A continuous time algorithm for quantum impurity models

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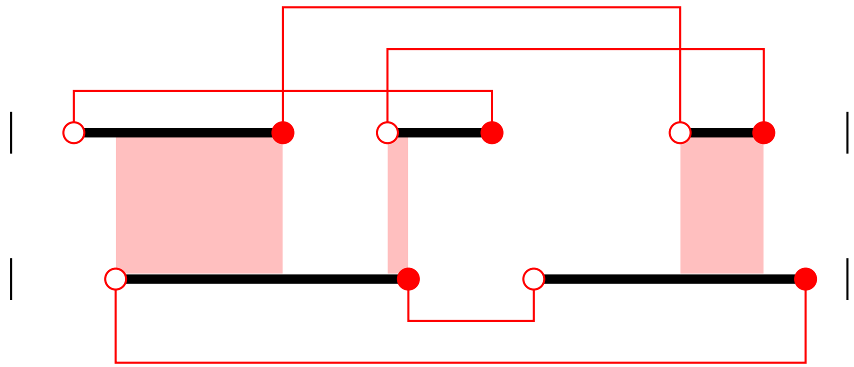


cond-mat/0512727

Outline

- Introduction
  - Dynamical mean field theory
  - Existing impurity solvers
- New approach
  - Diagrammatic expansion in the impurity-bath hybridization
  - Monte Carlo sampling
  - Scaling with temperature and interaction strength
- Applications
  - Temperature- and doping dependent Mott transition
  - Free energy calculation
- Generalization
  - Matrix formalism

Collaborators

- A. J. Millis, M. Troyer

Introduction

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

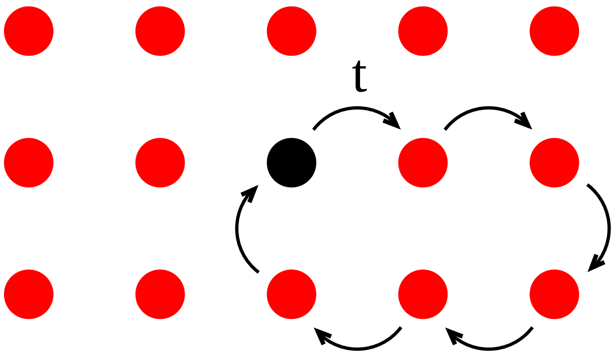
- Replace lattice problem by a single site effective problem
- Neglect spatial, keep dynamical fluctuations
- Becomes exact in the infinite coordination number limit

Introduction

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

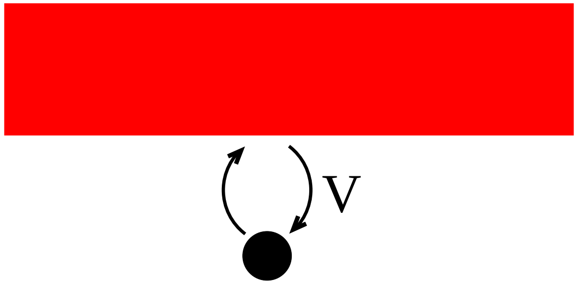
- Lattice model (Density of states $D(\epsilon)$, Self energy $\Sigma_{lat}(i\omega_n, k)$)

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



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

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



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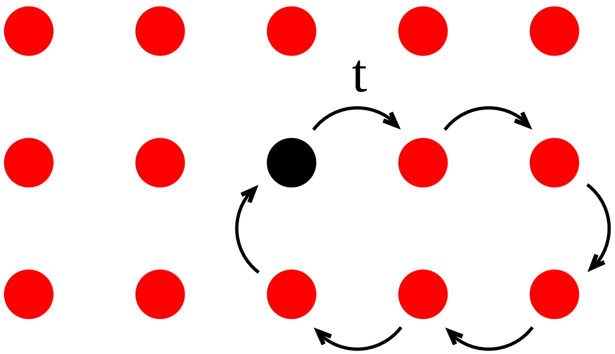
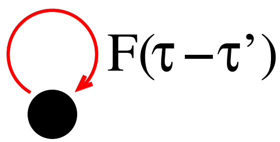


- Effective Action (Hybridization $F(\tau)$, Self energy $\Sigma_{imp}(i\omega)$)

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



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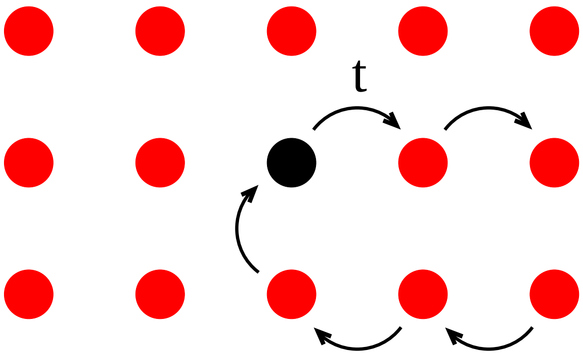

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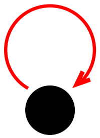


- Self-consistency

$$S \to \Sigma_{lat}(i\omega_n) \equiv \Sigma_{imp}(i\omega_n) \to G_{lat}(i\omega_n) = \int d\epsilon \frac{D(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_{lat}(i\omega_n)} \to S$$

Previous QMC approaches

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

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

$$S_F = -\sum_\sigma \int_0^\beta d\tau d\tau' c_\sigma(\tau) F_\sigma(\tau - \tau') c_\sigma^\dagger(\tau')$$

$$S_{loc} = -\mu \int_0^\beta d\tau (n_\uparrow + n_\downarrow) + U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

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

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

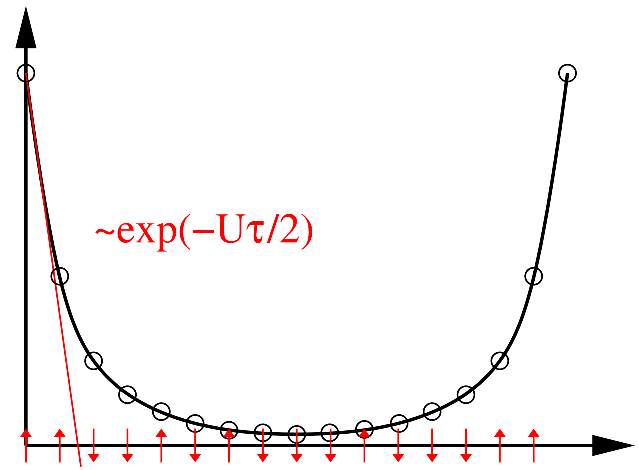
- Perform Gaussian integral

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

- 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 QMC approaches

Rubtsov solver *Rubtsov et al. (2005)*

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

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

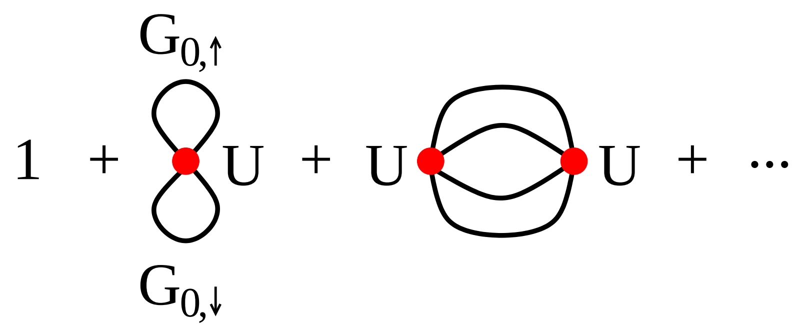
$$S_U = U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

