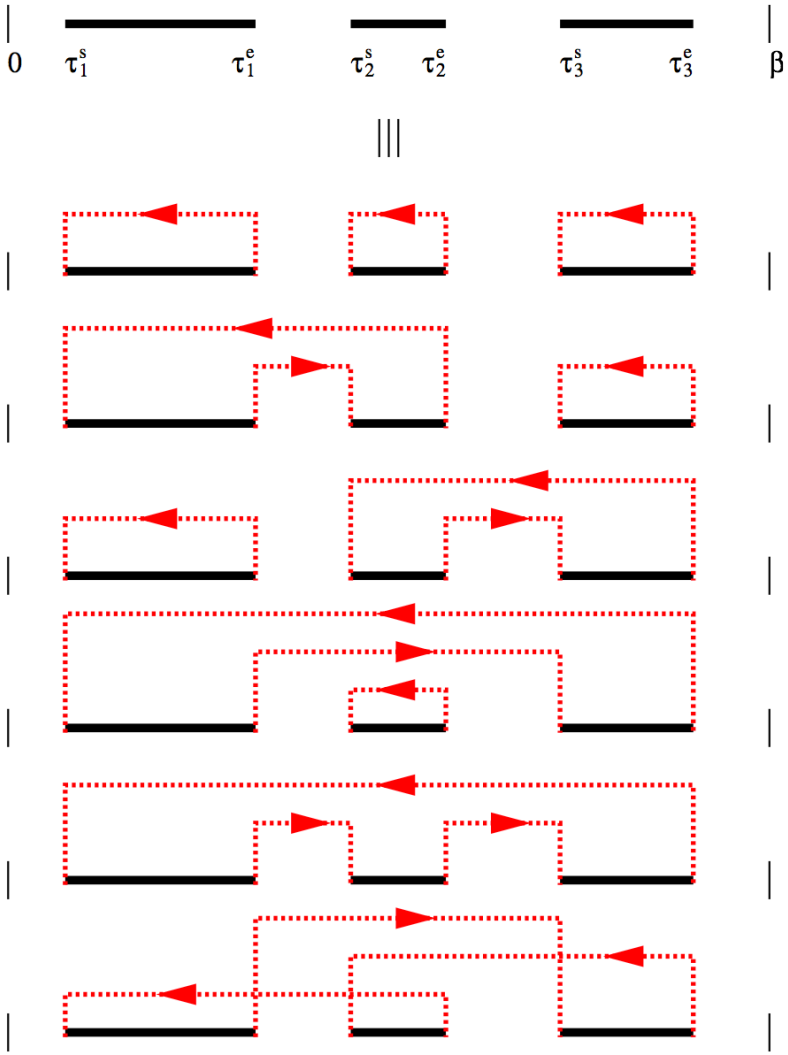
Continuous-time quantum Monte Carlo

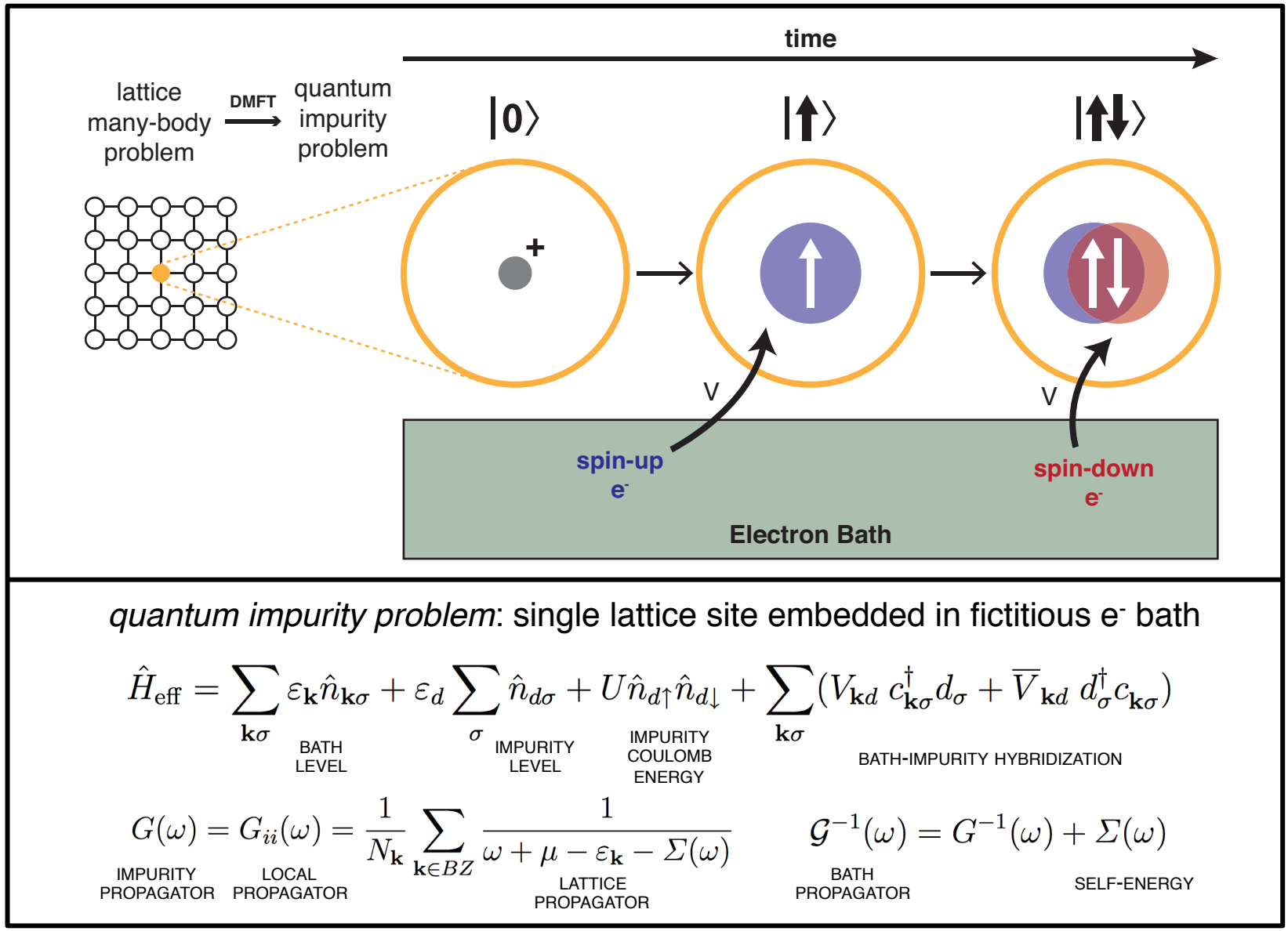


P. Werner et al., PRL **97**, 076405 (2006).

Eric Isaacs

Department of Applied Physics and Applied Math, Columbia University

Motivation: quantum impurity solver is needed for DMFT[1-3]



quantum impurity problem: single lattice site embedded in fictitious e⁻ bath

$$\hat{H}_{\text{eff}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma} + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\mathbf{k}\sigma} (V_{\mathbf{k}d}\, c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + \overline{V}_{\mathbf{k}d}\, d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma})$$

BATH LEVEL · IMPURITY LEVEL · IMPURITY COULOMB ENERGY · BATH-IMPURITY HYBRIDIZATION

$$G(\omega) = G_{ii}(\omega) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k} \in BZ} \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\omega)}$$

IMPURITY PROPAGATOR · LOCAL PROPAGATOR · LATTICE PROPAGATOR

$$\mathcal{G}^{-1}(\omega) = G^{-1}(\omega) + \Sigma(\omega)$$

BATH PROPAGATOR · SELF-ENERGY

[1] W. Metzner and D. Vollhardt, PRL **62**, 324 (1989). [2] A. Georges and G. Kotliar, PRB **45**, 6479 (1992). [3] G. Kotliar and D. Vollhardt, Phys. Today **57**, 53 (2004).

Quantum Monte Carlo

SOLVING A QUANTUM MECHANICAL PROBLEM

USING A RANDOMIZED ALGORITHM

types of QMC

(1) variational

$$\langle E(\{p\})\rangle = \frac{\int \Psi_T^*(R,\{p\})\hat{H}\Psi_T(R,\{p\})dR}{\int |\Psi_T(R,\{p\})|^2 dR}$$

parameterize ψ, use Monte Carlo to compute E, then minimize

(2) diffusion

$$-\frac{d\Psi(R,\tau)}{d\tau} = \hat{H}\Psi(R,\tau)$$

random walk for Schrödinger equation in imaginary time to find ψ

GROUND STATE

(3) determinantal (e.g. Hirsch-Fye)

$$Z = \int \mathcal{D}[\phi] \det G^{-1}(\{\phi\})$$

imaginary time discretization, Hubbard-Stratonovich transformation

(4) continuous-time

$$Z = \sum_k \int \mathcal{D}[\psi^\dagger\psi] e^{-S_0} \frac{(-1)^k}{k!} (\Delta S)^k$$

diagrammatic expansion of partition function

FINITE T

Types of CTQMC[1]

CT-INT[2] – *expand partition function in U*

