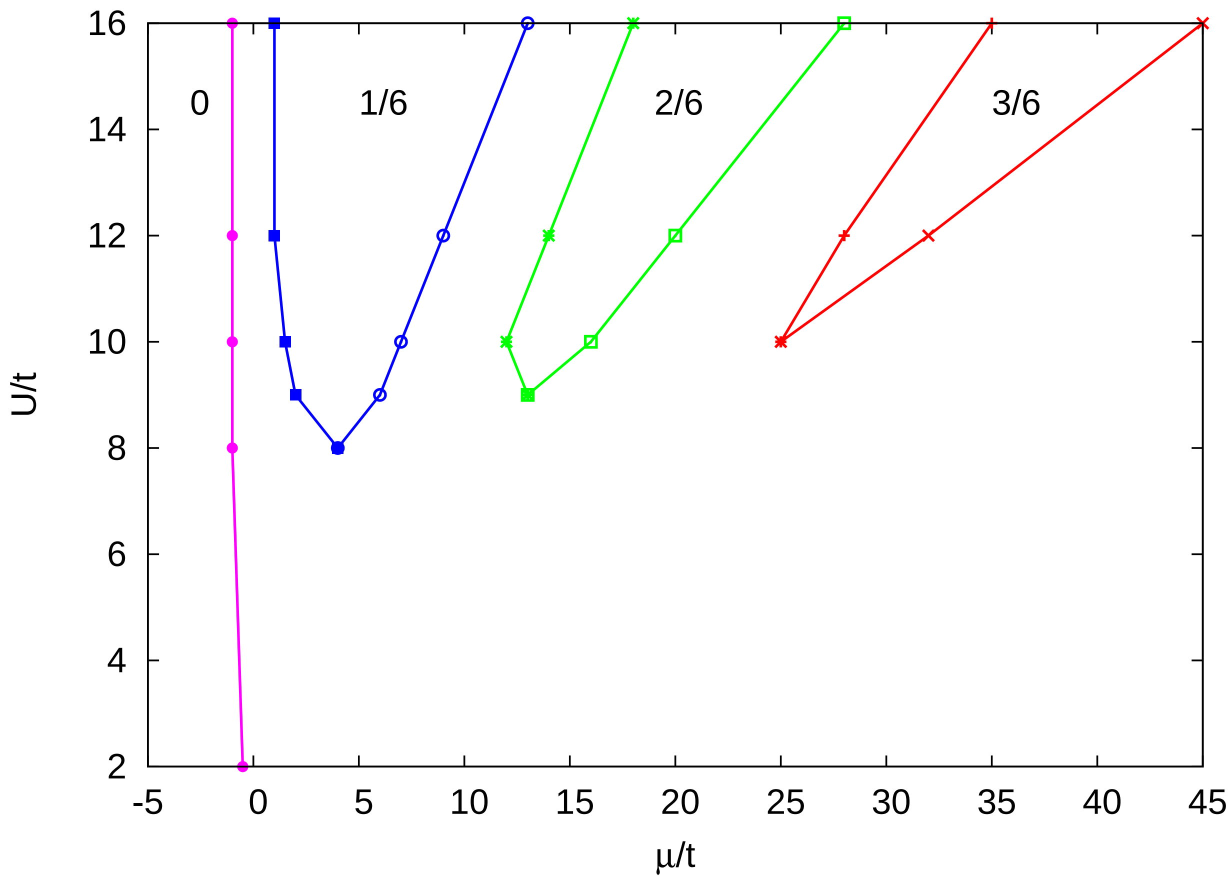




3-orbital model

- $H_{\text{loc}} = \sum_\alpha U n_{\alpha,\uparrow} n_{\alpha,\downarrow} + \sum_{\alpha\neq\beta,\sigma} U' n_{\alpha,\sigma} n_{\beta,-\sigma} + \sum_{\alpha\neq\beta,\sigma} (U'-J) n_{\alpha,\sigma} n_{\beta,\sigma}$
  $- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{\alpha,\uparrow} + \psi^\dagger_{\beta,\uparrow}\psi^\dagger_{\beta,\downarrow}\psi_{\alpha,\uparrow}\psi_{\alpha,\downarrow} + h.c.) - \sum_{\alpha,\sigma} \mu n_{\alpha,\sigma}$
- Bethe lattice with $\beta t = 50$, $U' = U - 2J$, $J = 0$





