Diagrammatic Monte Carlo simulation of quantum impurity models

Philipp Werner

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Outline

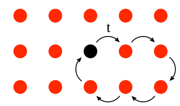
- Continuous-time auxiliary field method (CT-AUX)
  - Weak coupling expansion and auxiliary field decomposition
  - Application: electron pockets in the 2D Hubbard model
- Hybridization expansion
  - ``Strong coupling" method for general classes of impurity models
  - Application: spin freezing transition in a 3-orbital model
- Adaptation to non-equilibrium systems
  - quantum dots / non-equilibrium DMFT
- Collaborators
  - E. Gull, A. J. Millis, T. Oka, O. Parcollet, M. Troyer

Dynamical mean field theory

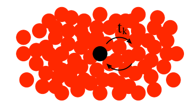
Metzner & Vollhardt, PRL (1989)
Georges & Kotliar, PRB (1992)

- Self-consistency loop

lattice model



impurity model



G_{latt} $\Longrightarrow$ H_{imp}

$G_{latt} \equiv G_{imp}$

$\int dk \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{latt}}$

impurity solver

Σ_{latt} $\Longleftarrow$ $G_{imp},\ \Sigma_{imp}$

$\Sigma_{latt} \equiv \Sigma_{imp}$

- Computationally expensive step: solution of the impurity model

Diagrammatic QMC

- General recipe:
  - Split Hamiltonian into two parts: $H = H_1 + H_2$
  - Use interaction representation in which $O(\tau) = e^{\tau H_1} O e^{-\tau H_1}$
  - Write partition function as time-ordered exponential, expand in powers of H_2

$$
\begin{aligned}
Z &= Tr\left[e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)}\right] \\
&= \sum_k \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \frac{(-1)^k}{k!} Tr\left[e^{-\beta H_1} T H_2(\tau_1) \ldots H_2(\tau_k)\right]
\end{aligned}
$$

- Weak-coupling expansion: *Rombouts et al., (1999), Rubtsov et al. (2005), Gull et al. (2008)*
  - expand in interactions, treat quadratic terms exactly
- Hybridization expansion: *Werner et al., (2006), Werner & Millis (2006), Haule (2007)*
  - expand in hybridizations, treat local terms exactly

CT-auxiliary field QMC

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

- Impurity model given by

$$\begin{aligned} H &= H_0 + H_U \\ H_0 &= K/\beta - (\mu - U/2)(n_\uparrow + n_\downarrow) + H_{hyb} + H_{bath} \\ H_U &= U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2) - K/\beta \end{aligned}$$

- Expand partition function into powers of the interaction term

$$Z = \sum_k \frac{(-1)^k}{k!} \int d\tau_1 \ldots \int d\tau_k Tr\left[T e^{-\beta H_0} H_U(\tau_1) \ldots H_U(\tau_k)\right]$$

- Decouple the interaction terms using *Rombouts et al., PRL (1999)*

$$-H_U = \frac{K}{2\beta} \sum_{s=\pm 1} e^{\gamma s (n_\uparrow - n_\downarrow)}, \qquad \cosh(\gamma) = 1 + \frac{\beta U}{2K}$$

CT-auxiliary field QMC

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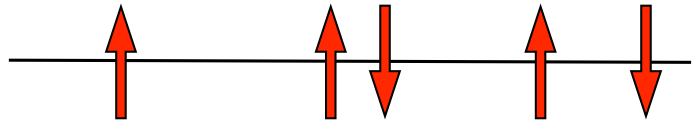
- Configuration space: all possible time-ordered spin configurations



- Weight: $$w(\tau_1, s_1; \ldots; \tau_k, s_k) = \left(\frac{K d\tau}{2\beta}\right)^k \prod_\sigma \det N_\sigma^{-1}(\{\tau_i, s_i\})$$
$$N_\sigma^{-1} = e^{\Gamma_\sigma} - G_{0\sigma}\left(e^{\Gamma_\sigma} - 1\right)$$
$$e^{\Gamma_\sigma} = \mathrm{diag}(e^{\gamma\sigma s_1}, \ldots, e^{\gamma\sigma s_k})$$

- Monte Carlo updates: random insertion/removal of a spin

- Equivalent to *Rubtsov et al.*, formally similar to *Hirsch-Fye*

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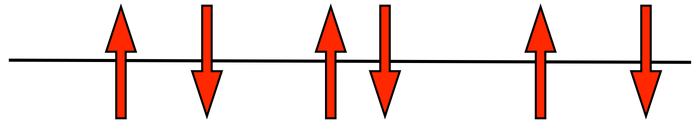

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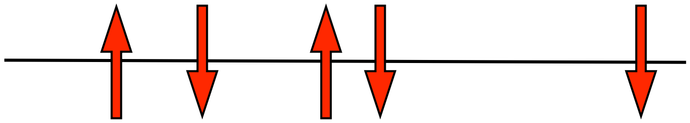

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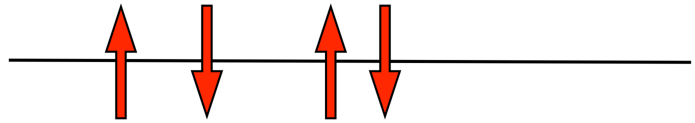

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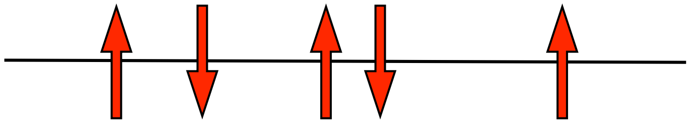

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M-I transition in the 2D Hubbard model