- 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 $e^{-U \int d\tau n_\uparrow n_\downarrow}$

$$Z = \sum_k \frac{(-U)^k}{k!} \int d\tau_1 \dots d\tau_k Tr \left[T_\tau e^{-S_0} n_\uparrow(\tau_1) n_\downarrow(\tau_1) \dots n_\uparrow(\tau_k) n_\downarrow(\tau_k) \right]$$

- Perform Gaussian integral

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



- MC sampling of vertices
  $\{n_\uparrow(\tau_i) n_\downarrow(\tau_i)\}_{i=1,2,\dots,k}$
- Matrix size: $\langle k \rangle \sim 0.5 \beta U$

New impurity solver

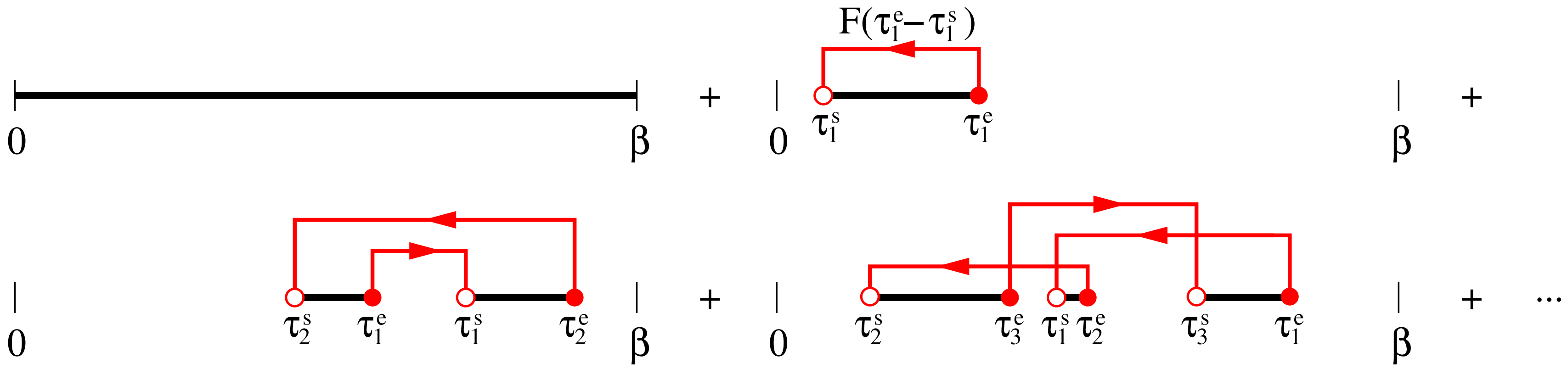
Expansion in the impurity-bath hybridization F (cond-mat/0512727)

- Non-interacting model: $Z = Tr T_\tau \exp(\int_0^\beta d\tau d\tau' c(\tau) F(\tau - \tau') c^\dagger(\tau'))$
- Expand exponential, evaluate in the occupation number basis $\{|0\rangle, |1\rangle\}$
- $Z = \frac{1}{0!} Tr 1$

$$+\frac{1}{1!} Tr T_\tau \int d\tau_1^s d\tau_1^e \; c(\tau_1^e) F(\tau_1^e - \tau_1^s) c^\dagger(\tau_1^s)$$

$$+\frac{1}{2!} Tr T_\tau \int d\tau_1^s d\tau_1^e d\tau_2^s d\tau_2^e \; c(\tau_1^e) F(\tau_1^e - \tau_1^s) c^\dagger(\tau_1^s) \; c(\tau_2^e) F(\tau_2^e - \tau_2^s) c^\dagger(\tau_2^s)$$

$$+ \dots$$



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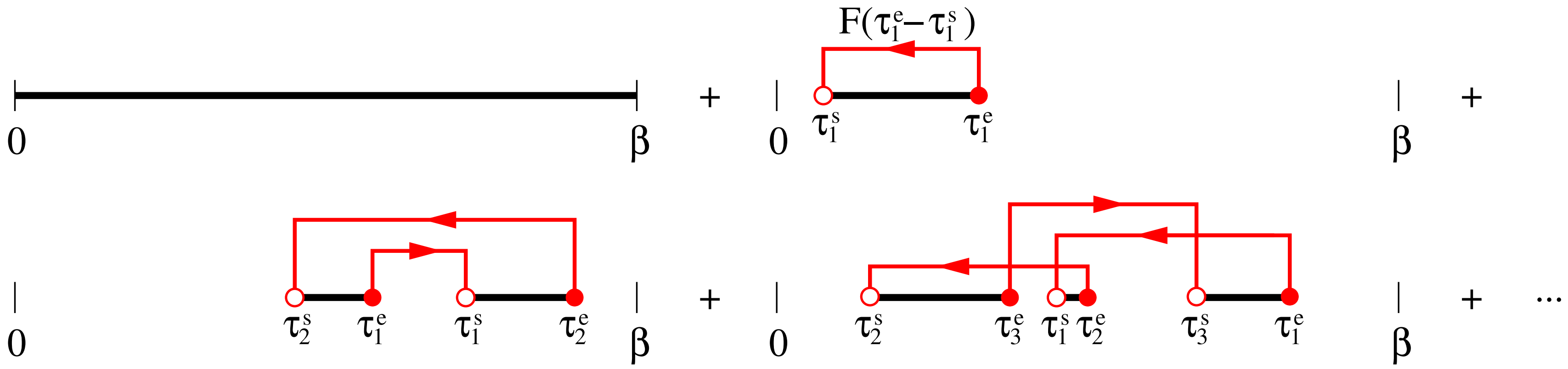
  $+\frac{1}{1!}TrT_\tau \int d\tau_1^s d\tau_1^e \; c(\tau_1^e)F(\tau_1^e-\tau_1^s)c^\dagger(\tau_1^s)$
  $+\frac{1}{2!}TrT_\tau \int d\tau_1^s d\tau_1^e d\tau_2^s d\tau_2^e \; c(\tau_1^e)F(\tau_1^e-\tau_1^s)c^\dagger(\tau_1^s)\; c(\tau_2^e)F(\tau_2^e-\tau_2^s)c^\dagger(\tau_2^s)$
  $+\ldots$



- Some diagrams have negative weight

New impurity solver

Expansion in the impurity-bath hybridization F (cond-mat/0512727)

- 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

$$Z_k(\tau_1^s,\tau_1^e;\tau_2^s,\tau_2^e;\ldots;\tau_k^s,\tau_k^e) = \det F^{(k)}\delta_{\tau_1^s}^{\tau_k^e}$$

