A solution for infinite variance problem of fermionic observables

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based on *"Infinite variance problem in fermion models"*
Phys. Rev. D **107**, 094502 (2022)

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Auxiliary Field for Fermionic Monte Carlo

- For fermionic quartic interactions, we use the Hubbard-Stratonovich(HS) transformation for Monte Carlo calculation

$$\int d\bar{\eta} d\eta \, e^{-\bar{\eta} M \eta} = \det M \rightarrow \text{No more Grassmann}$$

- Two ways:

1. Discrete

$$\exp[-\hat{n}_\uparrow \hat{n}_\downarrow] \propto \sum_{\sigma=\pm 1} \exp[2a\sigma(\hat{n}_\uparrow - \hat{n}_\downarrow) - \frac{1}{2}(\hat{n}_\uparrow + \hat{n}_\downarrow)]$$

2. Continuous

$$\exp[\frac{1}{2}\hat{X}^2] \propto \int d\phi \exp[-\frac{1}{2}\phi^2 - \phi\hat{X}]$$

J. Hirsch, Phys. Rev. B **28**, 4059(R) (1983)

Continuous Auxiliary Field is Needed

Hybrid Monte Carlo

- Higher acceptance rate
- Minimize correlation

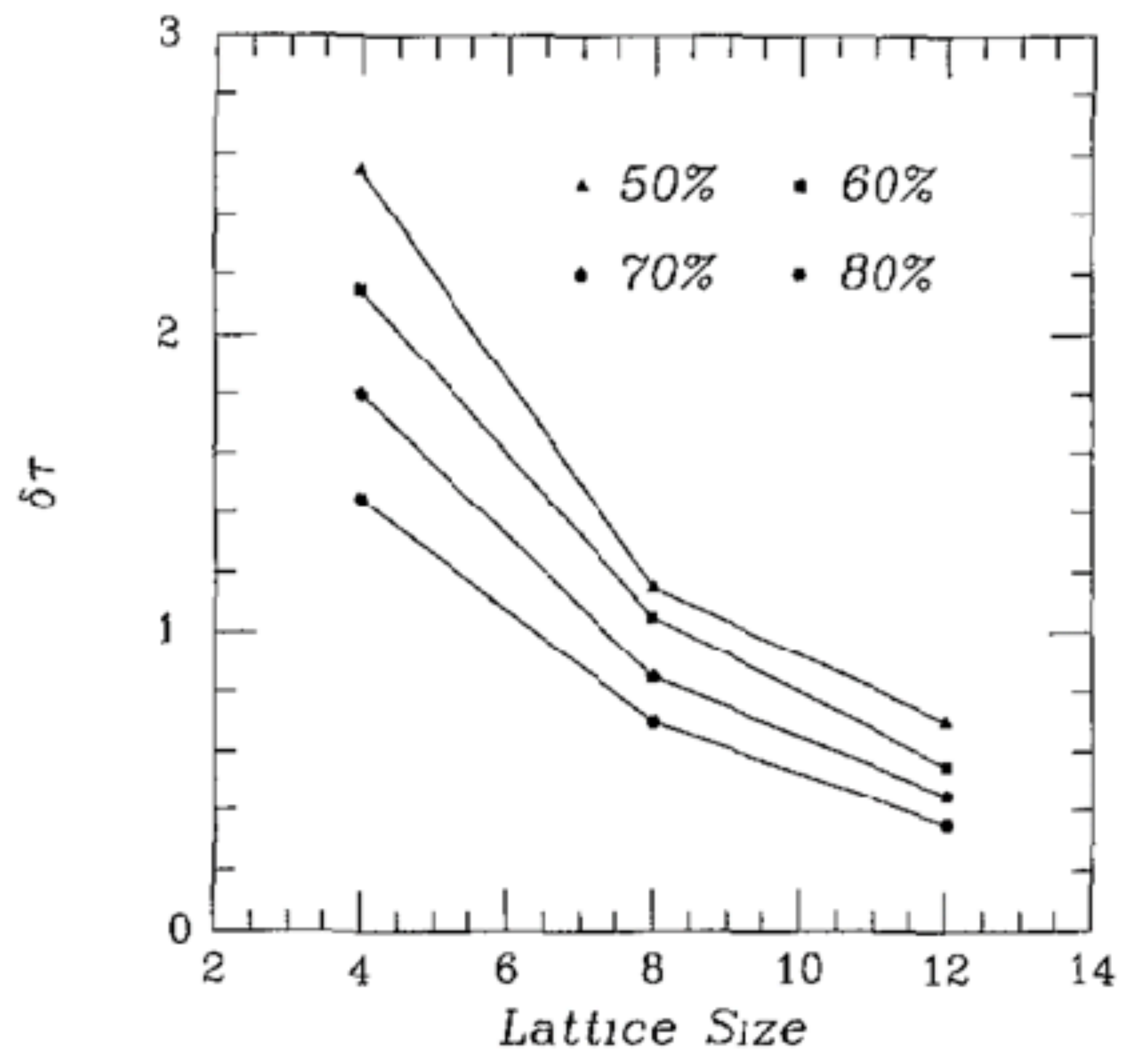
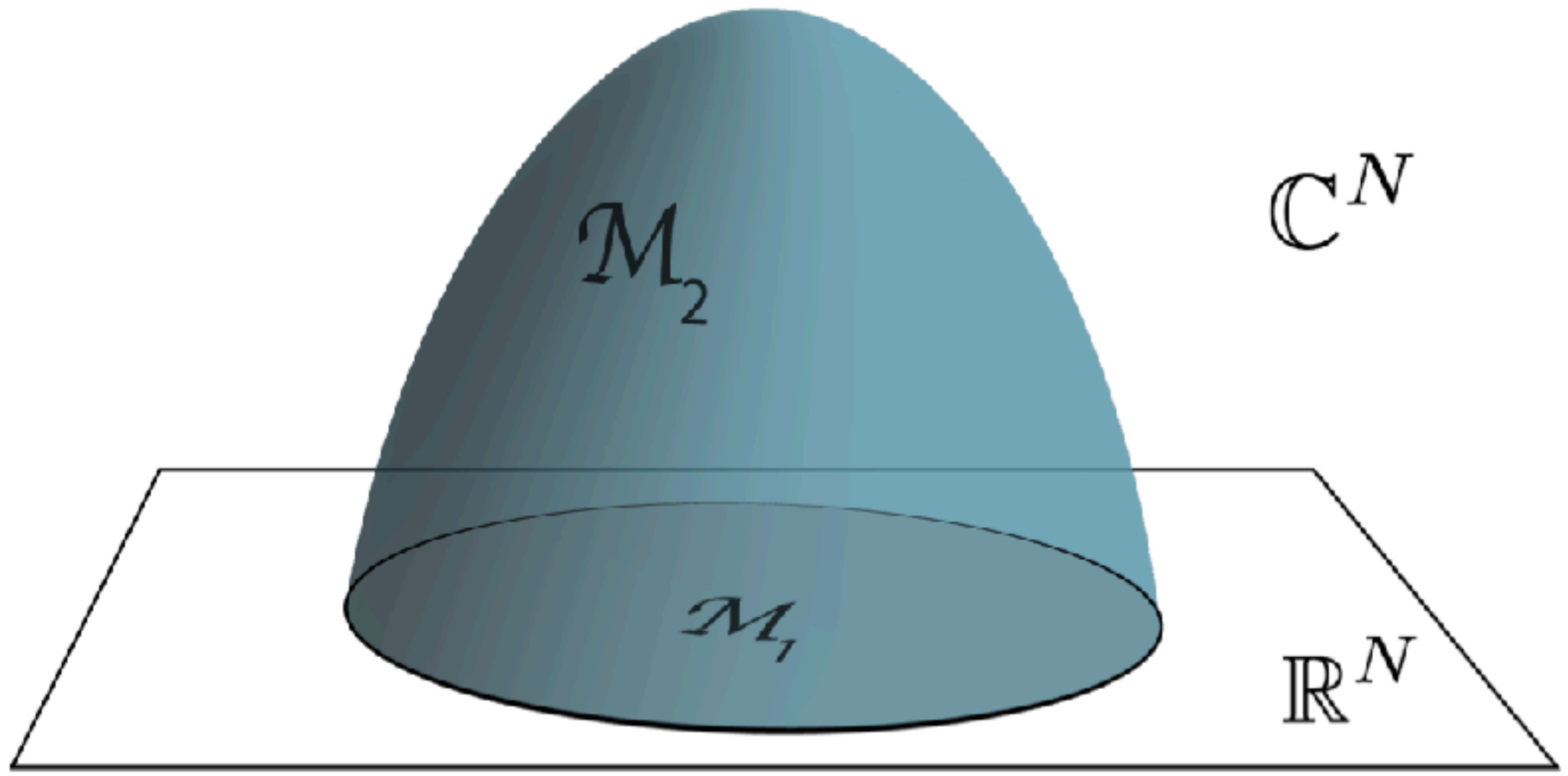