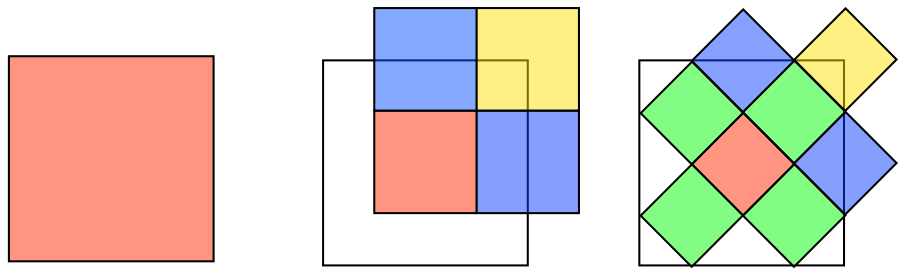
- Hubbard model with nn hopping *t*, nnn hopping *t'=0* (bandwidth *8t*)

$$H = \sum_{p,\alpha} \epsilon_p c^\dagger_{p,\alpha} c_{p,\alpha} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \qquad \epsilon_p = -2t(\cos(p_x) + \cos(p_y))$$

- DMFT: approximate momentum-dependence of the self-energy

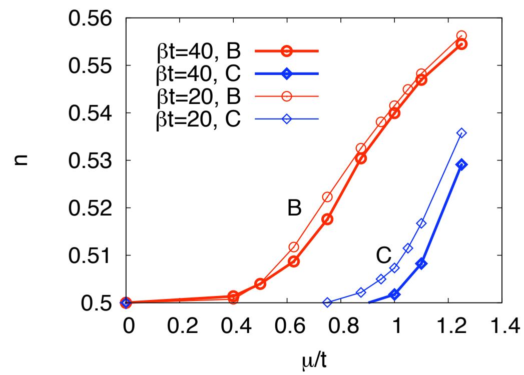
$$\Sigma(p,\omega) = \sum_a \phi_a(p) \Sigma_a(\omega)$$

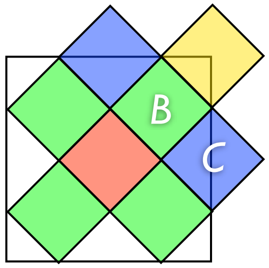
- DCA: ``tiling" of the Brillouin zone



M-I transition in the 2D Hubbard model

- Doping the insulator produces electron/hole pockets
- 8-site cluster has a ``tile" at the expected position of the pockets
- 8-site DCA-result at U/t=7: first 8% of dopants go into the *B* sector





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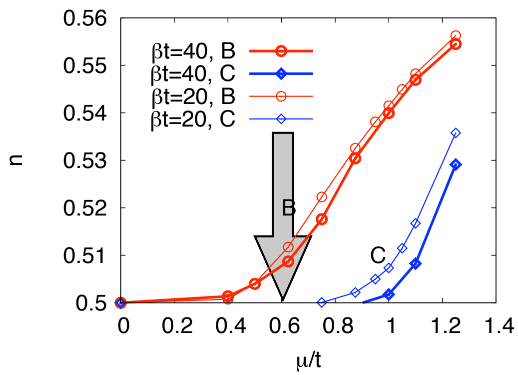

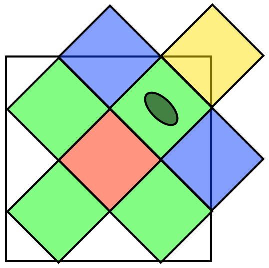

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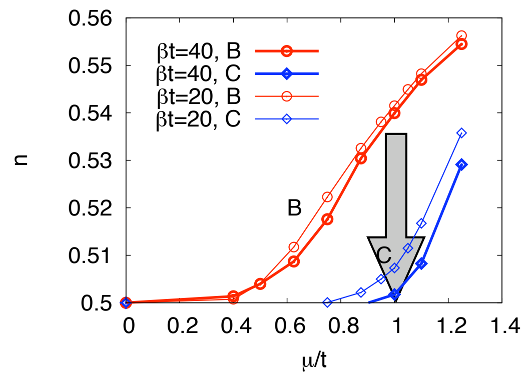

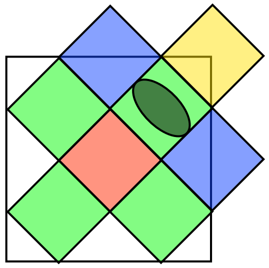

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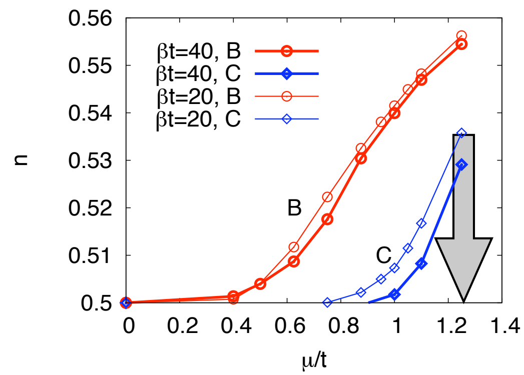

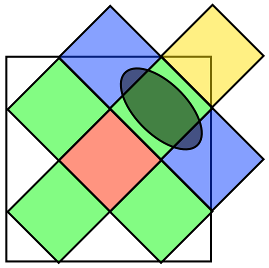

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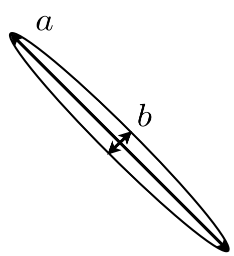
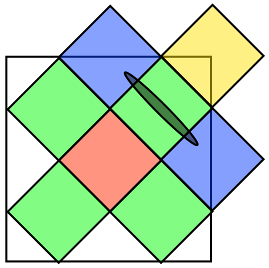
- 8-site cluster has a ``tile'' at the expected position of the pockets
- 8-site DCA-result at *U*/*t*=7: first 8% of dopants go into the *B* sector
- Assuming an ellipsoidal shape for the pocket, we can estimate the aspect ratio

$$\frac{b}{a} \approx \frac{1}{10}$$





Hybridization expansion

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

- Impurity model given by

$$
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H &= H_{loc} + H_{bath} + H_{hyb} \\
H_{loc} &= U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) \\
H_{hyb} &= \sum_{p,\sigma} t_p^\sigma c_\sigma^\dagger a_{p,\sigma} + h.c.
\end{aligned}
$$