$$Z/Z_0 = 1 + \frac{(-U)}{1!}\int_0^\beta d\tau_1 \langle n_\uparrow(\tau_1) n_\downarrow(\tau_1)\rangle_0 + \frac{(-U)^2}{2!}\iint_0^\beta d\tau_1 d\tau_2 \langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) n_\uparrow(\tau_2) n_\downarrow(\tau_2)\rangle_0 + \cdots$$

CT-AUX[3] – *like CT-INT but auxiliary field decomposition*

CT-HYB[4] – *expand partition function in Δ*

$$Z = \int D[\psi^\dagger \psi] e^{-S_c} \sum_k \frac{1}{k!}\left[\sum_{\alpha\alpha'}\int_0^\beta d\tau \int_0^\beta d\tau' \psi_{\alpha'}(\tau')\psi_\alpha^\dagger(\tau)\Delta_{\alpha\alpha'}(\tau,\tau')\right]^k$$

CT-J[5] – *for Kondo-like models; combines aspects of CT-INT and CT-HYB*

[1] E. Gull et al., Rev. Mod. Phys. **83**, 349 (2011). [2] A. N. Rubtsov et al., PRB **72**, 035122 (2005); A. N. Rubtsov and A. I. Lichtenstein, JETP Lett. **80**, 61 (2004). [3] E. Gull et al., Europhys. Lett. **82**, 57003 (2008). [4] P. Werner and A. J. Millis, PRB **74**, 155107 (2006); P. Werner et al., PRL **97**, 076405 (2006). [5] J. Otsuki et al., J. Phys. Soc. Jpn. **76**, 114707 (2007).

Terminology

Impurity	single lattice site on which we treat the correlations
Bath	auxiliary electron reservoir mimicking the effect of the discarded lattice sites
Hybridization	coupling b/w impurity and bath
Impurity Green function $G(\omega)$	Green function of the impurity problem
Lattice Green function $G(k,\omega)$	Green function of the lattice at a particular *k*-point
Local Green function $G_{ii}(\omega)$	Lattice Green function summed over *k*-points
Self-energy $\Sigma(\omega)$	interaction-induced shift (real part) and broadening (imaginary part) of 1-particle energy levels

Hybridization-expansion CTQMC[1]

$$Z = \int D[\psi^\dagger \psi] \exp\left[-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\alpha\alpha'} \psi^\dagger_\alpha(\tau) \Delta_{\alpha\alpha'}(\tau,\tau') \psi_{\alpha'}(\tau') \right]$$

partition function

$$Z = \mathrm{Tr}[e^{-\beta H}]$$

write as path integral

$$\int D[\psi^\dagger \psi] e^{-S}$$

Grassmann (anticommuting) variables

$$\psi, \psi^\dagger$$

local action (impurity energy and interaction)

hybridization action

bath action integrated out since noninteracting

β: inverse temperature

τ,τ′: imaginary time

Δ: hybridization function

α,α′: orbital+spin index

[1] K. Haule, Phys. Rev. B **75**, 155113 (2007).