Fig 2 Curves of constant acceptance rate are shown as a function of the integration step size $\delta\tau$ on the lattices of size 4^4, 8^4 and 12^4 in quenched QED at a coupling of $\beta = 0.97$.

Sign Problem

- **Contour deformation approach**



S. Duane et al, Phys. Lett. B. 195 (1987)

A. Alexandru et al, Rev. Mod. Phys. **94**, 015006 (2022)

Test Continuous Auxiliary Field

- Hubbard Model Hamiltonian with half-filling at $\mu = 0$:

$$H = \underbrace{-\kappa \sum_{\langle x,y \rangle} (\hat{\psi}^\dagger_{\uparrow,x}\hat{\psi}_{\uparrow,y} + \hat{\psi}^\dagger_{\downarrow,x}\hat{\psi}_{\downarrow,y})}_{\text{hopping}} + \underbrace{U \sum_x (\hat{\psi}^\dagger_{\uparrow,x}\hat{\psi}_{\uparrow,x} - \frac{1}{2})(\hat{\psi}^\dagger_{\downarrow,x}\hat{\psi}_{\downarrow,x} - \frac{1}{2})}_{\text{interaction}} - \underbrace{\mu \sum_x (\hat{\psi}^\dagger_{\uparrow,x}\hat{\psi}_{\uparrow,x} + \hat{\psi}^\dagger_{\downarrow,x}\hat{\psi}_{\downarrow,x} - 1)}_{\text{chemical potential}}$$

- We will first consider the $\mu = 0$ case, sign problem-free.

Path Integral Formulation

- Fermion coherent state formalism:

$$\mathrm{Tr}(e^{-\beta H}) = \int d\bar{\eta} d\eta \, e^{-\bar{\eta}\eta} \langle -\eta \,|\, e^{-\beta H} \,|\, \eta \rangle$$

$$= \int [d\bar{\eta} d\eta]_N \, e^{-\bar{\eta}\eta} \langle \eta_N \,|\, e^{-\epsilon H} \,|\, \eta_{N-1} \rangle \cdots \langle \eta_1 \,|\, e^{-\epsilon H} \,|\, \eta_0 \rangle \text{ with } \beta = \epsilon N$$

- The effective action:

$$S = S_0(\phi) - \log \det M_1(\phi) M_2(\phi) \text{ with } S_0(\phi) = -\beta \sum_{i=1}^{N} \cos(\phi_i)$$

common form (BSS)

