Universität Hamburg
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SFB
SFB 925: Light induced dynamics and control of strongly correlated quantum systems

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SFB 925 Workshop on Numerical Methods

Quantum Monte Carlo Methods
Focus: impurity solvers

Patryk Kubiczek

patryk.kubiczek@physik.uni-hamburg.de

I. Institute for Theoretical Physics
University of Hamburg

Monte Carlo

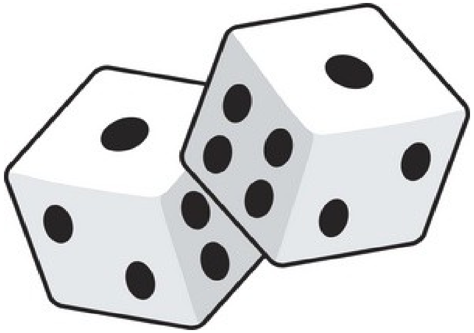
"Monte Carlo is an extremely bad method;
it should be used only when all
alternative methods are worse."

$$\text{error} \sim \frac{1}{\sqrt{N}}$$

Alan D. Sokal, *Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms* (1997)

"(…) these investigations share some of the features of ordinary **experimental work**, in that they are susceptible to both statistical and systematic errors. With regard to these matters, we believe that papers should meet much the same standards as are normally required for experimental investigations. "

W. W. Wood, J. J. Erpenbeck,
Ann. Rev. Phys. Chem. 27, 319 (1976)



Quantum Monte Carlo

- Iterative stochastic procedure to solve interacting quantum many-body problems
- **Idea:** replace summations over discrete quantum numbers and multi-dimensional integrals by Monte Carlo sampling
- However, the weights may not always be positive
  - Fermionic QMC hindered by the fermionic sign problem
  - Any real-time QMC hindered by the dynamical sign problem
- Exact up to statistical (and possible systematic) errors

Quantum Monte Carlo methods for fermions

- Zero temperature:
  - Variational Monte Carlo (VMC)
  - Diffusion Monte Carlo (DMC)
  - Full Configuration Interaction QMC (FCIQMC)

- Finite temperature
  - Determinant QMC (DQMC)
  - Hirsch-Fye QMC (HFQMC)
  - Continuous-time QMC (CT-QMC):
    - hybridization-expansion (CT-HYB-QMC)
    - interaction-expansion (CT-INT-QMC)
    - auxiliary-field interaction-expansion (CT-AUX-QMC)
  - Diagrammatic Monte Carlo (DiagMC)

Systematic errors due to time discretization (DQMC, HFQMC)

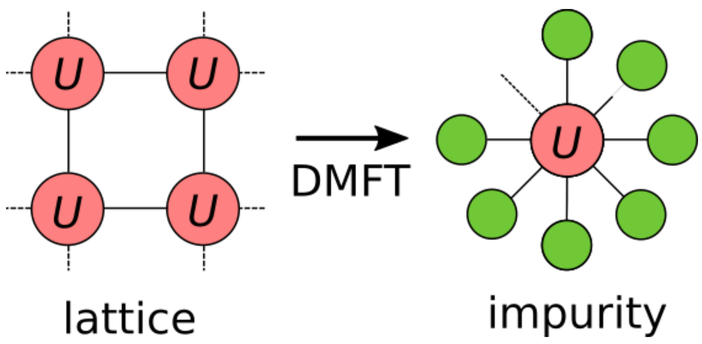
finite systems (VMC, DMC, FCIQMC, DQMC, HFQMC)

impurity models (HFQMC, CT-QMC)

thermodynamic limit (DiagMC)

Impurity models

- Consider a central interacting system coupled to one or several baths
- This setting describes many physically relevant situations such as
  - quantum dots coupled to leads
  - low-density magnetic impurities in metals
- Impurity problem can also serve as an auxiliary problem within **dynamical mean field theory (DMFT)** which provides an approximate solution to interacting lattice problems



Single impurity Anderson model (SIAM)

- Describes coupling of a single interacting electronic level *(d)* to a bath of noninteracting electrons *(c)*
- Maps to Hubbard model within DMFT approximation

$$H(t) = H_{\mathrm{loc}}(t) + \sum_{\sigma} \left[H_{\mathrm{bath},\sigma}(t) + H_{\mathrm{hyb},\sigma}(t) \right]$$

$$H_{\mathrm{loc}}(t) = \sum_{\sigma} \epsilon_{\sigma}(t)\, d^{\dagger}_{\sigma} d_{\sigma} + U(t)\, d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$

$$H_{\mathrm{bath},\sigma}(t) = \sum_{l} \varepsilon_{l\sigma}(t) c^{\dagger}_{l\sigma} c_{l\sigma}$$

$$H_{\mathrm{hyb},\sigma}(t) = \sum_{l} \left(V_{l\sigma}(t) c^{\dagger}_{l\sigma} d_{\sigma} + H.c. \right) \equiv H_{\mathrm{cd},\sigma}(t) + H^{\dagger}_{\mathrm{cd},\sigma}(t)$$

$$H_{\mathrm{cd},\sigma} = \sum_{l} V_{l\sigma}(t) c^{\dagger}_{l\sigma} d_{\sigma} \equiv C^{\dagger}_{\sigma}(t) d_{\sigma}$$

Quantum Monte Carlo solution of AIM: CT-HYB-QMC

- CT-HYB-QMC: continuous-time hybridization-expansion quantum Monte Carlo

review: E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, P. Werner, Rev. Mod. Phys. **83**, 349 (2011)

real-time: L. Mühlbacher, E. Rabani, Phys. Rev. Lett. **100**, 176403 (2008)
P. Werner, T. Oka, A. J. Millis, Phys. Rev. B **79**, 035320 (2009)
M. Schirò, Phys. Rev. B **81**, 085126 (2010)

- diagrammatic perturbation theory: expansion in the hybridization term

$$H(t) = H_{\mathrm{loc}}(t) + \sum_\sigma H_{\mathrm{bath},\sigma}(t) + \boxed{\sum_\sigma H_{\mathrm{hyb},\sigma}(t)}$$