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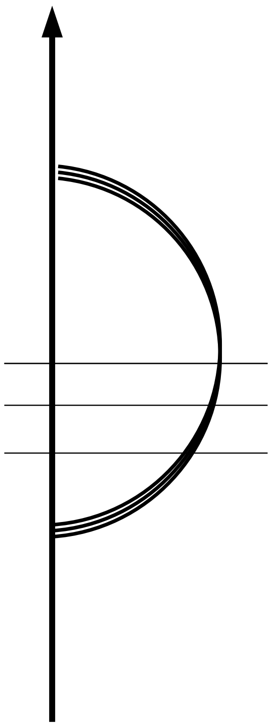
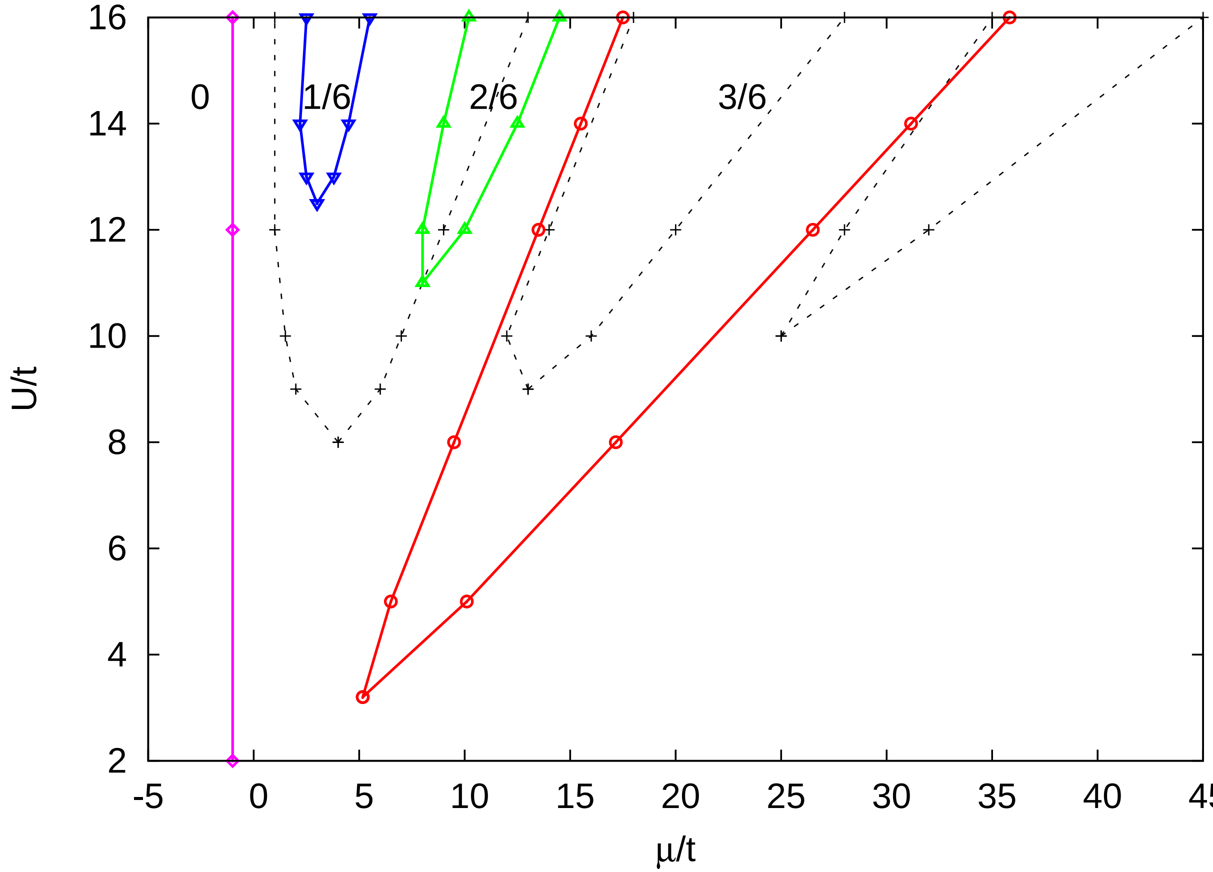
- Bethe lattice with $\beta t = 50$, $U' = U - 2J$, $J = U/6$





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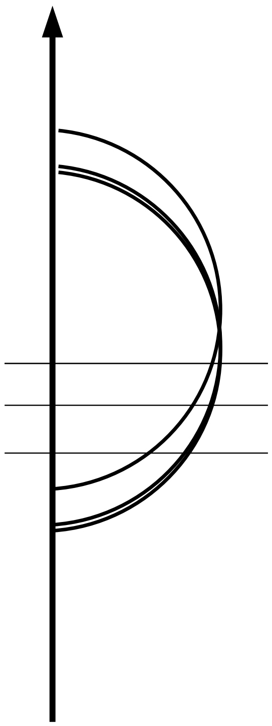