$$M_a(\phi) = \mathbf{1} + B_a(\phi_N) \cdots B_a(\phi_1)$$

Monte Carlo Method

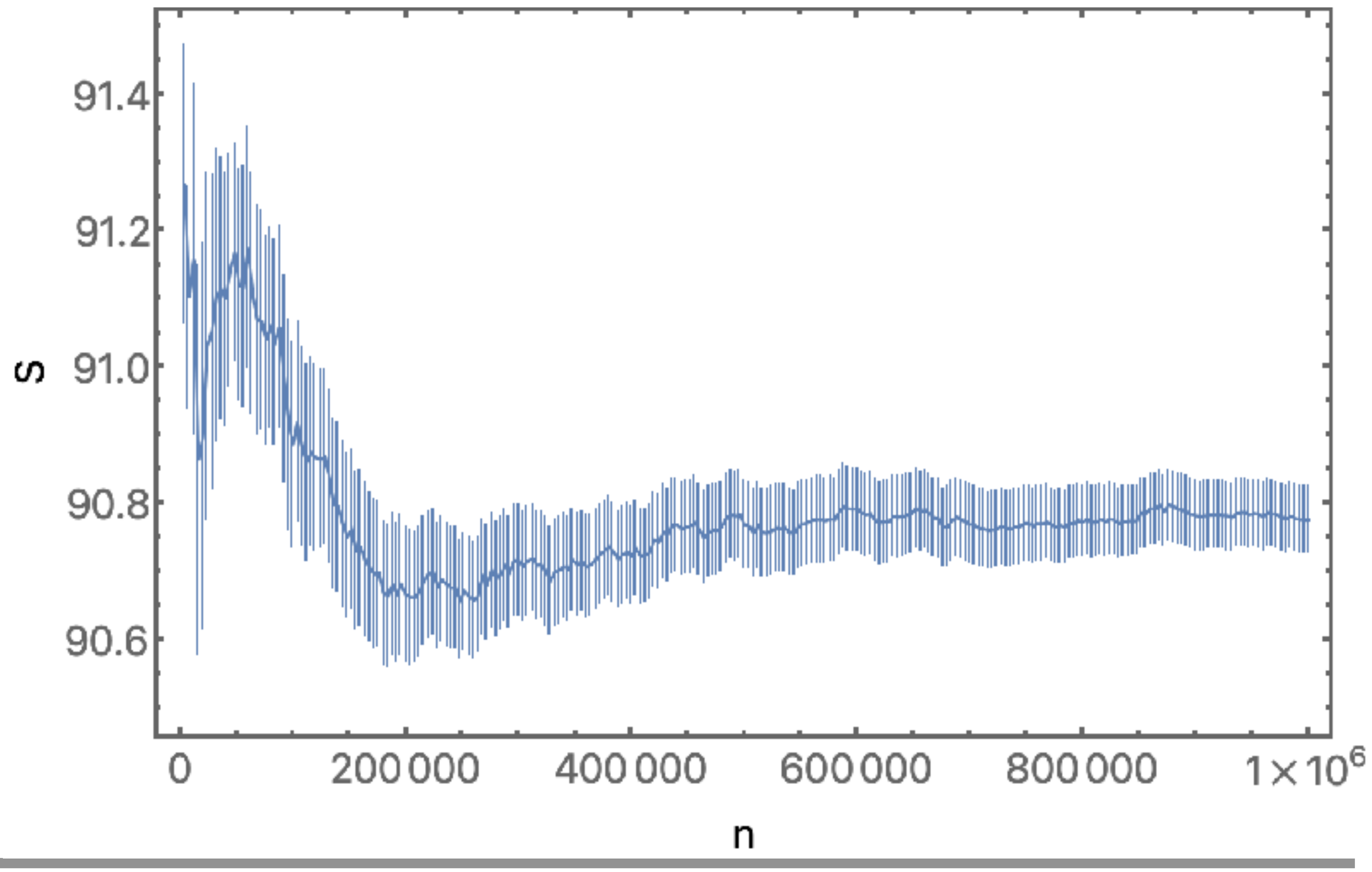
- With the importance sampling,

$$\bar{\mathcal{O}} = \int \mathcal{D}\phi \, \mathcal{O}(\phi) \frac{e^{-S[\phi]}}{\int \mathcal{D}\phi \, e^{-S[\phi]}} \simeq \frac{1}{n} \sum_{a=1}^{n} \mathcal{O}(\phi_a)$$

- As the number of samples increases,

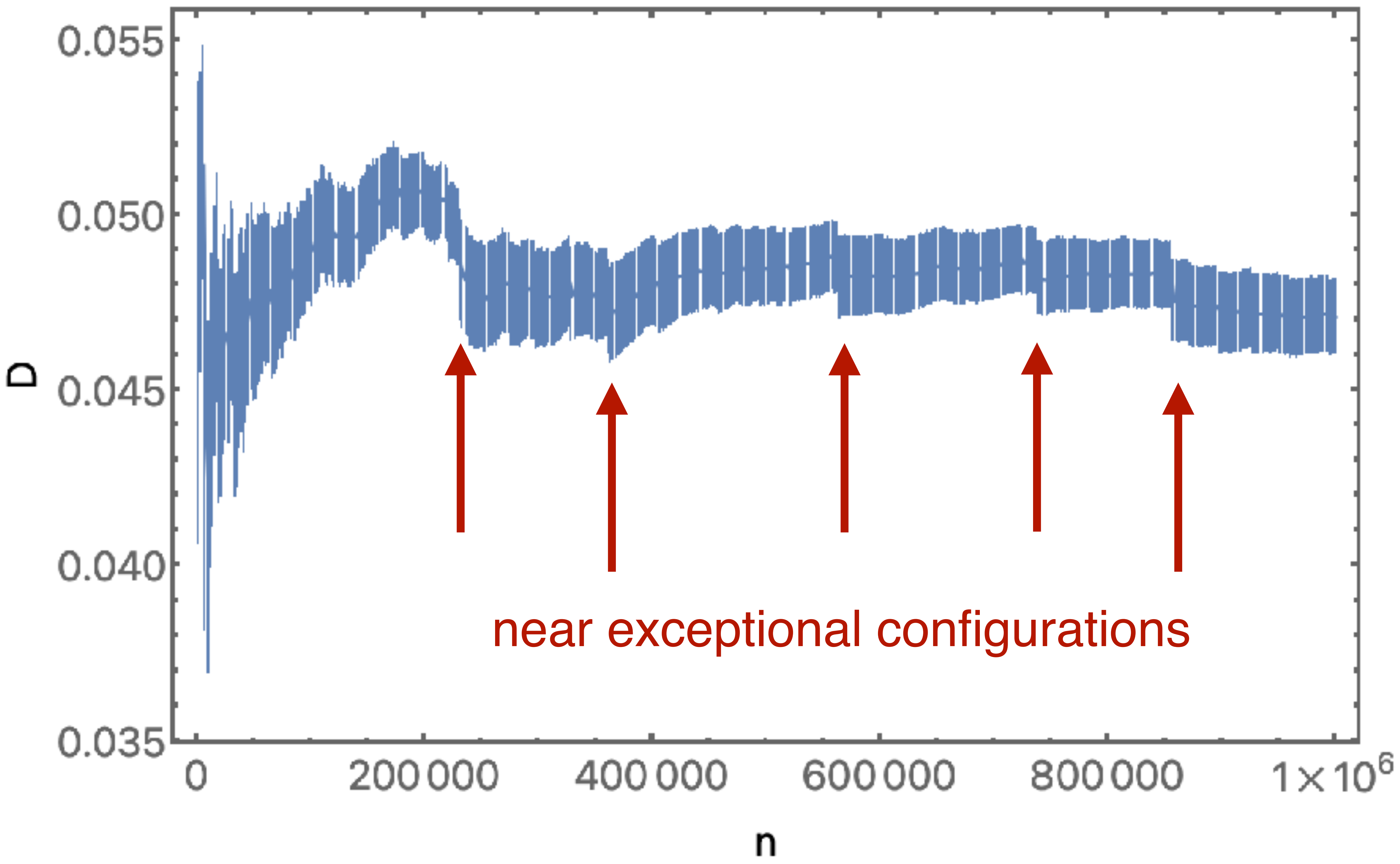
$$\bar{\mathcal{O}} = \langle \mathcal{O} \rangle + O(\frac{1}{\sqrt{n}})$$