- Sum up the important diagrams stochastically: Monte Carlo
- Numerical values of diagrams are not always real and positive: hence we use absolute values and sample the (complex) sign together with observables

$$\langle \mathcal{O}(t) \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left(e^{-\beta H(0)} \mathcal{T}_- e^{-i\int_t^0 ds H(s)} \mathcal{O}(t) \mathcal{T}_+ e^{-i\int_0^t ds H(s)} \right) = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left(\mathcal{T}_\mathcal{C}\, e^{-i\int_\mathcal{C} ds H(s)} \mathcal{O}(t) \right)$$

$$= \underbrace{\frac{\sum_c \langle \mathcal{O}(t) \rangle_c \,\mathrm{sgn}(w(c))\, |w(c)|}{\sum_c |w(c)|}}_{\text{MC average of } \langle \mathcal{O}(t) \rangle_c \,\mathrm{sgn}(w(c))} \cdot \underbrace{\frac{\sum_c |w(c)|}{\sum_c \mathrm{sgn}(w(c))\, |w(c)|}}_{\text{inverse average sign}}$$

CT-HYB-QMC: derivation

- Expand the dynamical partition function in spin-down hybridization

$$\mathcal{Z} = \mathrm{Tr}\left[\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt H(t)}\right]$$

$$= \mathrm{Tr}\left[\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt [H_{\mathrm{loc}}(t)+\sum_\sigma H_{\mathrm{bath},\sigma}(t)]}\, e^{-i\int_{\mathcal{C}} dt \sum_\sigma H^\dagger_{\mathrm{cd},\sigma}(t)}\, e^{-i\int_{\mathcal{C}} dt \sum_\sigma H_{\mathrm{cd},\sigma}(t)}\right]$$

$$= \prod_\sigma \left[\sum_{k_\sigma=0}^{\infty} (-1)^{k_\sigma} \int_{0_+}^{-i\beta} dt_1^{\mathrm{c}} \ldots \int_{t^{\mathrm{c}}_{k-1}}^{-i\beta} dt_k^{\mathrm{c}} \int_{0_+}^{-i\beta} dt_1^{\mathrm{a}} \ldots \int_{t^{\mathrm{a}}_{k-1}}^{-i\beta} dt_k^{\mathrm{a}}\right]$$

$$\mathrm{Tr}\left\{\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt [H_{\mathrm{loc}}(t)+\sum_\sigma H_{\mathrm{bath},\sigma}(t)]} \prod_\sigma \left[H^\dagger_{\mathrm{cd},\sigma}(t^{\mathrm{c}}_{k_\sigma}) \ldots H^\dagger_{\mathrm{cd},\sigma}(t^{\mathrm{c}}_1) H_{\mathrm{cd},\sigma}(t^{\mathrm{a}}_{k_\sigma}) \ldots H_{\mathrm{cd},\sigma}(t^{\mathrm{a}}_1)\right]\right\}$$

- Split the trace in two parts: local (d) + bath (c)

$$C^\dagger_\sigma(t) = \sum_l V_{l\sigma}(t) c^\dagger_{l\sigma}$$

$$\mathrm{Tr}\{\ldots\}$$

$$= \mathrm{Tr}_{\mathrm{d}}\left\{\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt H_{\mathrm{loc}(t)}} \prod_\sigma \left[d^\dagger_\sigma(t^{\mathrm{c}}_{k_\sigma}) d_\sigma(t^{\mathrm{a}}_{k_\sigma}) \ldots d^\dagger_\sigma(t^{\mathrm{c}}_1) d_\sigma(t^{\mathrm{a}}_1)\right]\right\}$$

W_{loc}

$$\prod_\sigma \mathrm{Tr}_{\mathrm{c}\sigma}\left[\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt H_{\mathrm{bath},\sigma}(t)} C_\sigma(t^{\mathrm{c}}_{k_\sigma}) C^\dagger_\sigma(t^{\mathrm{a}}_{k_\sigma}) \ldots C_\sigma(t^{\mathrm{c}}_1) C^\dagger_\sigma(t^{\mathrm{a}}_1)\right]$$

W_{bath}

CT-HYB-QMC: bath weight

- Bath weight is evaluated by means of Wick's theorem as a product of determinants of k_σ x k_σ matrices

$$w_{\rm bath} = w_{{\rm bath},\uparrow} w_{{\rm bath},\downarrow}$$

$$w_{{\rm bath},\sigma} = \left[\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt H_{{\rm bath},\sigma}(t)} C_\sigma(t_{k_\sigma}^{\sigma{\rm c}}) C_\sigma^\dagger(t_{k_\sigma}^{\sigma{\rm a}}) \ldots C_\sigma(t_1^{\sigma{\rm c}}) C_\sigma^\dagger(t_1^{\sigma{\rm a}})\right] = i^{k_\sigma} {\rm Det}\hat{\Delta}_\sigma$$

$$\hat{\Delta}_{\sigma ij} = -i\langle \mathcal{T}_{\mathcal{C}}\, C_\sigma(t_i^{\sigma{\rm c}}) C_\sigma^\dagger(t_j^{\sigma{\rm a}})\rangle_{{\rm c}_\sigma} = \Delta_\sigma(t_i^{\sigma{\rm c}}, t_j^{\sigma{\rm a}})$$

- The entries of the matrix are given by the hybridization function which is fully determined by the bath and the hybridization Hamiltonian

$$\Delta_\sigma(t,t') = -i\sum_l V_{l\sigma}^*(t)\langle \mathcal{T}_{\mathcal{C}}\, c_{l\sigma}(t) c_{l\sigma}^\dagger(t')\rangle_{{\rm c}_\downarrow} V_{l\sigma}(t') = \sum_l V_{l\sigma}^*(t) g_{l\sigma}(t,t') V_{l\sigma}(t'),$$

- During a QMC run fast updates for the determinant of Δ matrix are used such that the complexity is $O(k^2)$ and not $O(k^3)$

CT-HYB-QMC: local weight

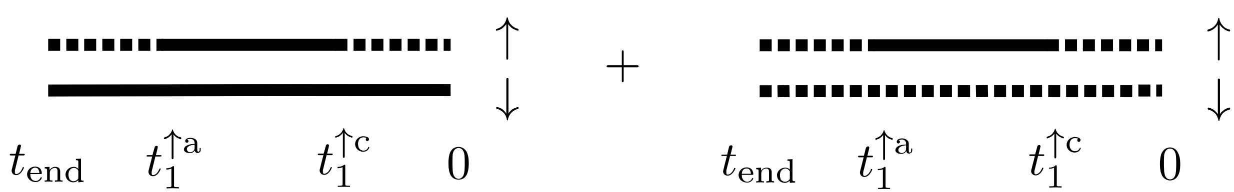
- Evaluation of a local weight is a many-body problem. However, it involves a small number of states, such that we can solve it exactly.

