Infinite variance problem in auxiliary-field quantum Monte Carlo:

Hao Shi
Center for Computational Quantum Physics, Flatiron Institute

- Introduction to auxiliary field quantum Monte Carlo method

- Infinite variance problem in determinantal quantum Monte Carlo
  - Origin of the diverging variance
  - Identify the infinite variance problem
  - Solution: bridge-link method

Shiwei Zhang

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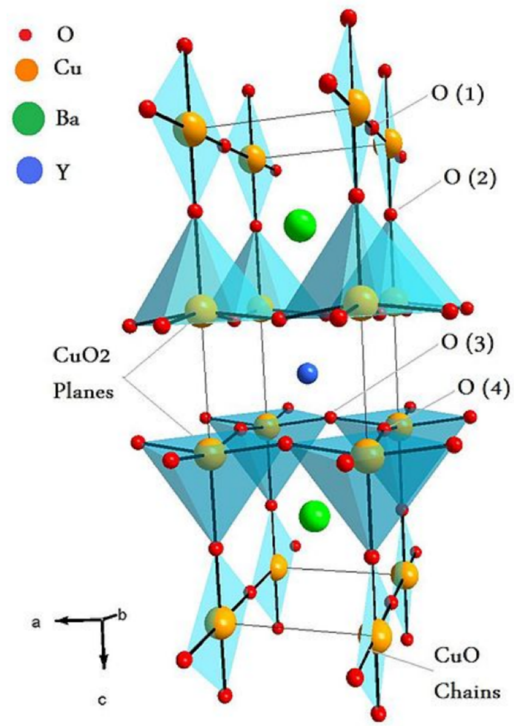
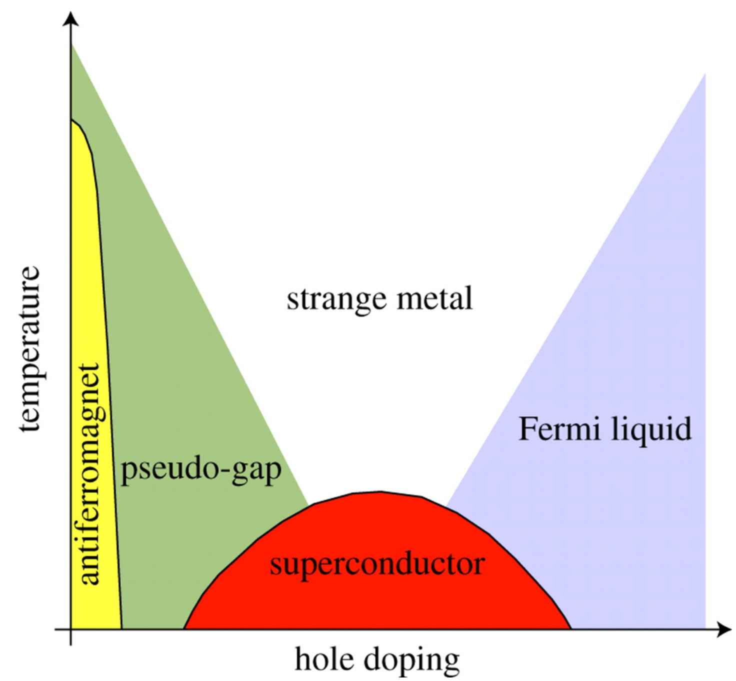
Auxiliary Field Quantum Monte Carlo Method

- Strongly-correlated quantum many-electron systems



YbaCuO (wikipedia)



Phase diagram

ab-initio

Lattice model

Molecular systems

Real material

Auxiliary Field Quantum Monte Carlo Method

- Hamiltonian in Second quantization

$$\hat{H} = \sum_{ij\sigma} T_{ij} C^{\dagger}_{i\sigma} C_{j\sigma} + \sum_{ijkl} V_{ijkl} C^{\dagger}_{i\sigma\rho} C^{\dagger}_{j\sigma} C_{k\sigma} C_{l\rho}$$

Basis

ab-initio

Auxiliary Field Quantum Monte Carlo Method

- Hamiltonian in Second quantization

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Basis

- Project to ground state:

$$|\psi_0\rangle \propto e^{-\tau \hat{H}} e^{-\tau \hat{H}} \cdots e^{-\tau \hat{H}} |\psi_T\rangle$$

Auxiliary Field Quantum Monte Carlo Method

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Single Determinant

Auxiliary Field Quantum Monte Carlo Method

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$$\sum_{\gamma} D_{\gamma} \hat{\rho}^2_{\gamma} \qquad \hat{\rho}_{\gamma} = \sum_{ij\sigma} \rho^{\gamma}_{ij} C^{\dagger}_{i\sigma} C_{j\sigma}$$

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$$\sum_\gamma D_\gamma \hat{\rho}^2_\gamma$$

$$e^{\hat{A}^2} = \int dx \frac{1}{\sqrt{2\pi}} e^{-x^2/2} e^{x\hat{A}}$$

Auxiliary Field Quantum Monte Carlo Method

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Basis

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- Integration of one body operators

$$e^{-\tau \hat{H}} = \int dx \; p(x) \hat{B}(x)$$

Auxiliary Field Quantum Monte Carlo Method

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Basis

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$$|\psi_0\rangle \propto e^{-\tau\hat{H}} e^{-\tau\hat{H}} \cdots e^{-\tau\hat{H}} |\psi_T\rangle$$

- High-dimensional integral

$$|\psi_0\rangle \propto \int dx_n \; p(x_n) \hat{B}(x_n) \ldots \int dx_1 \; p(x_1) \hat{B}(x_1) |\psi_T\rangle$$

Auxiliary Field Quantum Monte Carlo Method

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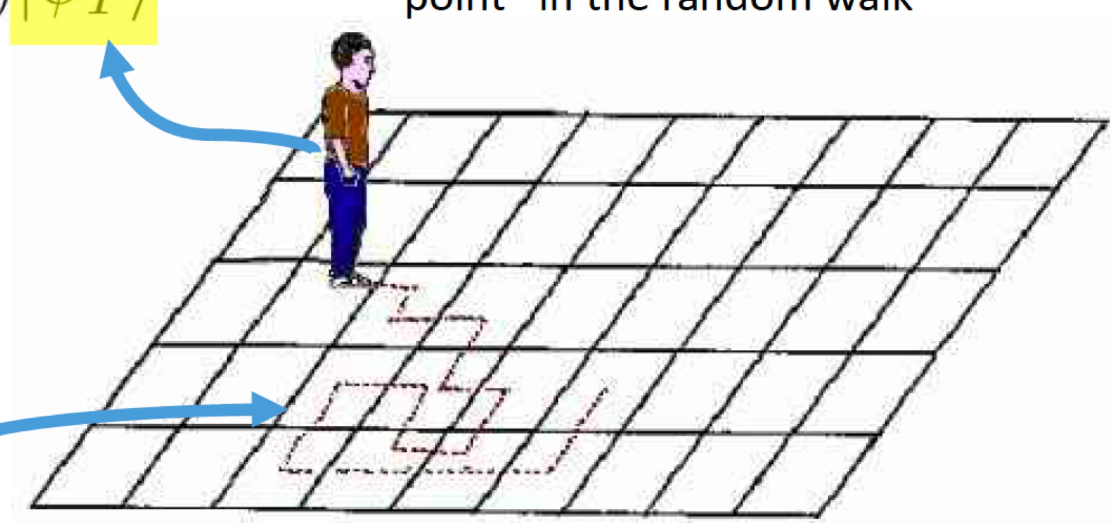
Single particle operator

Slater determinant

$$|\psi^n\rangle = \hat{B}(x_n) \ldots \hat{B}(x_2)\hat{B}(x_1)|\psi_T\rangle$$

The trial wave function is a “starting point” in the random walk



The random walk takes place inside the manifold of N particles Slater determinants

Auxiliary Field Quantum Monte Carlo Method

- Measure ground state property

$$\langle \hat{O} \rangle = \frac{\langle \psi_T | \exp(-\beta \hat{H}) \hat{O} \exp(-\beta \hat{H}) | \psi_T \rangle}{\langle \psi_T | \exp(-2\beta \hat{H}) | \psi_T \rangle}$$

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- General multi-dimensional integral:

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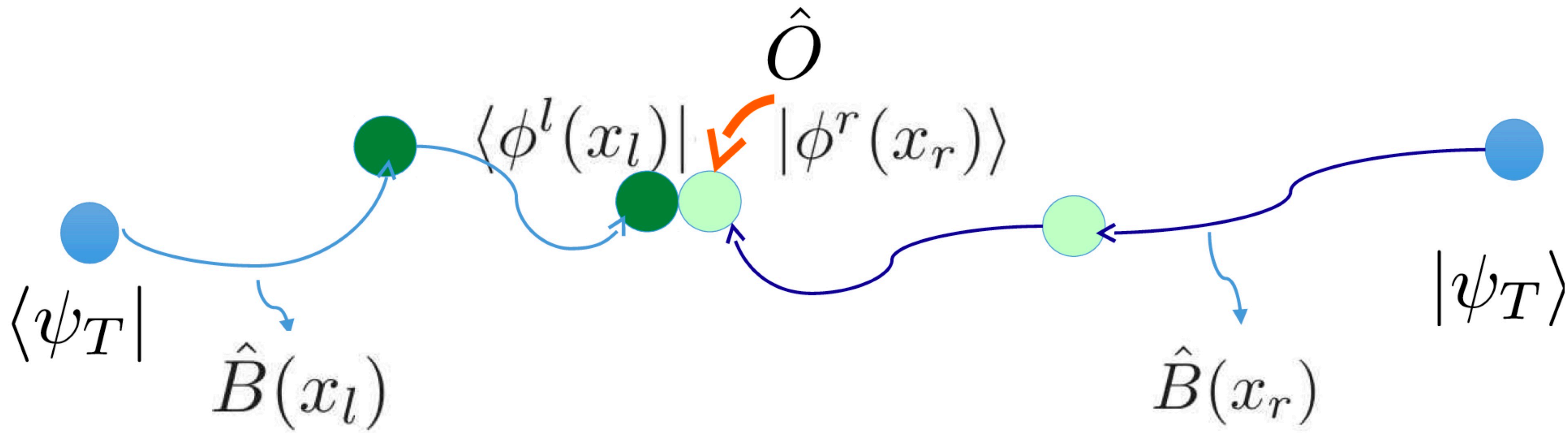
Auxiliary Field Quantum Monte Carlo Method

- Sampling configurations of the auxiliary field

- Estimate expectation values on the Ground State wave function



- Random walk in the manifold of N particles Slater Determinants that can be parametrized using complex matrices

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Infinite variance problem

•General Multi-dimensional integral:

Probability density function

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Phys. Rev. E 93, 033303 (2016)

Infinite variance problem

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•Sign problem free

$$W(X) \; \langle \phi^l(x_l) | \phi^r(x_r) \rangle \geqq 0$$

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- Half-filled repulsive Hubbard model

- The spin-balanced atomic Fermi gas

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QMC calculations are relied on to provide definitive answers.

