Diagrammatic Monte Carlo methods for Fermions

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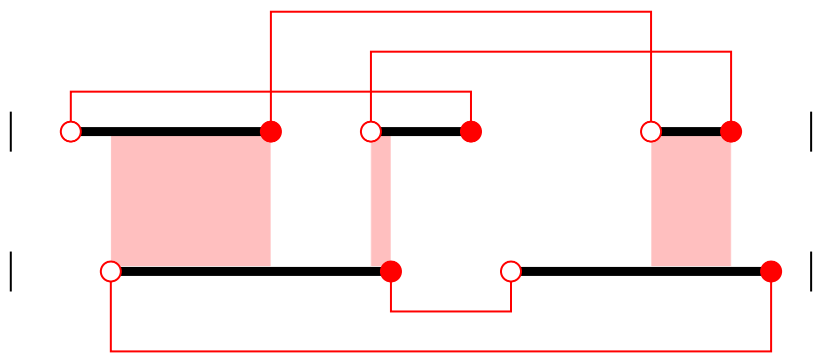

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Outline

- Motivation
  - Dynamical mean field theory for fermionic lattice models

    $\Rightarrow$ impurity models

- Recent advances im methodology
  - Diagrammatic Monte Carlo approach

    $\Rightarrow$ weak-coupling expansion

    $\Rightarrow$ expansion in hybridization

- Application
  - Metal-insulator transition in the Hubbard model
  - "Spin glass" transition in a 3-orbital model

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

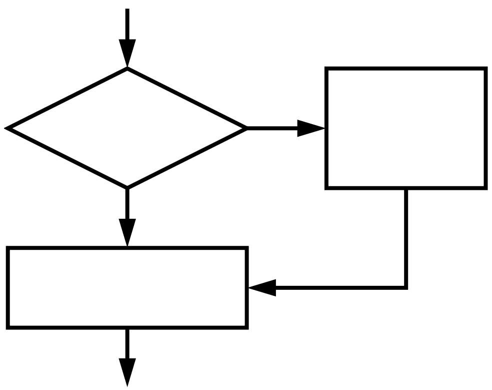
Introduction

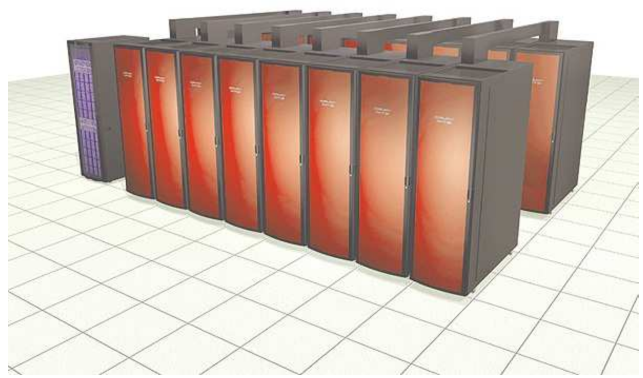
Theoretical Physics ⟷ Experimental Physics

Computational Physics

Computer science | Algorithms | Hardware

```
template
<class model,
  class lattice>
class simulation{
. . .
};
```





Introduction

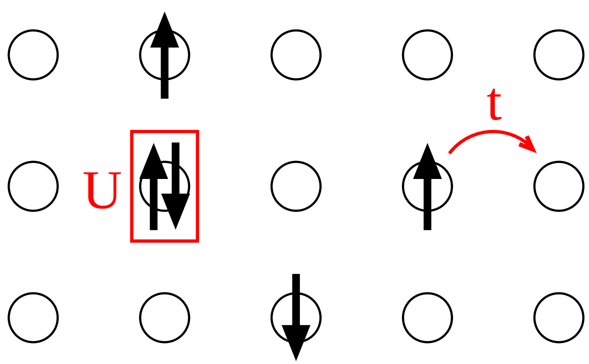
Theoretical Physics ⟷ Experimental Physics

Hubbard model

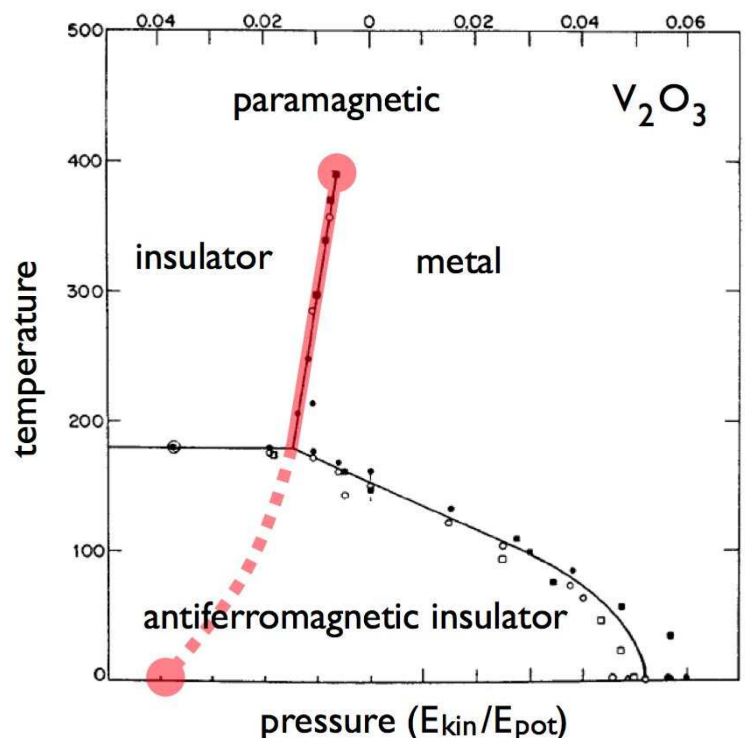
correlation driven
metal-insulator transition