$$w_{\mathrm{loc}} = \mathrm{Tr}_{\mathrm{d}} \left\{ \mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} dt H_{\mathrm{loc}(t)}} \prod_{\sigma} \left[d_\sigma^\dagger(t_{k_\sigma}^{\sigma \mathrm{c}}) d_\sigma(t_{k_\sigma}^{\sigma \mathrm{a}}) \dots d_\sigma^\dagger(t_1^{\sigma \mathrm{c}}) d_\sigma(t_1^{\sigma \mathrm{a}}) \right] \right\}$$

- Segment picture, example:

$$k_\uparrow = 1, k_\downarrow = 0$$

$w_{\mathrm{loc}} =$



$$= (-1) \cdot e^{-i\epsilon_\uparrow (t_1^{\uparrow\mathrm{a}} - t_1^{\uparrow\mathrm{c}})} \left[e^{-i\epsilon_\downarrow t_{\mathrm{end}}} e^{-iU(t_1^{\uparrow\mathrm{a}} - t_1^{\uparrow\mathrm{c}})} + 1 \right]$$

permutation sign
from time-ordering

CT-HYB-QMC: partition function configurations

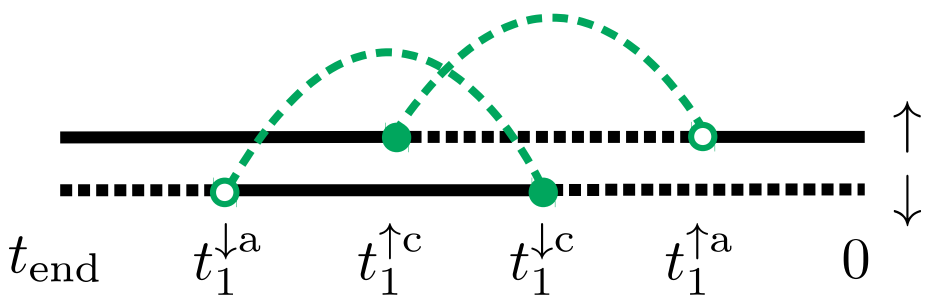
- During a QMC run we sample partition function diagrams

$$\mathcal{Z} = \prod_\sigma \left[\sum_{k_\sigma=0}^{\infty} (-1)^{k_\sigma} \int_{0_+}^{-i\beta} dt_1^{\sigma c} \ldots \int_{t_{k-1}^{\sigma c}}^{-i\beta} dt_k^{\sigma c} \int_{0_+}^{-i\beta} dt_1^{\sigma a} \ldots \int_{t_{k-1}^{\sigma a}}^{-i\beta} dt_k^{\sigma a} \right]$$

$$w_{\mathrm{loc}}(\{t_m^{\sigma c}\}, \{t_n^{\sigma a}\})\, w_{\mathrm{bath}}(\{t_m^{\sigma c}\}, \{t_n^{\sigma a}\})$$

$$= \sum_c w(c) = \sum_c \mathrm{sgn}(w(c))|w(c)|$$

- Example of a diagram (configuration) $k_\uparrow = 1, k_\downarrow = 1$



Markov process

- We generate diagrams (Monte Carlo configurations) using a Markov process

$$W_{ij} = \text{probability to go from } c_i \text{ to } c_j \text{ in one step}$$

$$\sum_j W_{ij} = 1$$

- The Markov process will converge to sampling diagrams with probabilities $|w(c)|$ if two conditions are satisfied
  - ergodicity: any configuration c_i should be possible to reach from any other configuration c_j in a finite number of steps
  - global balance: $\sum_i W_{ij} |w(c_i)| = |w(c_j)|$

Metropolis-Hastings algorithm

- Makes use of the detailed balance condition

$$\frac{W_{ij}}{W_{ji}} = \frac{|w(c_j)|}{|w(c_i)|}$$

- Decomposes update probability into proposal and acceptance probabilities

$$W_{ij} = W_{ij}^{\text{prop}} W_{ij}^{\text{acc}}$$

- Proposal probabilities can be chosen arbitrarily (as long as the ergodicity condition is satisfied) and then the detailed balance condition holds if

$$W_{ij}^{\text{acc}} = \min\left(1, R_{ij}\right)$$

$$R_{ij} = \frac{|w(c_j)| W_{ji}^{\text{prop}}}{|w(c_i)| W_{ij}^{\text{prop}}}$$

CT-HYB-QMC: updates

- Increase k_σ by adding two time points

$$W^{\text{prop}}_{k_\sigma \to k_\sigma+1} = \frac{dt^2}{\Delta t^2}$$

$$W^{\text{prop}}_{k_\sigma+1 \to k_\sigma} = \frac{1}{k_\sigma + 1}$$

$$R_{k_\sigma \to k_\sigma+1} = \frac{W^{\text{prop}}_{k_\sigma+1 \to k_\sigma}}{W^{\text{prop}}_{k_\sigma \to k_\sigma+1}} \cdot \frac{|w(c_{k_\sigma+1})| dt^2}{|w(c_{k_\sigma})|} = \frac{\Delta t^2}{k_\sigma + 1} \cdot \frac{|w(c_{k_\sigma+1})|}{|w(c_{k_\sigma})|}$$

- Decrease k_σ by removing two time points

$$R_{k_\sigma \to k_\sigma-1} = \frac{k_\sigma}{\Delta t^2} \cdot \frac{|w(c_{k_\sigma-1})|}{|w(c_{k_\sigma})|}$$

- Shift existing time points (not necessary for the ergodicity)

CT-HYB-QMC: measurement of observables

- During a QMC run we sample partition function diagrams

$$\mathcal{Z} = \prod_\sigma \left[\sum_{k_\sigma=0}^{\infty} (-1)^{k_\sigma} \int_{0_+}^{-i\beta} dt_1^{\sigma c} \dots \int_{t_{k-1}^{\sigma c}}^{-i\beta} dt_k^{\sigma c} \int_{0_+}^{-i\beta} dt_1^{\sigma a} \dots \int_{t_{k-1}^{\sigma a}}^{-i\beta} dt_k^{\sigma a} \right]$$

$$w_{\mathrm{loc}}(\{t_m^{\sigma c}\}, \{t_n^{\sigma a}\})\, w_{\mathrm{bath}}(\{t_m^{\sigma c}\}, \{t_n^{\sigma a}\})$$

$$= \sum_c w(c) = \sum_c \mathrm{sgn}(w(c))|w(c)|$$

- For each partition function diagram (configuration) we accumulate (measure) contributions to observables