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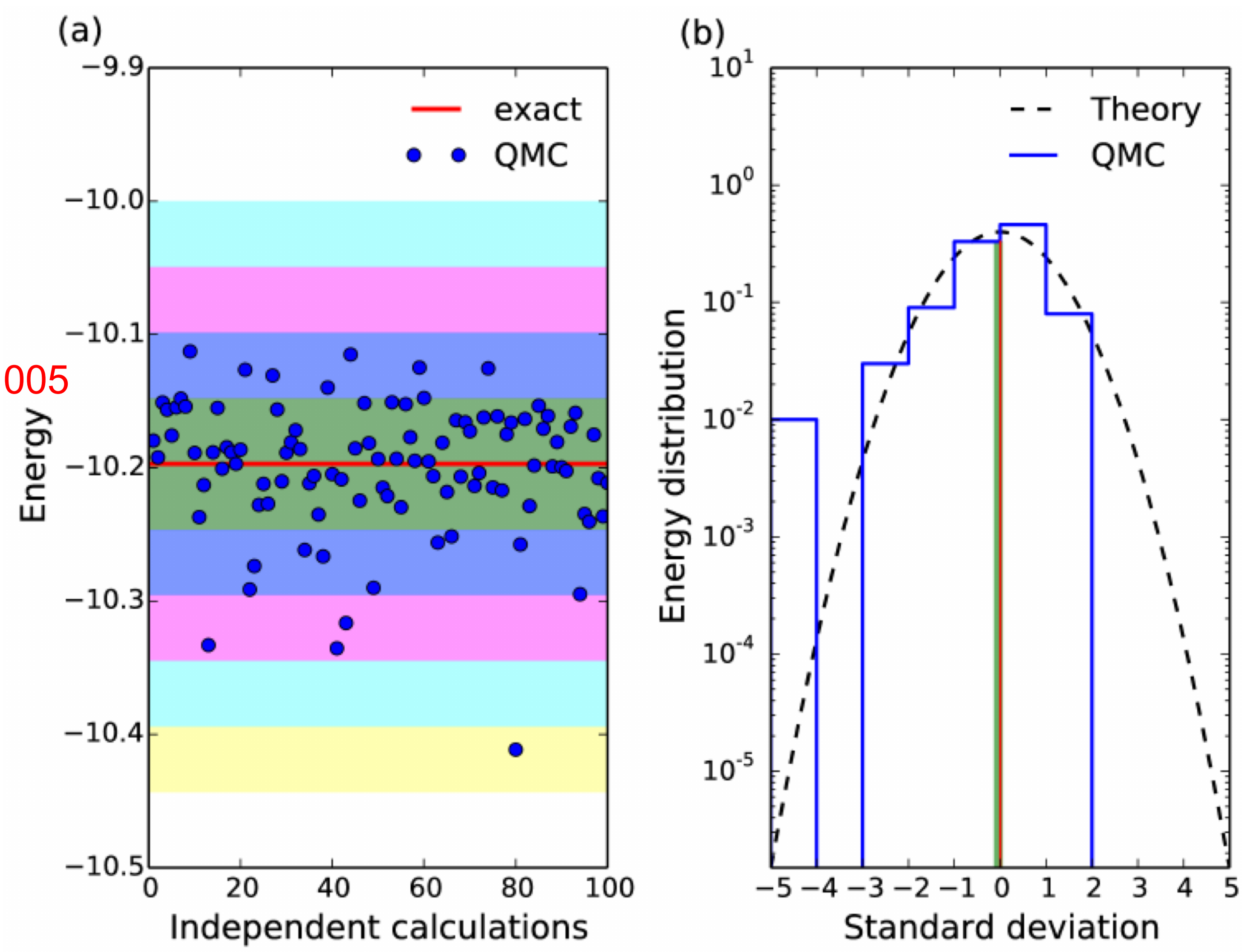
Infinite variance problem

Exact:
−10.197

QMC
−10.199 ± 0.005



Hubbard model: 2x4 U=4 k=(0.03,0.02) β=81 Δτ =0.01

Infinite variance problem

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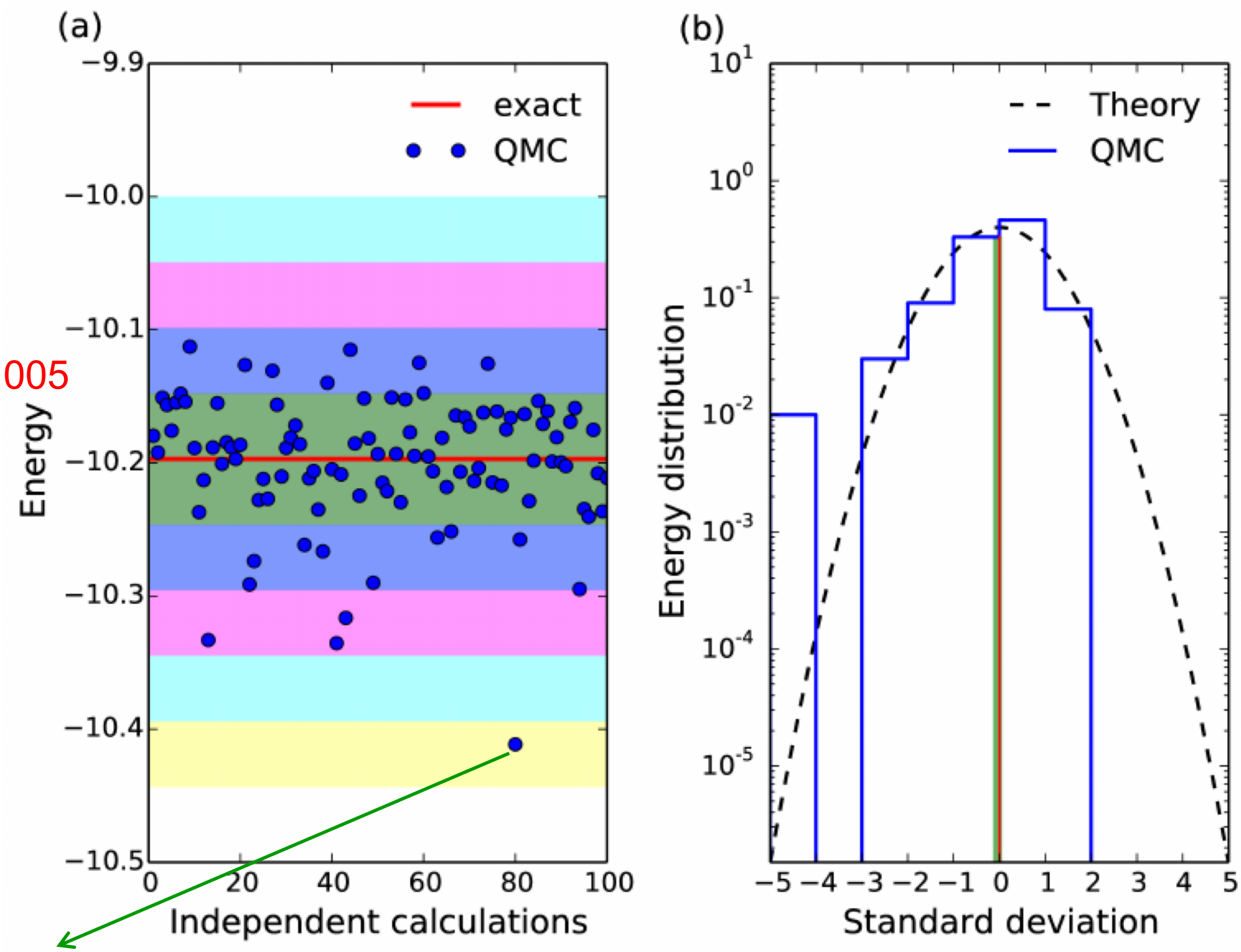

Less than 0.007%

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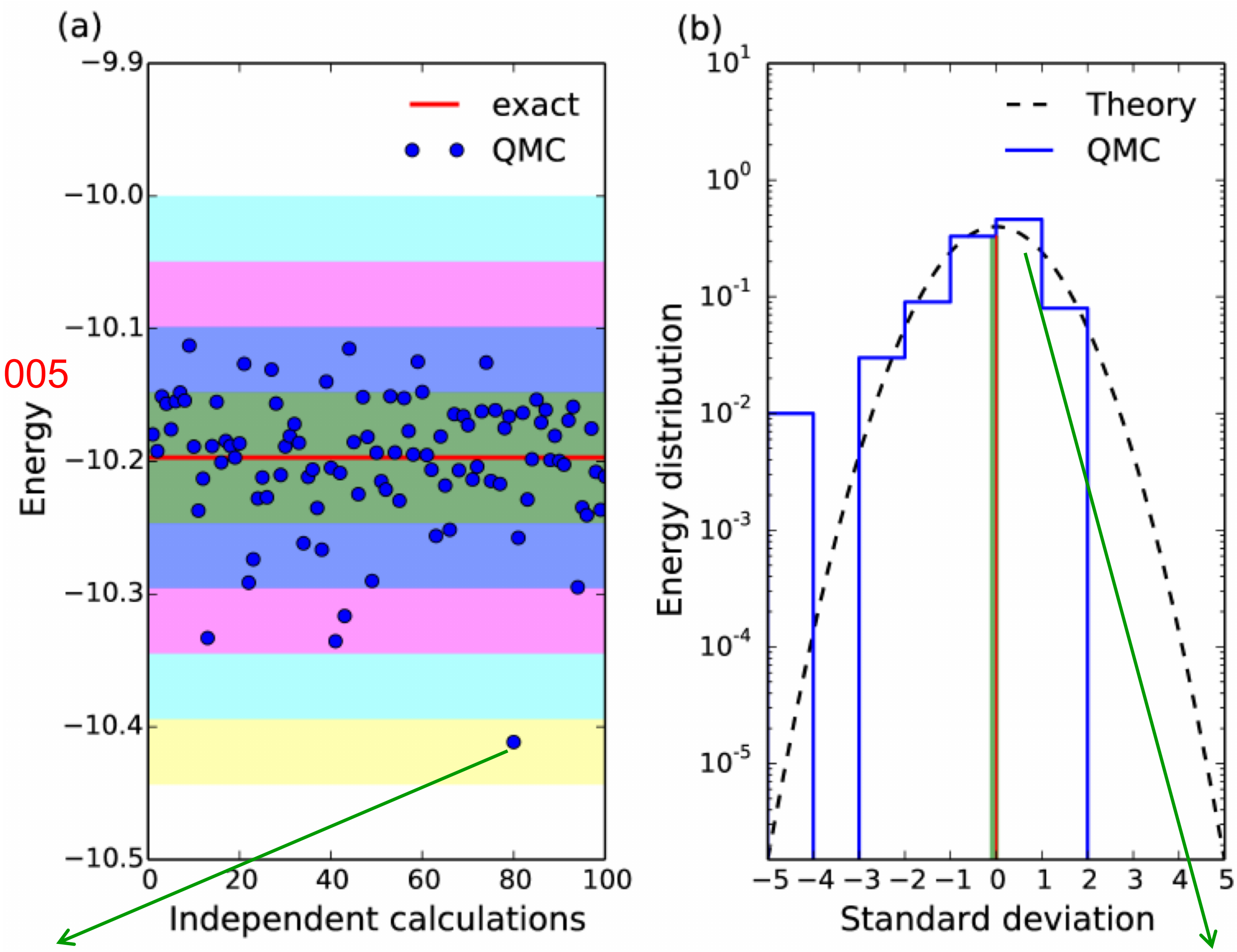