Computational Physics

$$H = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma}$$



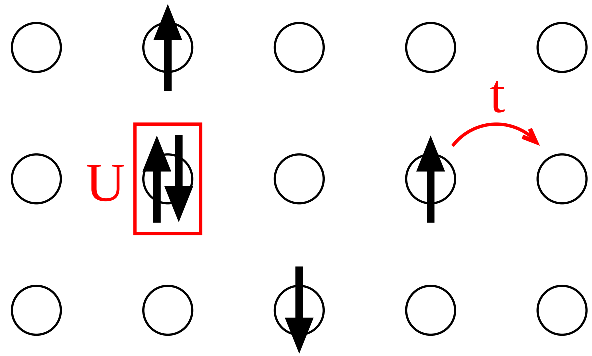
not analytically solvable



McWhan et al., (1973)

Introduction

Simulation of correlated lattice models



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

- Exact diagonalization: up to 20 sites
- Monte Carlo: fermion sign problem

$\Rightarrow$ Simulation of 2D, 3D lattice models not possible

$\Rightarrow$ Need new methods / approximate descriptions

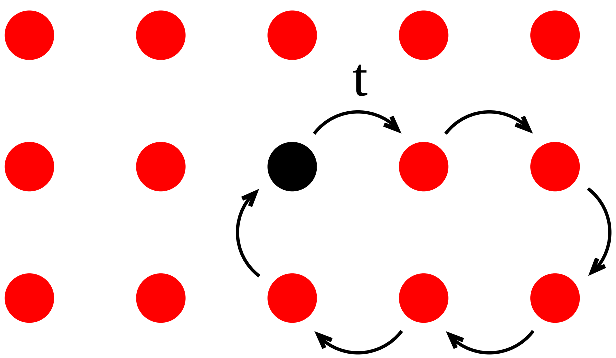
e. g. Dynamical Mean Field Theory (DMFT)

Motivation

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

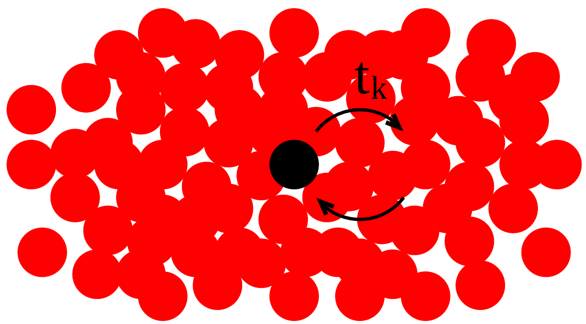
- Lattice model

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



- Quantum impurity model

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

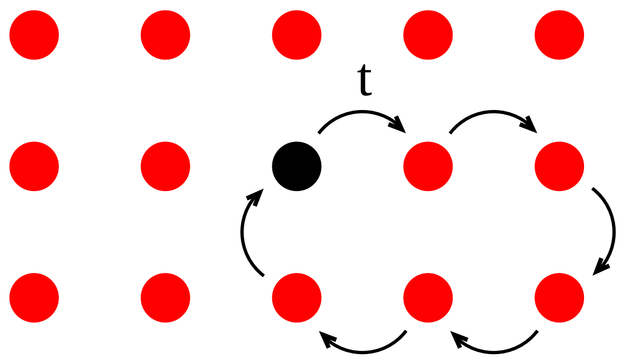


Motivation

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

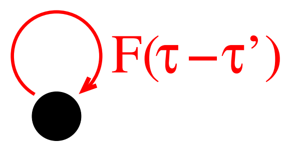
- Lattice model

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



- Effective action (hybridization function $F(\tau)$)

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



- Self-consistency condition

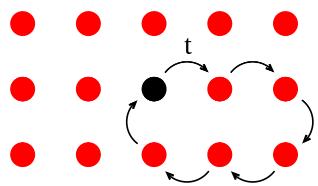
$$G^{\text{loc}}_{\text{latt}}(\tau) = G_{\text{imp}}(\tau)$$

Motivation

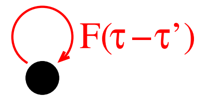
Dynamical mean field theory *Metzner & Vollhardt (1989), Georges & Kotliar (1992)*

- Self-consistency loop couples the impurity to the lattice

Lattice model



Impurity model



$\Rightarrow \Rightarrow \Rightarrow \Rightarrow \Rightarrow \Rightarrow$ $S_{\text{imp}}[F(\tau)]$