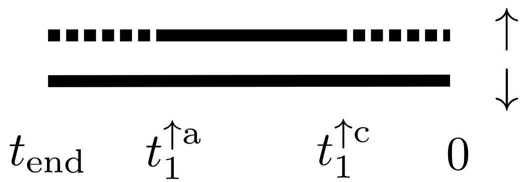
$$\langle \mathcal{O}(t) \rangle = \underbrace{\frac{\sum_c \langle \mathcal{O}(t) \rangle_c \, \mathrm{sgn}(w(c))\, |w(c)|}{\sum_c |w(c)|}}_{\text{MC average of } \langle \mathcal{O}(t) \rangle_c \, \mathrm{sgn}(w(c))} \cdot \underbrace{\frac{\sum_c |w(c)|}{\sum_c \mathrm{sgn}(w(c))\, |w(c)|}}_{\text{inverse average sign}}$$

- We expect for a finite (but large) number of measurements $\Delta \mathcal{O} = \sqrt{\frac{\mathrm{Var}\, \mathcal{O}}{N}}$

CT-HYB-QMC: measurement of observables

- Occupations and double occupancy easy to measure in segment picture

$$k_\uparrow = 1, k_\downarrow = 0$$



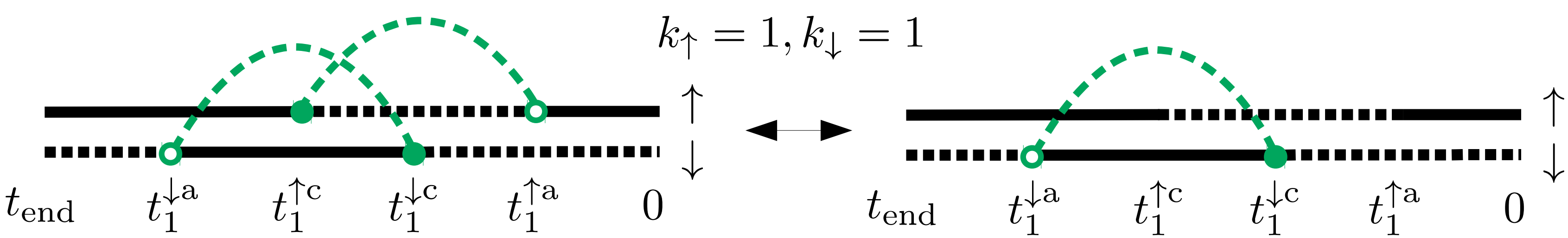
- Green functions – cut hybridizations lines

minors of matrix Δ

$$G_\sigma(t,t') = -i \left\langle \mathcal{T}_\mathcal{C}\, d_\sigma(t) d_\sigma^\dagger(t') \right\rangle = -\frac{1}{\mathcal{Z}} \frac{\delta \mathcal{Z}}{\delta \Delta_\sigma(t',t)}$$

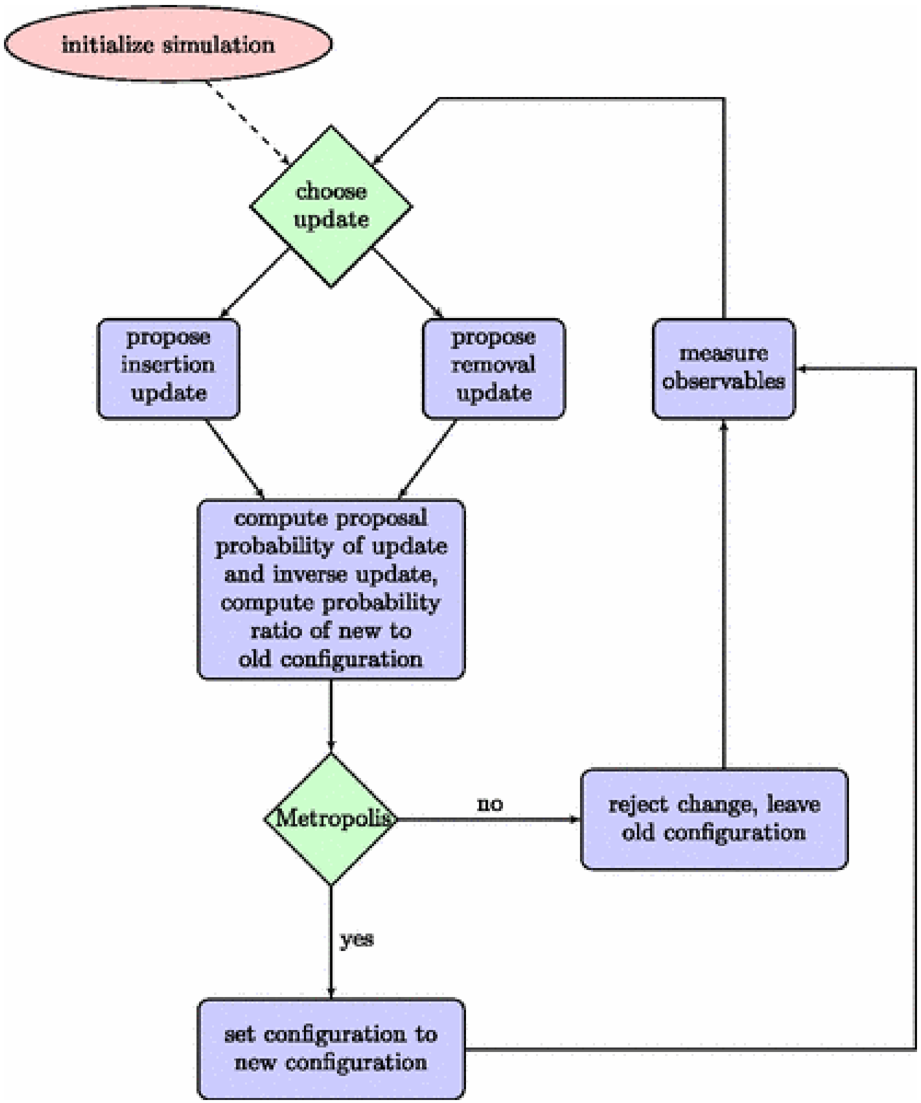
$$\langle G_\sigma(t,t') \rangle_c = -\frac{1}{w(c)} \frac{\delta w(c)}{\delta \Delta_\sigma(t',t)} = \sum_{ij}^{k_\sigma} \delta(t_i^{\sigma \text{c}} - t') \delta(t_j^{\sigma \text{a}} - t) \frac{(-1)^{i+j} M_{ij}}{\text{Det}\, \hat{\Delta}_\sigma}$$

$$k_\uparrow = 1, k_\downarrow = 1$$



$w(c)$ $\qquad$ $\left\langle G_\uparrow(t_1^{\uparrow \text{a}}, t_1^{\uparrow \text{c}}) \right\rangle_c w(c)$