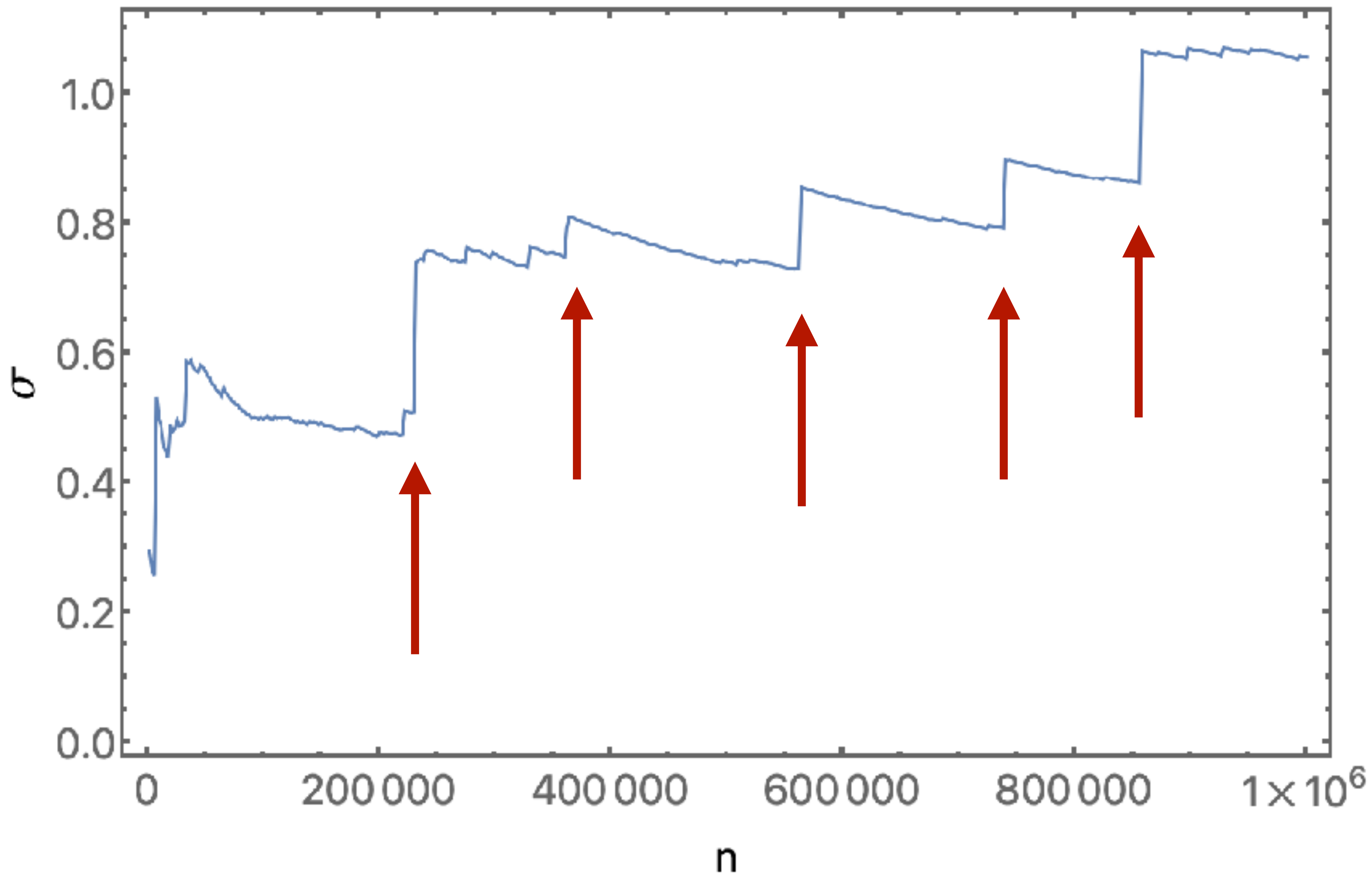
Number of samples



Infinite Variance Problem

- Error bar doesn't decrease / Variance doesn't converge

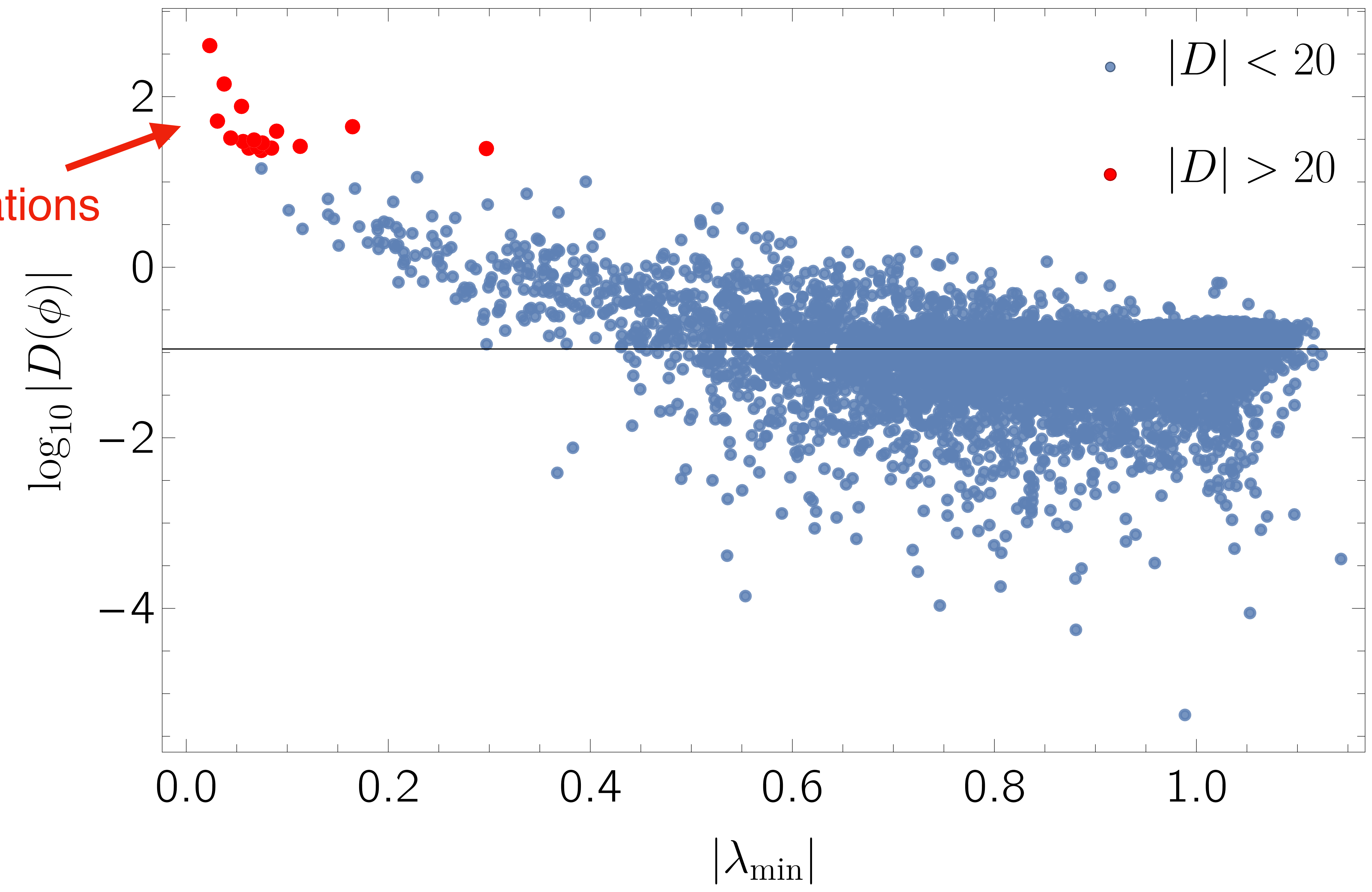




Determinant and Diverging Variance

- Monte Carlo sampling cannot choose $\det M = 0$ configuration, but the neighborhood of zero points is dangerous

Near exceptional configurations



A. Alexandru, P. Bedaque, A. Carosso, HO, Phys. Rev. D **107**, 094502 (2022)

Infinite Variance Problem

- For a fermionic observable $\mathcal{O}$,

$$\mathcal{O}(\phi) \sim \frac{1}{\det M} f(M_{ij}(\phi))\text{: large near } \det M = 0$$

- Expectation value is finite:

$$\langle \mathcal{O} \rangle \sim \int D\phi \, \mathrm{e}^{-S_0(\phi)} \det M \frac{1}{\det M} f(M_{ij}(\phi))$$

- Variance can be divergent:

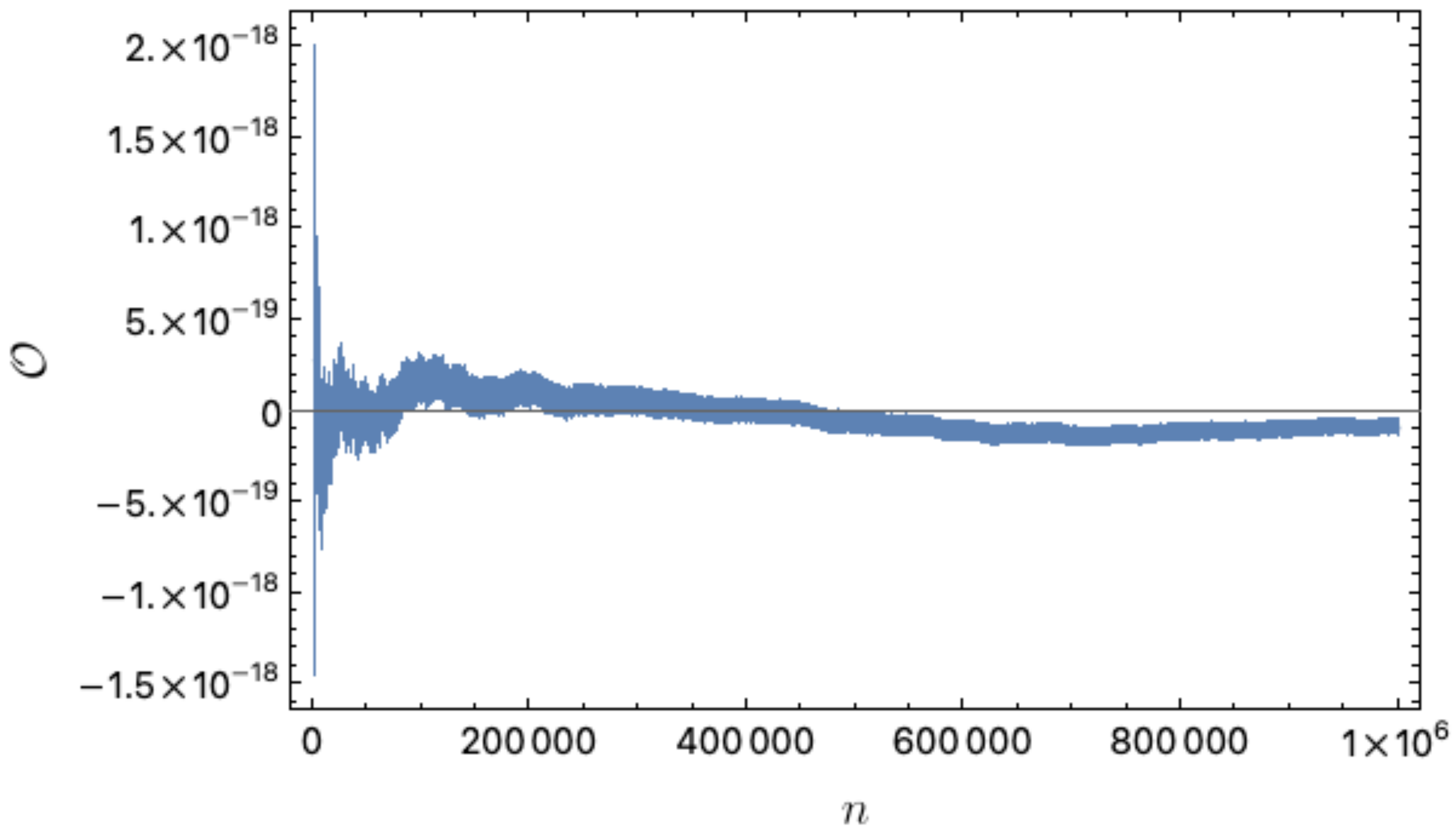
$$\langle \mathcal{O}^2 \rangle \sim \int D\phi \, \mathrm{e}^{-S_0(\phi)} \det M \frac{1}{(\det M)^2} f^2(M_{ij}(\phi)) \to \infty$$

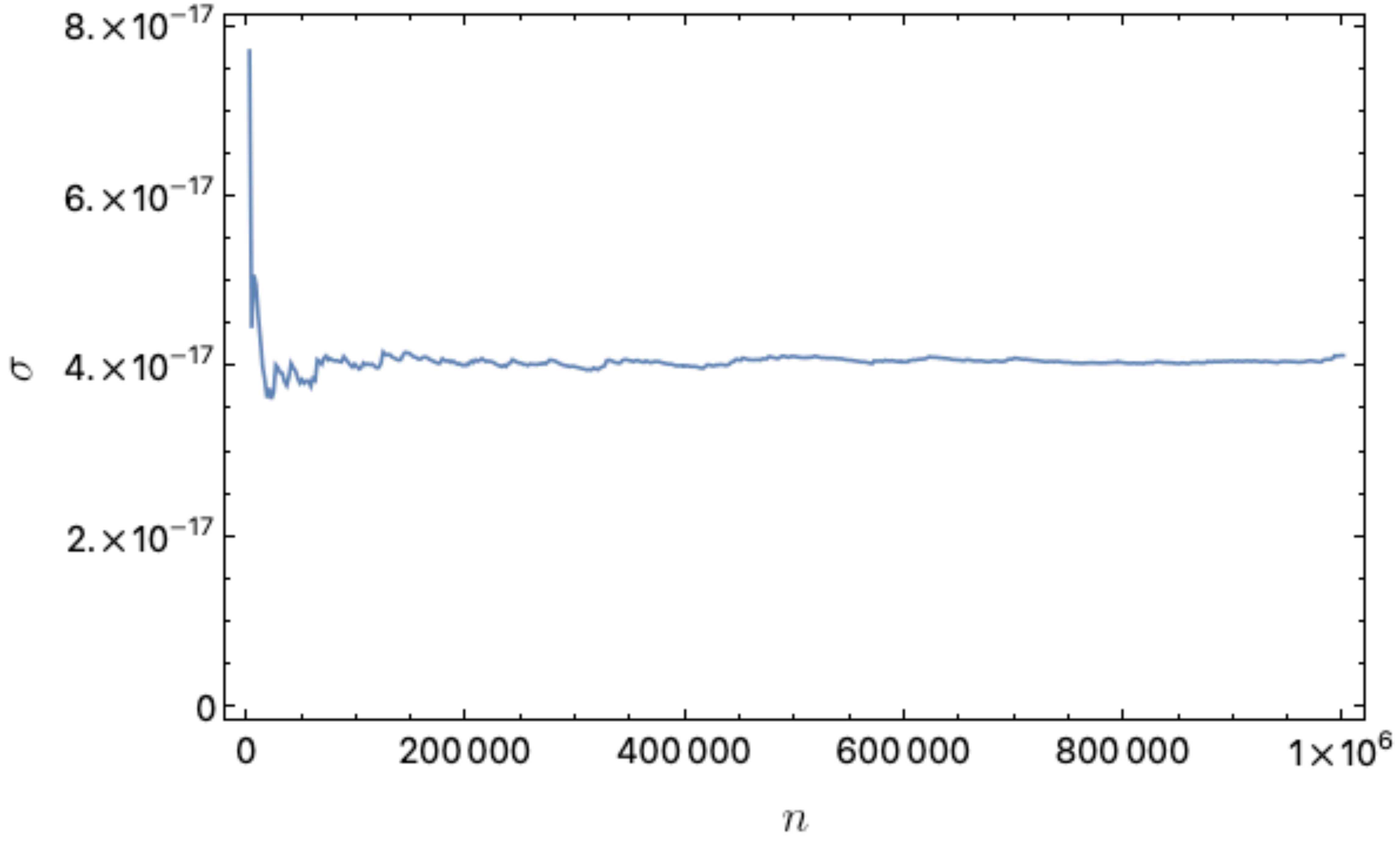
Fermionic Observable without Diverging Variance