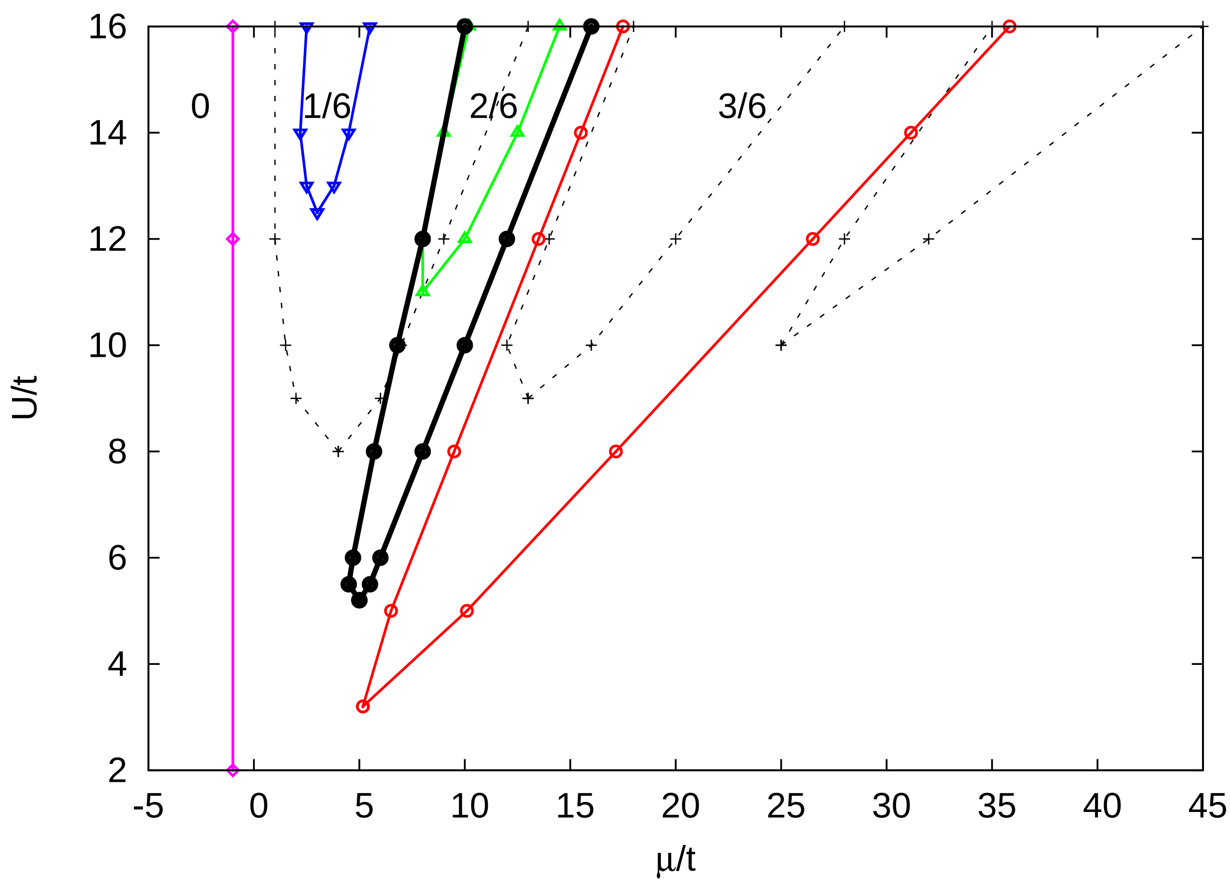

Outlook

Ongoing and future projects

- Applications: Multiorbital models, cluster DMFT, LDA+DMFT
  $\rightarrow$ More realistic models/parameter regimes can now be studied
  $\rightarrow$ Investigate "real materials" (band structure, filling, couplings, ...)
- Methodology: Explore limits and alternative approaches
  $\rightarrow$ Truncation of Hilbert space; Effective action methods
  $\rightarrow$ Krylov-space approach
  $\rightarrow$ Continuous-time auxiliary field method
- Beyond DMFT: Real time dynamics and non-equilibrium systems
  $\rightarrow$ Diagrammatic Monte Carlo on the Keldysh contour