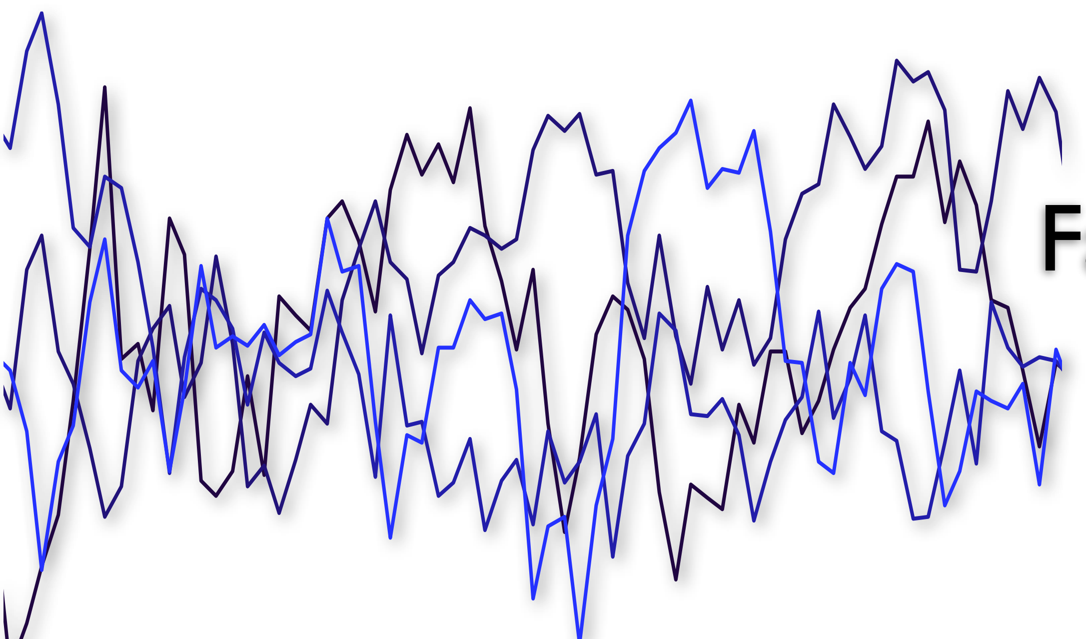
Gaussian Quantum Monte Carlo Method for Fermions with symmetry projection



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Joel Corney and Peter Drummond, PRL 93, 260401 (2004)

F.F. Assaad et al., PRB 72, 224518 (2005)

Attack the sign problem

Outline

- The idea of GQMC in short
- The Gaussian basis
- Derivation of stochastic differential equations (SDEs)
- Systematic errors: source and possible solutions
- Symmetry projection scheme
- Application: Hubbard ladders
- Conclusion

GQMC: A stochastic phase space method

Expansion of the density operator in a Gaussian operator basis:

Inverse temperature

Phase space variables

$$\hat{\rho}(\boldsymbol{\tau}) = \int d\underline{\boldsymbol{\lambda}} P(\underline{\boldsymbol{\lambda}}, \boldsymbol{\tau}) \hat{\Lambda}(\underline{\boldsymbol{\lambda}})$$

Density operator

Probability distribution

Gaussian operator basis

SDE

Stochastic Differential Equations

integration

Trajectories $\underline{\boldsymbol{\lambda}}(\tau)$ in phase space with positive weights

Observables: Functions of phase space variables $F(\underline{\boldsymbol{\lambda}})$

Expectation values: Weighted averages over trajectories

Gaussian operator basis

Basis: $\hat{\Lambda}(\mathbf{n}) = \det(\mathbf{1}-\mathbf{n}) : e^{-\hat{\mathbf{c}}^{\dagger}\left(\mathbf{2}+\left(\mathbf{n}^{T}-\mathbf{1}\right)^{-1}\right)\hat{\mathbf{c}}} :$

n is a NxN matrix of phase space variables
N: number of sites

Trace: $\mathrm{Tr}\left[\hat{c}_x^{\dagger}\hat{c}_y\hat{\Lambda}(\mathbf{n})\right] = n_{x,y}$

n correspond to the equal time Green functions

Expansion: $\hat{\rho}(\tau) = \sum_i P_i(\tau)\hat{\Lambda}(\mathbf{n}_i), \quad P_i \geq 0$

Positive expansion exists
Basis is overcomplete!

Introducing weight: $\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \Omega\hat{\Lambda}(\mathbf{n}), \ \underline{\boldsymbol{\lambda}} = (\Omega, \mathbf{n})$

Integral form: $\hat{\rho}(\tau) = \int d\underline{\boldsymbol{\lambda}} P(\underline{\boldsymbol{\lambda}}, \tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}})$

Derivation of the SDEs

$$\frac{d}{d\tau}\hat{\rho}(\tau) = -\tfrac{1}{2}\left[\hat{H}, \hat{\rho}(\tau)\right]_+$$

Introduce expansion

Differential properties

$$\hat{\mathbf{c}}^{\dagger T}\hat{\mathbf{c}}^T\hat{\Lambda} = \mathbf{n}\hat{\Lambda} + (\mathbf{1}-\mathbf{n})\frac{\partial\hat{\Lambda}}{\partial\mathbf{n}}\mathbf{n}$$

$$\frac{d}{d\tau}\int d\underline{\boldsymbol{\lambda}}P(\underline{\boldsymbol{\lambda}},\tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = -\frac{1}{2}\int d\underline{\boldsymbol{\lambda}}P(\underline{\boldsymbol{\lambda}},\tau)\left(\hat{H}\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) + \hat{\Lambda}(\underline{\boldsymbol{\lambda}})\hat{H}\right)$$

$$\int d\underline{\boldsymbol{\lambda}}\frac{d}{d\tau}P(\underline{\boldsymbol{\lambda}},\tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \int d\underline{\boldsymbol{\lambda}}P(\underline{\boldsymbol{\lambda}},\tau)L[\hat{\Lambda}(\underline{\boldsymbol{\lambda}})]$$

Contains first and second order derivatives.