- Hubbard Model: $\det M = \det M_1 \det M_2$

Only one of M's

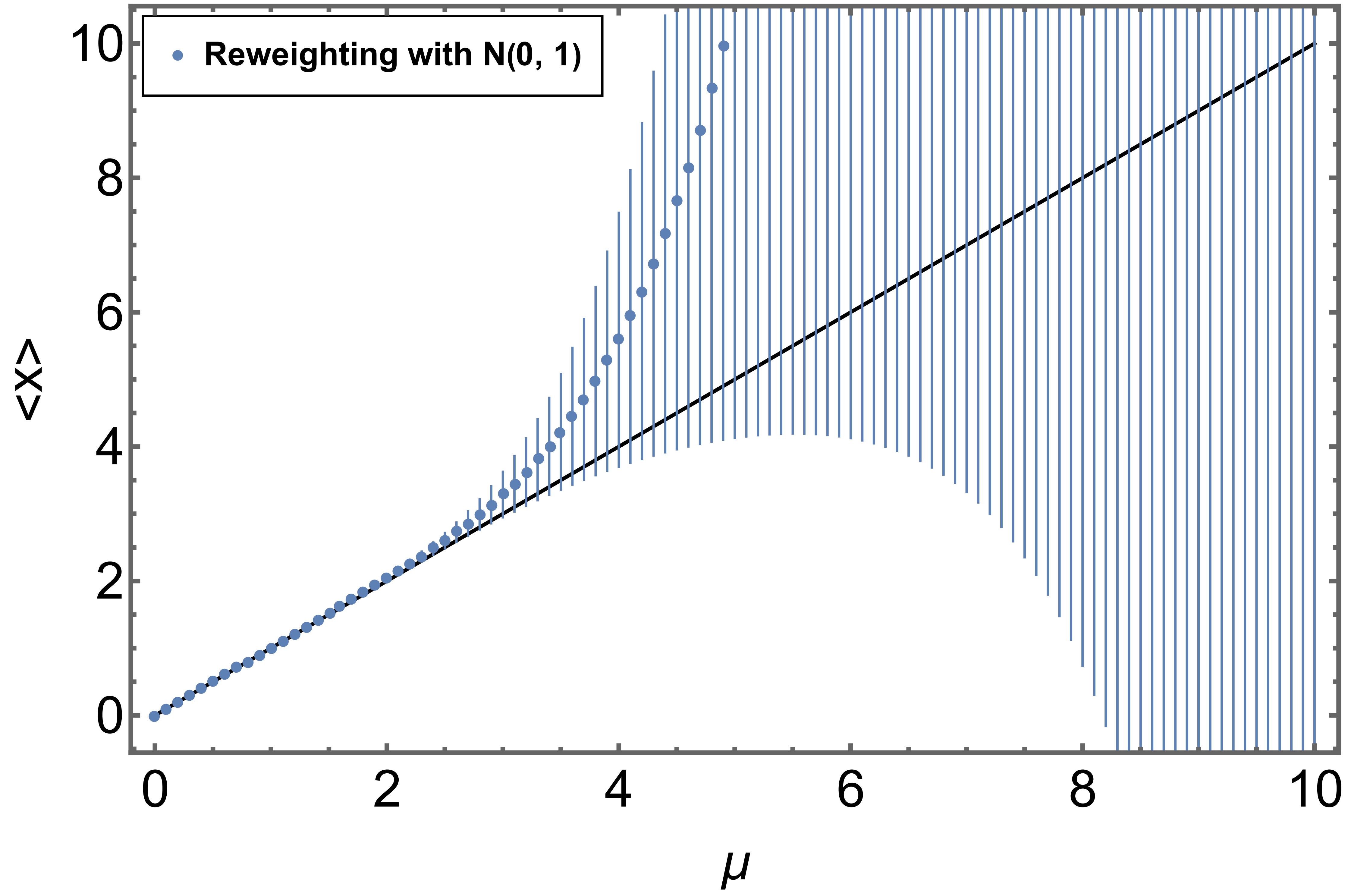
$$\text{Density } \mathcal{O}(\phi) = \frac{1}{V}\sum_x \langle n_\uparrow(x) + n_\downarrow(x)\rangle_F = \frac{1}{V}\sum_x [M_2^{-1}(\phi)_{x,x} - M_1^{-1}(\phi)_{x,x}]$$





Reweighting and Overlap Problem

- Reweighting: $\langle \mathcal{O} \rangle = \int D\phi\, \mathcal{O}(\phi) p(\phi) = \dfrac{\langle \mathcal{O}\, p/q \rangle_q}{\langle p/q \rangle_q}$
- If a new distribution is too different from the original, it cannot sample well



$$\langle x \rangle = \frac{\int dy\, y\, e^{-(y-\mu)^2}}{\int dy\, e^{-(y-\mu)^2}} = \mu$$

$$= \frac{\int dy\, y\, \frac{e^{-(y-\mu)^2}}{e^{-y^2}}\, e^{-y^2}}{\int dy\, \frac{e^{-(y-\mu)^2}}{e^{-y^2}}\, e^{-y^2}}$$

Extra Time Slice Method

- We want to use a different distribution from the original, but not too much
- Add one more auxiliary field along time direction:

$$Z = \int [\mathrm{d}\phi]_N \, \mathrm{e}^{-S_0(\phi)} \det M_N(\phi) \frac{F(\phi)}{F(\phi)} \quad (=1)$$

slightly lower temperature

$$= \int [\mathrm{d}\phi]_N \mathrm{d}\phi^* \; R(\phi) \; \mathrm{e}^{-S_0(\phi,\phi^*)} \det M_{N+1}(\phi, \phi^*)$$

with $$F(\phi) \equiv \int \mathrm{d}\phi^* \; \mathrm{e}^{-S_0(\phi^*)} \det M_{N+1}(\phi, \phi^*)$$

with $R(\phi) = \det M_N(\phi)/F(\phi)$

H. Shi and S. Zhang, Phys. Rev. E **93**, 033303 (2016)

Expansion Method

$R(\phi) = \det M_N(\phi)/F(\phi)$

- Integrate $F(\phi)$ analytically and expand it ($\epsilon = \beta/N$)

$$F(\phi) \equiv \int \mathrm{d}\phi^* \, \mathrm{e}^{-S_0(\phi^*)} \det M_{N+1}(\phi, \phi^*)$$

BSS Formula

$$= \mathrm{Tr}\left[\mathrm{e}^{-\tilde{H}_2}\mathrm{e}^{-\epsilon H_4} B(\phi_N)\cdots B(\phi_1)\right] = \mathrm{Tr}\left[(1 - \epsilon H) B(\phi_N)\cdots B(\phi_1)\right] + O(\epsilon^2)$$

$$= (1 - \epsilon H(\phi)) \det M_N(\phi) + O(\epsilon^2)$$

- Disadvantage:

1. Perturbative error
2. $F(\phi)$ can be 0 or negative
3. Difficult to calculate at higher orders

H. Shi and S. Zhang, Phys. Rev. E **93**, 033303 (2016)

Sub-Monte Carlo Method

- Estimate the integral using Monte Carlo

$$F(\phi) \equiv \int \mathrm{d}\phi^* \, \mathrm{e}^{-S_0(\phi^*)} \det M_{N+1}(\phi, \phi^*) \approx \frac{1}{n_{sub}} \sum_{i=1}^{n_{sub}} \det M_{N+1}(\phi, \phi_i^*)$$

$$M_a(\phi) = \mathbf{1} + B_a(\phi_{N+1}) \boxed{B_a(\phi_N) \cdots B_a(\phi_1)}$$

fixed!