$\Uparrow$ $G_{\text{latt}}^{\text{loc}} = G_{\text{imp}}$ $\Downarrow$

Hilbert transform | impurity solver

$\Uparrow$ $\Sigma_{\text{latt}} = \Sigma_{\text{imp}}$ $\Downarrow$

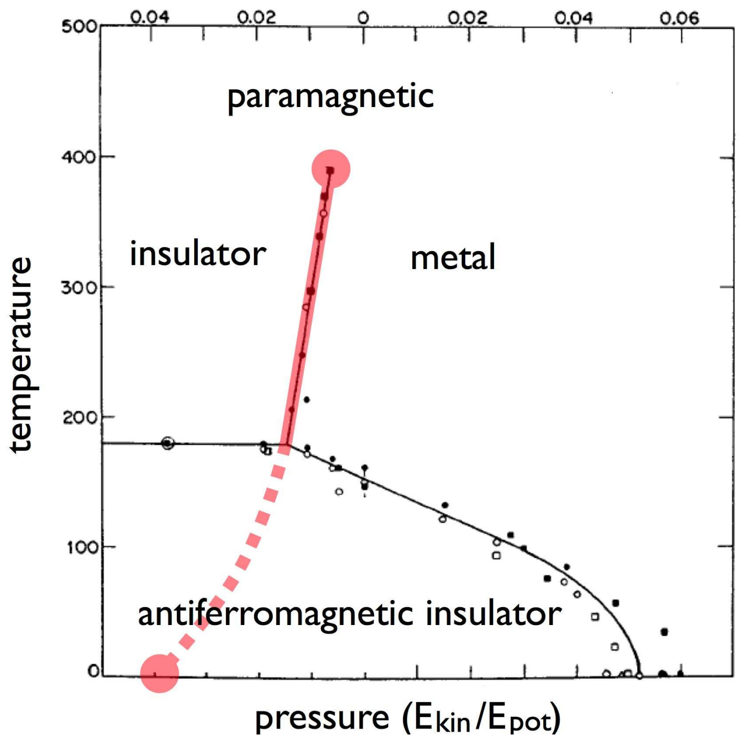
$\Leftarrow \Leftarrow \Leftarrow \Leftarrow \Leftarrow \Leftarrow$ $G_{\text{imp}}(\tau)$

- Computationally expensive step: solution of the impurity problem

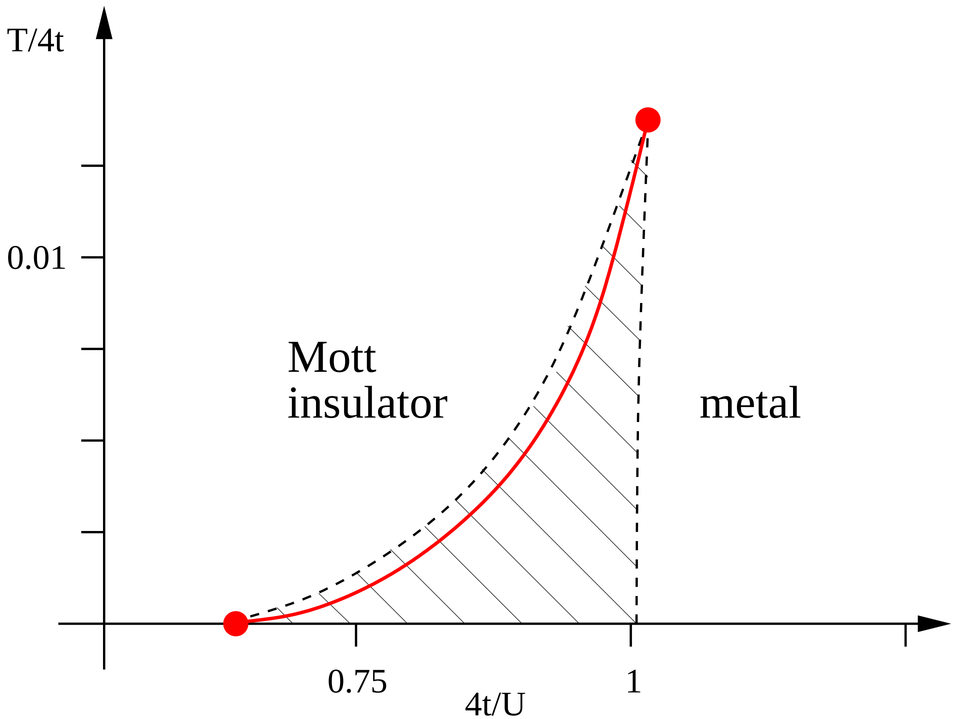
Example: Hubbard model

Correlation driven metal-insulator (Mott) transition

- Phasediagram for V_2O_3
  McWhan et al., (1973)



paramagnetic DMFT solution
1-band Hubbard model
Georges & Krauth (1993), Blümer (2002)



- More realistic multi-band simulation requires powerful impurity solvers

Diagrammatic Monte Carlo

Weak coupling vs. strong coupling approach

- Diagrammatic QMC = stochastic sampling of Feynman diagrams
- Hubbard model: $Z = Tr T_\tau e^{-S}$ with action

$$S = \underbrace{-\sum_\sigma \int_0^\beta d\tau d\tau' c_\sigma(\tau) F_\sigma(\tau-\tau') c_\sigma^\dagger(\tau')}_{S_F} \underbrace{+U \int_0^\beta d\tau n_\uparrow n_\downarrow}_{S_U}$$

  - Weak-coupling expansion

    Rombouts et al., PRL (1999); Rubtsov et al., PRB (2005); Gull et al., EPL (2008)

    Treat quadratic part (S_F) exactly, expand Z in powers of S_U
  - Hybridization expansion

    Werner et al., PRL (2006); Werner & Millis, PRB (2006); Haule, PRB (2007); Werner & Millis, PRL (2007)

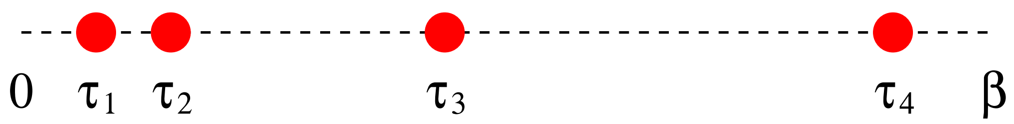
    Treat local part (S_U) exactly, expand Z in powers of S_F

Diagrammatic Monte Carlo

Expansion in U + auxiliary field decomposition

Rombouts et al., PRL (1999), Gull et al., EPL (2008)