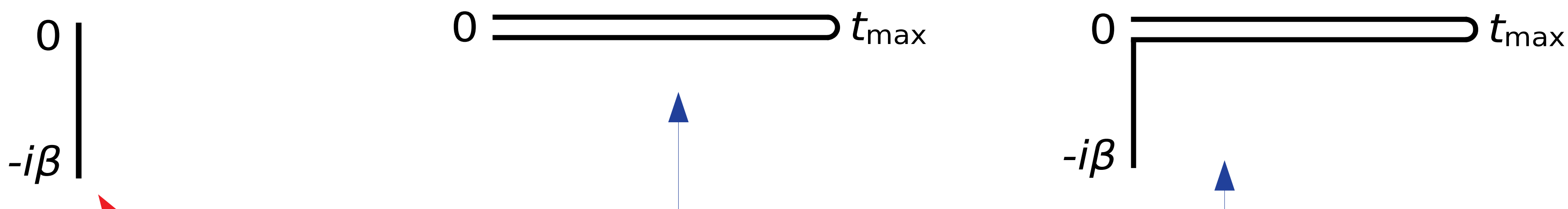
CT-HYB-QMC: flow diagram



Rev. Mod. Phys. **83**, 349 (2011)

CT-HYB-QMC: choice of contour

$$\langle \mathcal{O}(t) \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr} \left(e^{-\beta H(0)} \mathcal{T}_- e^{-i \int_t^0 ds H(s)} \mathcal{O}(t) \mathcal{T}_+ e^{-i \int_0^t ds H(s)} \right) = \frac{1}{\mathcal{Z}} \mathrm{Tr} \left(\mathcal{T}_\mathcal{C} \, e^{-i \int_C ds H(s)} \mathcal{O}(t) \right)$$



non-equilibrium physics
with no bath-impurity coupling
in the initial state

equilibrium physics
(analytical continuation
of Green functions necessary)

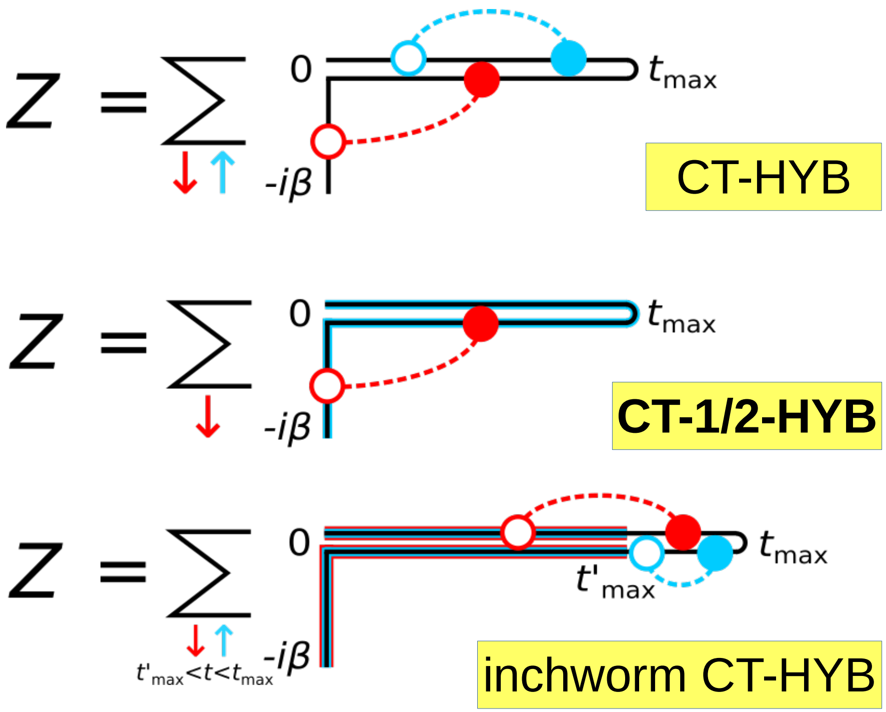
$$G(\tau) = -\int d\omega \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} A(\omega)$$

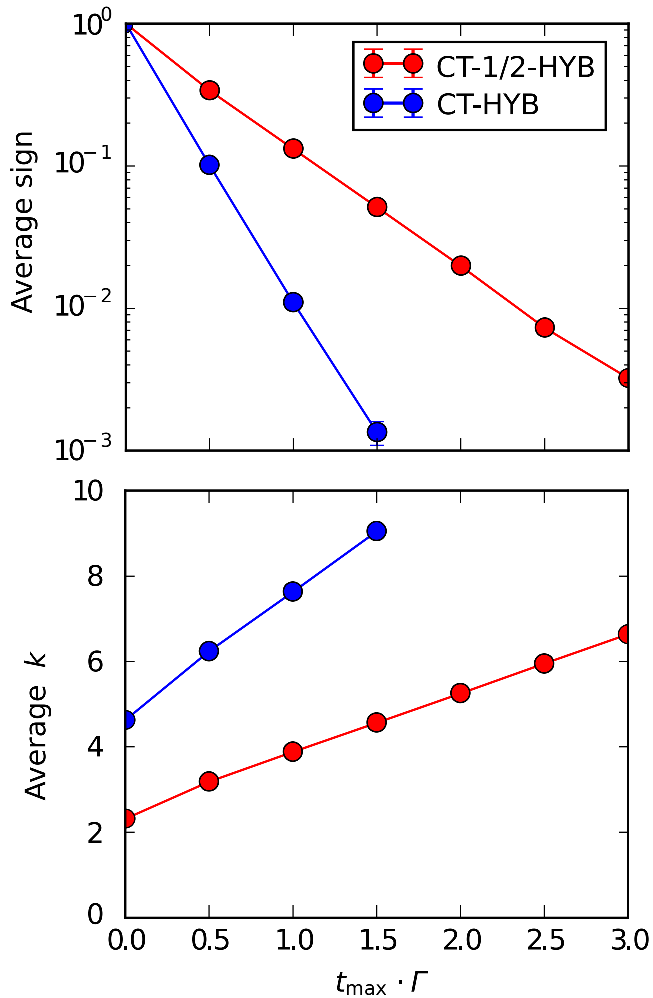
non-equilibrium physics
with initially coupled bath-impurity
thermal state