Hybridization-expansion CTQMC

Taylor expansion of the exponential function for the hybridization part

$$Z = \int D[\psi^\dagger \psi] e^{-S_c} \sum_k \frac{1}{k!} \left[\sum_{\alpha\alpha'} \int_0^\beta d\tau \int_0^\beta d\tau' \, \psi_{\alpha'}(\tau') \psi^\dagger_\alpha(\tau) \Delta_{\alpha\alpha'}(\tau, \tau') \right]^k$$

rearrange terms to separate cluster and bath contributions

$$Z = \int D[\psi^\dagger \psi] e^{-S_c} \sum_k \frac{1}{k!} \int_0^\beta \prod_{i=1}^k d\tau_i \int_0^\beta \prod_{i=1}^k d\tau_i' \sum_{\alpha\alpha'} \prod_{i=1}^k [\psi_{\alpha_i'}(\tau_i') \psi^\dagger_{\alpha_i}(\tau_i)] \prod_{i=1}^k \Delta_{\alpha_i \alpha_i'}(\tau_i, \tau_i')$$

average over impurity d.o.f.

average over bath d.o.f.

trick is to combine all terms of the same order (both crossing and noncrossing) into a determinant to minimize sign problem

k: perturbation order

Hybridization-expansion CTQMC

essentially we are perturbing from the atomic limit

$$Z = Z_c \sum_k \frac{1}{k!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \cdots \int_0^\beta d\tau_k \int_0^\beta d\tau_k' \sum_{\alpha_1 \alpha_1', \ldots, \alpha_k, \alpha_k'} \langle T_\tau \psi_{\alpha_1'}(\tau_1') \psi^\dagger_{\alpha_1}(\tau_1) \cdots \psi_{\alpha_k'}(\tau_k') \psi^\dagger_{\alpha_k}(\tau_k) \rangle_{cluster}$$

$$\times \frac{1}{k!} \det \begin{pmatrix} \Delta_{\alpha_1 \alpha_1'}(\tau_1, \tau_1') & \Delta_{\alpha_1 \alpha_2'}(\tau_1, \tau_2') & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \Delta_{\alpha_k \alpha_1'}(\tau_k, \tau_1') & \cdots & \cdots & \Delta_{\alpha_k \alpha_k'}(\tau_k, \tau_k') \end{pmatrix}$$

bath part represents contributions from all Feynman diagrams of order *k*

$$Z_c = \int D[\psi^\dagger \psi] e^{-S_c}$$

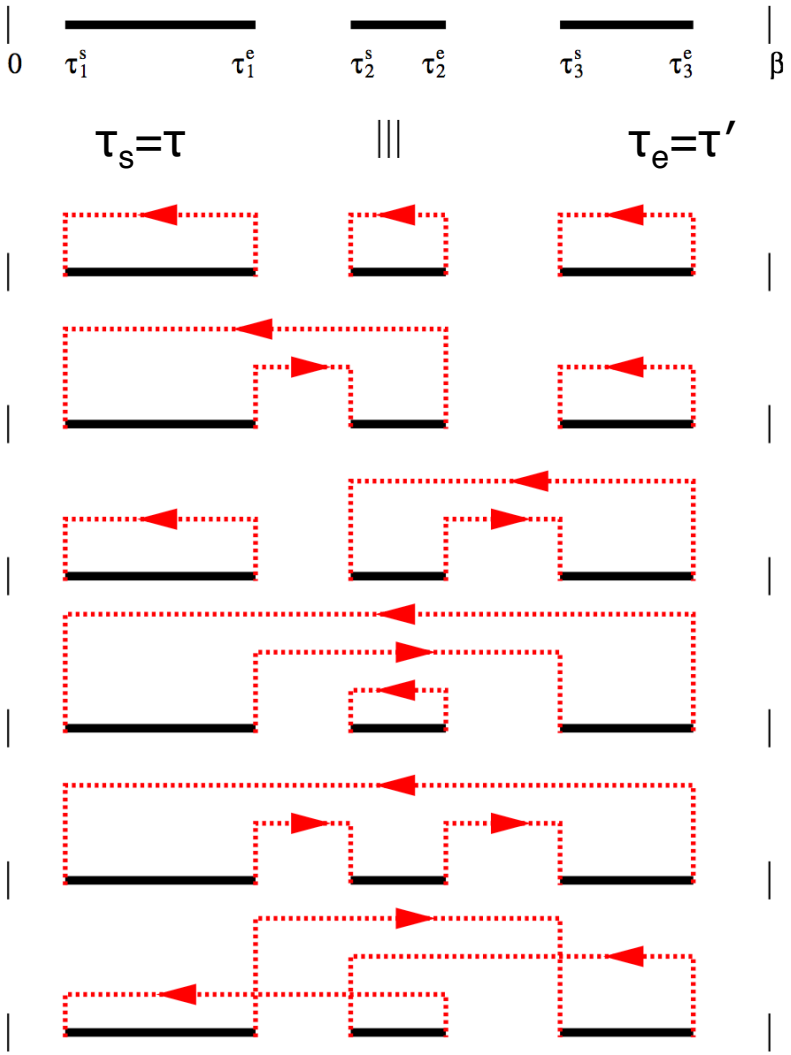
$$\langle O \rangle_{cluster} = \frac{1}{Z_c} \int D[\psi^\dagger \psi] e^{-S_c} O$$

average over cluster d.o.f.