- Expand partition function into powers of the hybridization term

$$Z = \sum_k \frac{1}{2k!} \int d\tau_1 \ldots \int d\tau_{2k} Tr\left[T e^{-\beta(H_{loc}+H_{bath})} H_{hyb}(\tau_1) \ldots H_{hyb}(\tau_{2k})\right]$$

- Trace over bath degrees of freedom yields determinant of hybridization functions *F*

$$Tr_{bath}[\ldots] = \prod_\sigma \det M_\sigma^{-1}, \qquad M_\sigma^{-1}(i,j) = F_\sigma(\tau_i^{(c)} - \tau_j^{(c^\dagger)})$$

$$F_\sigma(-i\omega_n) = \sum_p \frac{|t_p^\sigma|^2}{i\omega_n - \epsilon_p}$$

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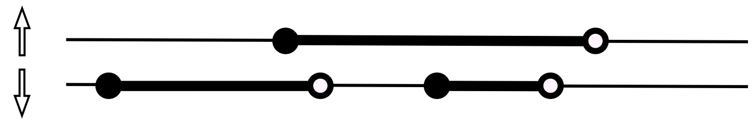
- Monte Carlo configurations consist of segments for spin up and down



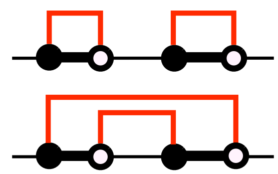
- Monte Carlo updates: random insertion/removal of (anti-)segments

- Weight of a segment configuration:

$$w\left(\tau_1^{\sigma(c)}, \tau_1^{\sigma(c^\dagger)}; \ldots; \tau_{k_\sigma}^{\sigma(c)}, \tau_{k_\sigma}^{\sigma(c^\dagger)}\right) = \underbrace{e^{-Ul_{overlap}+\mu(l_\uparrow+l_\downarrow)}}_{Tr_{imp}[\ldots]} \prod_\sigma \underbrace{\det M_\sigma^{-1}}_{Tr_{bath}[\ldots]} d\tau^{2k_\sigma}$$

- Determinant of a *k x k* matrix resums *k!* diagrams

$$\det \begin{pmatrix} F_\sigma(\tau_1^{(c)} - \tau_1^{(c^\dagger)}) & F_\sigma(\tau_1^{(c)} - \tau_2^{(c^\dagger)}) \\ F_\sigma(\tau_2^{(c)} - \tau_1^{(c^\dagger)}) & F_\sigma(\tau_2^{(c)} - \tau_2^{(c^\dagger)}) \end{pmatrix}$$



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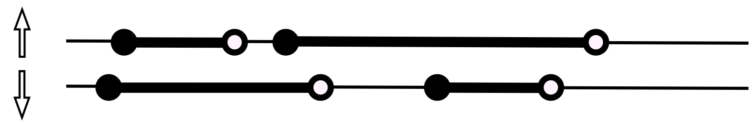

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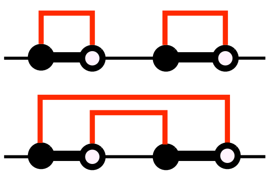

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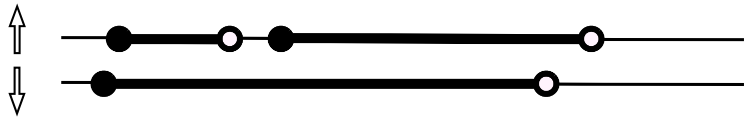

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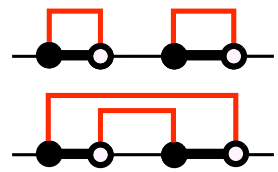

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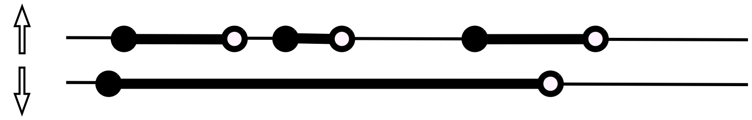

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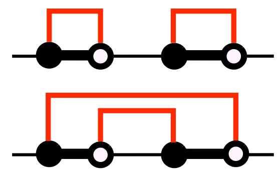

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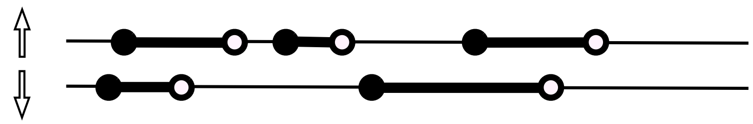

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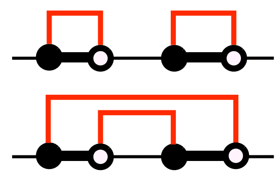


Spin freezing transition in a 3-orbital model

Werner et al., PRL (2008)

- 1 site, 3 degenerate orbitals (semi-circular DOS, bandwidth *4t*)

$$H_{\rm loc} = -\sum_{\alpha,\sigma} \mu n_{\alpha,\sigma} + \sum_{\alpha} U n_{\alpha,\uparrow} n_{\alpha,\downarrow}$$
$$+ \sum_{\alpha>\beta,\sigma} U' n_{\alpha,\sigma} n_{\beta,-\sigma} + (U'-J) n_{\alpha,\sigma} n_{\beta,\sigma}$$
$$- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{\alpha,\uparrow} + \psi^\dagger_{\beta,\uparrow}\psi^\dagger_{\beta,\downarrow}\psi_{\alpha,\uparrow}\psi_{\alpha,\downarrow} + h.c.)$$