Partial integration

$$\int d\underline{\boldsymbol{\lambda}}\frac{d}{d\tau}P(\underline{\boldsymbol{\lambda}},\tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \int d\underline{\boldsymbol{\lambda}}L'[P(\underline{\boldsymbol{\lambda}},\tau)]\hat{\Lambda}(\underline{\boldsymbol{\lambda}})$$

Assume no boundary terms!

Compare both integrands

$$\frac{d}{d\tau}P(\underline{\boldsymbol{\lambda}},\tau) = L'[P(\underline{\boldsymbol{\lambda}},\tau)]$$

→ **Fokker-Planck equation**

Derivation of the SDEs

$$L' = -\sum_{\alpha} \frac{\partial}{\partial \lambda_\alpha} A_\alpha + \frac{1}{2} \sum_{\alpha\beta z} \frac{\partial}{\partial \lambda_\alpha} B_\alpha^z \frac{\partial}{\partial \lambda_\beta} B_\beta^z$$

Fokker-Planck eq: $\frac{d}{d\tau} P(\underline{\boldsymbol{\lambda}}, \tau) = L'[P(\underline{\boldsymbol{\lambda}}, \tau)]$

SDE: $d\lambda_\alpha(\tau) = A_\alpha(\underline{\boldsymbol{\lambda}})d\tau + \sum_k B_\alpha^k(\underline{\boldsymbol{\lambda}})dW_k(\tau)$

(Stratonovich)

Drift term Diffusion term

Noise terms (Wiener increments) drawn from normal distribution

$$\langle dW_k(\tau) dW_{k'}(\tau') \rangle = d\tau \delta_{kk'} \delta_{\tau\tau'}$$

$$\langle dW_k(\tau) \rangle = 0$$

Integration: Forward Euler, (semi-) implicit, higher order schemes

SDEs are not unique! There are several "gauge" choices.

$$\hat{n}_{ii\sigma}^2 - \hat{n}_{ii\sigma} = 0$$

- Does not change the Hamiltonian. But changes the SDE!
- Crucial trick for Hubbard model to get positive weights!

→ No explicit manifestation of the negative sign problem!

Example: Hubbard model

$$\hat{H}_{\text{Hub}} = -t \sum_{\langle i,j\rangle,\sigma} \hat{n}_{ij\sigma} + U \sum_{i} \hat{n}_{ii\uparrow}\hat{n}_{ii\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{ii\sigma}$$

$\hat{n}_{ij\sigma} \rightarrow \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}$

Final form of the SDEs: $2N^2+1$ coupled equations:

$$\frac{d\boldsymbol{n}_\sigma}{d\tau} = \frac{1}{2}\{(\mathbf{I}-\boldsymbol{n}_\sigma)\boldsymbol{\Delta}^{(1)}_\sigma \boldsymbol{n}_\sigma + \boldsymbol{n}_\sigma \boldsymbol{\Delta}^{(2)}_\sigma (\mathbf{I}-\boldsymbol{n}_\sigma)\}$$

→ full matrix-matrix multiplication

$$\boldsymbol{\Delta}^{(\mathbf{r})}_{\sigma}{}_{\mathbf{ij}\sigma} = \mathbf{t_{ij}} - \delta_{\mathbf{ij}}\{\mathbf{U}\mathbf{n}_{\mathbf{jj}-\sigma} - \mu + \mathbf{f}\xi^{(\mathbf{r})}_{\mathbf{j}}\}$$