This is the central equation of CT-HYB

Hybridization-expansion CTQMC

The basic idea is that we use a Monte Carlo (Metropolis) algorithm to "visit" the diagrams associated with a set of imaginary times



P. Werner et al., PRL **97**, 076405 (2006).

example

k=3 segments of τ corresponding to occupied fermion states

dotted lines connecting segments represent the hybridization function

3!=6 diagrams are combined into a determinant to minimize sign

application of ψ or $\psi^\dagger$ is referred to as a "kink" in the time evolution

CT-HYB Monte Carlo moves

insertion of two kinks τ_{new} and τ_{new}' at random times (one creation, one destruction) of same spin

determinants

$$P_{add} = min\left[\left(\frac{\beta N_b}{k+1}\right)^2 \frac{\mathcal{Z}_{new}}{\mathcal{Z}_{old}} \frac{\mathcal{D}_{new}}{\mathcal{D}_{old}}, 1\right]$$

$$\mathcal{Z}_{new} = \langle T_\tau \psi_{\alpha'_{new}}(\tau'_{new}) \psi^\dagger_{\alpha_{new}}(\tau_{new}) \psi_{\alpha'_1}(\tau'_1) \psi^\dagger_{\alpha_1}(\tau_1) \psi_{\alpha'_k}(\tau'_k) \psi^\dagger_{\alpha_k}(\tau_k) \rangle_{cluster}$$

removal of two kinks τ_{new} and τ_{new}' at random times (one creation, one destruction) of same spin

$$P_{remove} = min\left[\left(\frac{k}{\beta N_b}\right)^2 \frac{\mathcal{Z}_{new}}{\mathcal{Z}_{old}} \frac{\mathcal{D}_{new}}{\mathcal{D}_{old}}, 1\right]$$

shift of one operator in time and insertion/removal of multiple kinks are not necessary but are used to reduce sampling time

CT-HYB Monte Carlo moves

sketch of how P_{add} is derived

trial-step probability: $\omega_{X\to X'}$ acceptance probability: $A_{X\to X'}$

detailed balance: $$\frac{A_{X\to X'}}{A_{X'\to X}} = \frac{\rho(X')}{\rho(X)}\frac{\omega_{X'\to X}}{\omega_{X\to X'}}$$

$$\frac{\omega_{X\to X'}}{\omega_{X'\to X}} = \frac{(k+1)^2}{\beta^2}$$

from which creation kink to add from k+1 options and which removal kink to remove from k+1 options

from prob. of choosing particular τ and τ′ in [0,β] x [0,β] space

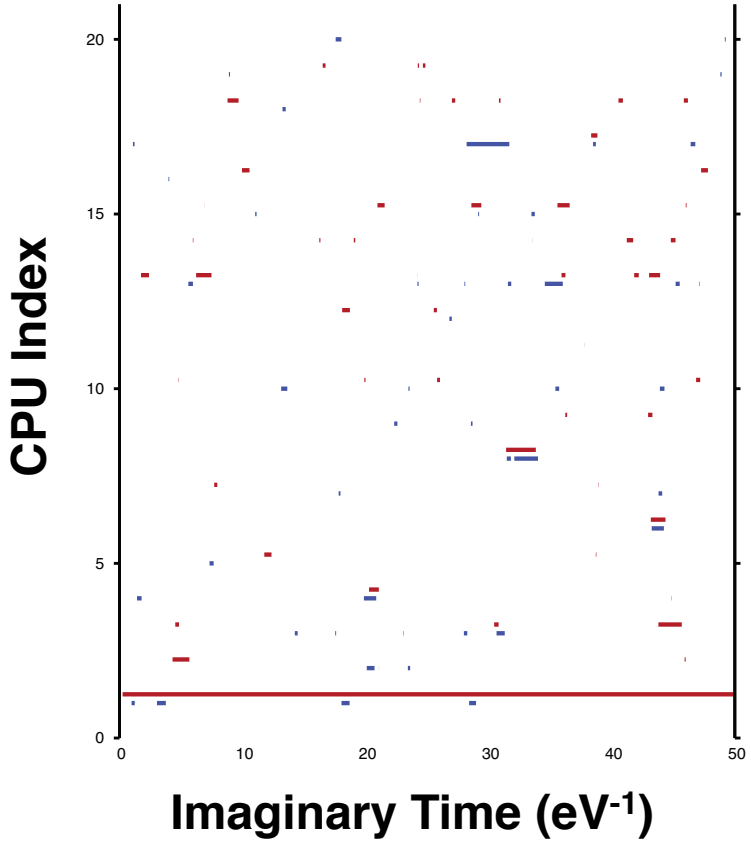
$\beta^2 \to (N_b\beta)^2$ when non-unity bath dimensionality

$$\frac{\rho(X')}{\rho(X)} = \frac{\mathcal{Z}_{new}}{\mathcal{Z}_{old}}\frac{\mathcal{D}_{new}}{\mathcal{D}_{old}}$$