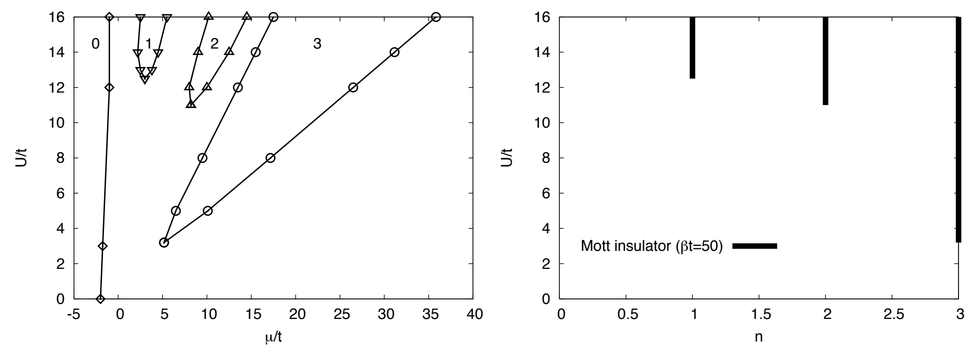
- Captures essential physics of *$SrRuO_3$*

- Similar models for other transition metal oxides, actinide compounds, *Fe* / *Ni* based superconductors, ...

Spin freezing transition in a 3-orbital model

Werner et al., PRL (2008)

- Phase diagram for $U' = U = 2J, J/U = 1/6, \beta t = 50$



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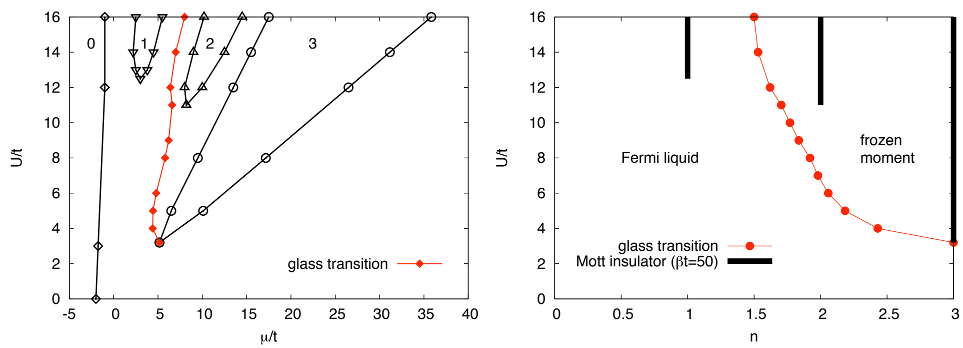


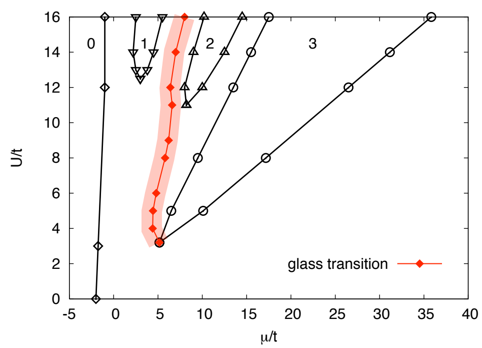
- Mott insulating ``lobes'' with 1, 2, 3, (4, 5) electrons

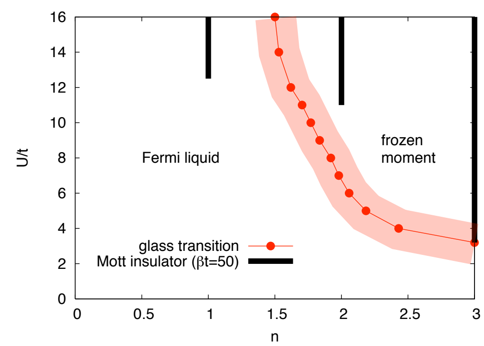
- In the metallic phase: transition from Fermi liquid to ``spin glass''

Spin freezing transition in a 3-orbital model

Werner et al., PRL (2008)

- Phase diagram for $U' = U = 2J, J/U = 1/6, \beta t = 50$





- Critical exponents associated with the transition can be seen in a wide quantum critical regime

- e. g. non Fermi-liquid self-energy $\mathrm{Im}\Sigma/t \sim (i\omega_n/t)^\alpha, \ \alpha \approx 0.5$

Spin freezing transition in a 3-orbital model

Werner et al., PRL (2008)

- A self-energy with frequency dependence $\Sigma(\omega) \sim \omega^{1/2}$ implies an **optical conductivity** $\sigma(\omega) \sim 1/\omega^{1/2}$

VOLUME 81, NUMBER 12 PHYSICAL REVIEW LETTERS 21 SEPTEMBER 1998

Non-Fermi-Liquid Behavior of $SrRuO_3$: Evidence from Infrared Conductivity

P. Kostic, Y. Okada,* N. C. Collins, and Z. Schlesinger
Department of Physics, University of California, Santa Cruz, California 95064

J. W. Reiner, L. Klein,† A. Kapitulnik, T. H. Geballe, and M. R. Beasley
Edward L. Ginzton Laboratories, Stanford University, Stanford, California 94305
(Received 13 March 1998)

The reflectivity of the itinerant ferromagnet $SrRuO_3$ has been measured between 50 and 25 000 cm^{-1} at temperatures ranging from 40 to 300 K, and used to obtain conductivity, scattering rate, and effective mass as a function of frequency and temperature. We find that at low temperatures the conductivity falls unusually slowly as a function of frequency (proportional to $1/\omega^{1/2}$), and at high temperatures it even appears to increase as a function of frequency in the far-infrared limit. The data suggest that the charge dynamics of $SrRuO_3$ are substantially different from those of Fermi-liquid metals.