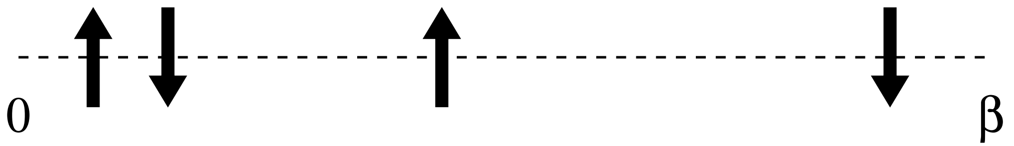
- Expand Z in powers of $K/\beta - U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2)$



- Decouple "interaction vertices" using *Rombouts et al., PRL (1999)*

$$K/\beta - U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2) = (K/2\beta) \sum_{s=-1,1} e^{\gamma s (n_\uparrow - n_\downarrow)}$$

$$\cosh(\gamma) = 1 + (\beta U/2K)$$



Diagrammatic Monte Carlo

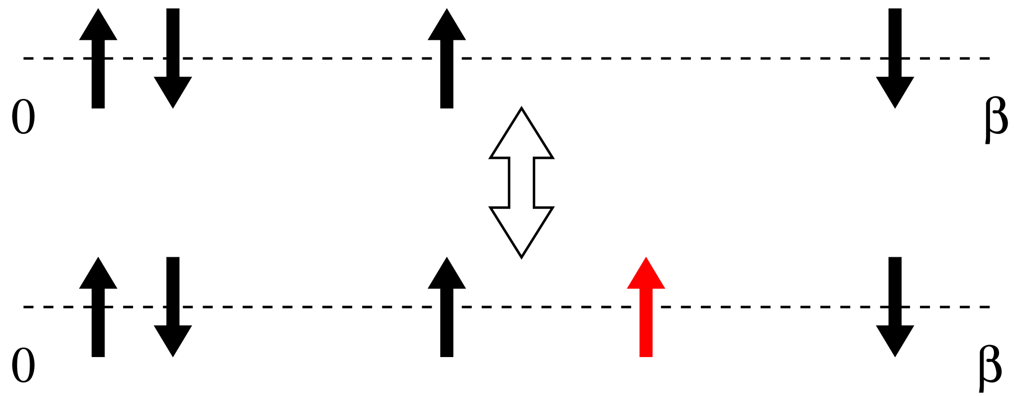
Expansion in U + auxiliary field decomposition

Rombouts et al., PRL (1999), Gull et al., EPL (2008)

- Weight of the configuration ($\Gamma_\sigma = \text{diag}(\gamma\sigma s_1, ...), (G_0)_{ij} = g_0(\tau_i - \tau_j)$)

$$w(\{s_i, \tau_i\}) = \left(\frac{K d\tau}{2\beta}\right)^n \prod_\sigma \det\left(e^{\Gamma_\sigma} - G_{0\sigma}(e^{\Gamma_\sigma} - I)\right)$$

- Local updates: insertion/removal of an auxiliary spin



- Advantage: less spins than Hirsch-Fye method

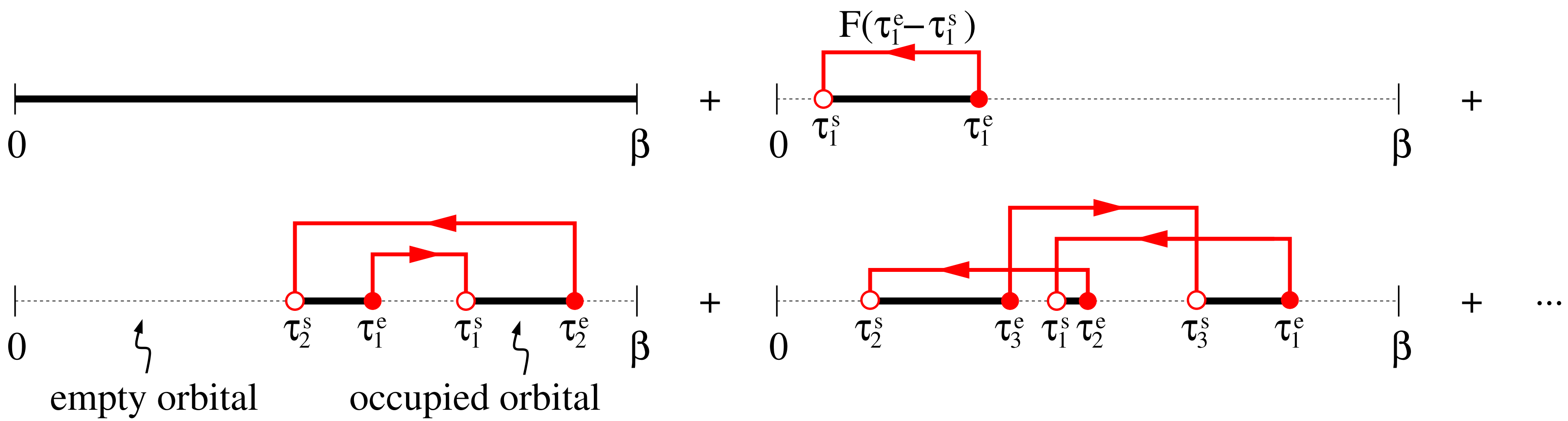
  $\Rightarrow$ faster updates, shorter autocorrelation (thermalization) times

Diagrammatic Monte Carlo

Expansion in the impurity-bath hybridization F *Werner et al., PRL (2006)*

- Non-interacting model: $Z = Tr T_\tau \exp\left[\int_0^\beta d\tau d\tau' c(\tau) F(\tau-\tau') c^\dagger(\tau')\right]$