Quantum Monte Carlo sign problem

- QMC sign problem occurs when the average sign gets too small
- There are two types of the sign problem: **fermionic** and **dynamical**
- **Fermionic sign problem** results from the sign change after the interchange of fermionic operators
  - miraculously for SIAM every interchange of *d* operators is accompanied by an interchange of *c* operators leading to no net sign change
- **Dynamical sign problem** results from phases generated by time-evolution operators exp(-*itH*) – it is not present in equilibrium QMC where one samples the expansion of statistical operator exp(-*βH*)
- In general both sign problems get worse with an increasing dominant order of the perturbative expansion
- **Goal**: reduce expansion order by (semi-)analytically summing as many diagrams as possible
  - bold CT-HYB-QMC, inchworm CT-HYB-QMC, **CT-1/2-HYB-QMC**

Extensions of CT-HYB-QMC

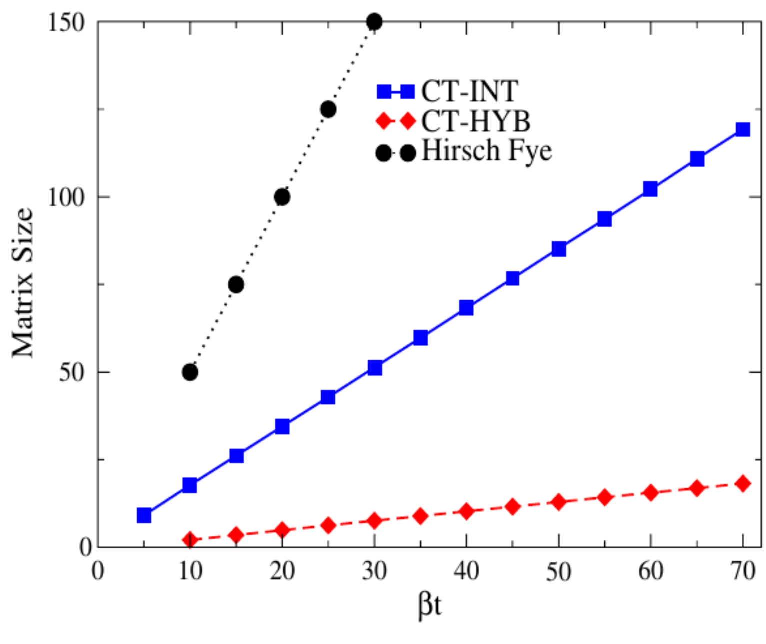


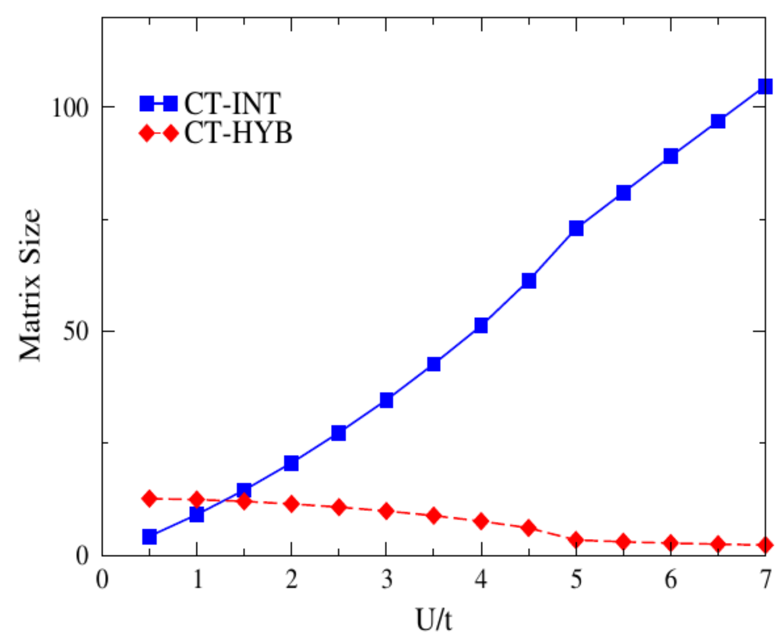


Comparison of different QMC impurity solvers

Scaling algorithm	CT-INT	CT-AUX	CT-HYB (segment)	CT-HYB (matrix)
Diagonal hybridization	$N(\beta U)^3$	$N(\beta U)^3$	$N\beta^3$	$ae^N\beta^2 + bN\beta^3$, $a \gg b$
Nondiagonal hyb.	$(N\beta U)^3$, sign prob.	$(N\beta U)^3$, sign prob.	$(N\beta)^3$, sign prob.	$ae^N\beta^2 + b(N\beta)^3$, $a \gg b$, sign prob.
Diagonal interaction	$(N\beta U)^3$, sign prob.	$(N\beta U)^3$, sign prob.	$(N\beta)^3$, sign prob.	$ae^N\beta^2 + b(N\beta)^3$, $a \gg b$, sign prob.
General U_{ijkl}	$(N^2\beta U)^3$, sign prob.	N/A	N/A	$ae^N\beta^2 + b(N\beta)^3$, $a \gg b$, sign prob.

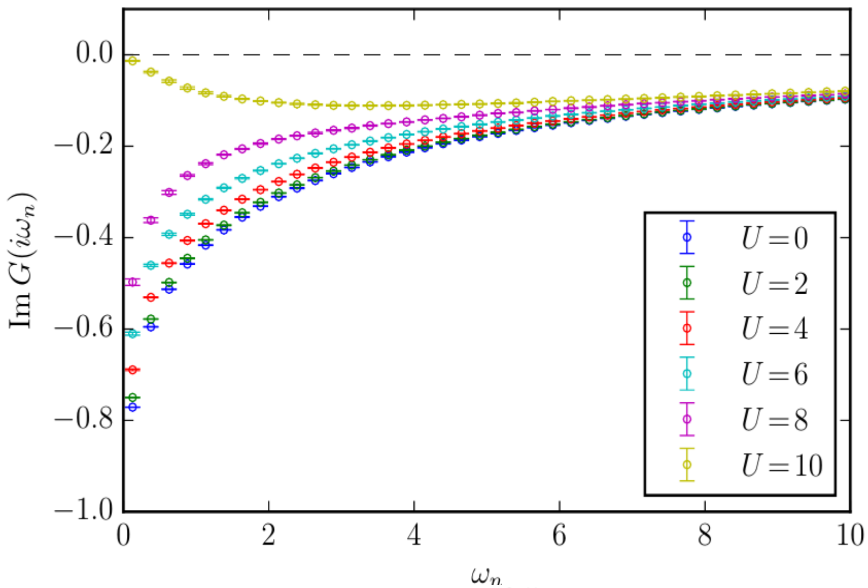
Rev. Mod. Phys. **83**, 349 (2011)