Real-time formalism

Muehlbacher & Rabani (2008)
Schmidt et al. (2008)
Schiro & Fabrizio (2008)
Werner et al. (2008)

- Quantum dot coupled to two infinite leads

$$
\begin{aligned}
H &= H_{\text{dot}} + H_{\text{leads}} + H_{\text{mix}} \\
H_{\text{dot}} &= \epsilon_d (n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow} \\
H_{\text{leads}} &= \sum_{\alpha=L,R} \sum_{p\sigma} (\epsilon^{\alpha}_{p\sigma} - \mu_\alpha) a^{\alpha\dagger}_{p\sigma} a^{\alpha}_{p\sigma} \\
H_{\text{mix}} &= \sum_{\alpha=L,R} \sum_{p,\sigma} (V^{\alpha}_{p} a^{\alpha\dagger}_{p\sigma} d_\sigma + h.c.)
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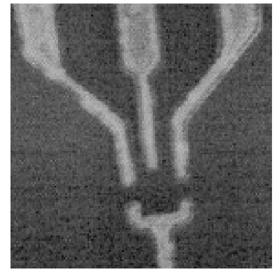

Goldhaber-Gordon (1998)

- Initial preparation of the dot: $\rho_{0,\text{dot}}$
- Non-interacting leads: $\rho_{0,\text{leads}}$ (DOS, Fermi distribution function)
- Level broadening: $\Gamma^\alpha(\omega) = \pi \sum_p |V^\alpha_p|^2 \delta(\omega - \epsilon^\alpha_p)$

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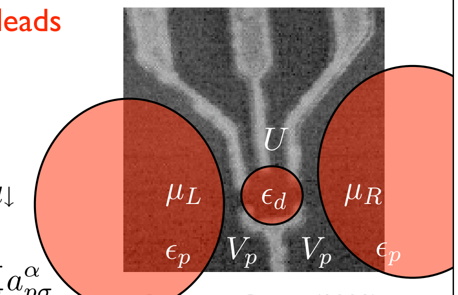

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- Interaction picture

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\langle \mathcal{O}(t) \rangle &= Tr\Big[\rho_0 e^{iHt}\mathcal{O}e^{-iHt}\Big] \\
&= Tr\Big[\rho_0 \Big(\tilde{T} e^{i\int_0^t ds H_2(s)}\Big)\mathcal{O}(t)\Big(T e^{-i\int_0^t ds H_2(s')}\Big)\Big]
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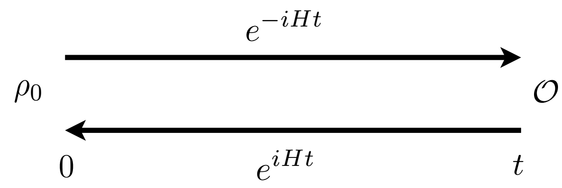
$$

- ``Keldysh contour''



- Expand time evolution operators in powers of H_2

Real-time formalism

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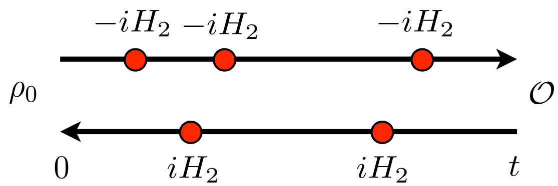
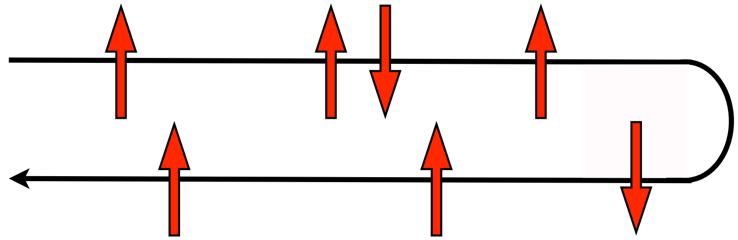


- Expand time evolution operators in powers of H_2

Weak-coupling expansion

Werner, Oka & Millis, PRB (2009)

- Configuration space: all possible spin configurations on the Keldysh contour



- Weight: analogous to imaginary-time CT-AUX with

$$G_{0,\sigma}(t'_K, t''_K) = \begin{cases} G^{<}_{0,\sigma}(t', t'') & t'_K < t''_K \\ G^{>}_{0,\sigma}(t', t'') & t'_K \geq t''_K \end{cases}$$

$$G_0^{</>}(t', t'') = \pm i \int \frac{d\omega}{2\pi} e^{-i\omega(t'-t'')} \frac{\sum_{\alpha=L,R} \Gamma^\alpha \left(1 \mp \tanh\left(\frac{\omega-\mu_\alpha}{2T}\right)\right)}{(\omega - \epsilon_d - U/2)^2 + \Gamma^2}$$

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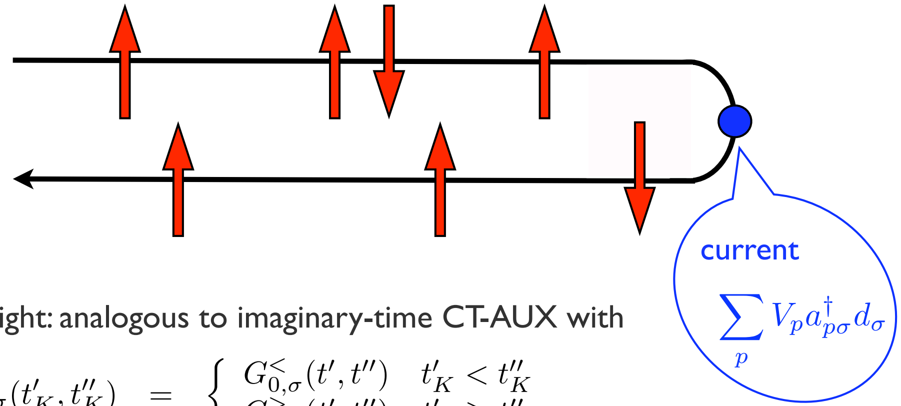

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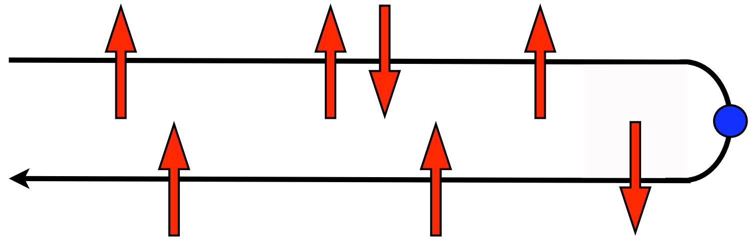
Weak-coupling expansion