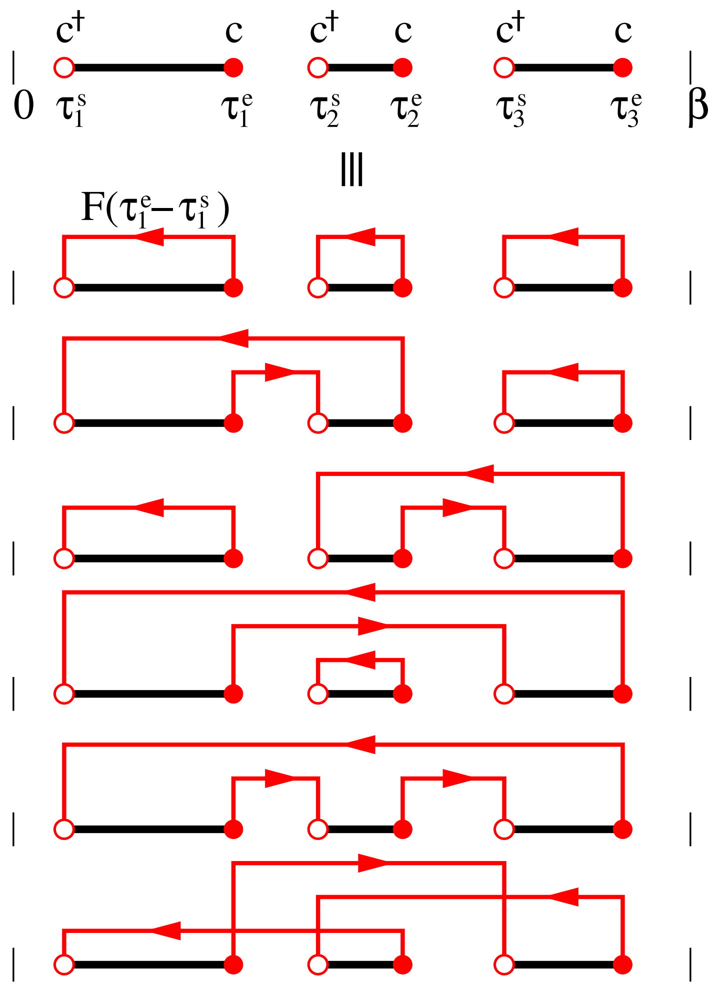
$$F^{(k)}_{m,n} = F(\tau_m^e - \tau_n^s)$$

$\rightarrow$ resums huge numbers of diagrams

$\rightarrow$ eliminates the sign problem

- Z_k can be visualized as a configuration of k segments on a circle
- $Z = 2 + \sum_{k=1}^\infty \int_0^\beta d\tau_1^s \ldots \int_{\tau_{k-1}^e}^\beta d\tau_k^s \int_{\tau_k^s}^{\circ\tau_1^s} d\tau_k^e$

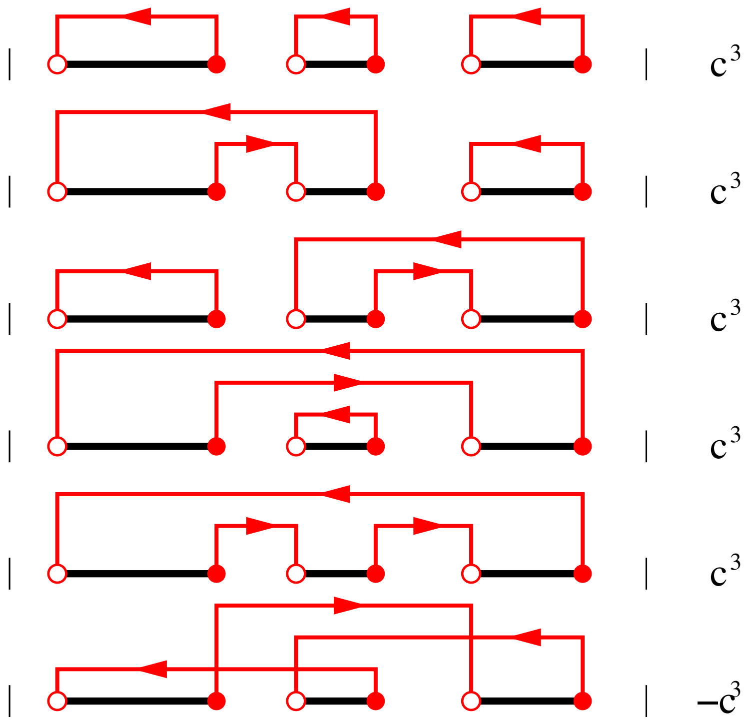
$$\times Z_k(\tau_1^s,\tau_1^e;\tau_2^s,\tau_2^e;\ldots;\tau_k^s,\tau_k^e)$$

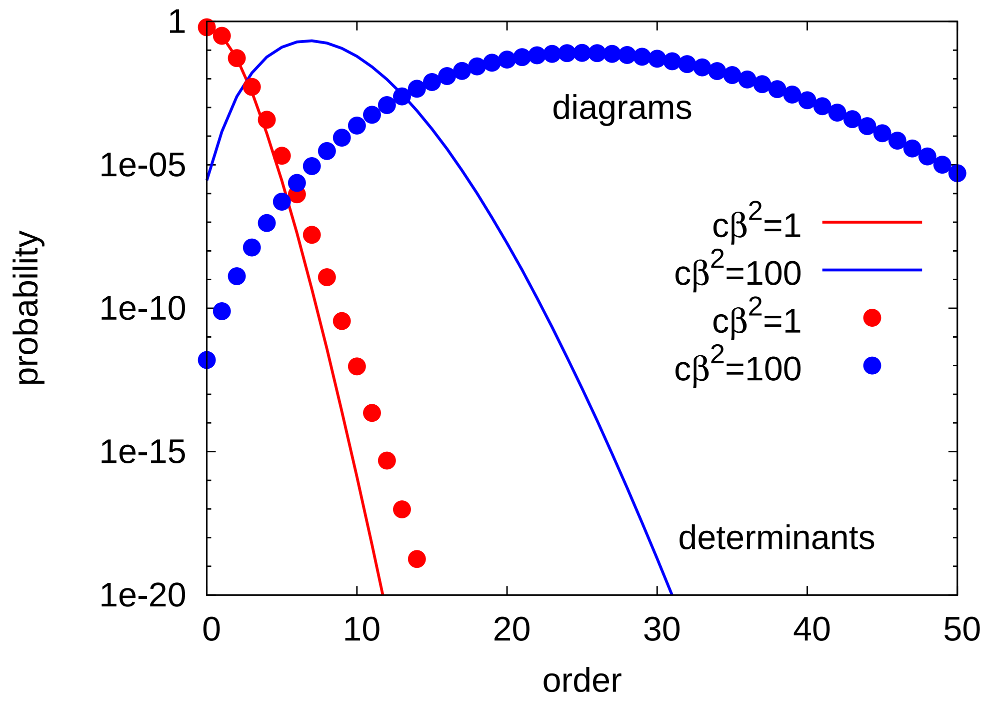


Sign problem

Expansion in the impurity-bath hybridization F (cond-mat/0512727)