- Expand exponential in powers of F

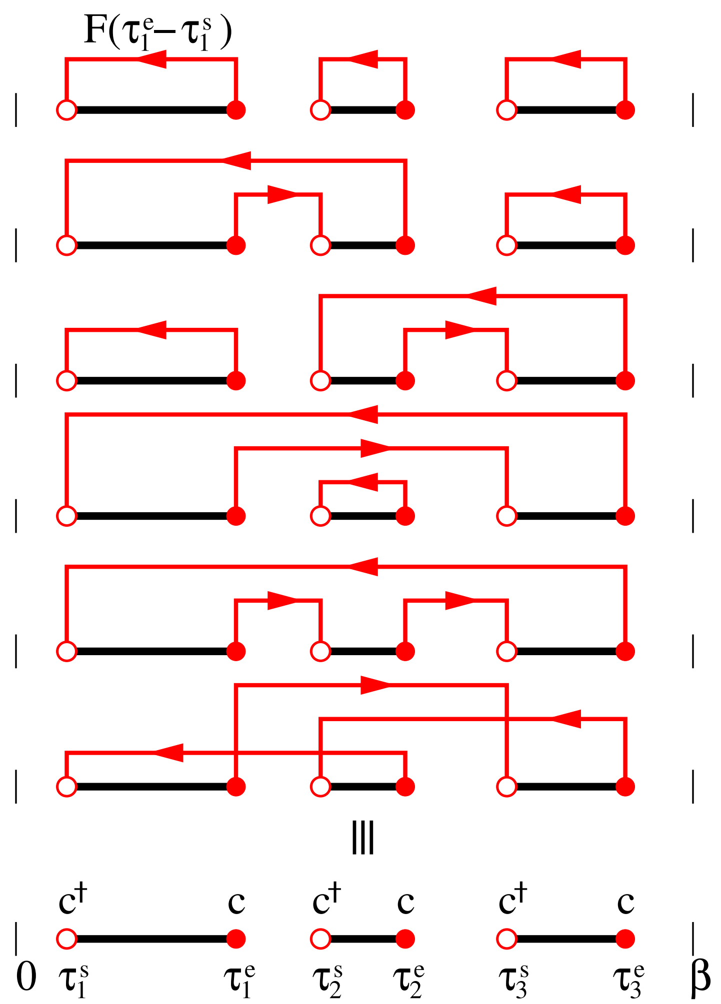


- Some diagrams have negative weight

  $\Rightarrow$ sampling individual diagrams leads to a severe sign problem

Diagrammatic Monte Carlo

Expansion in the impurity-bath hybridization F *Werner et al., PRL (2006)*



- Collect the diagrams with the same $\{c(\tau_i^s), c^\dagger(\tau_i^e)\}$ into a determinant

$$\det \mathcal{F}$$

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

$\rightarrow$ resums huge numbers of diagrams ($100! = 10^{158}$)

$\rightarrow$ eliminates the sign problem

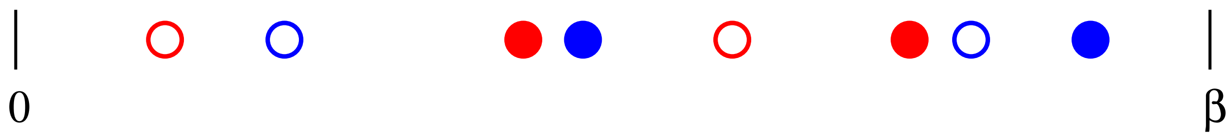
- $Z =$ sum of all operator sequences

Diagrammatic Monte Carlo

Generalizations

- Arbitrary interactions: $U^{\alpha\beta\gamma\delta} c^\dagger_\alpha c_\beta c^\dagger_\gamma c_\delta,\ \vec{S}\cdot c^\dagger_\alpha \vec{\sigma}_{\alpha,\beta} c_\beta,\ \vec{S}\cdot\vec{L}, \ldots$

  Werner & Millis, PRB (2006); Haule, PRB (2007)



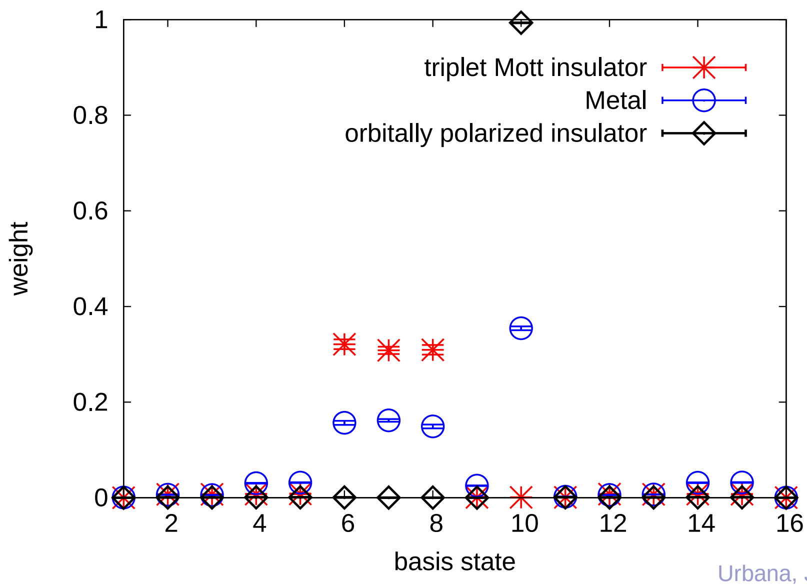
$$w = Tr\left[e^{-H_{\text{loc}}\tau_1}\psi^\dagger_\uparrow e^{-H_{\text{loc}}(\tau_2-\tau_1)}\psi^\dagger_\downarrow e^{-H_{\text{loc}}(\tau_3-\tau_2)}\psi_\uparrow \ldots\right] \det \mathcal{F}_\uparrow \det \mathcal{F}_\downarrow$$