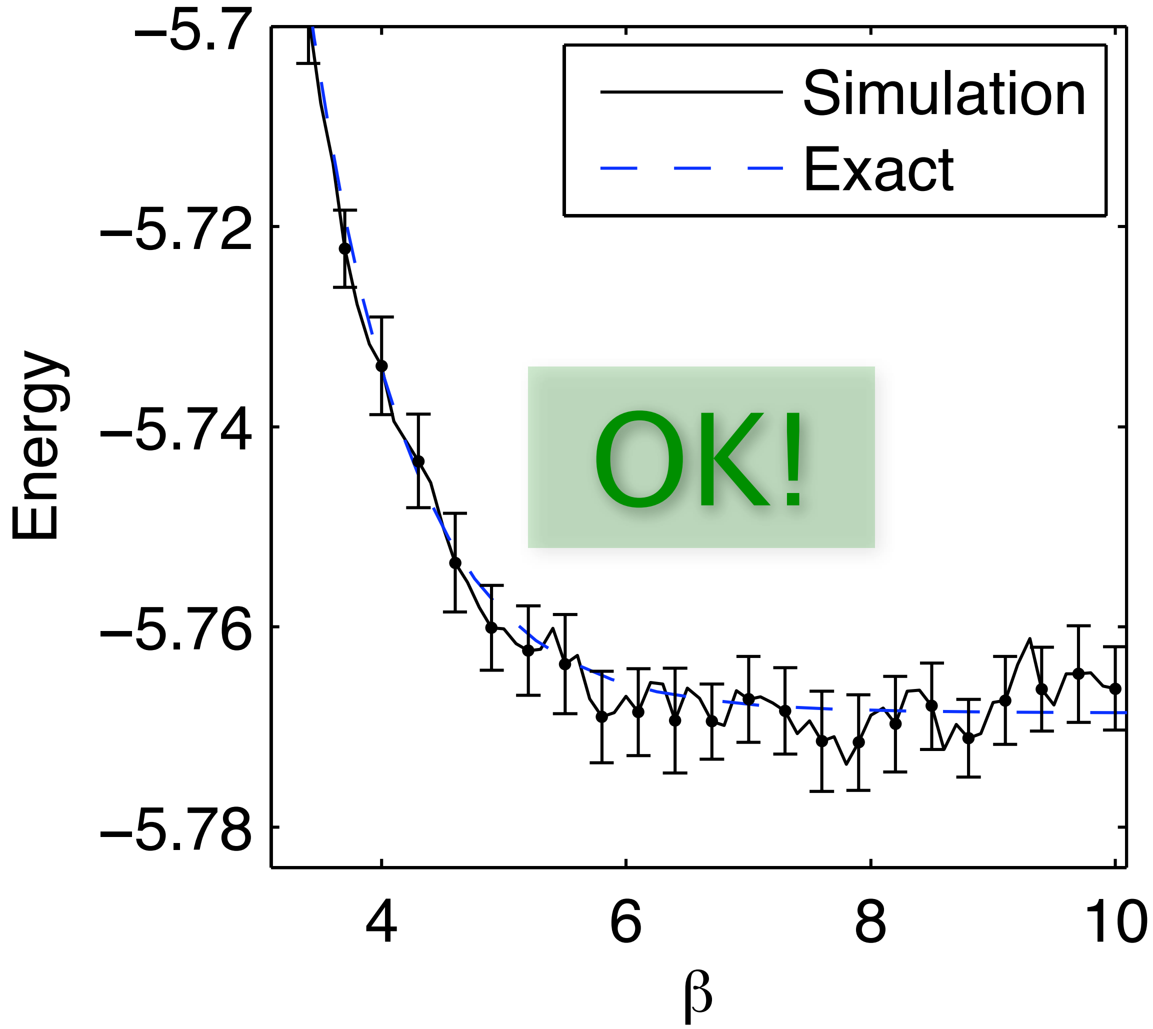
$f = -\text{sign}(U)$ for $\sigma = \downarrow$

$$\frac{d\Omega}{d\tau} = -\Omega H(\boldsymbol{n}_\uparrow, \boldsymbol{n}_\downarrow)$$

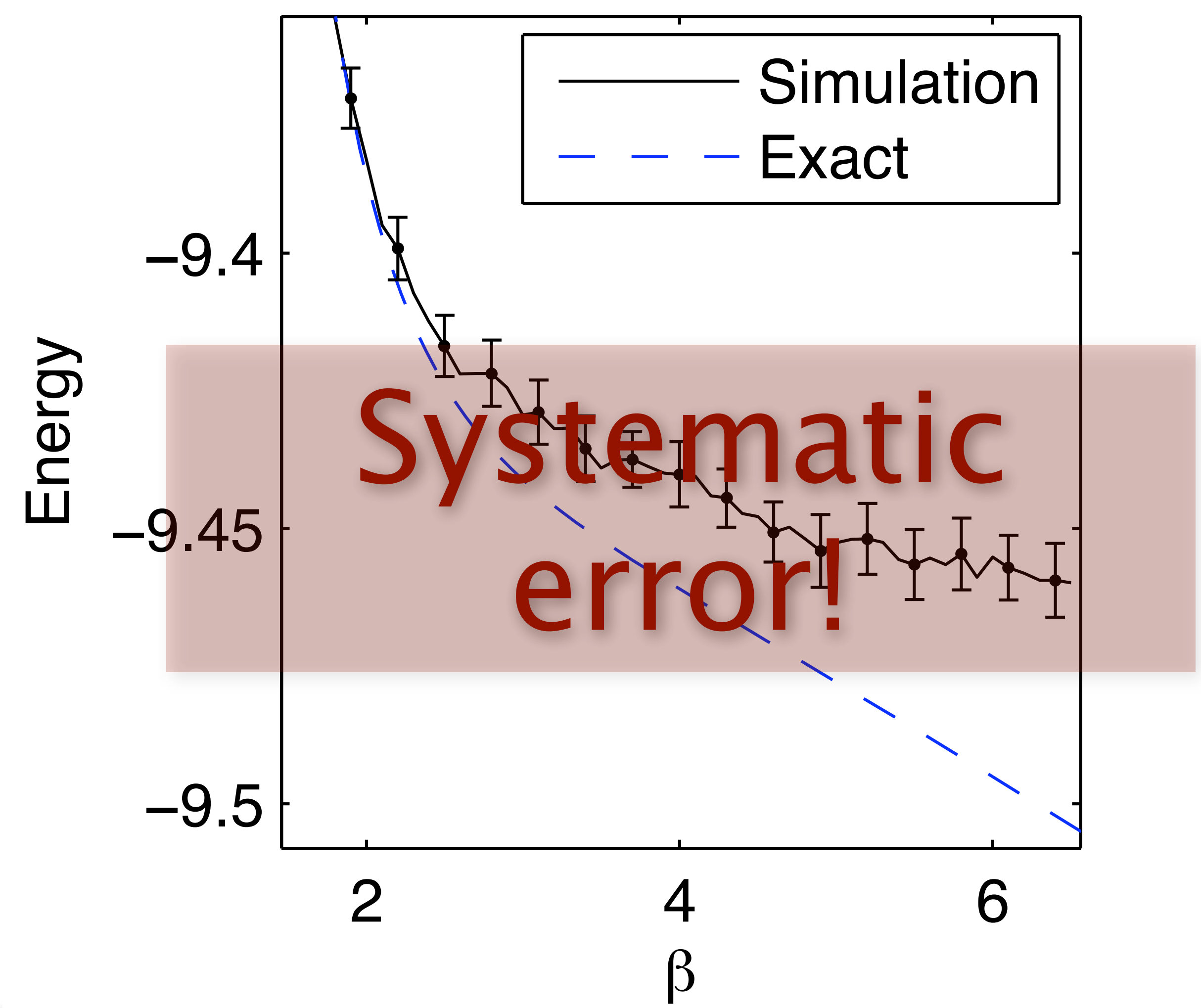
$$< \xi^{(r)}_j(\tau)\xi^{(r')}_{j'}(\tau') >= 2|U|\delta(\tau-\tau')\delta_{jj'}\delta_{rr'}$$