Less than 0.007%

chi-square 342.1

Hubbard model: 2x4 U=4 k=(0.03,0.02) β=81 Δτ =0.01

Infinite variance problem

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orthogonal

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$$W(X) \; \langle \phi^l(x_l) | \phi^r(x_r) \rangle \rightarrow 0$$ **orthogonal**

$$W(X) \; \langle \phi^l(x_l) | \hat{O} | \phi^r(x_r) \rangle \neq 0$$ **Quantum connection**

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Infinite variance problem

- General Multi-dimensional integral:

$$\langle \hat{O} \rangle = \frac{\int dX \; W(X) \; \langle \phi^l(x_l)|\phi^r(x_r)\rangle \frac{\langle \phi^l(x_l)|\hat{O}|\phi^r(x_r)\rangle}{\langle \phi^l(x_l)|\phi^r(x_r)\rangle}}{\int dX \; W(X) \; \langle \phi^l(x_l)|\phi^r(x_r)\rangle}$$

Diverge

- Sign problem free

$$W(X) \; \langle \phi^l(x_l)|\phi^r(x_r)\rangle \geqq 0$$

$$W(X) \; \langle \phi^l(x_l)|\phi^r(x_r)\rangle \rightarrow 0$$ **orthogonal**

$$W(X) \; \langle \phi^l(x_l)|\hat{O}|\phi^r(x_r)\rangle \neq 0$$ **Quantum connection**

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$$W(X)\ \langle \phi^l(x_l)|\phi^r(x_r)\rangle \to 0$$

orthogonal

$$W(X)\ \langle \phi^l(x_l)|\hat{O}|\phi^r(x_r)\rangle \neq 0$$

Quantum connection

zero is never sampled

how fast overlap approach zero?

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Simple Example

- One dimensional integral: sample $x/(\int_\alpha^1 dx\ x)$

$$y(\alpha) = \frac{\int_\alpha^1 x\ \frac{x+2}{x}\, dx}{\int_\alpha^1 x\, dx}$$

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- When a $\longrightarrow$ 0, $y(\alpha) \longrightarrow$ 5, variance will diverge as $-8\log(\alpha)$
- MC error bar will be unreliable!
- It's hard to see problem in a normal MC calculations.

block size	Mean value	Error bar
5000	5.0290	0.0227
20000	5.0104	0.0125

Infinite Variance I

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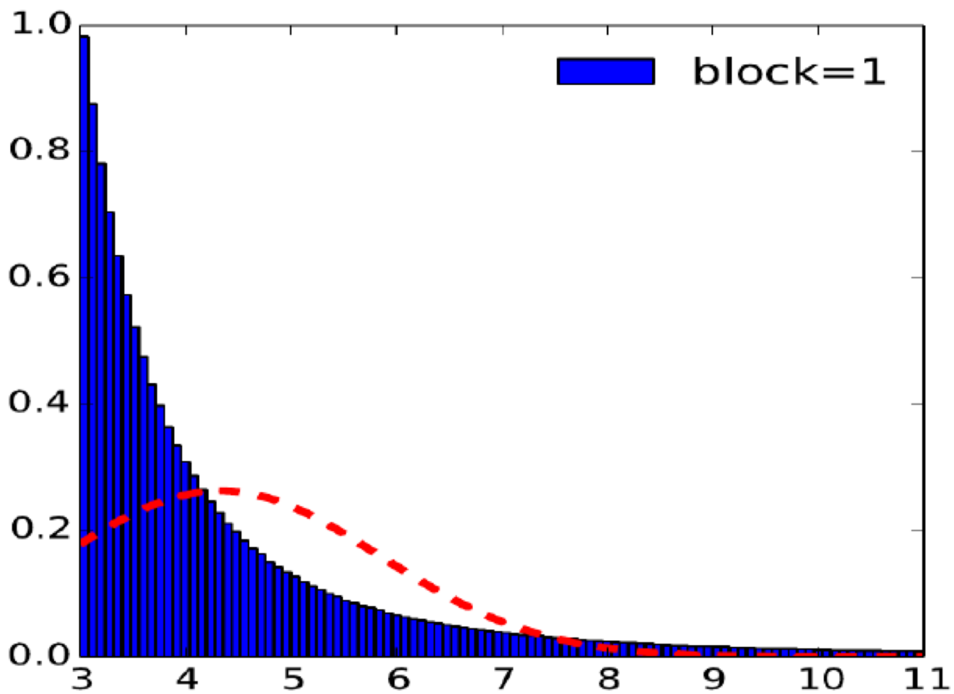
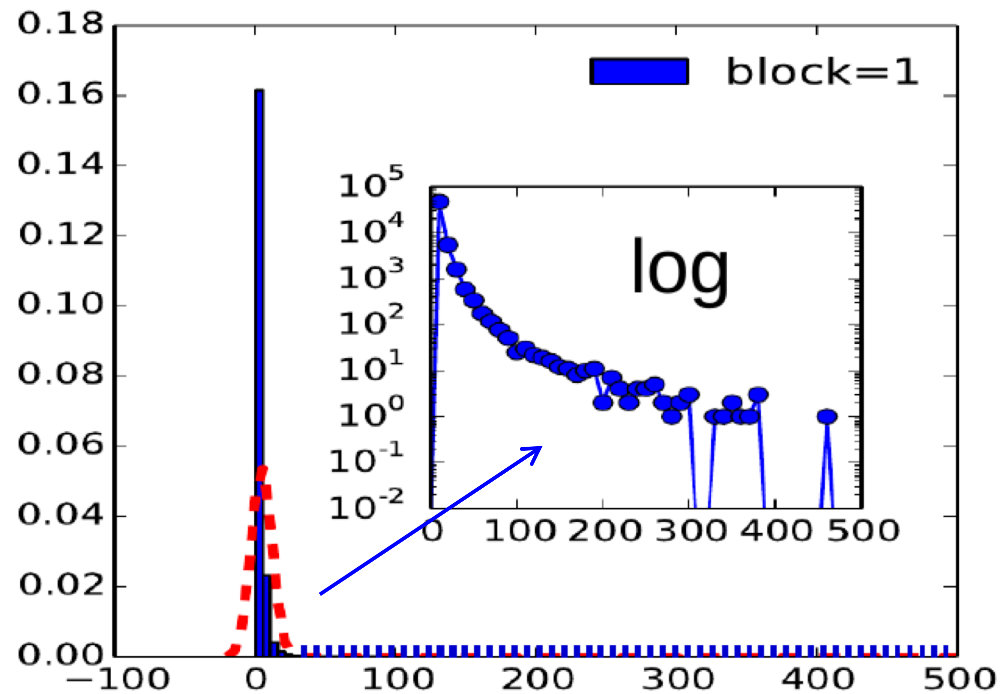
- Central limit theorem:
  - Finite variance: **Gaussian**
  - Infinite variance: **Not Gaussian**

Finite variance α=0.2



Infinite variance α=0.0



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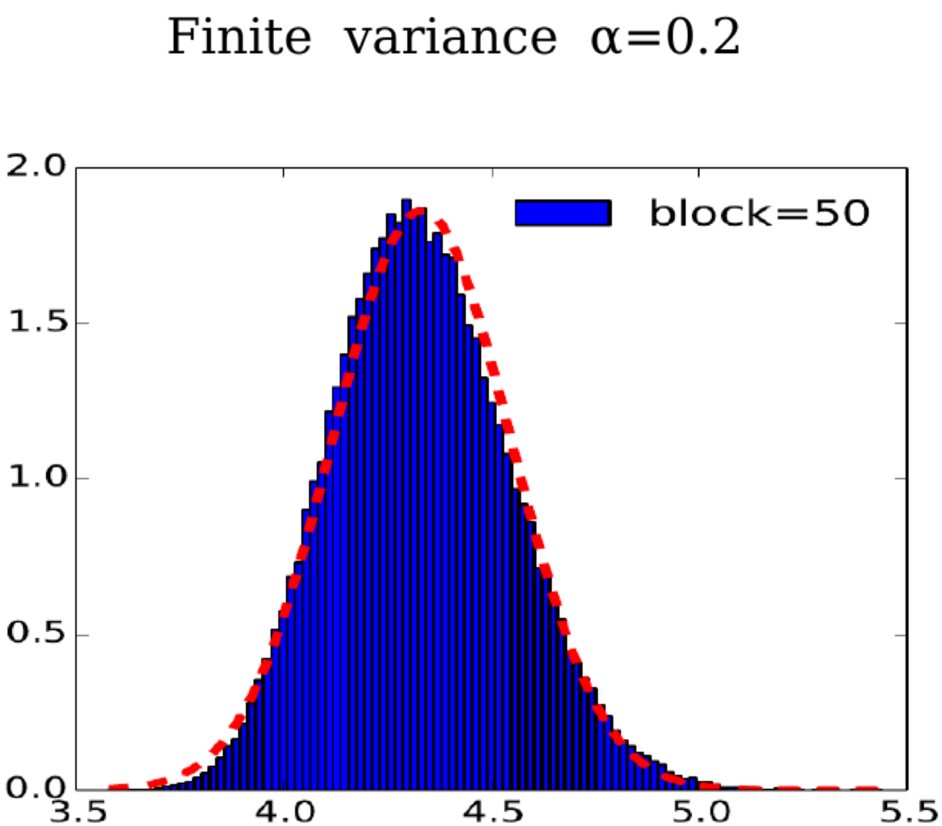