Werner, Oka & Millis, PRB (2009)

- Monte Carlo sampling: random insertion/removal of spins



- Current measurement:

$$I = -2\mathrm{Im}\sum_\sigma \sum_c w_c^{I_\sigma} = -2\mathrm{Im}\sum_\sigma \left[\left\langle \frac{w_c^{I_\sigma}}{|w_c|} \right\rangle_{|w_c|} \frac{1}{\langle \phi_c \rangle_{|w_c|}} \right]$$

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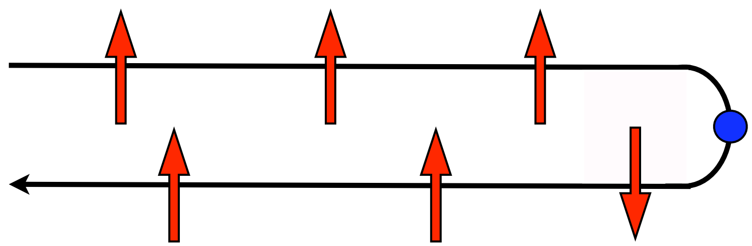

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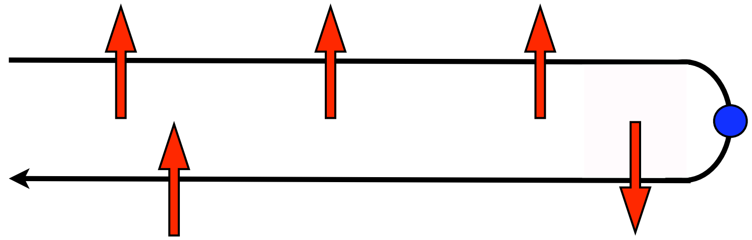

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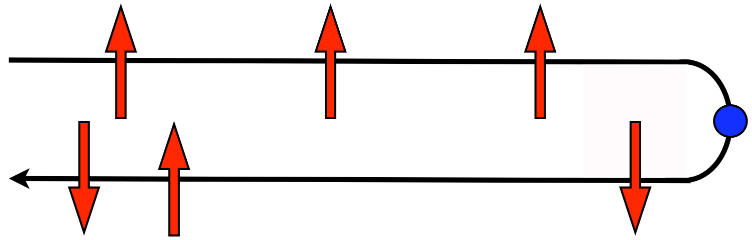

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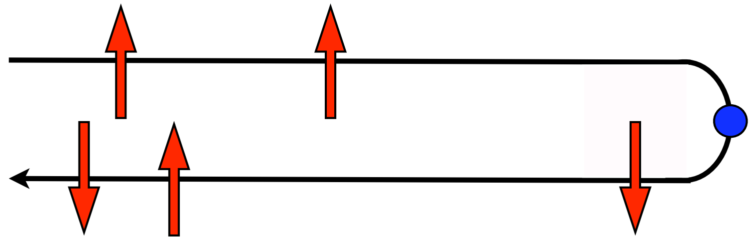

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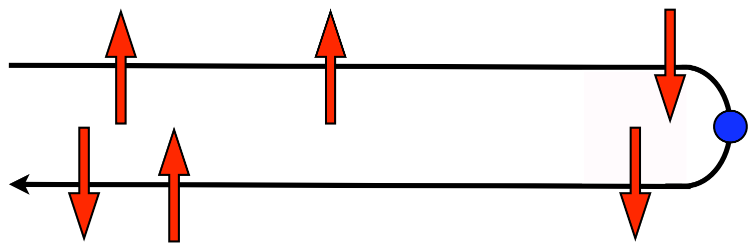

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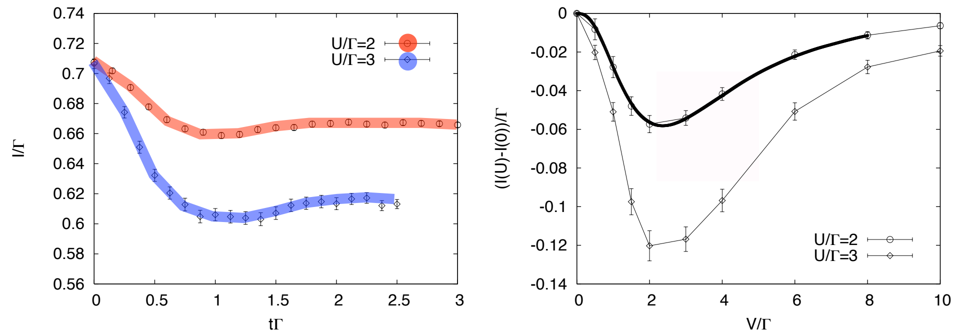
Weak-coupling expansion

Werner, Oka & Millis, PRB (2009)

- Interaction and voltage dependence of the current

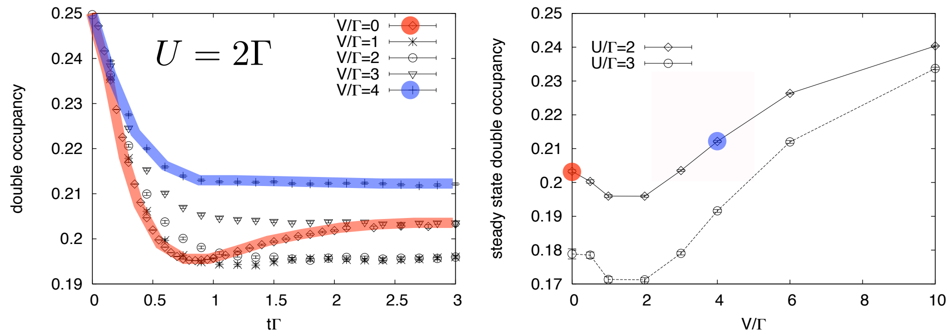


- Interaction suppresses the current
- Correction largest for $V \approx U$
- 4th order perturbation theory by *Fujii & Ueda* identical to MC for $U = 2\Gamma$