Weight grows exponentially, but remains positive

Results for Hubbard model



2x2 system, U=1, t=1, <n>=0.5, 40’000 trajectories



2x2 system, U=4, t=1, <n>=0.875, 480000 trajectories

Use higher order integrator

Use different quantization axis

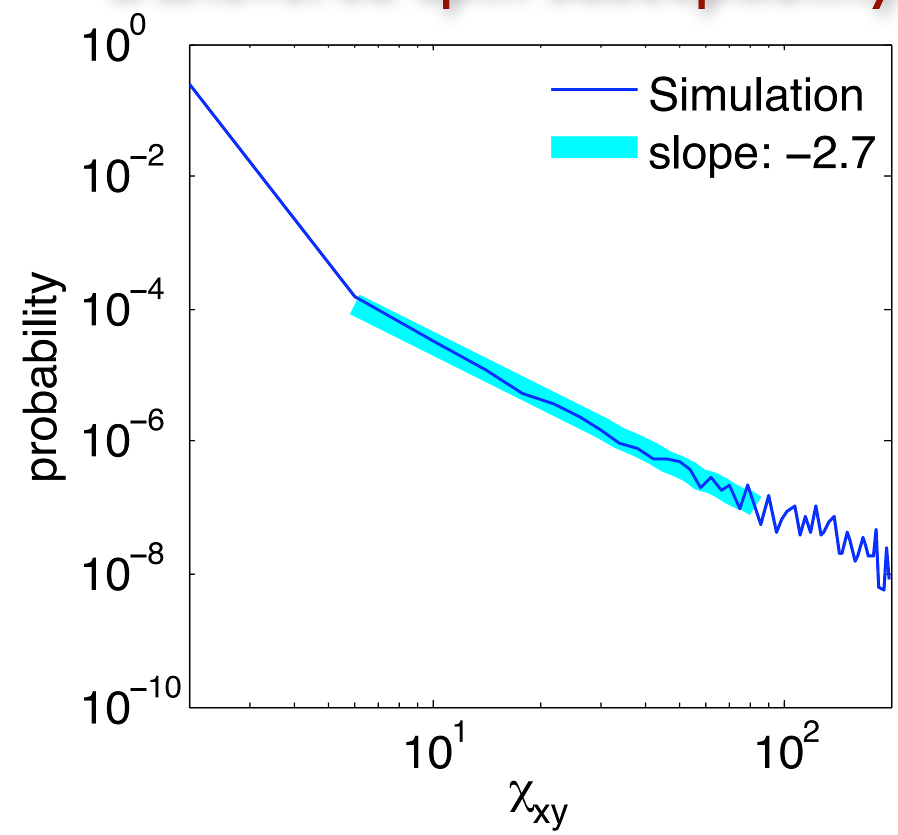
additional noise

Change integration timestep

more trajectories

Fat tailed distributions

Diverging variance of the transverse spin susceptibility



Some Monte Carlo measurements seem to be ill defined (diverging error bars).

➡ Fat tailed distributions can become a problem in derivation of SDE's: **Boundary Terms!**

Go back to derivation:

Fat power law tails!

$$\int d\underline{\boldsymbol{\lambda}} \frac{d}{d\tau} P(\underline{\boldsymbol{\lambda}},\tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \int d\underline{\boldsymbol{\lambda}} P(\underline{\boldsymbol{\lambda}},\tau) L[\hat{\Lambda}(\underline{\boldsymbol{\lambda}})]$$

Partial integration

$$\int d\underline{\boldsymbol{\lambda}} \frac{d}{d\tau} P(\underline{\boldsymbol{\lambda}},\tau)\hat{\Lambda}(\underline{\boldsymbol{\lambda}}) = \int d\underline{\boldsymbol{\lambda}} L'[P(\underline{\boldsymbol{\lambda}},\tau)]\hat{\Lambda}(\underline{\boldsymbol{\lambda}})$$