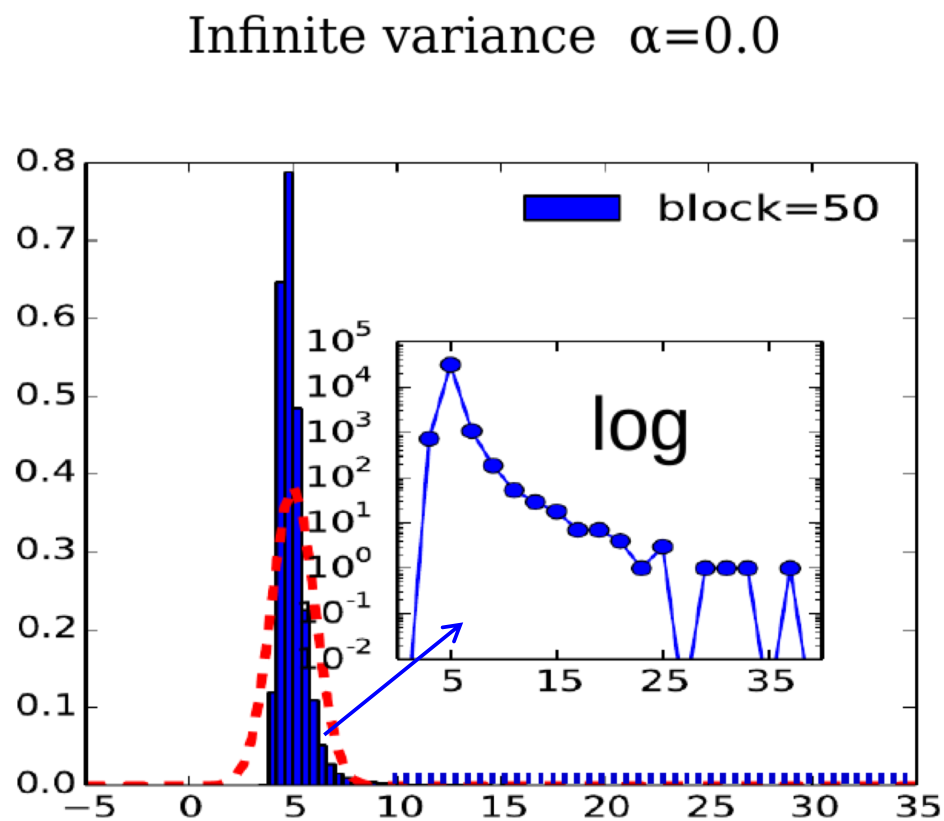

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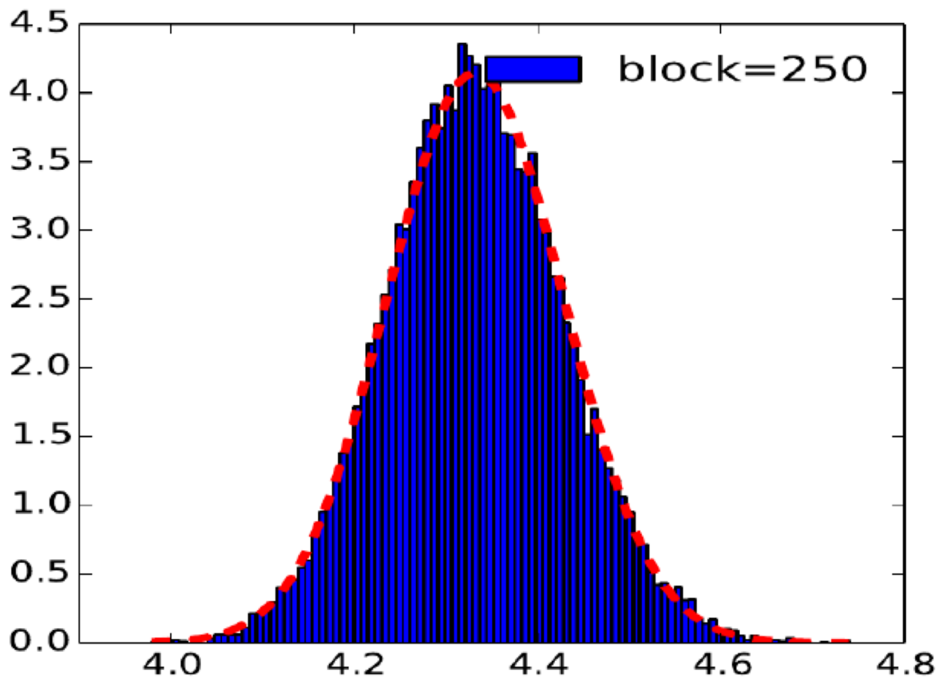

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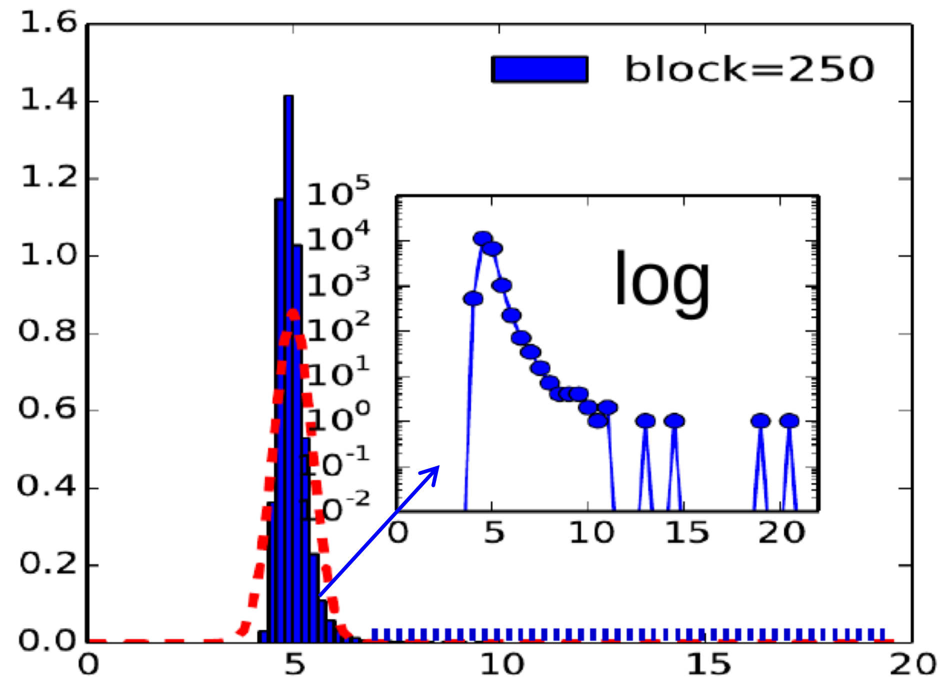

Infinite Variance II

- Measure standard deviation

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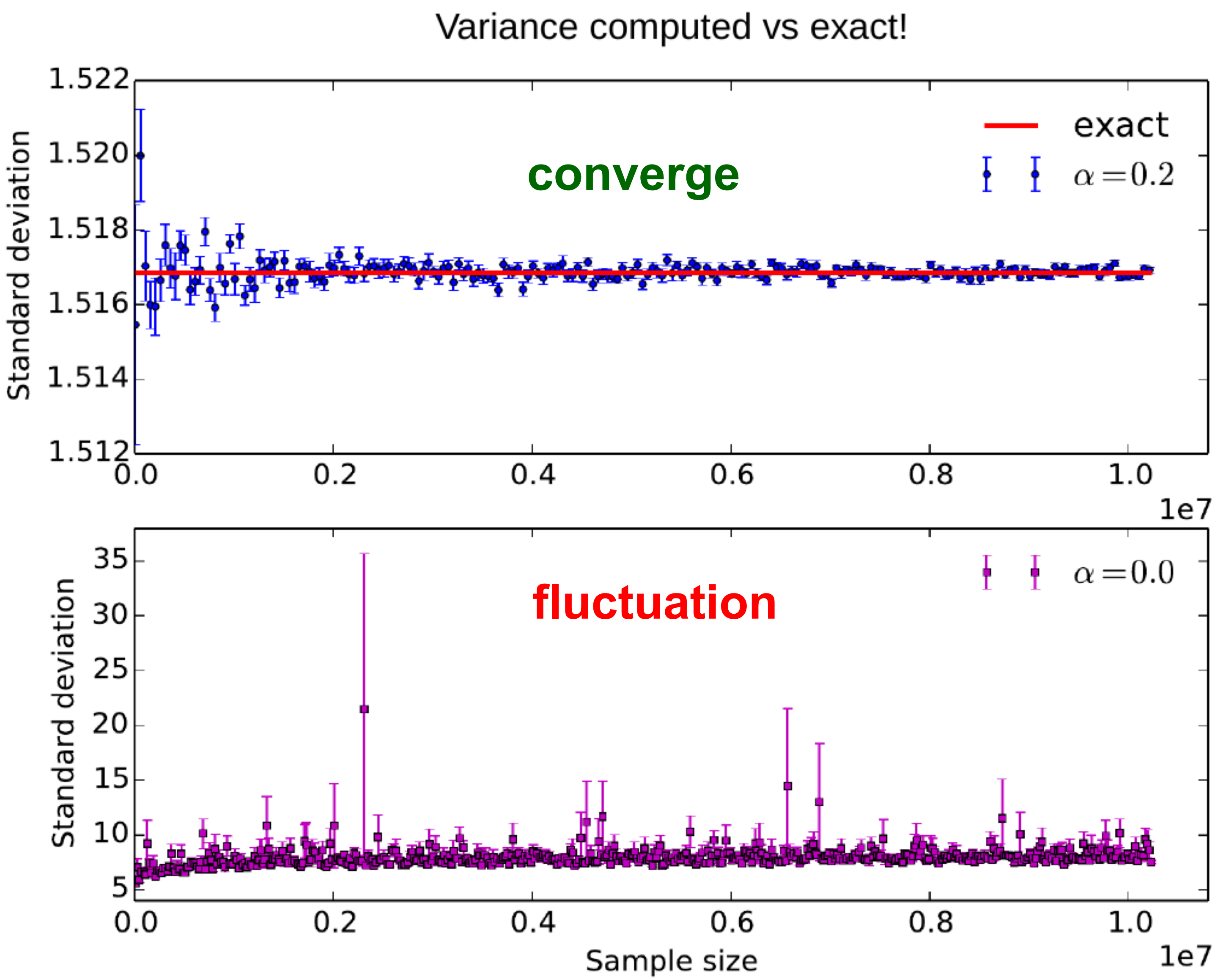