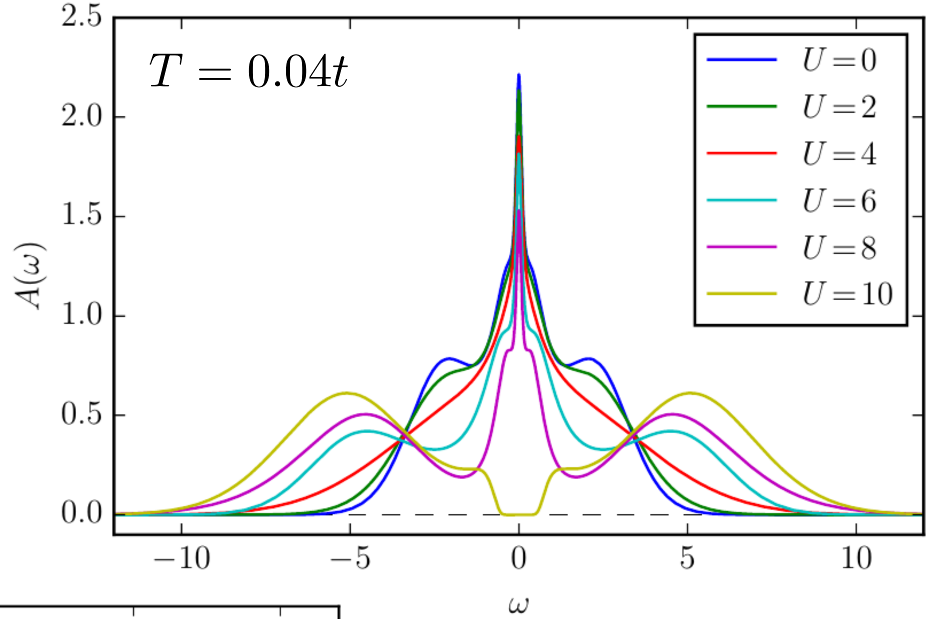


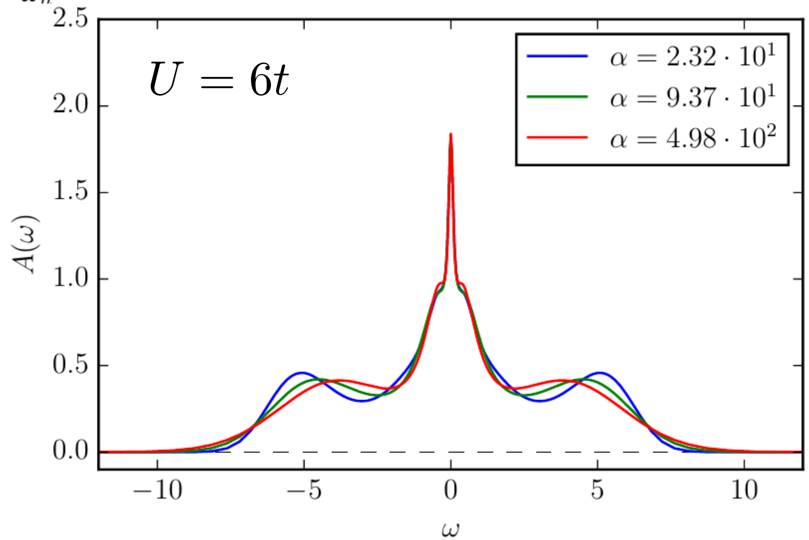


Gull, E., P. Werner, A. Millis, and M. Troyer, Phys. Rev. **B** 76, 235123 (2007)

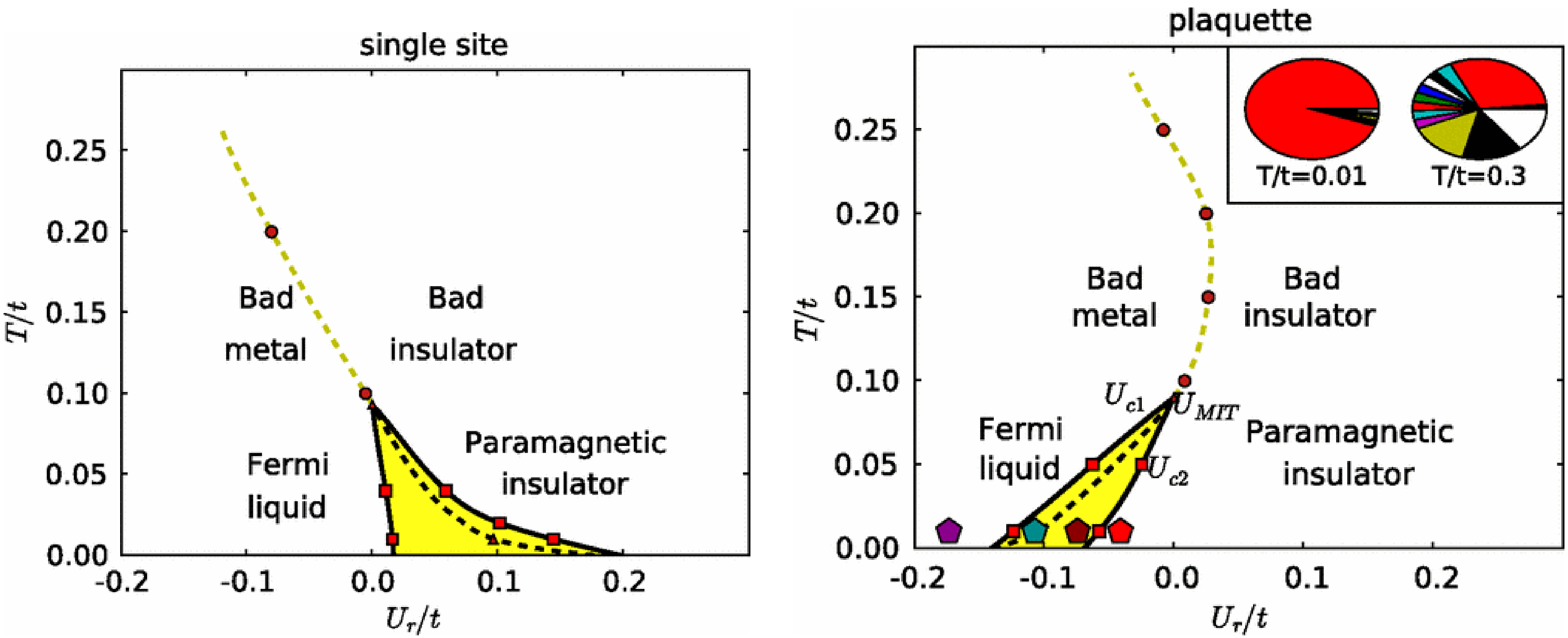
DMFT with CT-HYB-QMC: square-lattice Hubbard model