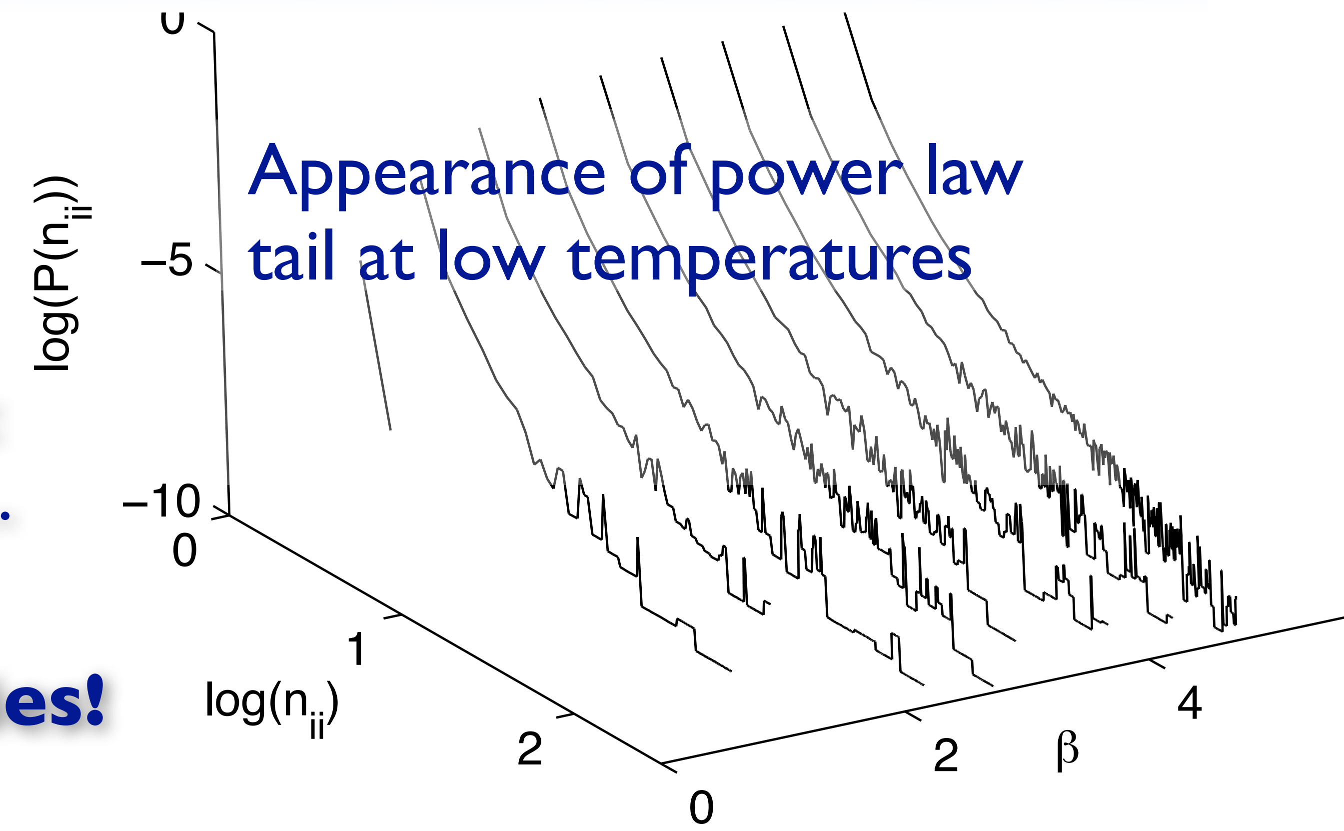
+ boundary terms

➡ Assumption is wrong!
➡ SDE's are no longer valid!!!!