New Method to Control Variance

- Change the PDF:

$$\langle \phi^l(x_l) | \phi^r(x_r) \rangle + \Delta\tau \langle \phi^l(x_l) | \hat{O} | \phi^r(x_r) \rangle$$

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$$\Downarrow$$

$$\langle \phi^l(x_l)|1 + \Delta\tau\hat{O}|\phi^r(x_r)\rangle$$

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$$\langle \phi^l(x_l) | 1 + \Delta\tau \hat{O} | \phi^r(x_r) \rangle$$

$$\Downarrow$$

$$\langle \phi^l(x_l) | \exp(\Delta\tau \hat{O}) | \phi^r(x_r) \rangle$$

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$$\langle\phi^l(x_l)|1+\Delta\tau\hat{O}|\phi^r(x_r)\rangle$$

$$\Downarrow$$

$$\langle\phi^l(x_l)|\exp(\Delta\tau\hat{O})|\phi^r(x_r)\rangle$$

$$\Downarrow$$

$$\langle\phi^l(x_l)|\exp(\Delta\tau\hat{H})|\phi^r(x_r)\rangle$$

New Method to Control Variance

- Change the PDF:

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- For auxiliary field QMC:

$$\langle \psi_T | \hat{B}(x_1) \ldots \hat{B}(x_{L/2}) \exp(\Delta\tau \hat{H}) \hat{B}(x_{L/2+1}) \ldots \hat{B}(x_L) | \psi_T \rangle$$

New Method to Control Variance

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$\hat{B}(x_{L/2}) \rightarrow \exp(-\Delta\tau\hat{H})$

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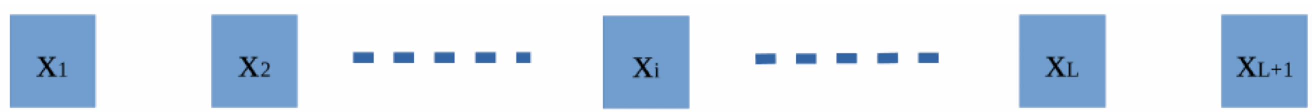
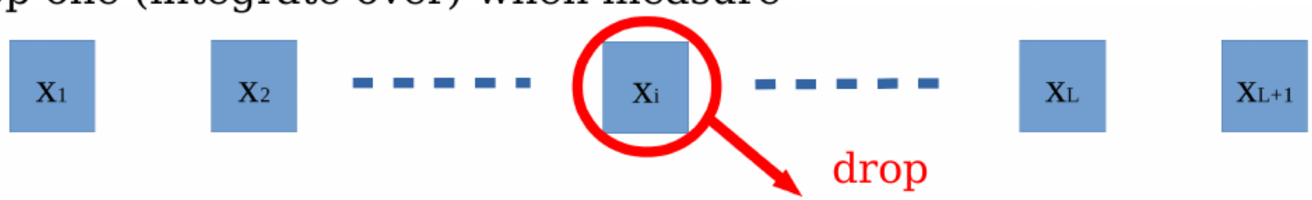
- Conveniently implemented in path integral:

-Sample L+1 slices



-Drop one (integrate over) when measure

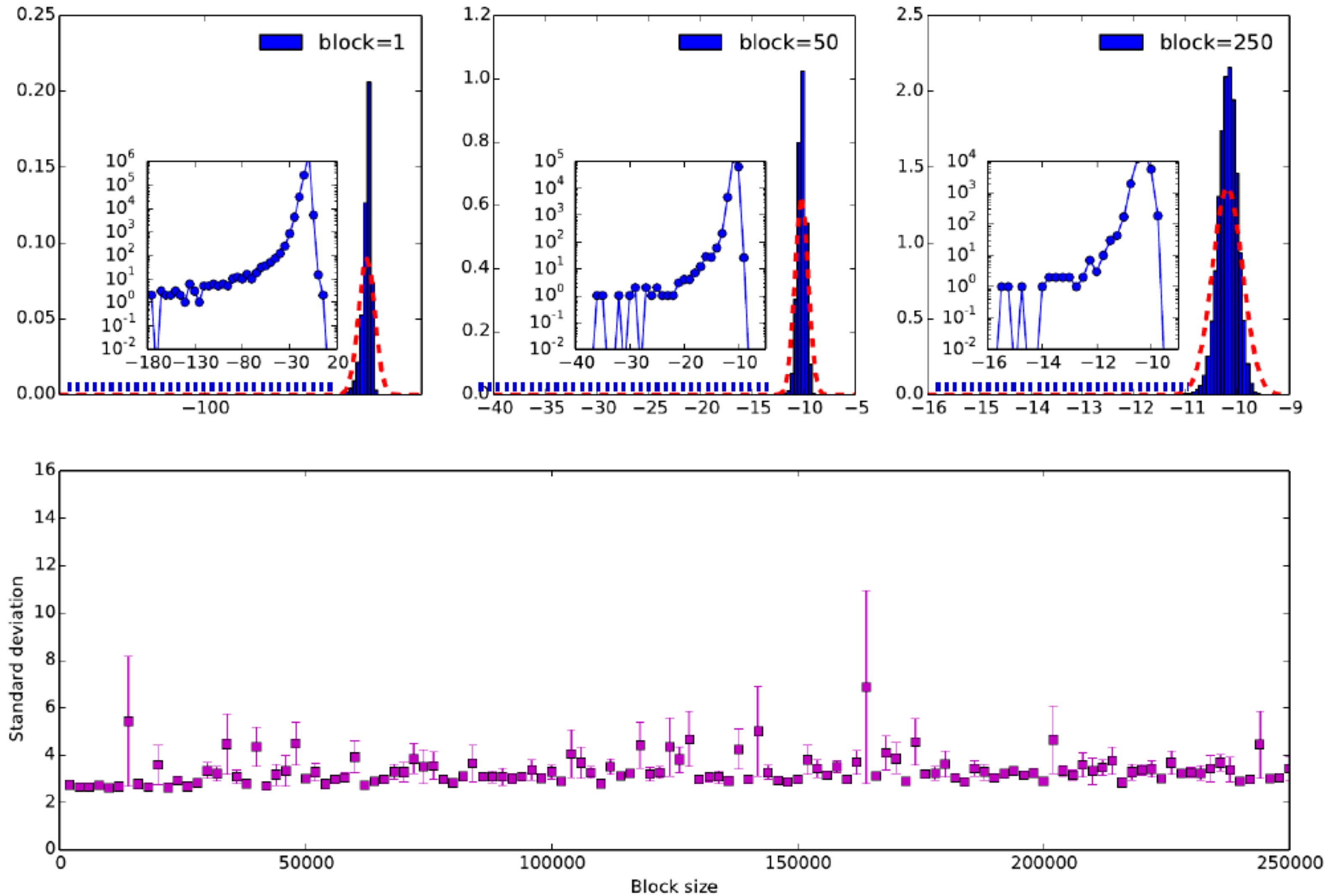


-Dropped link is dynamic

Apply the New Method

Hubbard model:
2x4
U=4 k=(0.03,0.02)
β=81
Δτ =0.01

Before:



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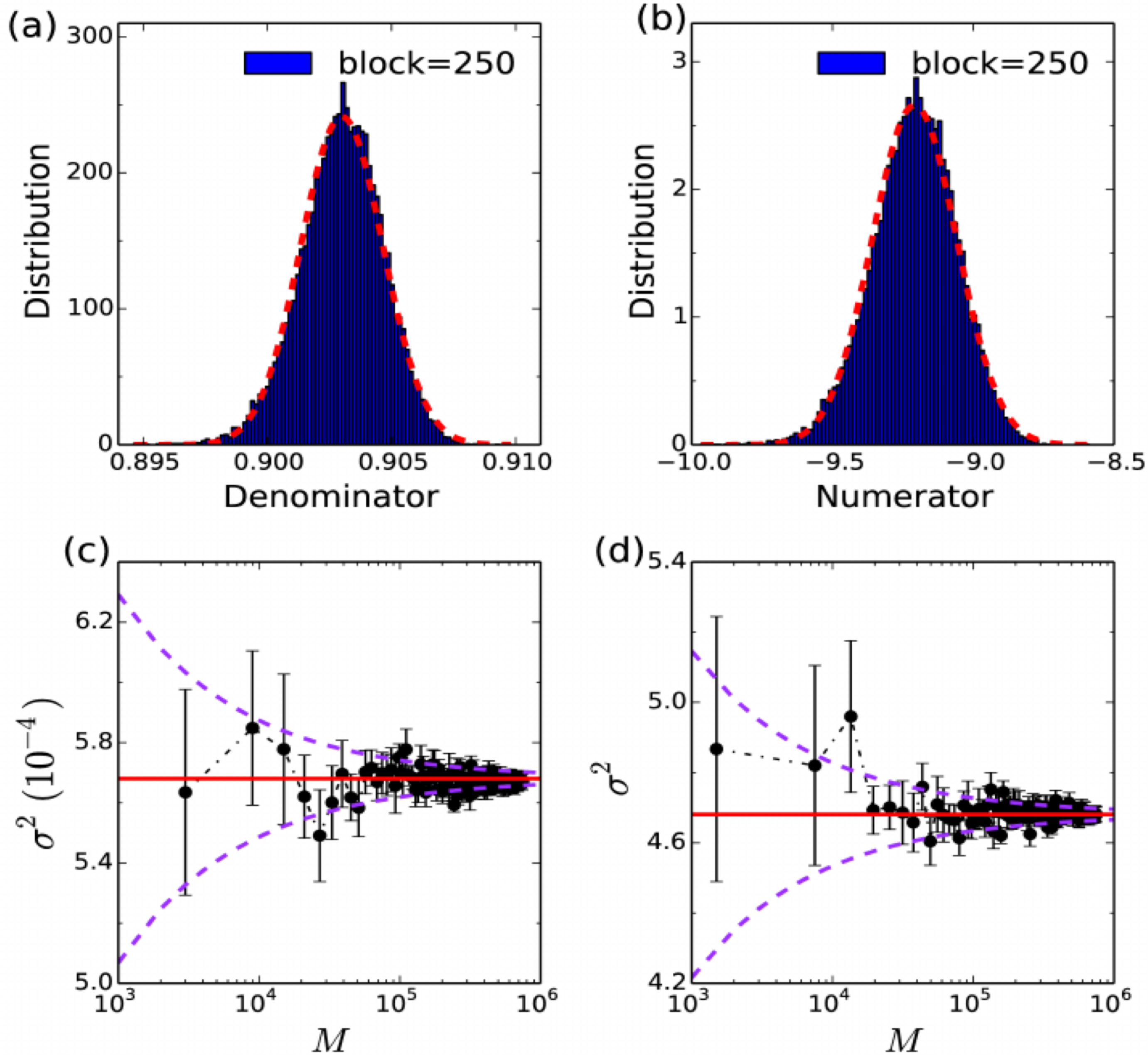
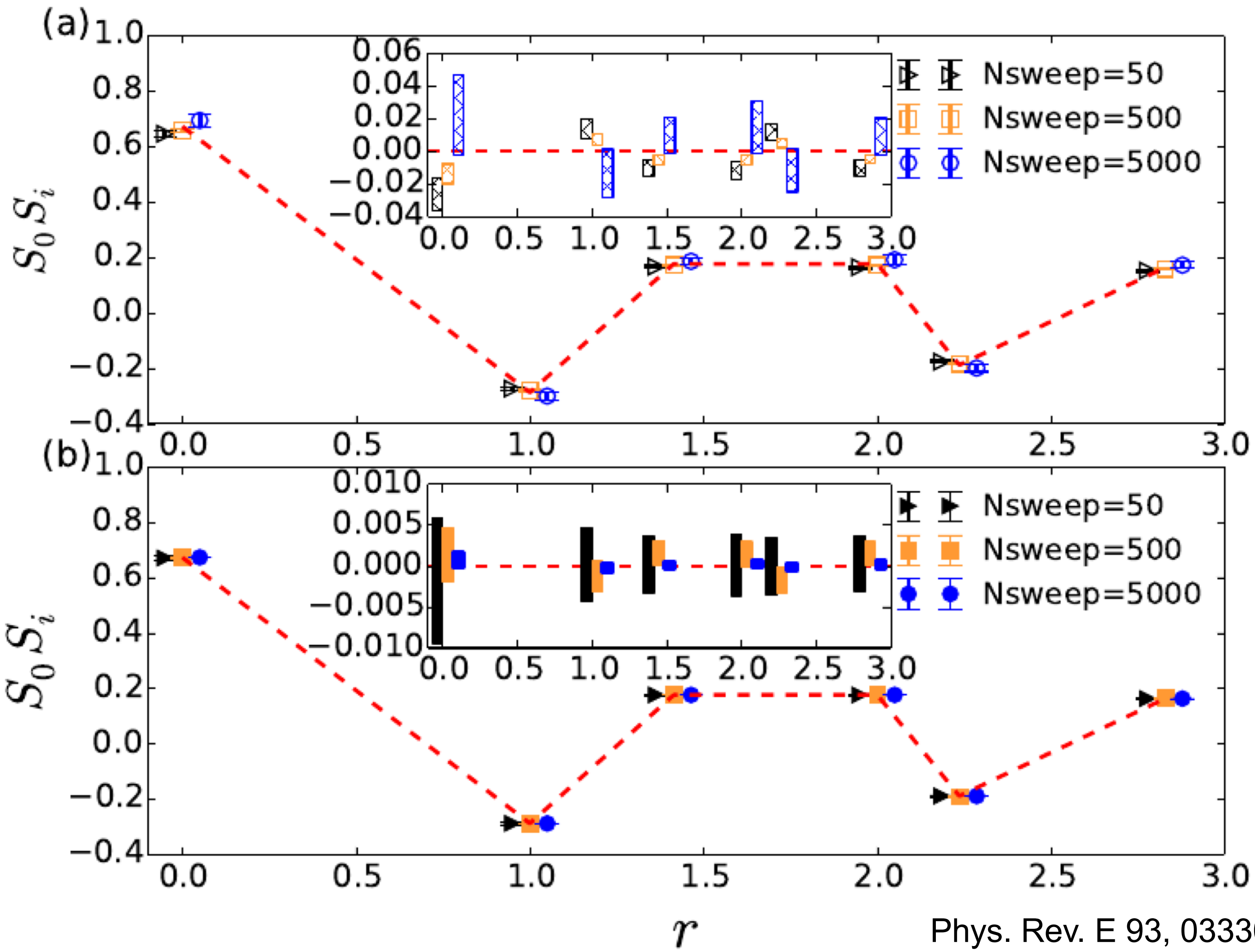


Application

- Spin-spin correlation, reduce error bar

4x4
U=8t
N=16



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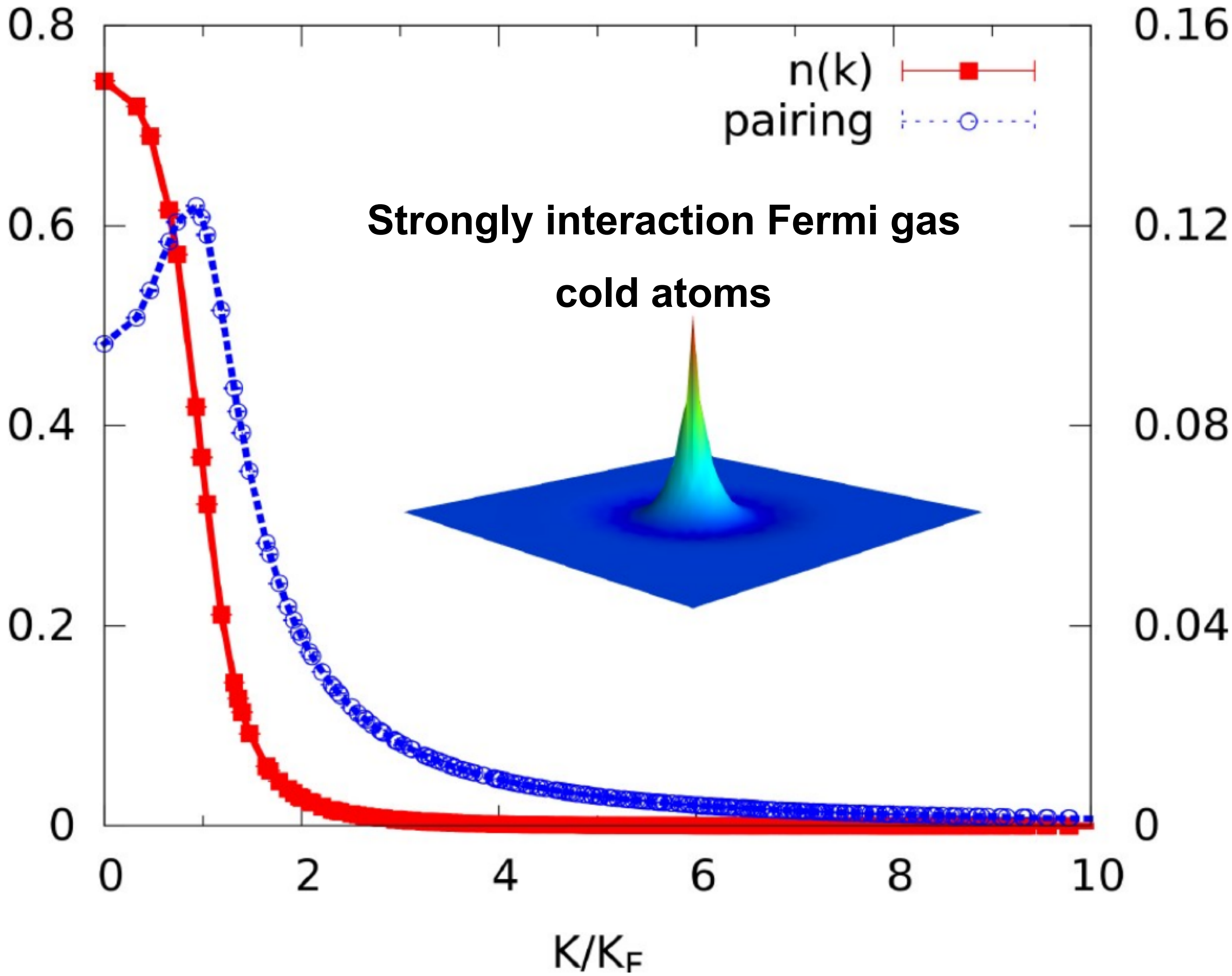
Application

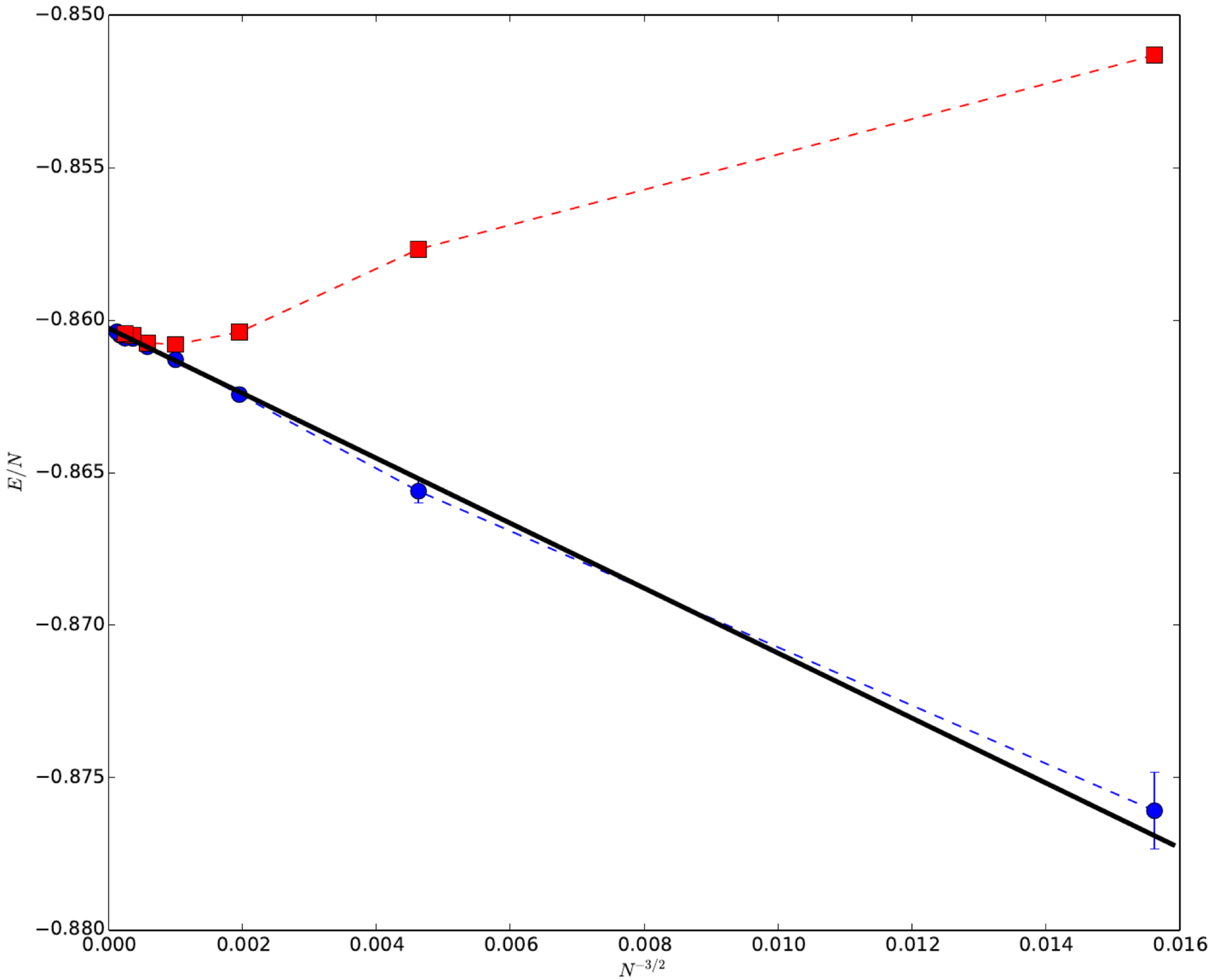
- large system, large interaction and long β