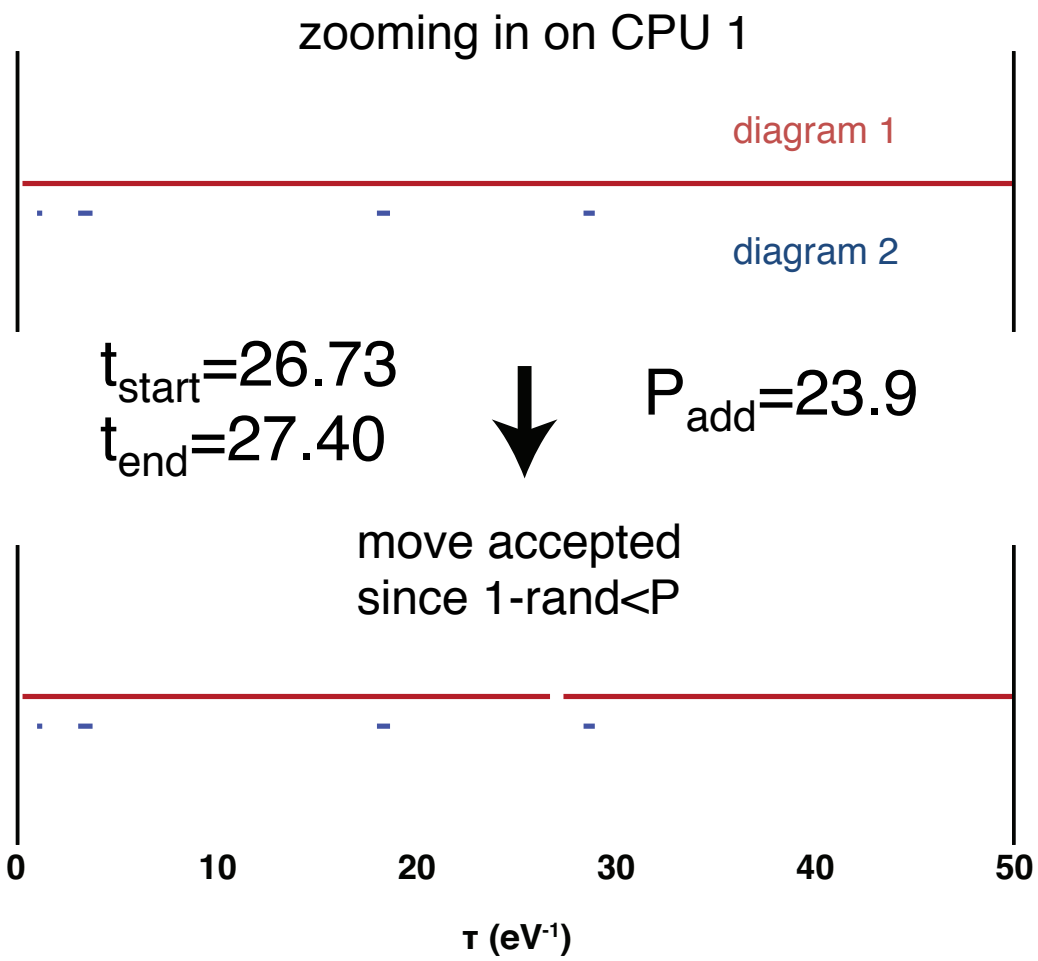
$$P_{add} = min\left[\left(\frac{\beta N_b}{k+1}\right)^2 \frac{\mathcal{Z}_{new}}{\mathcal{Z}_{old}}\frac{\mathcal{D}_{new}}{\mathcal{D}_{old}}, 1\right]$$

CT-HYB Monte Carlo moves

Example of 1 move from an actual run



state for 20 cores



Codes

- Kristjan Haule's **CTQMC** (part of dmft_w2k code on his website) has CT-HYB

- **ALPS** (Algorithms and Libraries for Physics Simulations)

- **TRIQS** (a Toolbox for Research on Interacting Quantum Systems)

Tricks to speed things up in Haule's code

$$\mathcal{Z}_D = \mathrm{Tr}\left(T_\tau \exp\left[-\int_0^\beta d\tau H_c(\tau) \right] \psi_{\alpha_1}(\tau_1') \right.$$

$$\left. \times \psi^\dagger_{\alpha_2}(\tau_2) \cdots \psi_{\alpha_{n-1}}(\tau'_{n-1}) \psi^\dagger_{\alpha_n}(\tau_n) \right)$$

$$= \sum_{\{m\}} e^{-E_{m_1}\tau_1'} (F^{\alpha_1})_{m_1 m_2} e^{-E_{m_2}(\tau_2 - \tau_1')}$$

$$\times (F^{\dagger\alpha_2})_{m_2 m_3} \cdots (F^{\alpha_{n-1}})_{m_{n-1} m_n} e^{-E_{m_n}(\tau'_{n-1} - \tau_n)}$$

$$\times (F^{\dagger\alpha_n})_{m_n m_1} e^{-E_{m_1}(\beta - \tau_n)}$$

typical form of cluster component of the partition function

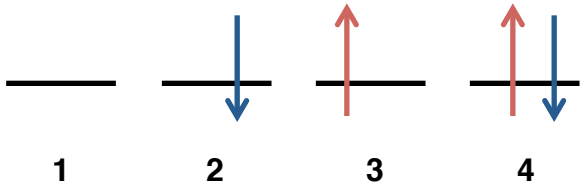
$$(F^{\alpha\dagger})_{m'm} \equiv \langle j | \langle m' | \psi^\dagger_\alpha | m \rangle | i \rangle$$

- *F* matrices can be very large (e.g. 2^{14} states for *f* shell
- Large **matrix mult** is the bottleneck, particularly when we go beyond density-density interactions (non-Ising like *J*)
- Atomic states with same N, S_z, and K are grouped together (**superstates**) so can avoid many zero matrix elements
- Insertion of a kink is fairly local in time so the code **stores chains of products** in the eqn to the left from both sides
- Sampled average of probability of atomic states is used to **eliminate low-probability states** dynamically