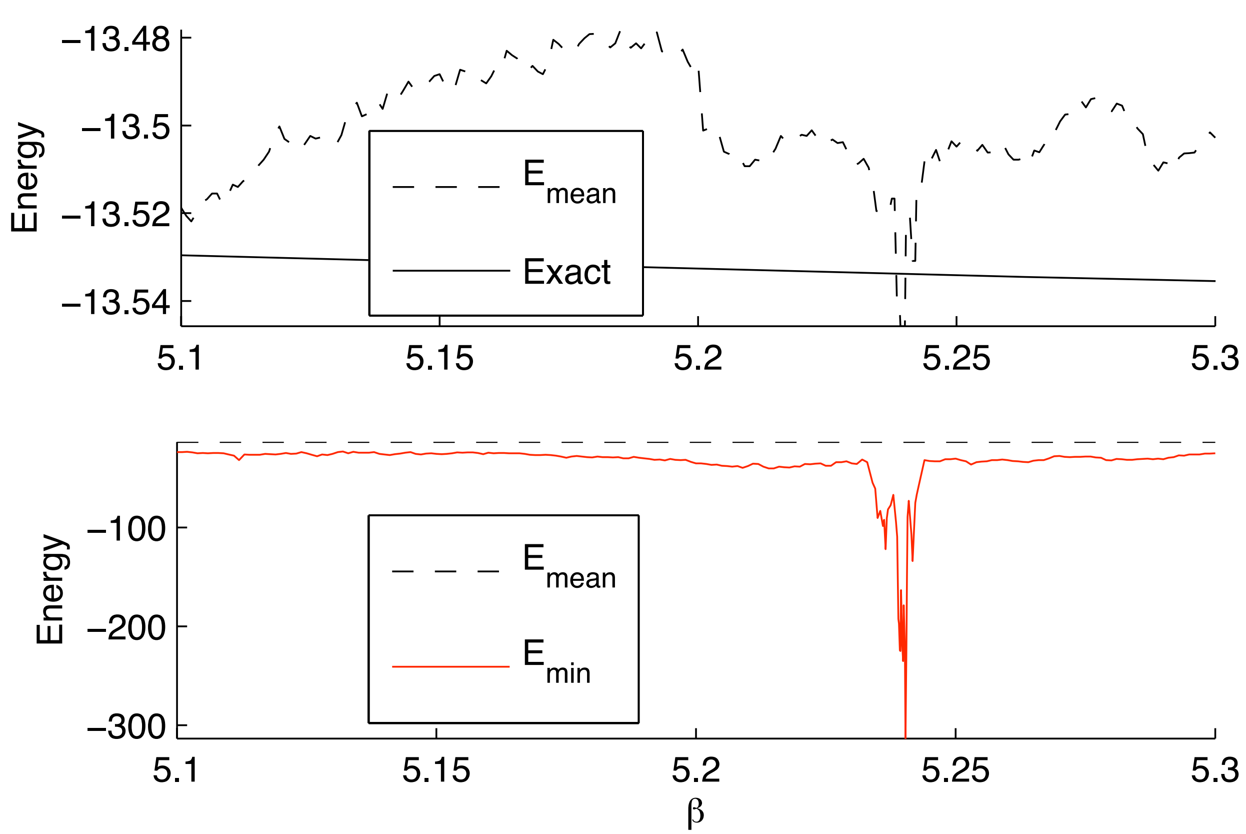
Boundary terms

This is a known problem!

Gilchrist, Gardiner and Drummond, PRA, 55(4), 3014, 1997:
Boundary terms found in some examples: single-mode laser, anharmonic oscillator, ...



Another indicator: **spiking trajectories!**



➡ presence of nearly singular trajectories

➡ indicator, when boundary terms become non-negligible

➡ **Consistency**: systematic errors appear only after a certain ß.

Possible solutions

- The SDE's are not unique: Use gauges to change distribution P!
  - "Fermi" gauges (like $\hat{n}_{ii\sigma}^2 - \hat{n}_{ii\sigma} = 0$)
  - Additional noise terms (diffusion gauge)
  - Arbitrary drift functions (drift gauges)

$$d\lambda_\alpha(\tau) = A_\alpha d\tau + \sum_k B_\alpha^k \left[dW_k(\tau) - g_k d\tau\right]$$

$$d\Omega(\tau) = A_0 d\tau + \Omega g_k dW_k(\tau)$$

BUT AT THE SAME TIME WEIGHTS HAVE TO REMAIN POSITIVE!!!

  - Change basis

➡ **work in progress**

- In case of small systematic errors, use a **symmetry projection** scheme to calculate ground state properties

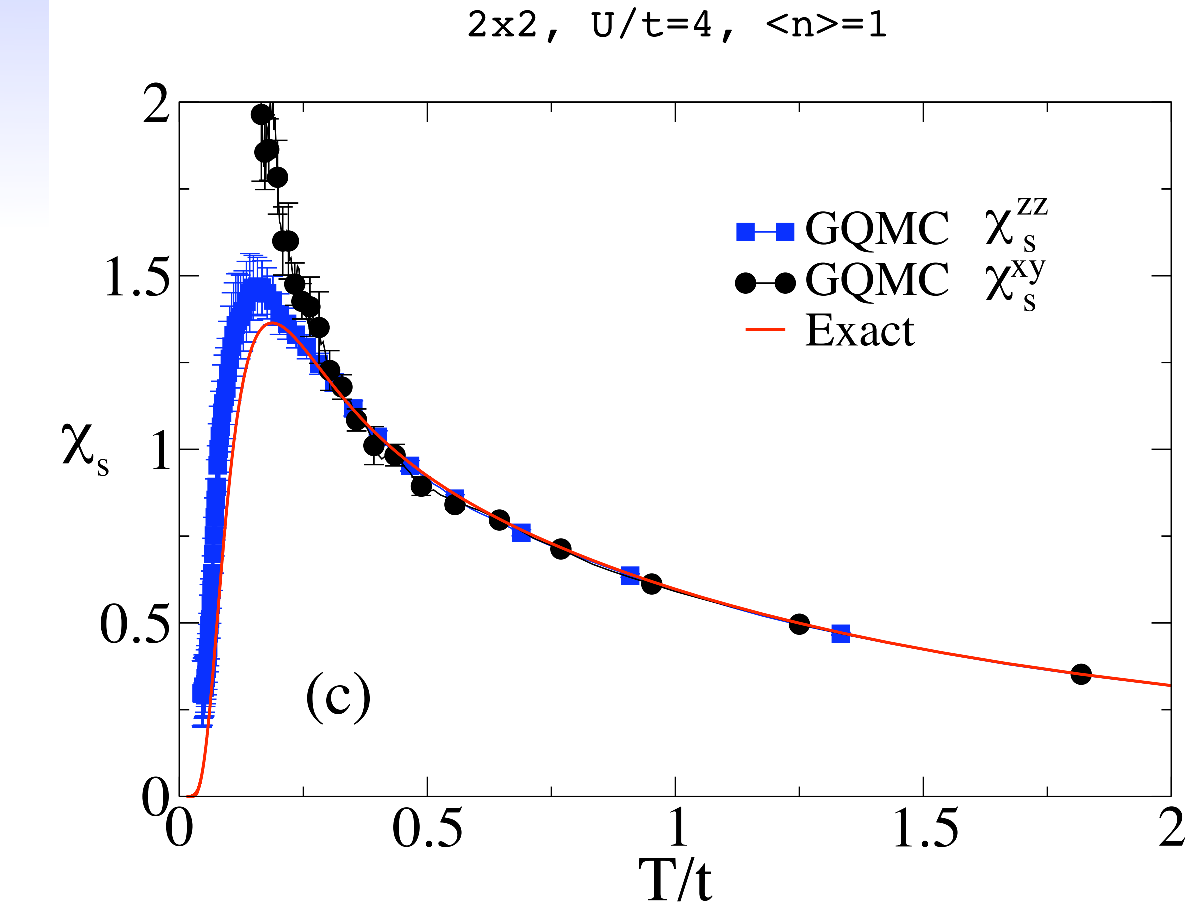
Assaad et al., PRB 72, 224518 (2005)