45x45
N=58
β=320
Δτ=0.025



Application

- Hubbard Model Half-filling **Thermodynamic Limit**



U=4

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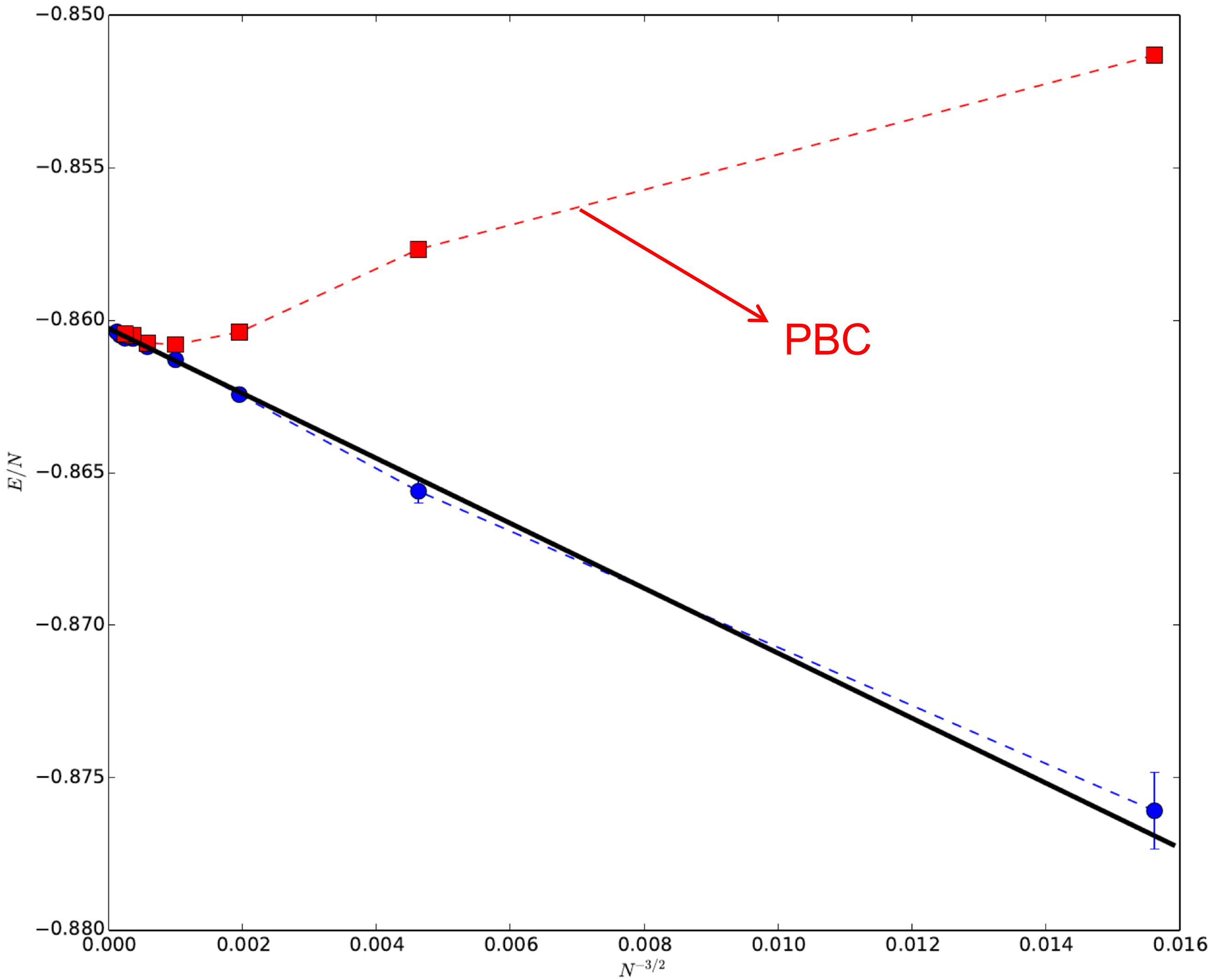

U=4

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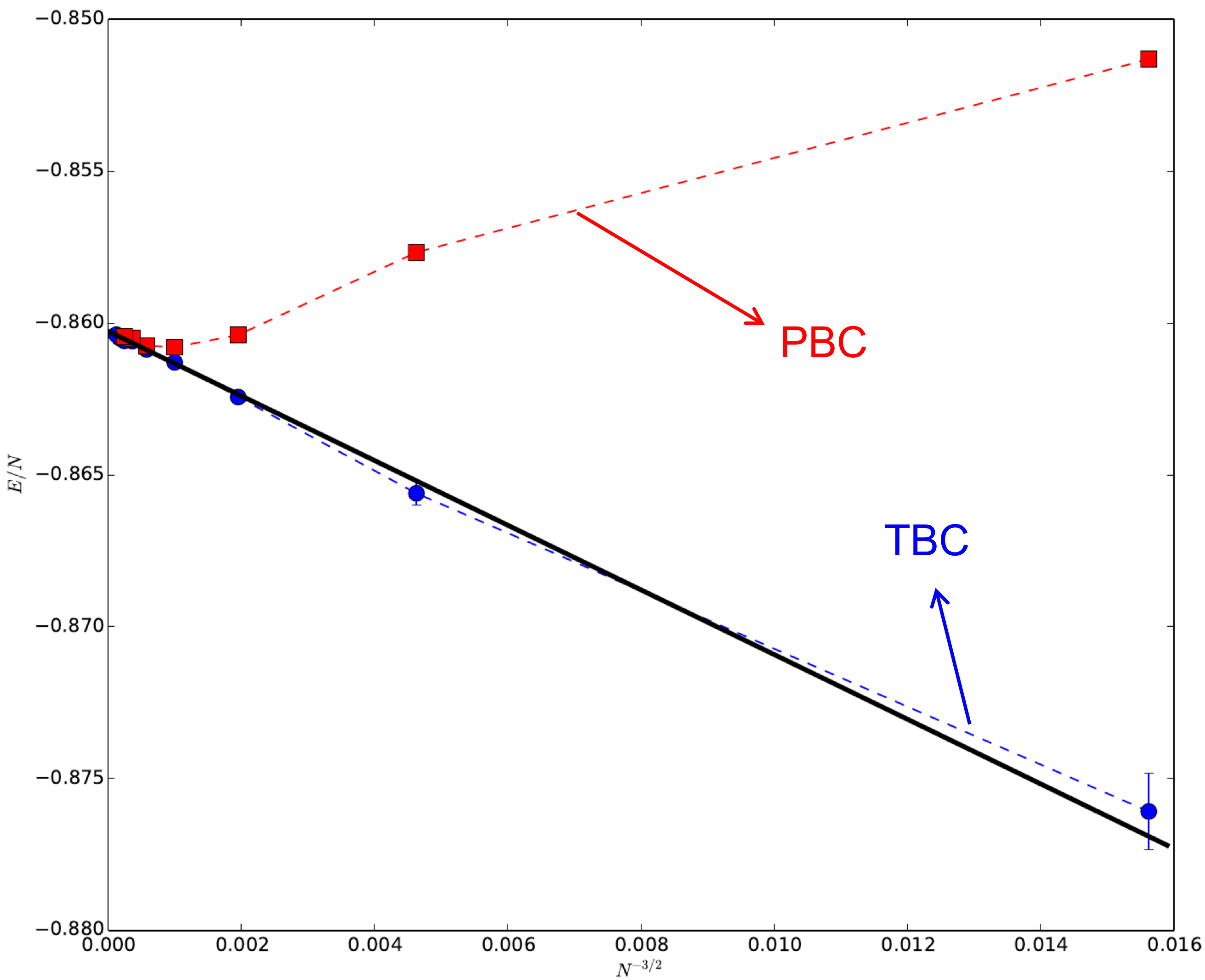