Weak-coupling expansion

Werner, Oka & Millis, PRB (2009)

- Interaction and voltage dependence of the double occupancy



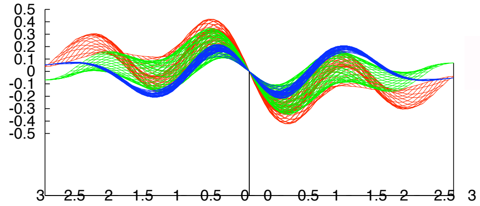
- Convergence to steady state faster for larger voltage bias

Weak-coupling expansion

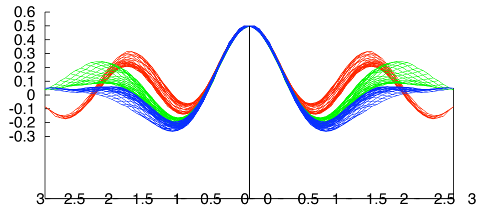
- Non-equilibrium DMFT
- Dynamics of the Hubbard model after a ``quantum quench"

Eckstein and Werner (work in progress)

$\mathrm{Re}G(t,t')$



$\mathrm{Im}G(t,t')$



Weak-coupling expansion

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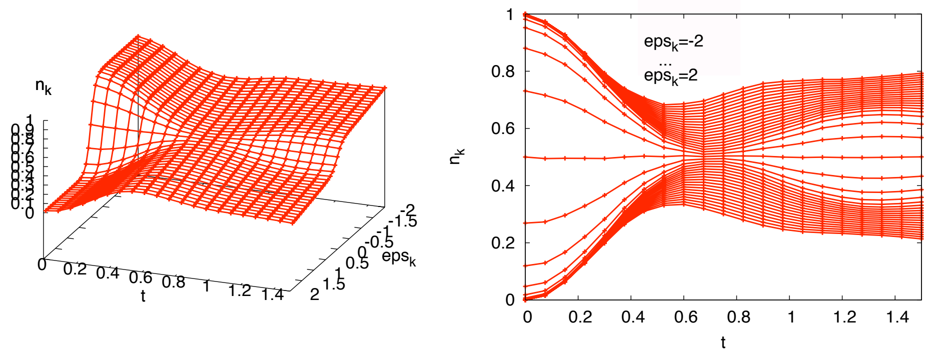
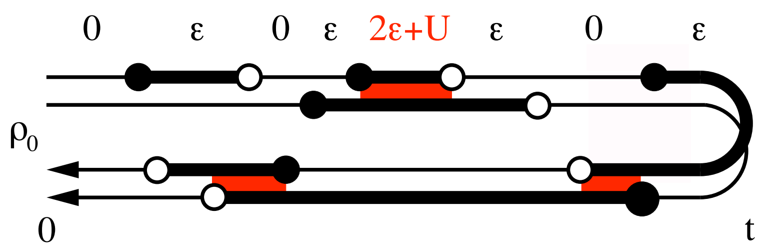


Hybridization expansion

Muehlbacher & Rabani (2008)
Schmidt et al. (2008)
Schiro & Fabrizio (2008)
Werner et al. (2008)

- Configuration space: all possible segment configurations on the (doubled) Keldysh contour



- Hybridization matrix becomes $\begin{pmatrix} \Sigma^<(t_1 - t_1') & \Sigma^<(t_2 - t_1') & \dots \\ \Sigma^>(t_1 - t_2') & \Sigma^<(t_2 - t_2') & \dots \\ \dots & \dots & \dots \end{pmatrix}$

- Monte Carlo sampling: random insertions/removals of segments

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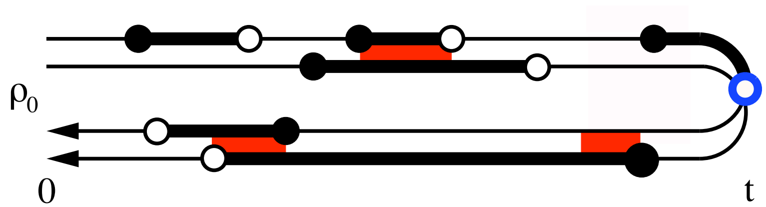

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Hybridization expansion

Muehlbacher & Rabani (2008)
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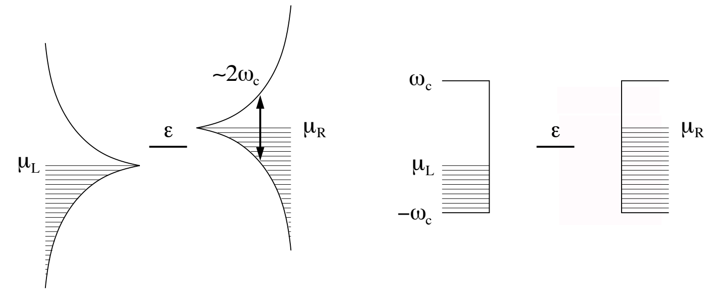
Werner et al. (2008)

- $\Sigma^{<,>}$ depends on the DOS and voltage bias



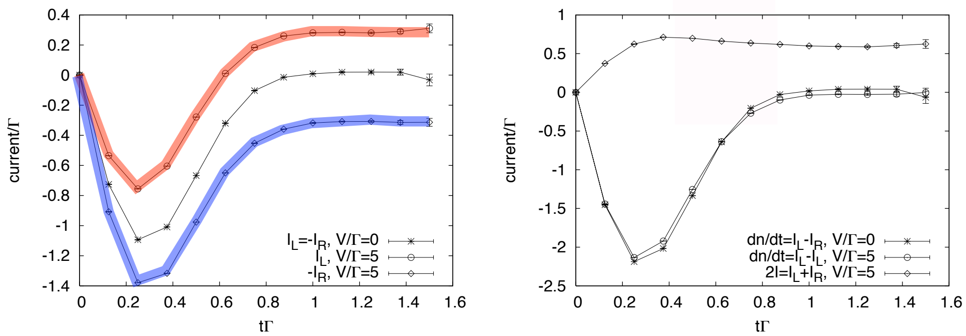
- soft cutoff: $$\Sigma^{<,>}_{\text{soft}}(t) = \Gamma \frac{\cos(\frac{V}{2})}{\beta \sinh(\frac{\pi}{\beta}(t \pm i/\omega_c))}$$