$\oplus$ local problem treated exactly

$\Rightarrow$ flexible

$\Rightarrow$ histogram of relevant states

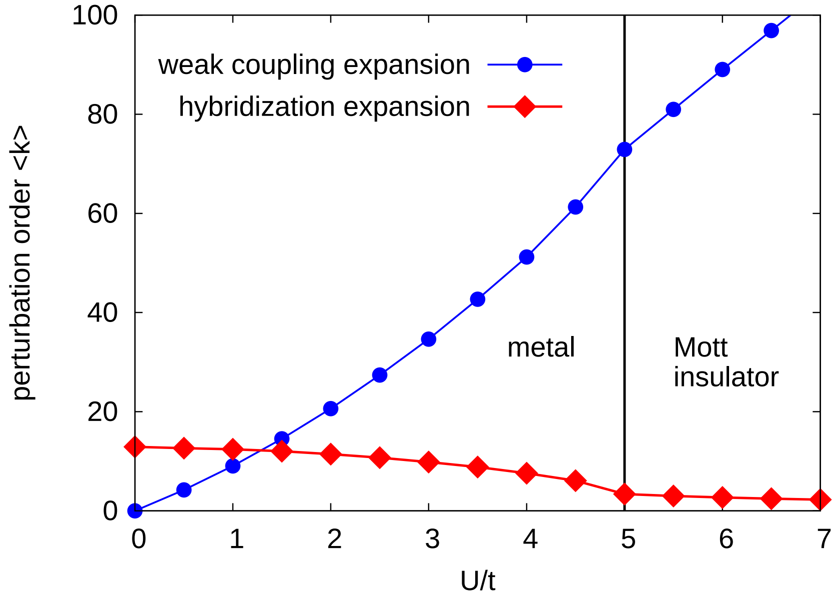
$\ominus$ scales exponentially with
sites, orbitals



Efficiency

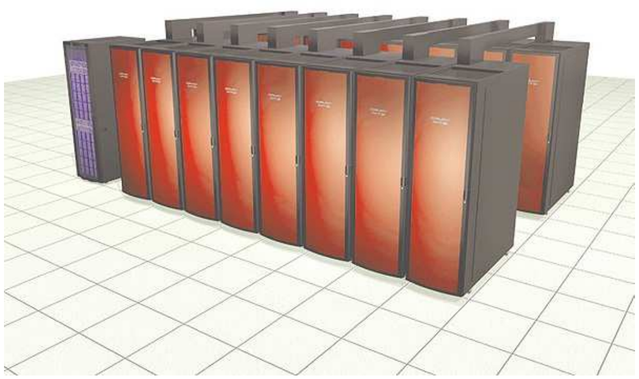
Scaling of the average perturbation order $\langle k \rangle$ *Gull et al, PRB (2007)*

- Computational effort grows $O(k^3)$ with size k of determinants
- Weak coupling expansion: $\langle k \rangle \sim U$
- Hybridization expansion: $\langle k \rangle$ decreases with increasing U



$\Rightarrow$ In the strong correlation regime, speed-ups of 10^4-10^5

$\Leftrightarrow$



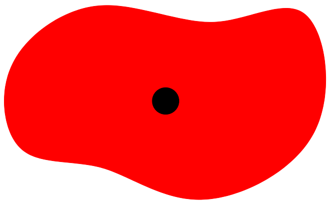
1-band Hubbard model

Metal-insulator transition on the 2D square lattice (bandwidth $= 8t$)

Gull et al, EPL (2008)

- Single site DMFT: $H_{\text{loc}} = U n_\uparrow n_\downarrow$

  $\Rightarrow$ "Mott" transition at $U_c \approx 12t$

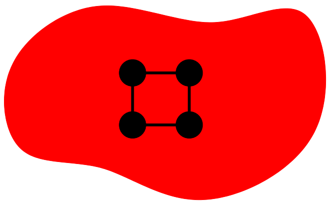


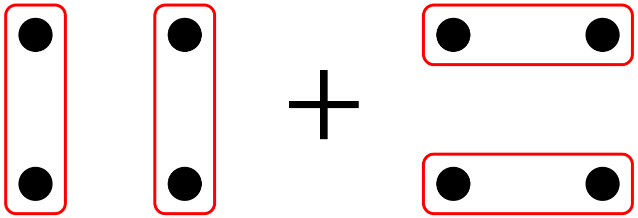
- 4 site DMFT:

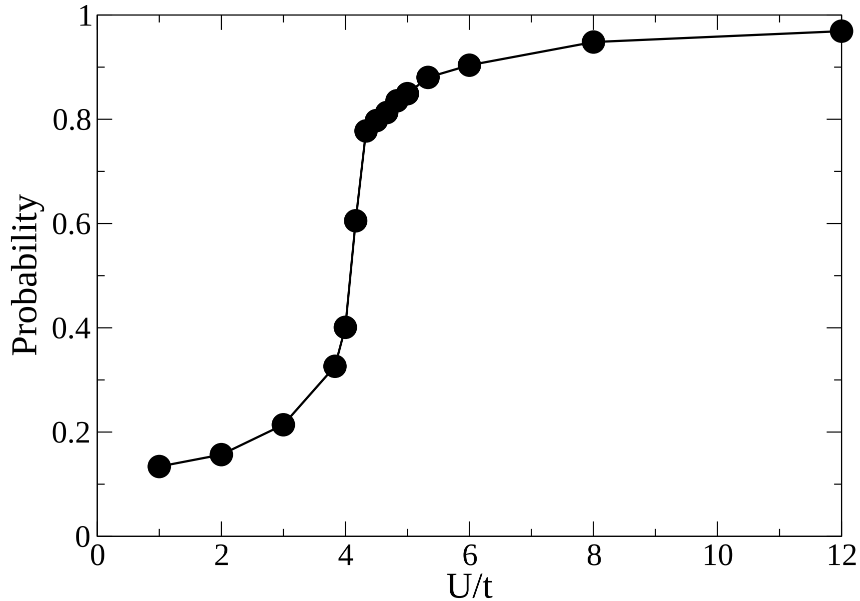
  $H_{\text{loc}} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_i U n_\uparrow n_\downarrow$