- Advantage:

1. No approximation
2. $F(\phi) > 0$ since $\det M \geq 0$

Biased Estimation

- We need to calculate $1/F(\phi)$, not $F(\phi)$ ($R(\phi) \equiv \det M_N(\phi)/F(\phi)$)
- Just taking an inverse is biased:

$$\left\langle \frac{1}{A} \right\rangle = \frac{1}{\langle A \rangle} - \underbrace{\left\langle \frac{\bar{A} - \langle A \rangle}{\langle A^2 \rangle} \right\rangle}_{=0} + \underbrace{\left\langle \frac{(\bar{A} - \langle A \rangle)^2}{\langle A \rangle^3} \right\rangle}_{\neq 0} + \cdots$$

$$= \frac{1}{\langle A \rangle} + O\left(\frac{1}{n}\right) \longrightarrow \text{wrong value}$$

Unbiased Estimation

- Unbiased estimator of $1/\langle A \rangle$:

$$\hat{\xi}_A \equiv \frac{w}{q_n} \prod_{i=1}^{n} (1 - wA_i)$$

- Optimized choice of w and q_n (with respect to cost minimization):

$$w = \min\left\{ \frac{1}{k\bar{A}}, \frac{\bar{A}}{\overline{A^2}}, \frac{1}{A_{\max}} \right\},$$

$$p = 1 - \left[1 - 2w\bar{A} + w^2\overline{A^2}\right]^{\frac{1}{2}}, \ q_n = p(1-p)^n$$