Symmetry breaking

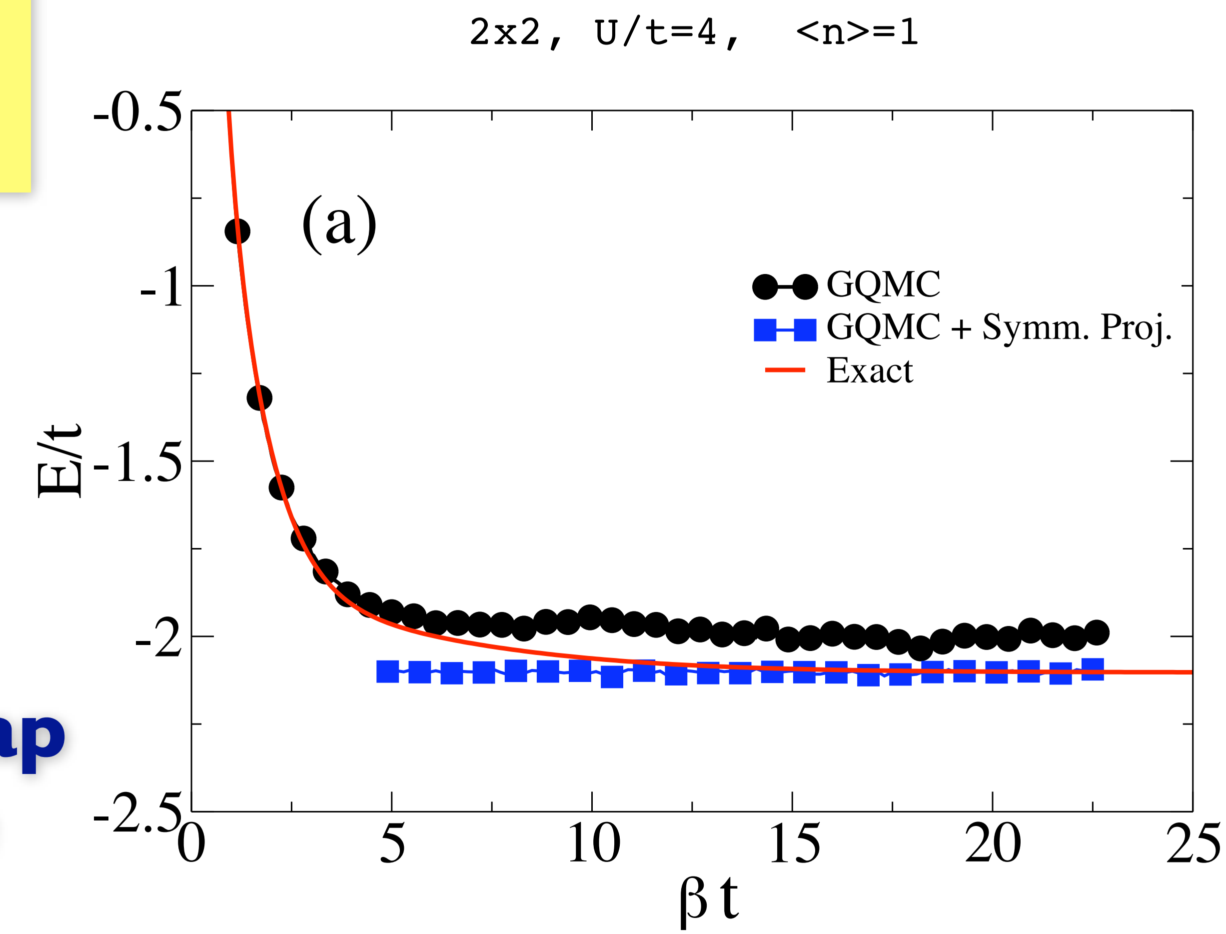
- The SU(2) spin symmetry is not preserved in the cases with systematic errors

Idea: Take density matrix from simulation and project it onto the ground state symmetry sector.

Mizusaki, Imada, Phys. Rev. B 69, 125110 (2004)



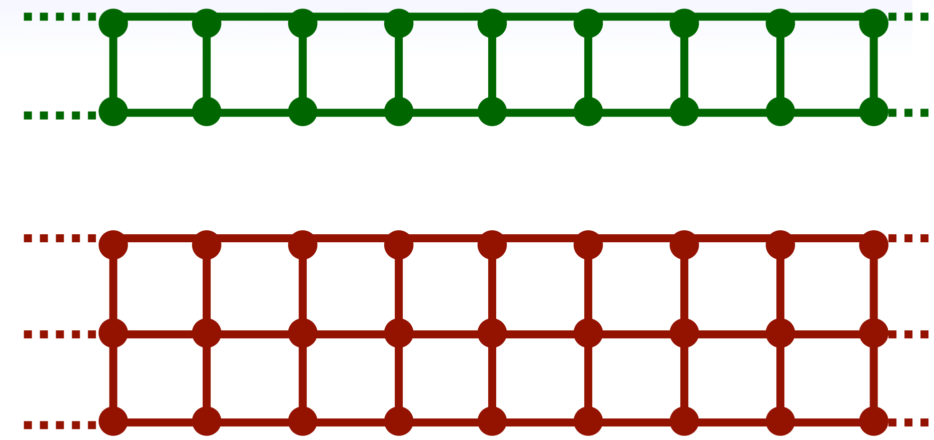
PGQMC $$\hat{\rho}_{Pr} = \hat{P}\hat{\rho}_{sim}\hat{P}^{\dagger}$$