- hard cutoff: $$\Sigma^{<,>}_{\text{hard}}(t) = \Gamma \left(\frac{\cos(\frac{V}{2}t)}{\beta \sinh(\frac{\pi}{\beta}t)} - \frac{e^{\pm i \omega_c t}}{\nu \sinh(\frac{\pi}{\nu}t)} \right)$$

Hybridization expansion

Muehlbacher & Rabani (2008)
Schmidt et al. (2008)
Schiro & Fabrizio (2008)
Werner et al. (2008)

- Initial state: dot decoupled from the leads
- Time evolution of the left, right and average current $(U/\Gamma = 8)$

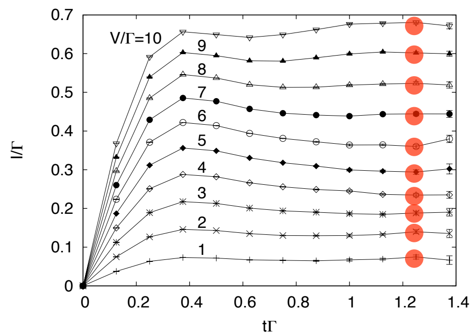


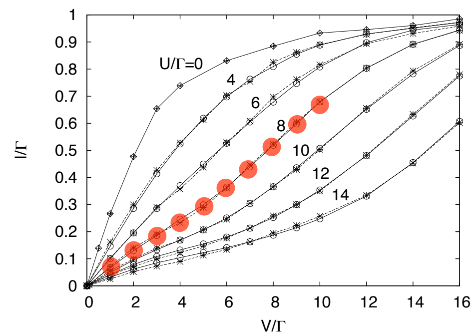
- Initially, electrons rush to the dot from both leads; after $t\Gamma \gtrsim 2$ a ``steady state'' is established with $I_L = -I_R$

Hybridization expansion

Muehlbacher & Rabani (2008)
Schmidt et al. (2008)
Schiro & Fabrizio (2008)
Werner et al. (2008)

- Current-Voltage characteristic of a strongly interacting dot ($U/\Gamma = 8$) measured at $t\Gamma = 1,\ 1.25$



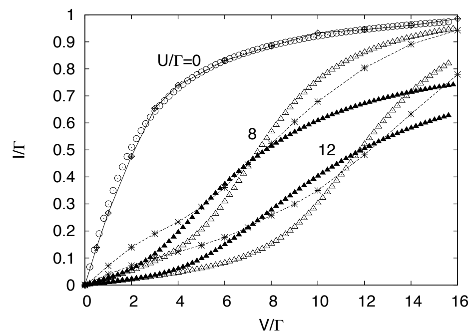


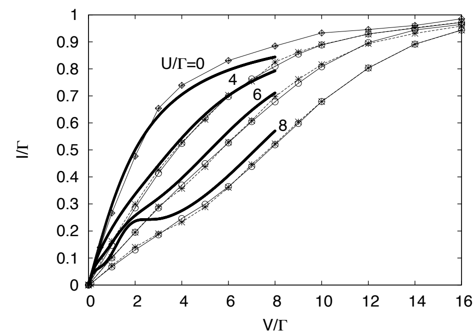
- Is $t\Gamma = 1,\ 1.25$ close enough to steady state ?
- Probably not for small voltage bias

Hybridization expansion

Muehlbacher & Rabani (2008)
Schmidt et al. (2008)
Schiro & Fabrizio (2008)
Werner et al. (2008)

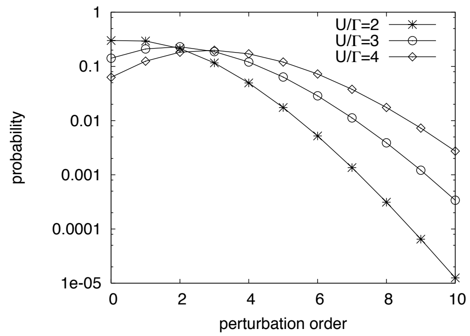
- Comparison to ``fixed gap calculation” and 4th order perturbation theory

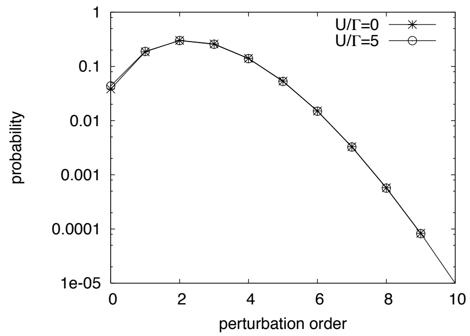




(Dis)advantages of the two approaches

- Perturbation order: weak-coupling (left), hyb-expansion (right)





- Weak-coupling: restricted to small *U*, but can reach steady state
- Hybridization expansion: cannot quite reach steady state for U>0, requires finite bandwidth, but can treat strong interactions
- Both: sign problem which grows exponentially with time

Summary and Conclusions

- Diagrammatic QMC impurity solvers
  - Enable efficient DMFT simulations of fermionic lattice models
  - Weak-coupling solver scales favorably with number of sites/ orbitals: ideal for large impurity clusters
  - Hybridization expansion allows to treat multi-orbital models with complicated interactions

- Keldysh implementation of diagrammatic QMC
  - Enables the study of transport and relaxation dynamics
  - Sign problem prevents the simulation of long time intervals
  - Impurity solver for non-equilibrium DMFT