  $\Rightarrow$ "Slater" transition at $U_c \approx 4t$

  collapse into plaquette singlet state





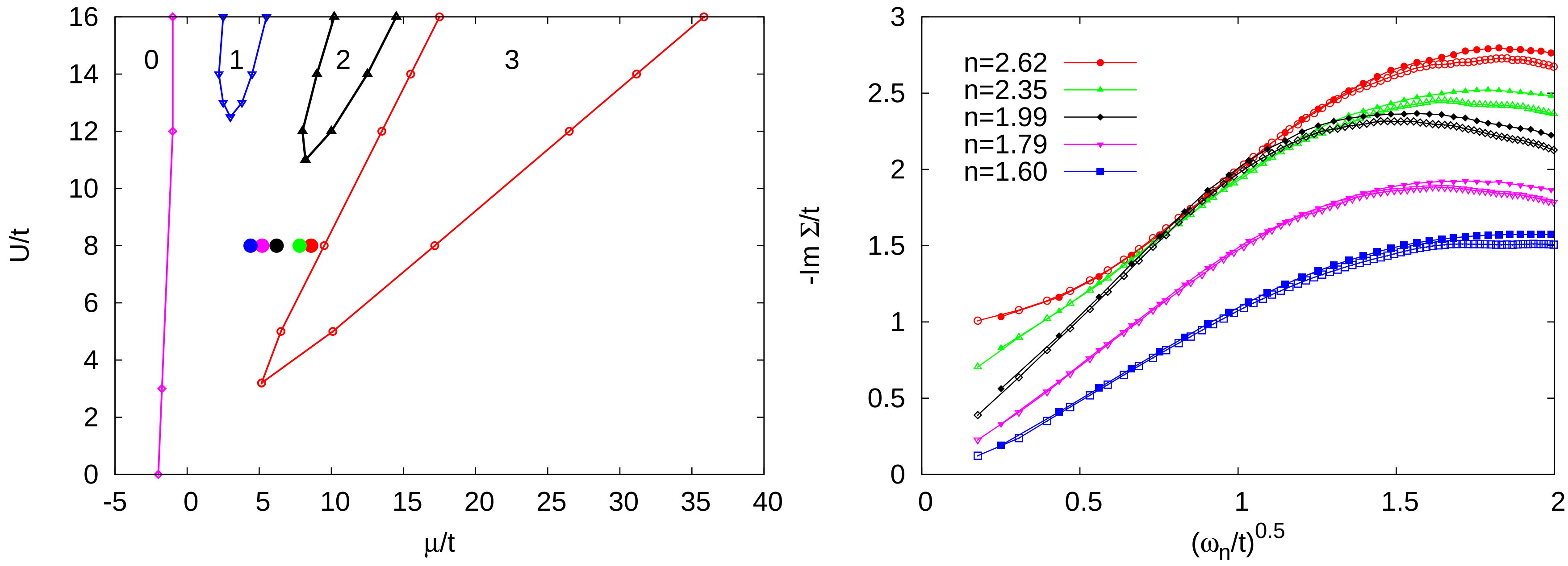


3-orbital model

Non-Fermi liquid behavior in multi-orbital models with Hund coupling

Werner et al, arXiv:cond-mat/0806.2621

- $H_{\text{loc}} = \sum_\alpha U n_{\alpha,\uparrow} n_{\alpha,\downarrow} + \sum_{\alpha\neq\beta,\sigma} U' n_{\alpha,\sigma} n_{\beta,-\sigma} + \sum_{\alpha\neq\beta,\sigma} (U'-J) n_{\alpha,\sigma} n_{\beta,\sigma}$
  $- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{\alpha,\uparrow} + \psi^\dagger_{\beta,\uparrow}\psi^\dagger_{\beta,\downarrow}\psi_{\alpha,\uparrow}\psi_{\alpha,\downarrow} + h.c.) - \sum_{\alpha,\sigma} \mu n_{\alpha,\sigma}$
- Bethe lattice with bandwidth $4t$, $U' = U - 2J$
- Phase diagram for $J = U/6$ (left) and self-energy at $U/t = 8$ (right)