- Example: $F(\tau) = c$, β-antiperiodic $\quad \leftrightarrow \quad F(i\omega_n) = \frac{c}{i\omega_n}$
- Diagrams: $p(k) \sim k! \frac{(c\beta^2)^k}{(2k)!}$
- Determinants: $p(k) \sim 2^k \frac{(c\beta^2)^k}{(2k)!}$





Monte Carlo sampling

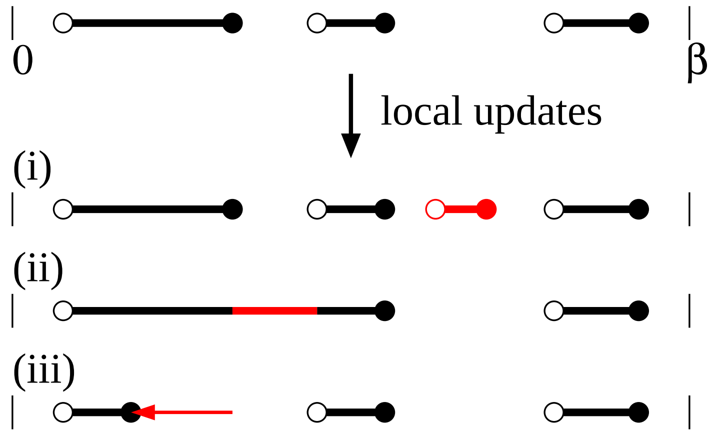
Expansion in the impurity-bath hybridization F (cond-mat/0512727)

- Sampling of Z through local updates

  (i) insertion/removal of segments

  (ii) insertion/removal of anti-segments

  (iii) shifts of the segment end points



- Detailed balance

$$s_k \rightarrow s_{k+1} = s_k + \tilde{s} \qquad \frac{p_{ins}(\tilde{s})}{p_{rem}(\tilde{s})} = \frac{Z_{k+1}(s_{k+1})}{Z_k(s_k)} \frac{\beta l_{max}}{k+1} e^{\tilde{l}\mu}$$

- Store and update the matrix $M = F^{-1}$

  $\rightarrow$ access to determinant ratios

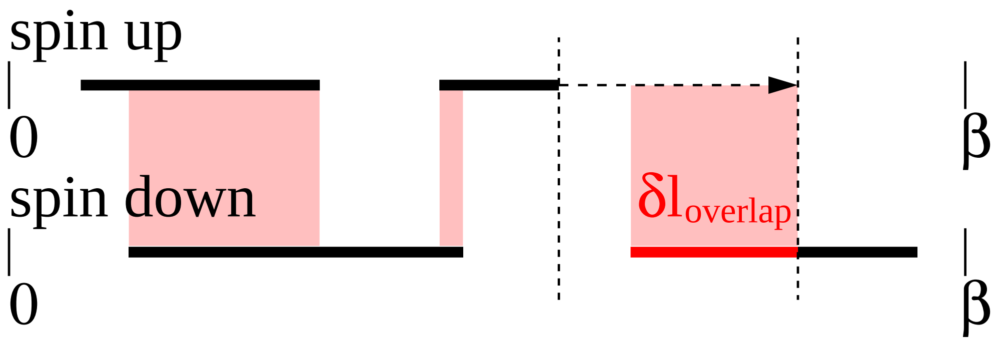
  $\rightarrow$ efficient computation of G

$$G(\tau) = \left\langle \frac{1}{\beta} \sum_{i,j} M_{j,i} \Delta(\tau, \tau_i^e - \tau_j^s) \right\rangle$$

Monte Carlo sampling

Expansion in the impurity-bath hybridization F (cond-mat/0512727)

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



- Acceptance rate for MC moves now also depends on segment overlap
- Detailed balance

$$s \rightarrow \tilde{s} \qquad \frac{p(s \rightarrow \tilde{s})}{p(\tilde{s} \rightarrow s)} = \frac{Z_k(\tilde{s})}{Z_k(s)} e^{(\tilde{l}-l)\mu - U\delta l_{overlap}}$$

- Obviously: $E_{pot} = U\langle l_{overlap}^{total}\rangle$

$$n_\sigma = G_\sigma(\beta) = \beta^{-1}\langle l_\sigma^{total}\rangle$$

$$\ldots$$

Number of segments

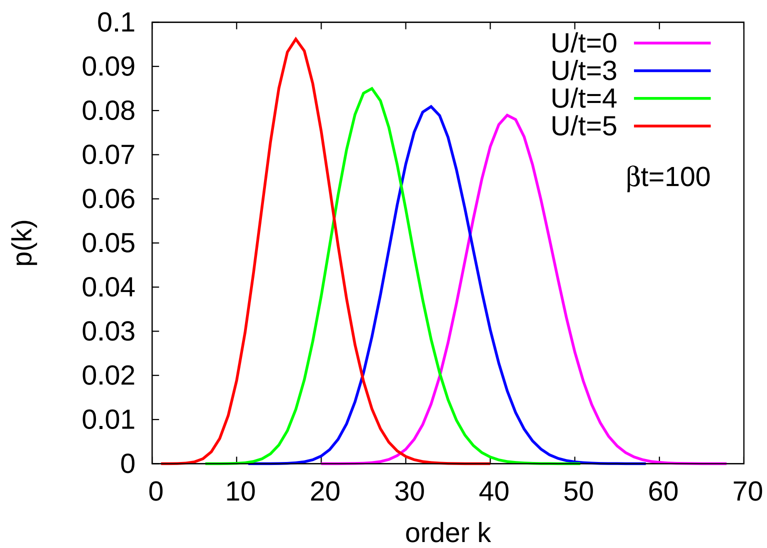
Expansion in the impurity-bath hybridization F (cond-mat/0512727)

- Efficiency of the algorithm depends on the matrix size k

- Computational effort $O(k^3)$
- Order of diagrams $\langle k \rangle \sim \beta$
- $\langle k \rangle$ decreases with increasing U