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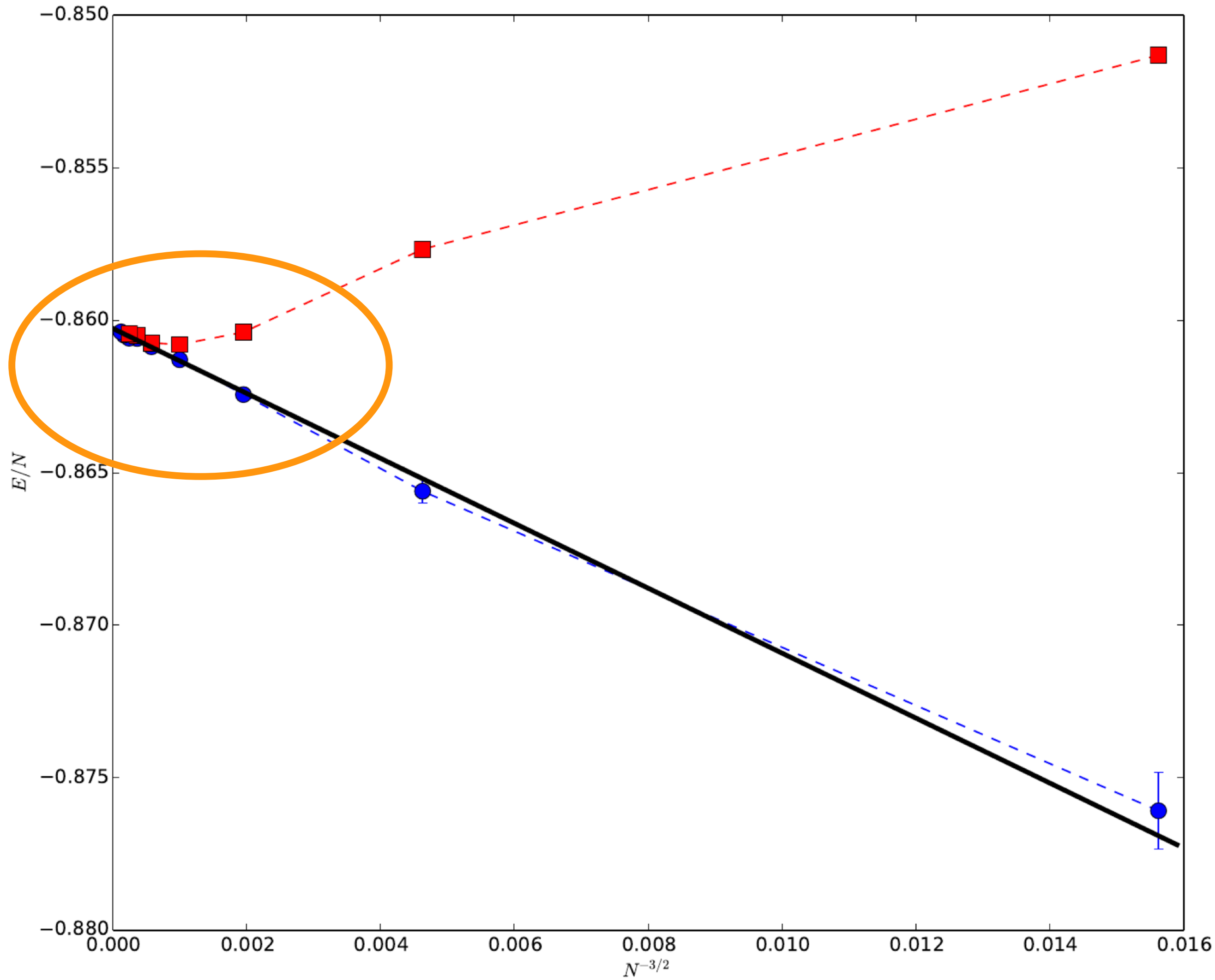

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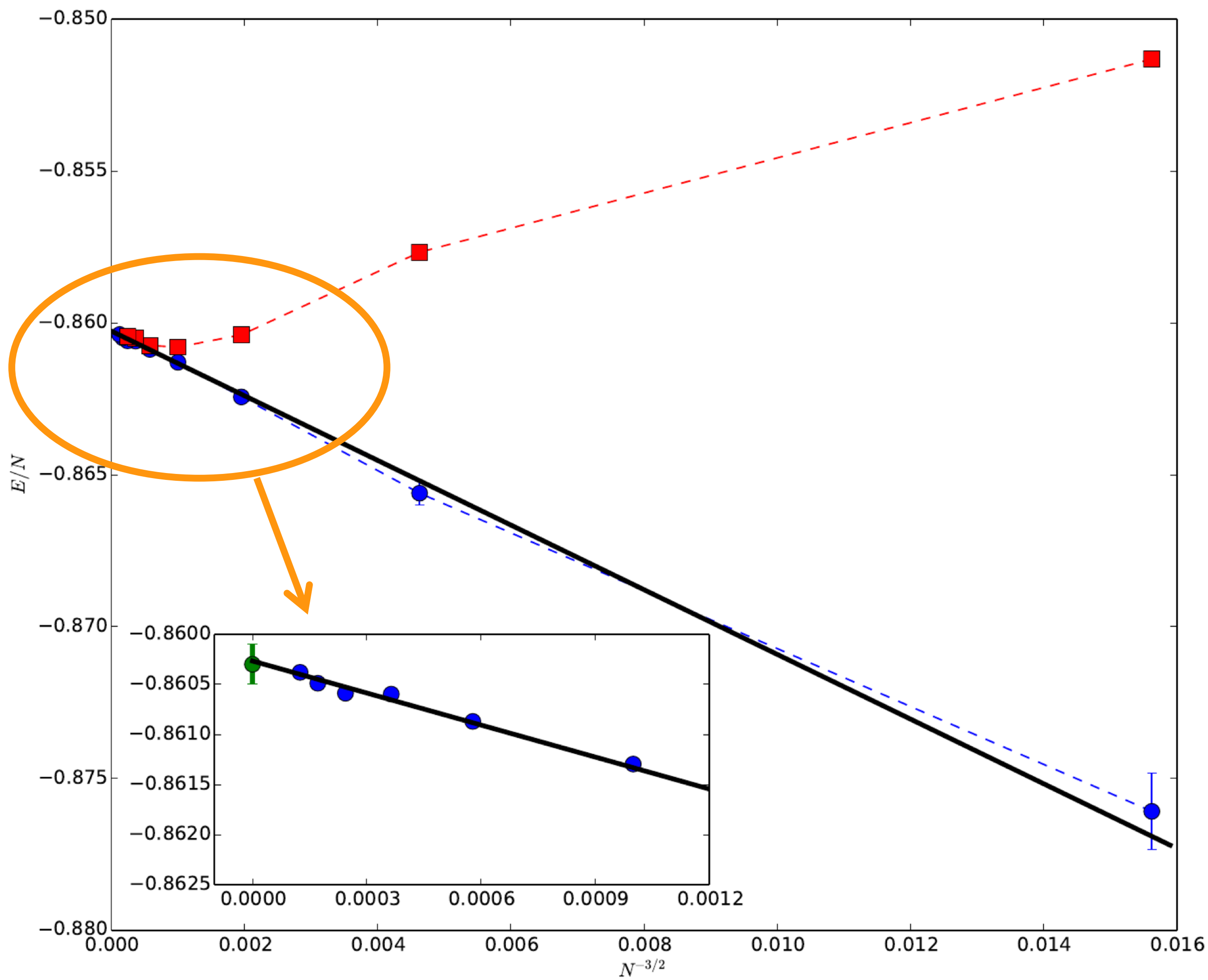

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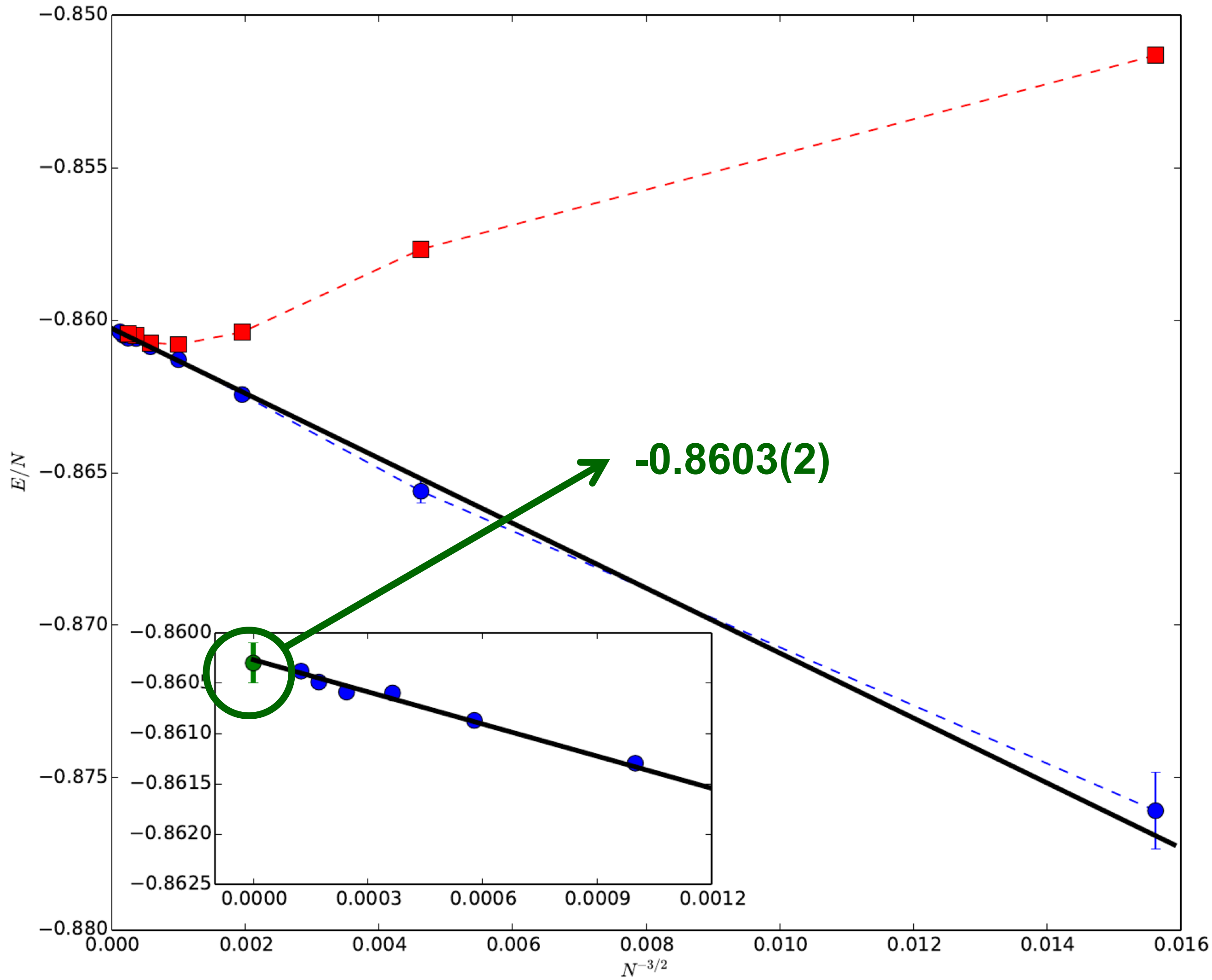

U=4

Conclusion

- There is an infinite variance problem in standard determinantal QMC.

- A method is proposed to eliminate the problem.

- The issues are very general. Our approach applies to other MC methods.

When sign problem is present, we usually have infinite variance problem.