Simple Example

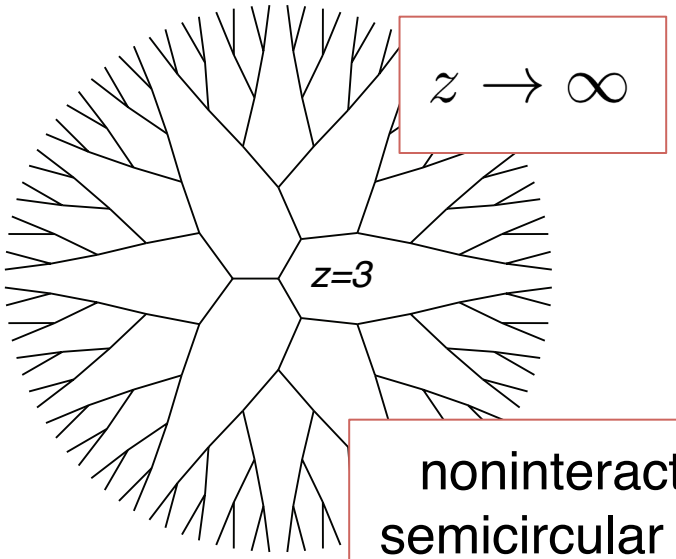
1-band Hubbard model

$$H = \sum_{\sigma} \sum_{i,j} t_{i,j} c^{\dagger}_{i\sigma} c_{n\sigma} + \sum_{i} U n_{i,\uparrow} n_{i,\downarrow}$$



four possible states

Bethe lattice (Cayley tree)



noninteracting
semicircular DOS

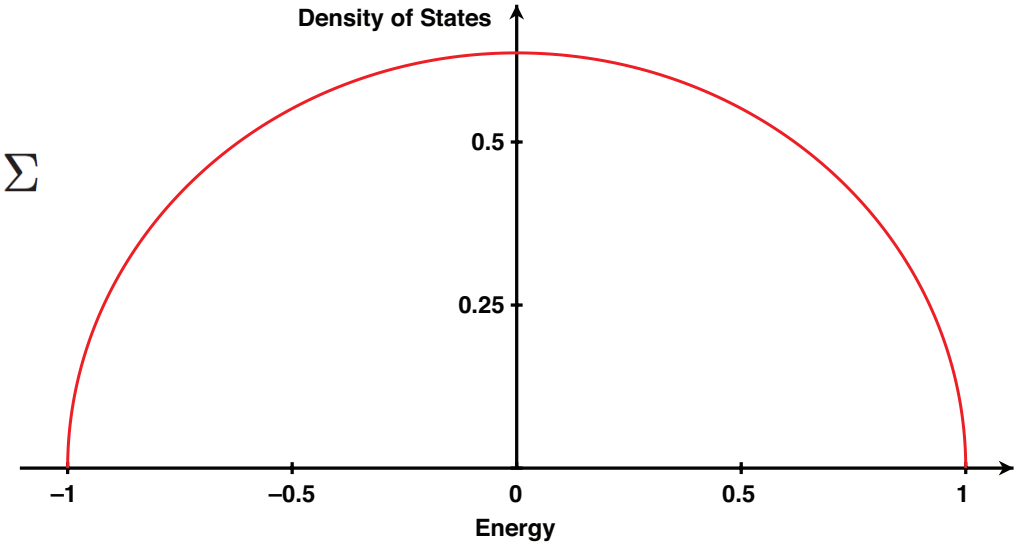
G(ω) $G_{ii}(\omega)$

$$\frac{1}{\omega - E_{imp} - \Sigma - \Delta} = \int d\epsilon \frac{D(\epsilon)}{\omega + \mu - \epsilon - \Sigma}$$

$$G = 2(z - \sqrt{z^2 - 1}) \quad z = \omega + \mu - \Sigma$$

DMFT self-consistency condition $\Delta = \frac{1}{4} G$

μ=U/2 for half filling, E_{imp}=-μ, t=1/2



Simple Example

```
# Cix file for cluster DMFT with CTQMC
# cluster_size, number of states, number of baths, maximum matrix size
1 4 2 1
# baths, dimension, symmetry, global flip
0       1 0 0
1       1 0 0
# cluster energies for unique baths, eps[k]
0 0
#   N   K   Sz size F^{+,dn}, F^{+,up}, Ea  S
1   0   0    0   1   2       3       0   0
2   1   0 -0.5   1   0       4       0   0.5
3   1   0  0.5   1   4       0       0   0.5
4   2   0    0   1   0       0       0   0
```

impurity energy absorbed into chemical potential

atomic states

applying spin-up bath to state 1 yields state 2

Simple Example

```
                # matrix elements
F†,down         1  2  1  1    1    # start-state,end-state, dim1, dim2, <2|F^{+,dn}|1>
F†,up           1  3  1  1    1    # start-state,end-state, dim1, dim2, <3|F^{+,up}|1>
F†,down         2  0  0  0
F†,up           2  4  1  1   -1    # start-state,end-state, dim1, dim2, <4|F^{+,up}|2>
F†,down         3  4  1  1    1
F†,up           3  0  0  0
F†,down         4  0  0  0
F†,up           4  0  0  0
```

start state

end state

matrix element(s)

$$(F^{\alpha\dagger})_{m'm} \equiv \langle j|\langle m'|\psi_\alpha^\dagger|m\rangle|i\rangle$$

(only 1 for i and j here since atomic superstates are 1D)