  $\rightarrow$ small matrices

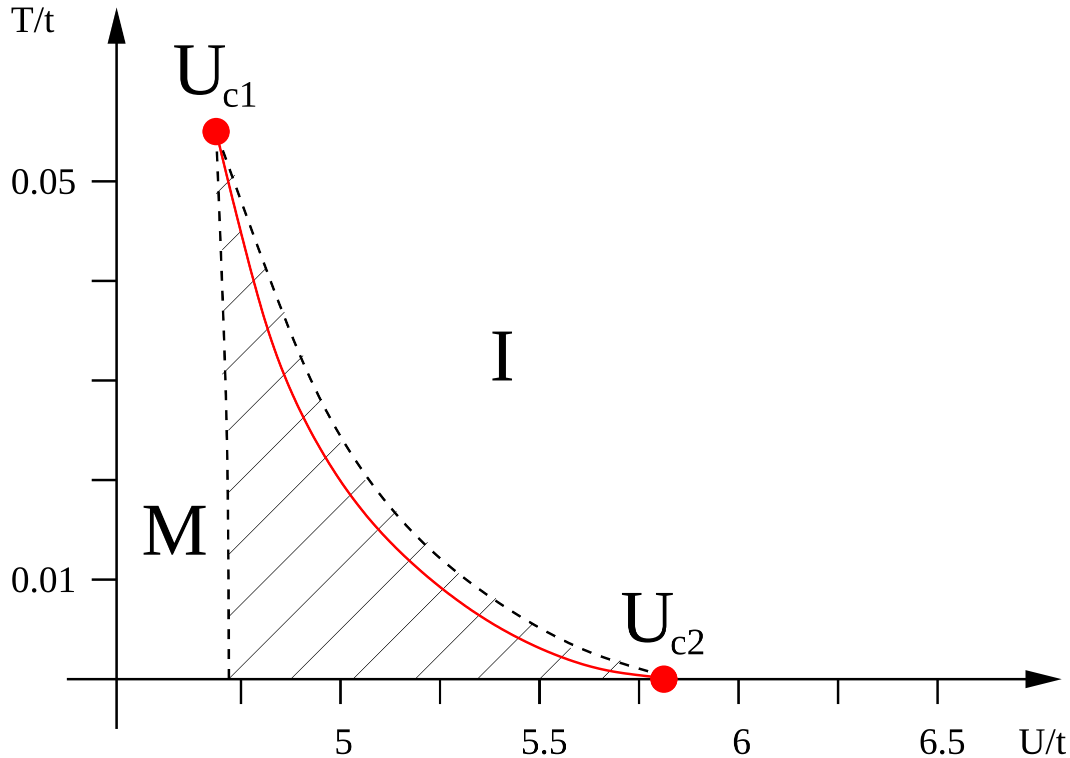
  $\rightarrow$ works even at very low T



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

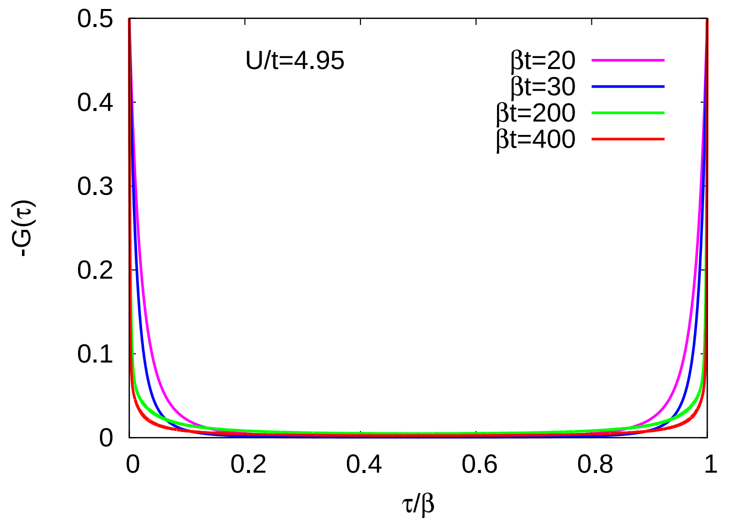
Results

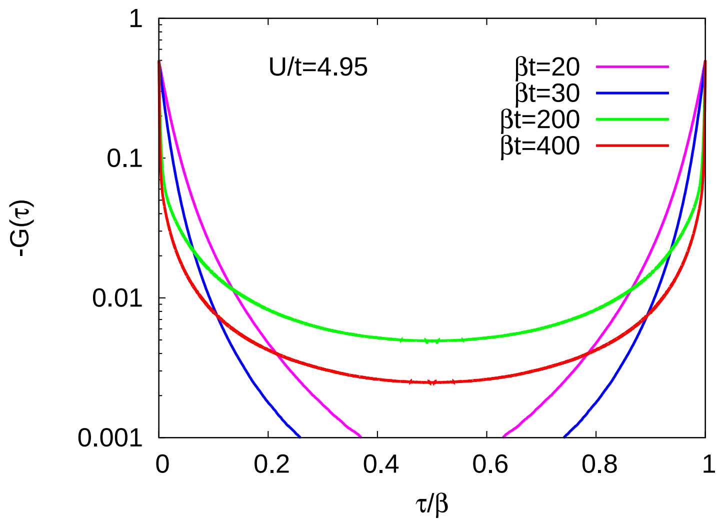
- Semi-circular density of states (Bethe lattice) with band width 4t
- Enforce paramagnetic phase
- Self-consistency condition: $F(\tau) = t^2 G(-\tau)$
- Phase diagram (sketch)

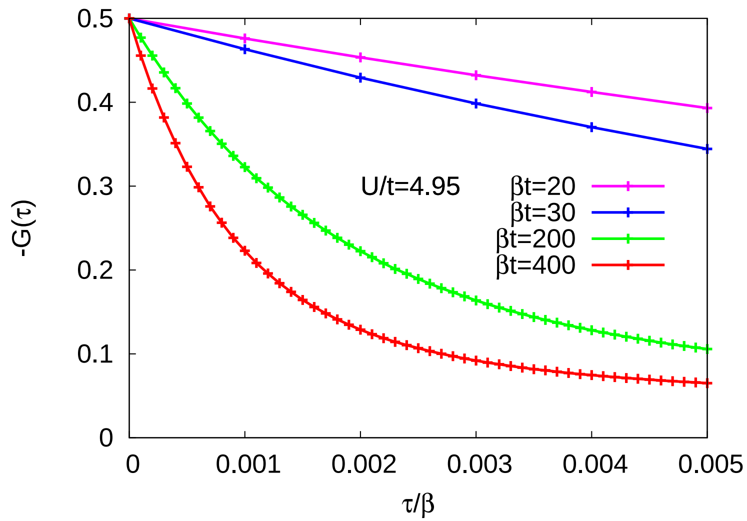


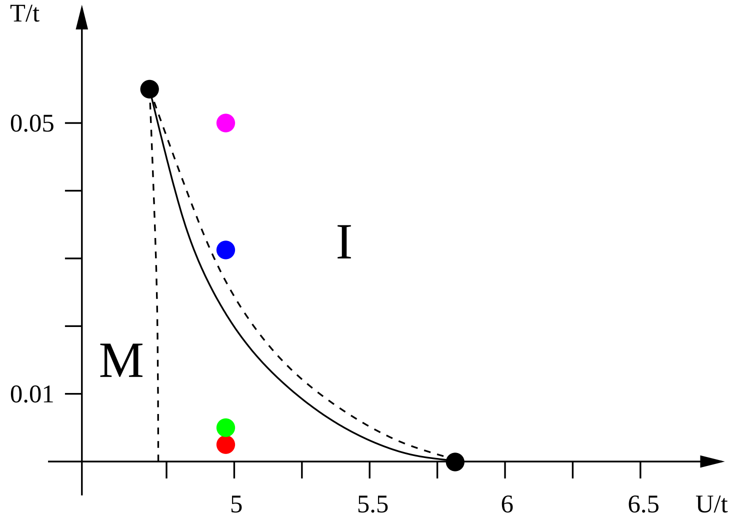
Results - Green functions

- Can map out steep drop of $G(\tau)$ with almost perfect resolution
- Different large-τ behavior for metallic/insulating Green functions