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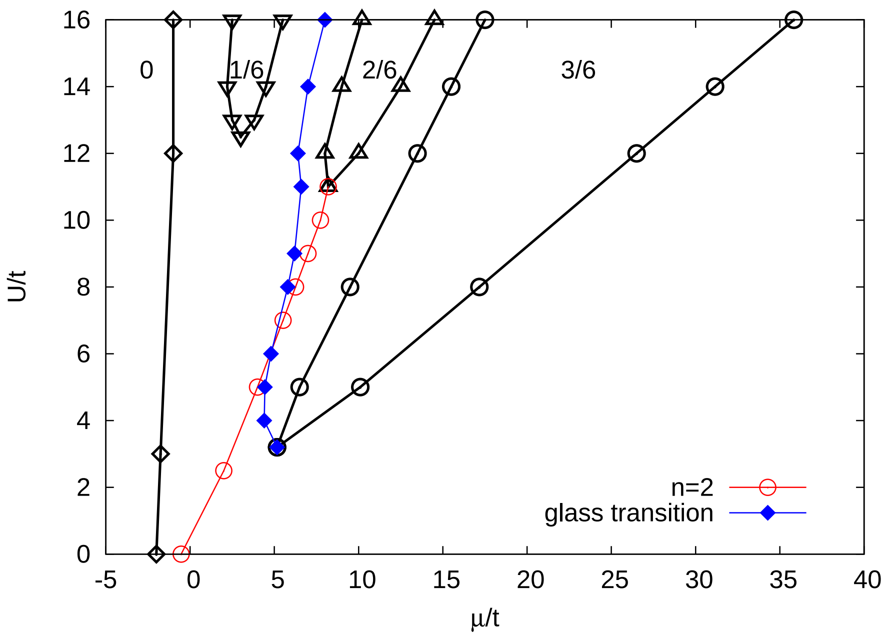
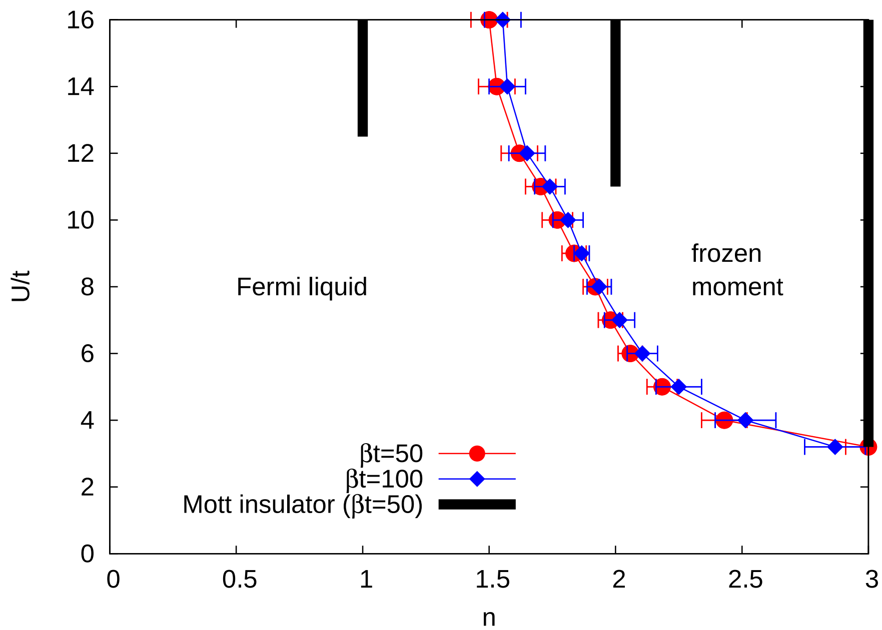
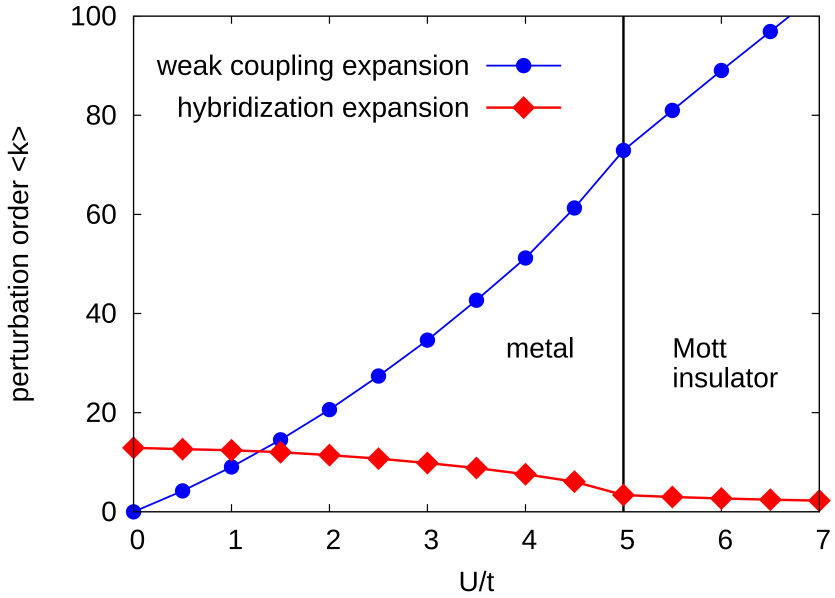
  $- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{\alpha,\uparrow} + \psi^\dagger_{\beta,\uparrow}\psi^\dagger_{\beta,\downarrow}\psi_{\alpha,\uparrow}\psi_{\alpha,\downarrow} + h.c.) - \sum_{\alpha,\sigma} \mu n_{\alpha,\sigma}$
- Transition to a phase with frozen moments
- Broad quantum critical regime $\Rightarrow$ Im$\Sigma \sim \sqrt{\omega_n} \Rightarrow \sigma(\Omega) \sim 1/\sqrt{\Omega}$





Conclusions & Outlook

- Diagrammatic MC simulation of impurity models:
  - Weak-coupling method for large impurity clusters
  - "Strong-coupling" method for multi-orbital models



- On-going projects:
  - LDA+DMFT simulation of transition metal oxides and actinide compounds
  - Adaptation of the diagrammatic approach to real-time dynamics (non-equilibrium systems)

- Job openings: PhD and postdoc position at ETH Zürich