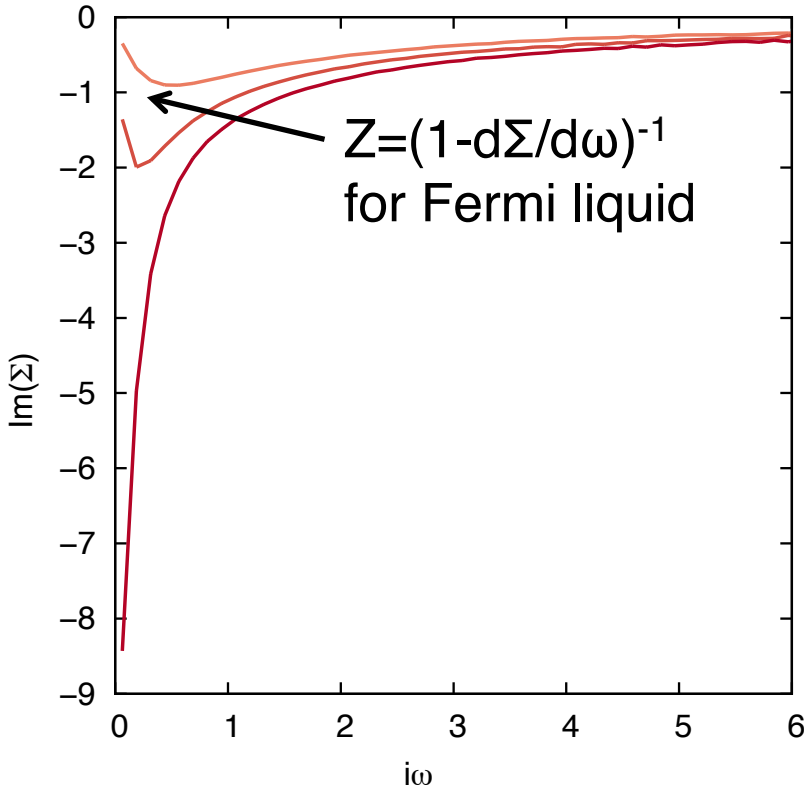
Simple Example

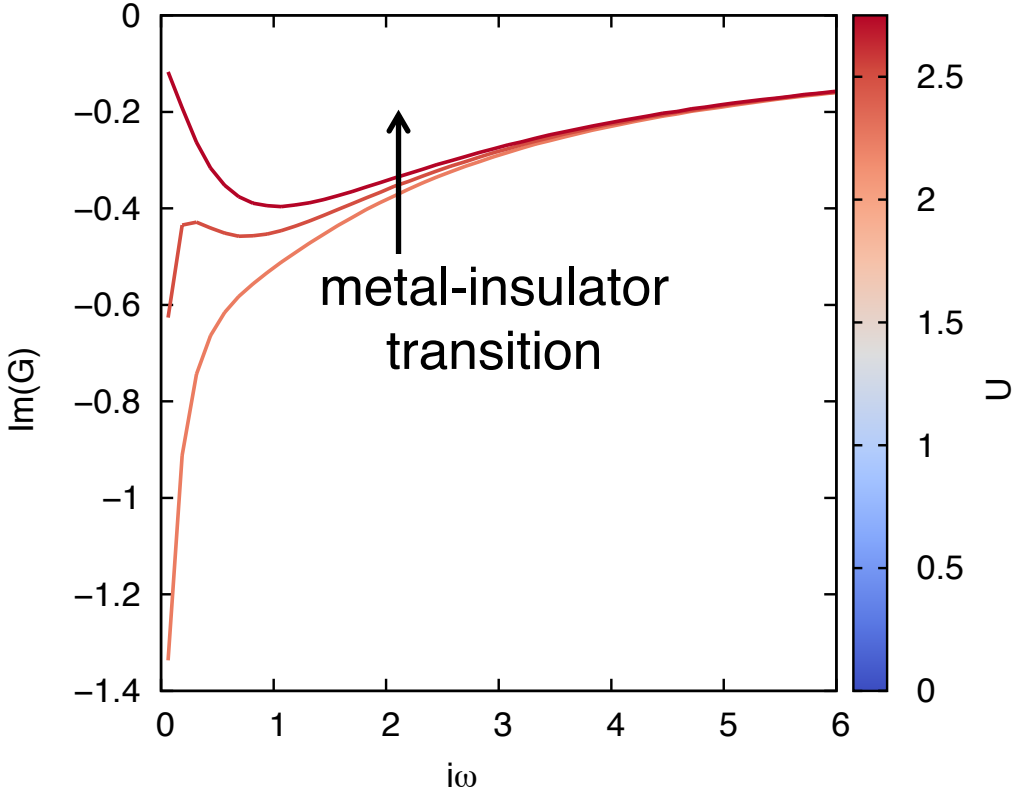
Ran 3 *U* values for 7 temperatures each with 8 DMFT iterations