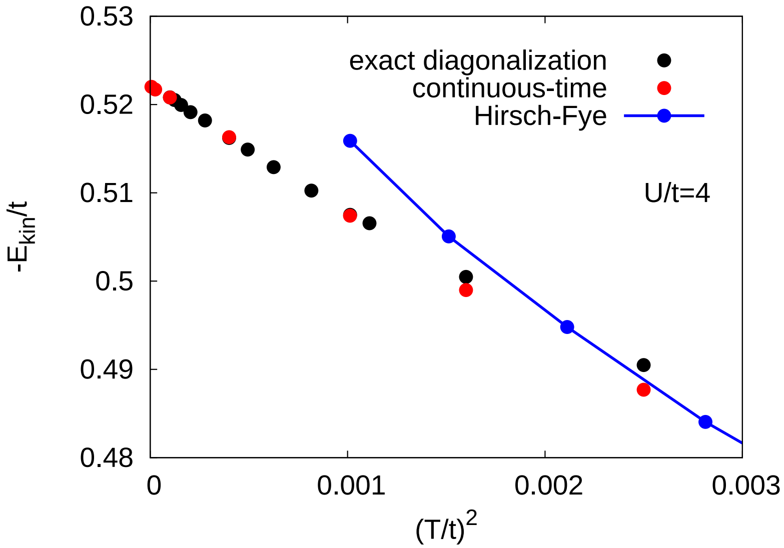


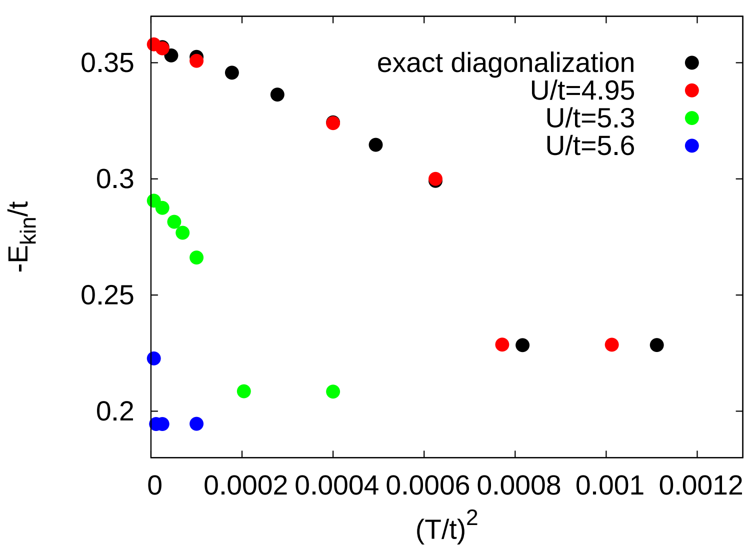




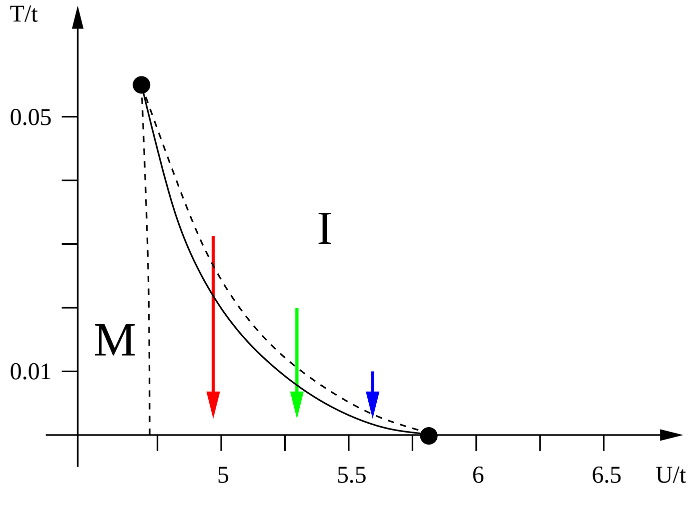
Results - Kinetic energy

- Low temperature physics near Mott transition easily accessible
- Hirsch-Fye: systematic errors due to insufficient time-resolution





$$E_{kin} = -2t^2 \int d\tau G(\tau)^2$$



ED method:

M. Capone et al., cond-mat/0512484

Results - Free energy

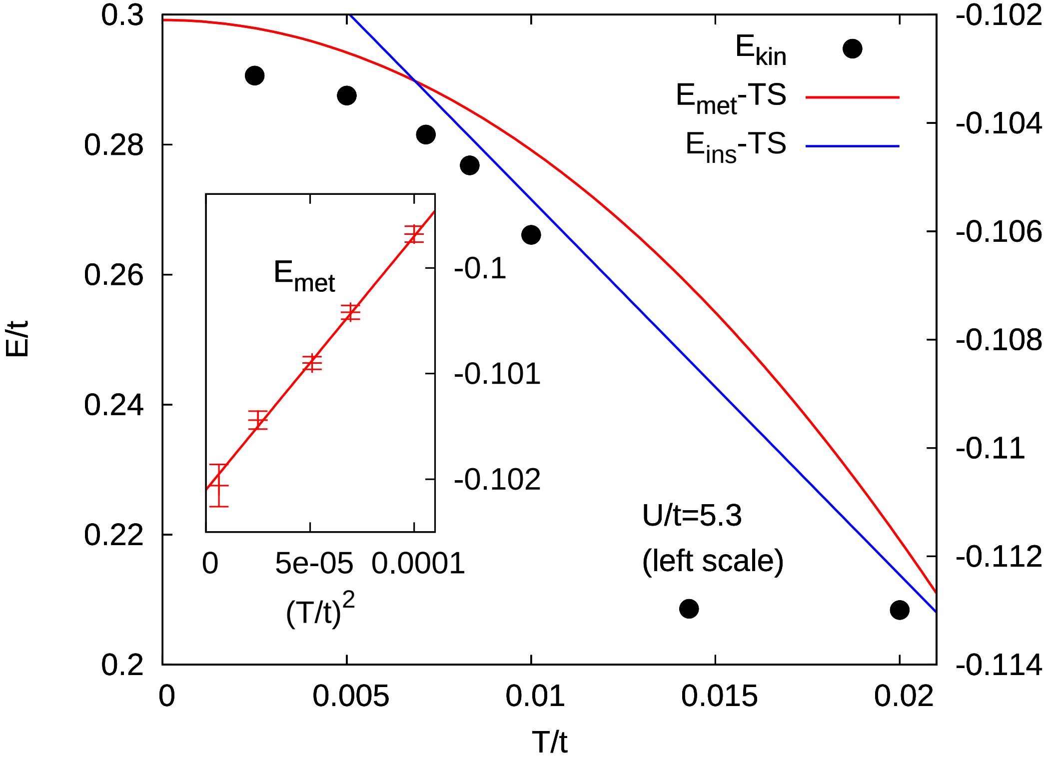
- Access to low temperature allows to compute the entropy