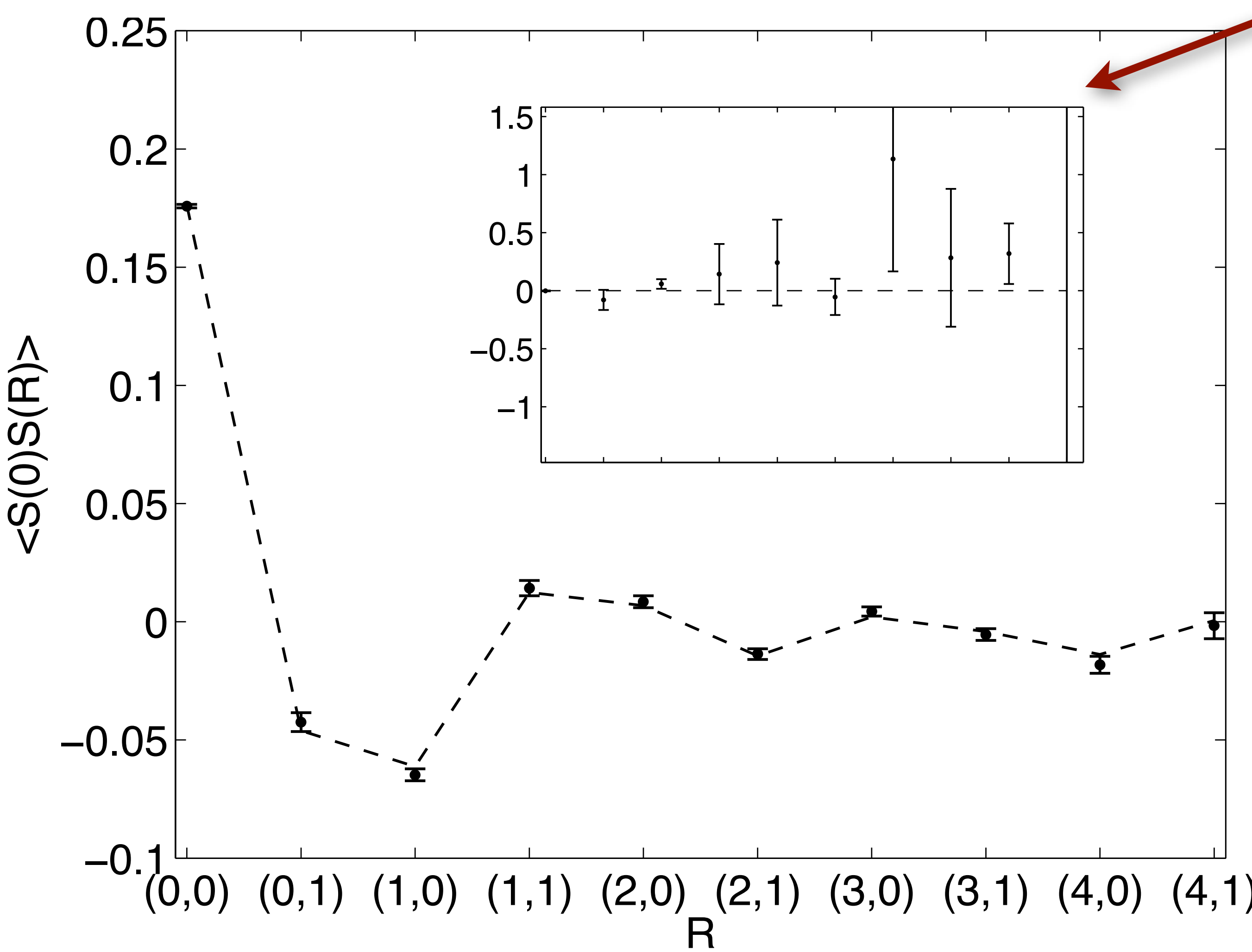
- Ground state properties (not finite temperature)
- Projection is done a posteriori
- Good agreement in many cases
- $Tr\hat{\rho}_{Pr}/Tr\hat{\rho}_{sim}$ measures the **overlap** between density matrix and ground state sector

Results: Hubbard ladders

- Simulation of 2xL and 3xL Hubbard ladders with different fillings n, interaction U
- Comparison of GQMC and PGQMC to Density Matrix Renormalization Group (DMRG) results (high precision)



8x2, U/t=4, n_{tot}=14, PGQMC



Inset: Relative errors
One standard deviation (σ) error bars. Exact result should be within 2σ

Results agree with DMRG

Conclusion

- Once more: the sign problem is **not solved** (yet).

- GQMC is an elegant finite temperature method for fermions. Further application examples are needed!

- Systematic errors in GQMC in SOME cases. But we have **indicators** for their presence: fat tailed distributions, spiking trajectories, broken symmetries...

- Fat tails may disappear with appropriate choice of **gauges.**

- Symmetry projection allows to obtain ground state properties. In many cases it corrects the systematic errors of GQMC. There are examples, where we could go beyond auxiliary field QMC!

Outlook: Recent news

- Projection method can be incorporated into the sampling.
  Aimi and Imada, cond-mat/0704.3792

- Importance sampling (Metropolis algorithm) which favors the ground state symmetry sector

- Better results than with projection a posteriori. Promising!

- Projected weights can become negative. Sign problem? For doped systems with large U (>8).

- Work in progress!