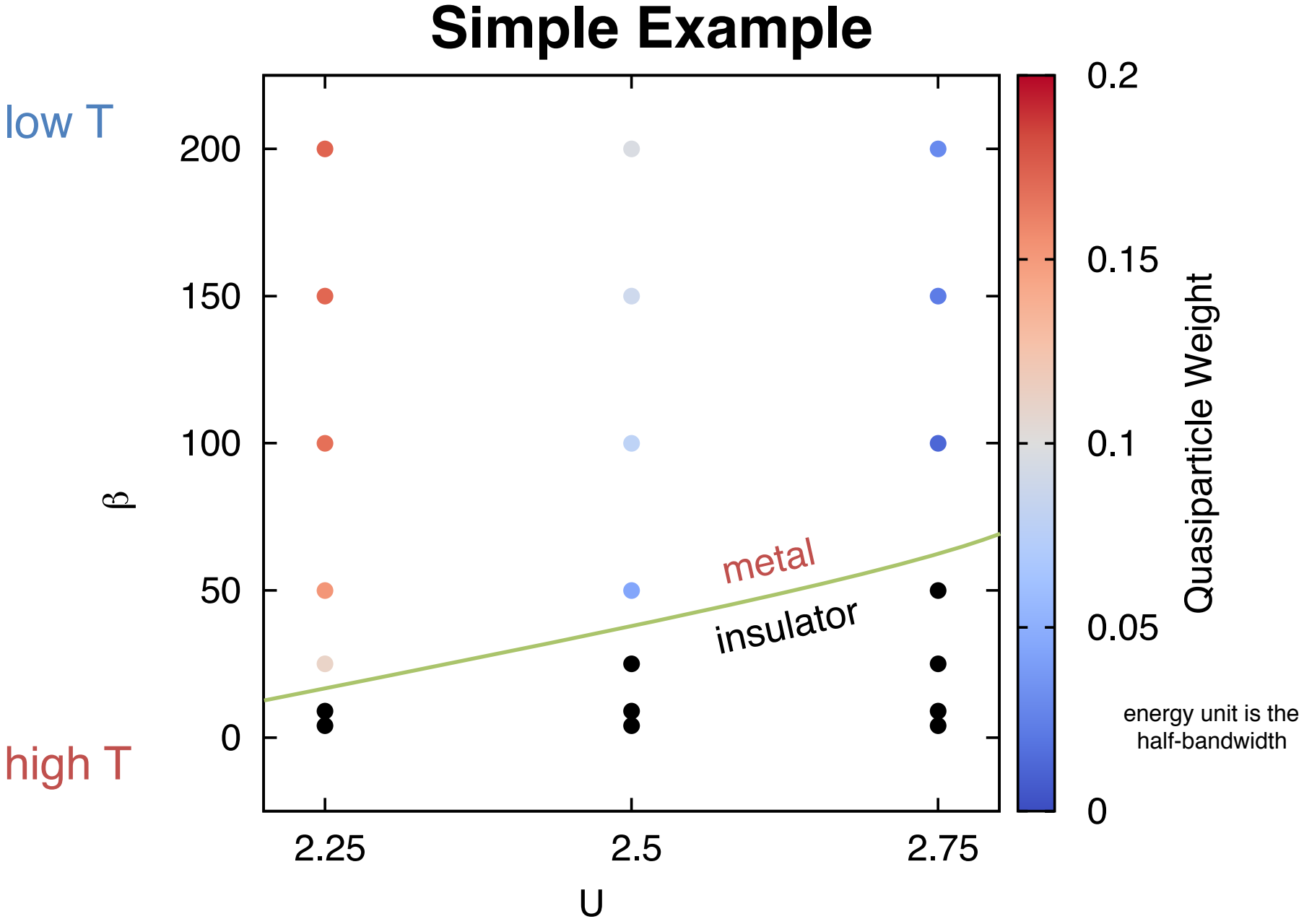
For each iteration CTQMC employs 100 million Monte Carlo steps/core on the 20 cores of our dual-socket machines

Example of results for β=50:

energy unit is the half-bandwidth



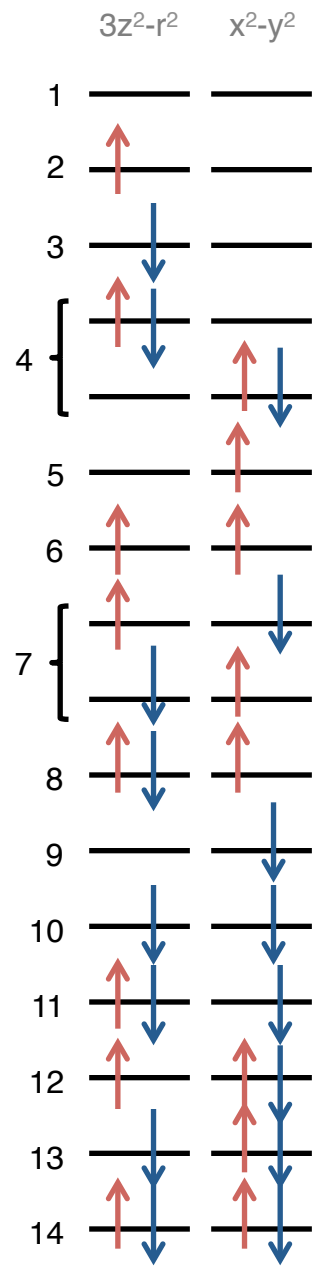




metal-insulator transition for increasing T and increasing U

2-orbital CIX file example: $LaNiO_3$ E_g

```
# CIX file for ctqmc!
# cluster_size, number of states, number of baths, maximum_matrix_size
1 14 4 2
# baths, dimension, symmetry
0    1 0 0
1    1 0 0
2    1 1 1
3    1 1 1
# cluster energies for non-equivalent baths, eps[k]
0.0 -0.03108101
#   N   K   Sz size
  1   0  0  0.0  1    2   3   5   9    0.0       0.0
  2   1  0  0.5  1    0   4   6   7    0.0       0.0
  3   1  0 -0.5  1    4   0   7  10    0.0       0.0
  4   2  0  0.0  2   12  13   8  11    -1.031563908   0.969401887996      0.0   0.5
  5   1  0  0.5  1    6   7   0   4    -0.03108101      0.0
  6   2  0  1.0  1    0   8   0  12    -3.03108101      0.0
  7   2  0  0.0  2    8  11  12  13    -3.03108101   -1.03108101      0.0   0.5
  8   3  0  0.5  1    0   0   0  14    -5.03108101      0.0
  9   1  0 -0.5  1    7  10   4   0    -0.03108101      0.0
 10   2  0 -1.0  1   11   0  13   0    -3.03108101      0.0
 11   3  0 -0.5  1    0   0  14   0    -5.03108101      0.0
 12   3  0  0.5  1    0  14   0   0    -5.06216202      0.0
 13   3  0 -0.5  1   14   0   0   0    -5.06216202      0.0
 14   4  0  0.0  1    0   0   0   0    -10.06216202     0.0
# matrix elements
  1   2   1  1  1.0
  1   3   1  1  1.0
[…]
```



Future Work

1) Better understand how the CIX file is constructed for more complicated cases

2) Try ALPS implementation of CT-HYB

3) Use this solver to study Li_xCoO_2 and Li_xFePO_4

Acknowledgements

Thanks to Jia, Hyowon, and Chris for useful discussions