$$C_{met}(T) = dE_{met}/dT$$

$$S_{met}(T) = \int_0^T dT' \frac{C_{met}(T')}{T'}$$

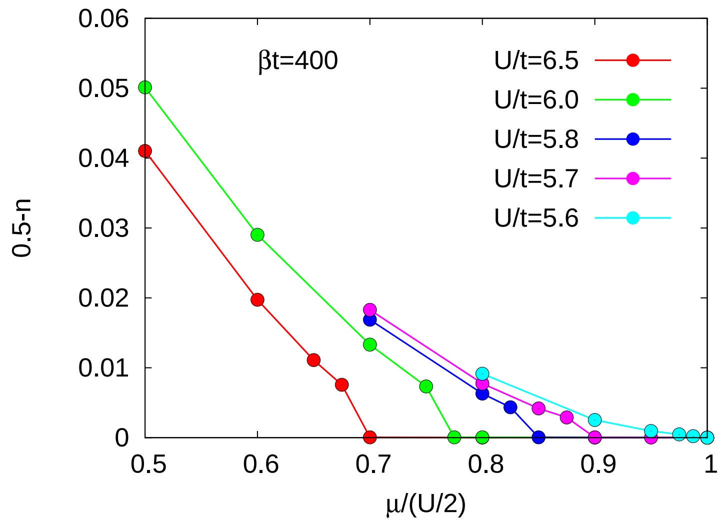
$$S_{ins}(T) = \ln(2)$$

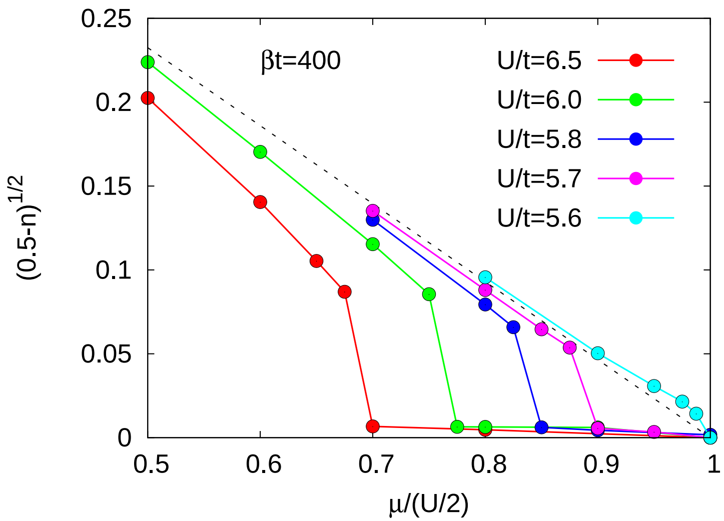
- Crossing of free energy curves yields first order transition point

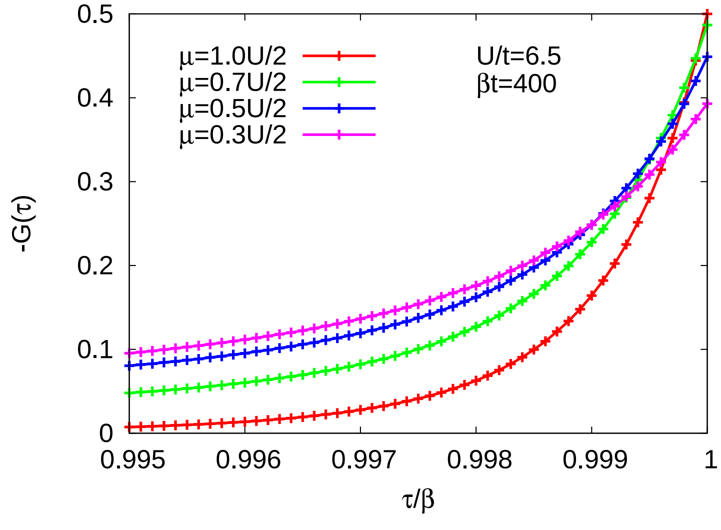


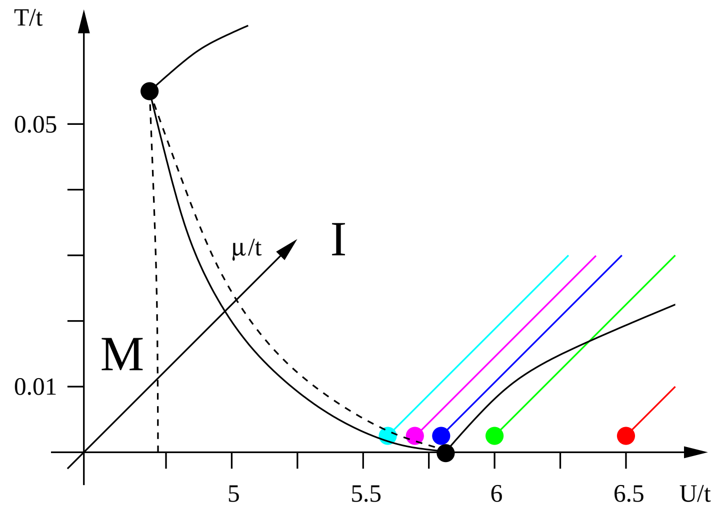
Results - Doping dependence

- Algorithm works away from half filling $\rightarrow$ compute $n(\mu)$ for $U \gtrsim U_{c2}$.
- Doping dependent Mott transition (for $T > 0$) is first order