DMFT with CT-HYB-QMC: square-lattice Hubbard model



$U_{\rm MIT} = 9.35t$ $\qquad U_r = \dfrac{U_r - U_{\rm MIT}}{U_{\rm MIT}}$ $\qquad U_{\rm MIT} = 6.05t$

Park, H., K. Haule, and G. Kotliar, Phys. Rev. Lett. **101**, 186403 (2008)

Error estimation, autocorrelation time

- Because the subsequent Monte Carlo configurations are correlated the knowledge of the autocorrelation "time" N_{auto} is needed to properly estimate the error

$$\Delta\mathcal{O} = \sqrt{\frac{\operatorname{Var}\mathcal{O}}{N}\left(1 + 2N_{\text{auto}}(\mathcal{O})\right)}$$

$$N_{\text{auto}}(\mathcal{O}) = \frac{\sum_{i=1}^{\infty}\left(\langle\mathcal{O}_1\mathcal{O}_{1+i}\rangle - \langle\mathcal{O}\rangle^2\right)}{\langle\mathcal{O}^2\rangle - \langle\mathcal{O}\rangle^2}$$

- Binning analysis

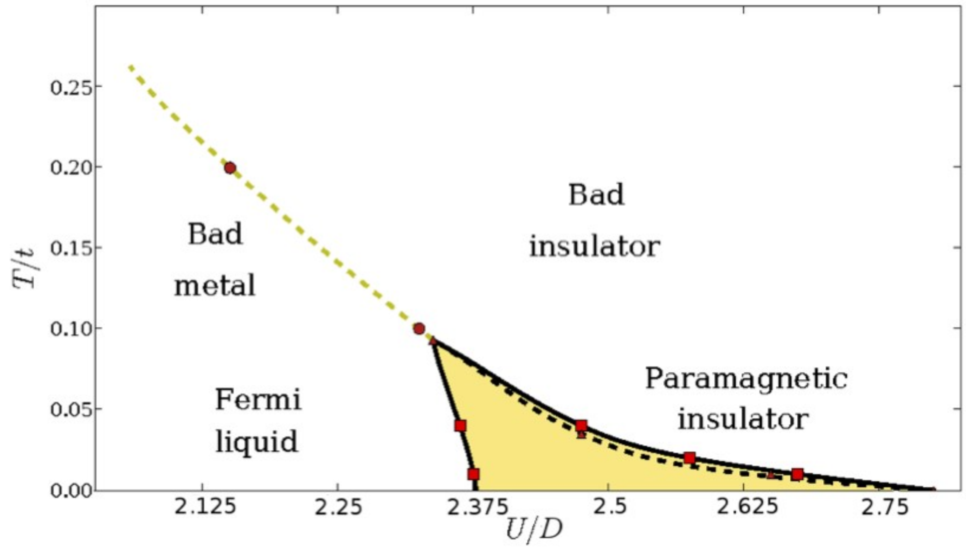
$$N_{\text{auto}}(\mathcal{O}) = \frac{1}{2}\left\{\left[\frac{\Delta\mathcal{O}(l)}{\Delta\mathcal{O}(0)}\right]^2 - 1\right\}$$

QMC packages

- TRIQS (http://triqs.ipht.cnrs.fr)
- ALPS (http://alps.comp-phys.org)
- ALF (http://alf.physik.uni-wuerzburg.de)
- iQist (http://github.com/iqist/iqist)
- w2dynamics (http://w2dynamics.physik.uni-wuerzburg.de)

Exercises (CT-HYB-QMC)

- Flat-band SIAM: observe Kondo peak
- Bethe lattice Hubbard model: reproduce phase diagram using DMFT
- Estimation of the autocorrelation time in SIAM



K. Haule, hauleweb.rutgers.edu

DQMC (determinant QMC)

- Discrete Hubbard-Stratonovitch transformation

$$e^{-\Delta\tau U\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)} = \frac{e^{-\frac{U}{4}\Delta\tau}}{2}\sum_{\xi_i=\pm 1} e^{-\Delta\tau\xi_i\lambda(n_{i\uparrow}-n_{i\downarrow})}$$

$$\cosh\left(\Delta\tau\lambda\right) = e^{\frac{\Delta\tau U}{2}}$$

- Single particle problem specified by configuration $\{\xi_{1,0},\ldots,\xi_{N,M}\}$

$$\mathrm{Tr}_c\left[\mathcal{T}e^{-i\int dt\,\sum_{ab} c_i^\dagger h_{ij}(t)c_j}\right] = \mathrm{Det}\left[1+\mathcal{T}e^{-i\int dt\,h(t)}\right]$$

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_c \mathrm{Det}L_\uparrow(c)\,\mathrm{Det}L_\downarrow(c)$$

BSS algorithm: R. Blankenbecler, D. J. Scalapino,and R. L. Sugar, Phys. Rev. **D** 24, 2278 (1981)

Summary

- Quantum Monte Carlo algorithms are powerful methods to study interacting quantum systems in equilibrium
- They usually employ Markov chain processes with Metropolis-Hastings sampling
- QMC suffer from sign problems: fermionic and dynamical
- The best impurity solver in the strong-coupling regime is CT-HYB-QMC
- CT-HYB-QMC can treat general many-body interactions, therefore has been successfully used in numerous DFT + DMFT studies
- We still lack efficient QMC methods for the study of non-equilibrium dynamics due to the dynamical sign problem

Thank you for your attention!

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