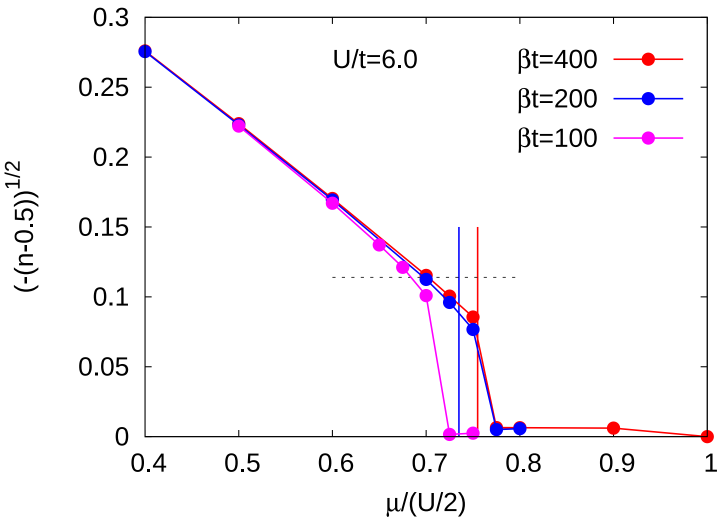


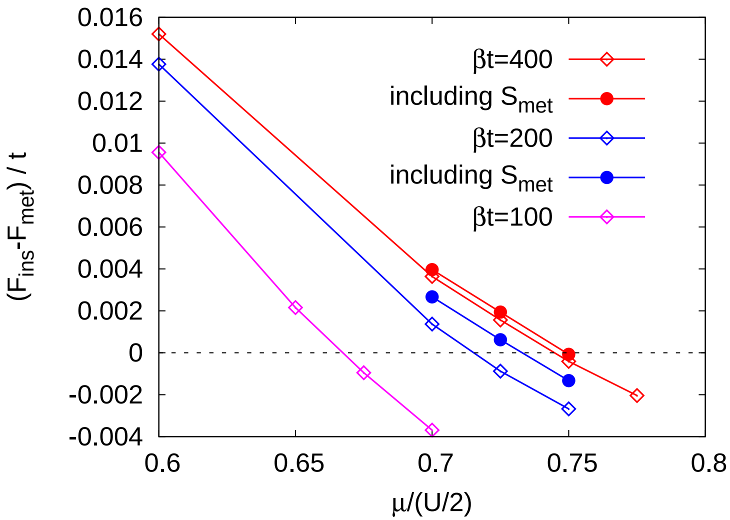


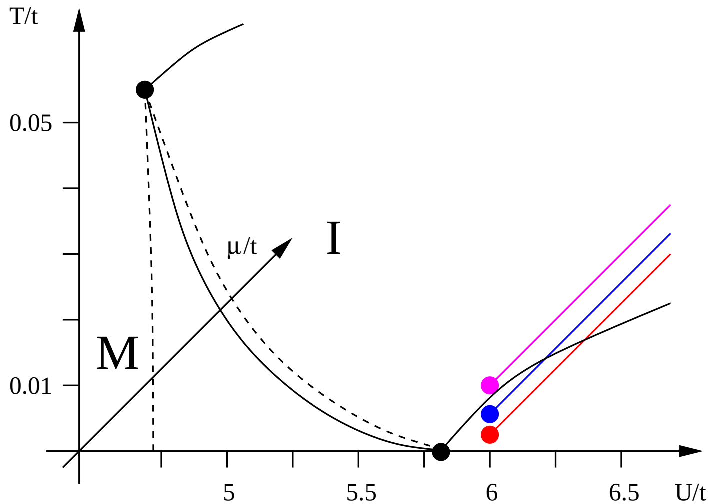


Results - Doping dependence

- Doping dependent Mott transition remains first order down to $T = 0$
- Change in $F = E - TS - \mu n$ yields precise location of the transition







General formalism

Expansion in the impurity-bath hybridization function

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

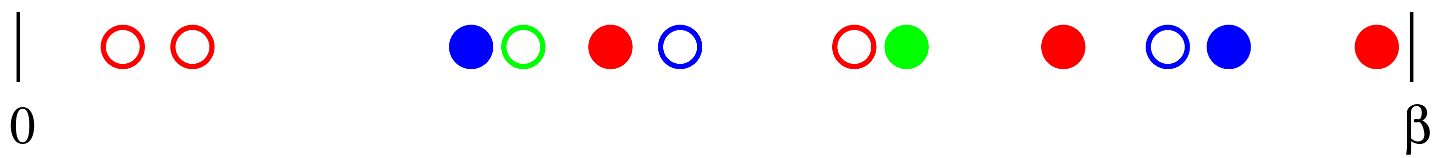
$$S_F = -\sum_a \int_0^\beta d\tau d\tau' \psi_a(\tau) F_a(\tau - \tau') \psi_a^\dagger(\tau')$$

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

- Expand in F_a, resum diagrams into determinants

$$Z = TrT_\tau e^{-S_{loc}} \prod_a \sum_{k_a=0}^{\infty} \int d\tau_{a_1}^s \dots d\tau_{a_{k_a}}^e \det(F_a^{(k_a)}(\{\tau_a\})) \times \psi_a^\dagger(\tau_{a_1}^s)\psi_a(\tau_{a_1}^e) \dots \psi_a^\dagger(\tau_{a_{k_a}}^s)\psi_a(\tau_{a_{k_a}}^e)$$

- Configurations consist of k_a creation (annihilation) operators at times $\tau_{a_1}^s < \dots < \tau_{a_{k_a}}^s$ $(\tau_{a_1}^e < \dots < \tau_{a_{k_a}}^e)$



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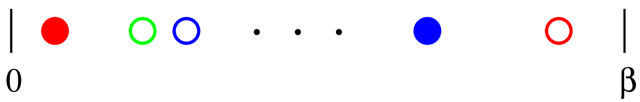
$$S_{loc} = -\int_0^\beta d\tau \underbrace{(\psi^\dagger Q \psi \cdot T + U^{abcd} \psi_a^\dagger \psi_b^\dagger \psi_c \psi_d)}_{H_{loc}}$$

- Weight of 

is ($K(\tau) = e^{-H_{loc}\tau}$)

$$w \sim \prod_f \det(F_f^{(k_f)}) Tr[K(\beta - \tau^e_{a_{k_a}}) \psi_a(\tau^e_{a_{k_a}}) K(\tau^e_{a_{k_a}} - \tau^s_{b_{k_b}}) \psi_b^\dagger(\tau^s_{b_{k_b}}) \ldots$$

$$\ldots \psi_b(\tau^e_{b_1}) K(\tau^e_{b_1} - \tau^e_{c_1}) \psi_c(\tau^e_{c_1}) K(\tau^e_{c_1} - \tau^s_{a_1}) \psi_a^\dagger(\tau^s_{a_1}) K(\tau^s_{a_1})]$$

- K, ψ, $\psi^\dagger$ are $n \times n$ matrices

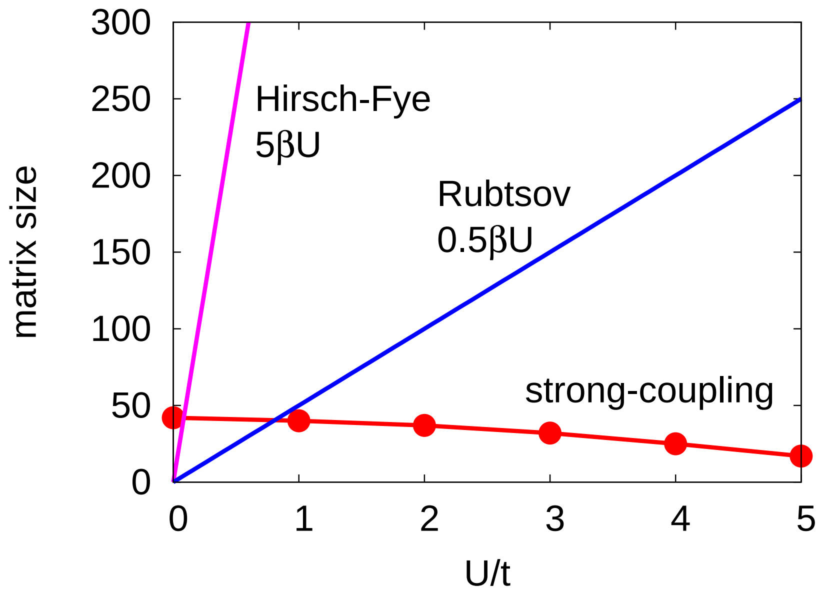
- Use eigenbasis of K

$$K(\tau) = \text{diag}(e^{-\alpha_1 \tau}, e^{-\alpha_2 \tau}, \ldots, e^{-\alpha_n \tau})$$

Conclusions

- Strong-coupling continuous-time impurity solver, based on a diagrammatic expansion in the impurity-bath hybridization

- Matrix size $\langle k \rangle$ decreases with increasing U
- Allows access to low T, even at large U
- No detectable sign problem
- Can be generalized to models with exchange $\rightarrow$ Conference talk



- On-going and future projects
  - Multi-orbital models and clusters
  - Small (or truncated) systems using matrix formalism
  - Large systems using double expansion in F and J