where n is from the geometric distribution with p

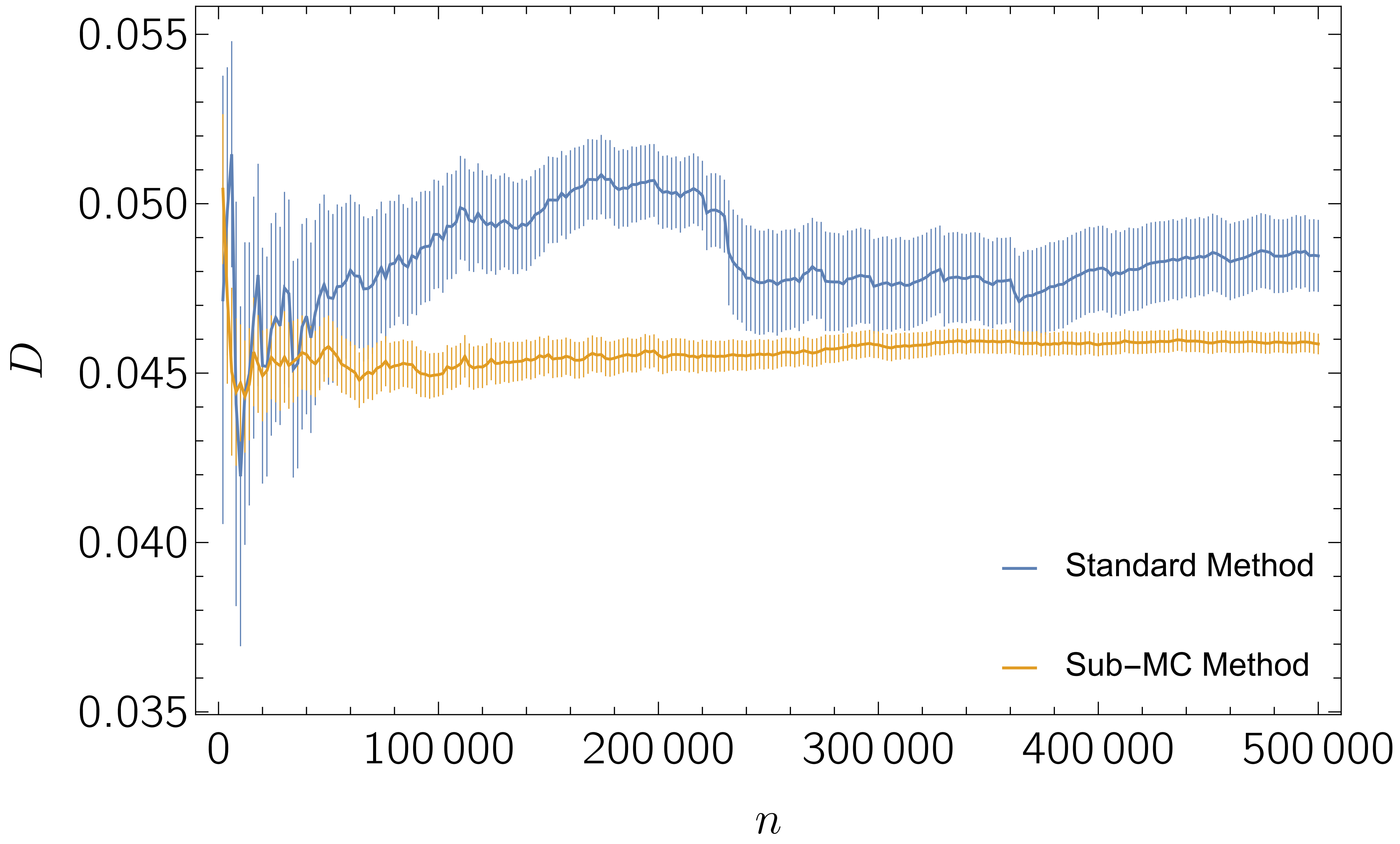
Moka et al, arXiv:1907.01843

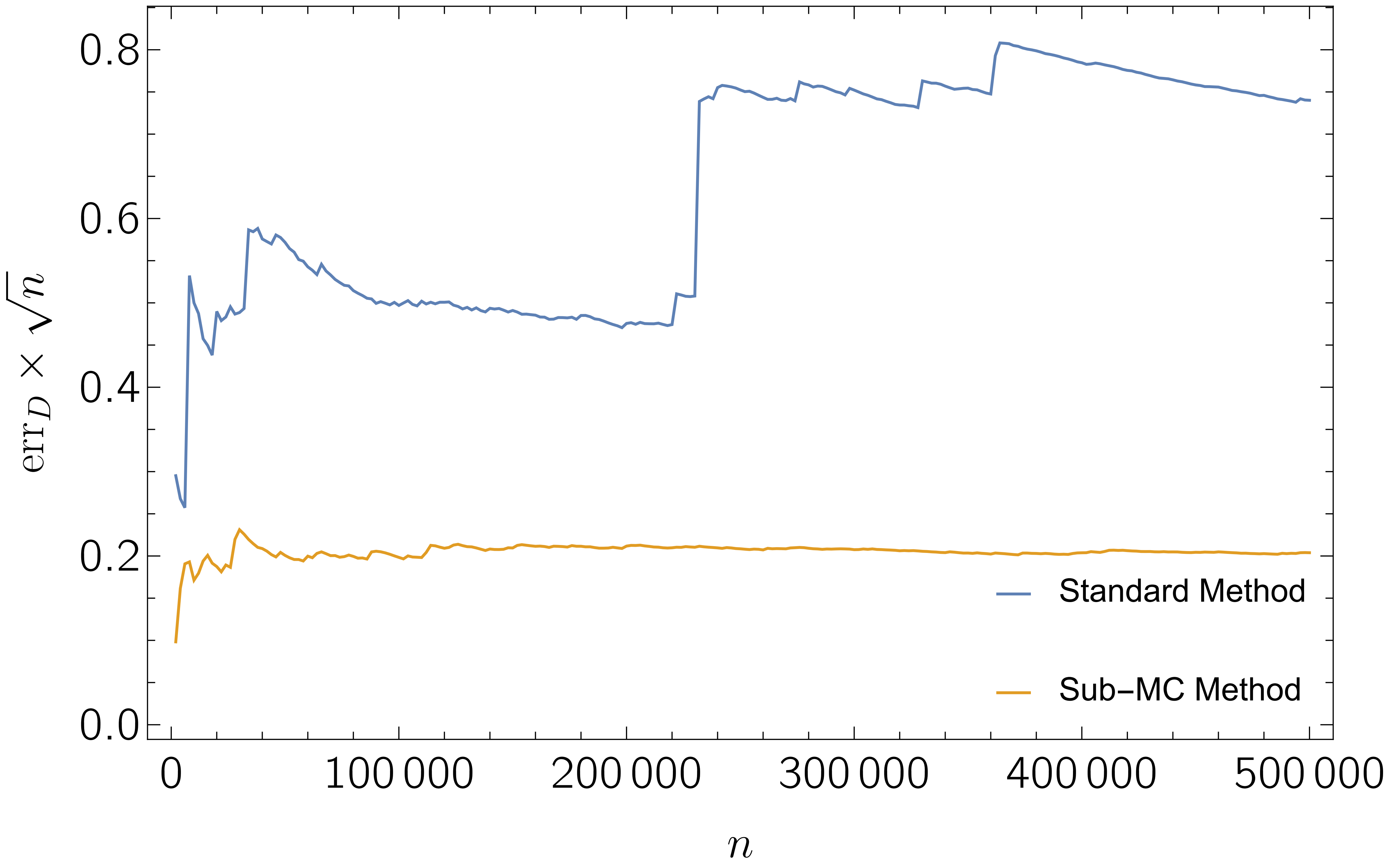
Result

Finite Variance

- Variance is not diverging

$$D(\phi) = \frac{1}{V}\sum_x \langle n_\uparrow(x) n_\downarrow(x)\rangle_F$$
$$= \frac{1}{V}\sum_x [1 - M_1^{-1}(\phi)_{x,x}] M_2^{-1}(\phi)_{x,x}$$





4x4 lattice, $U/\kappa = 8$, $T/\kappa = 0.5$, $\mu = 0$

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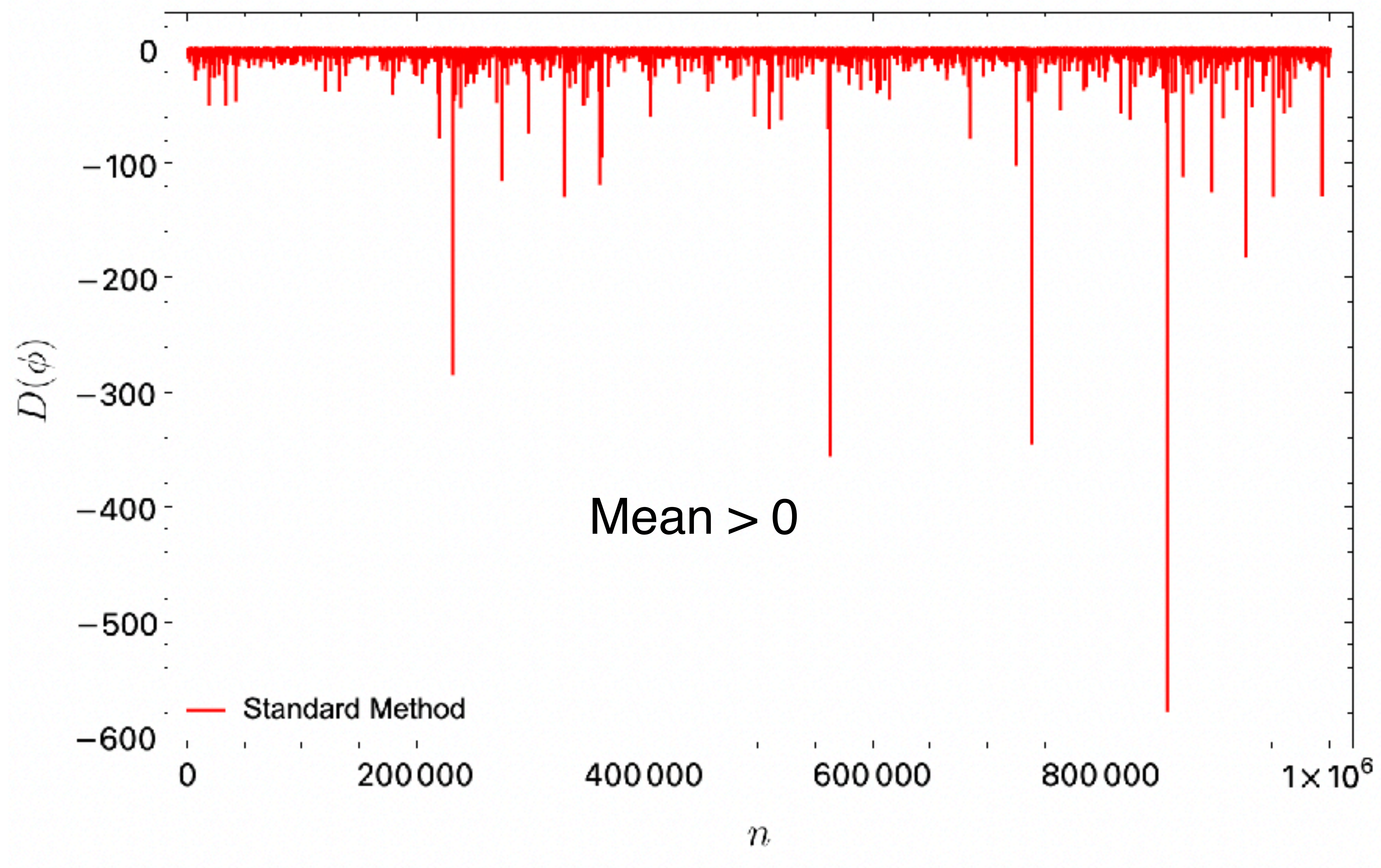
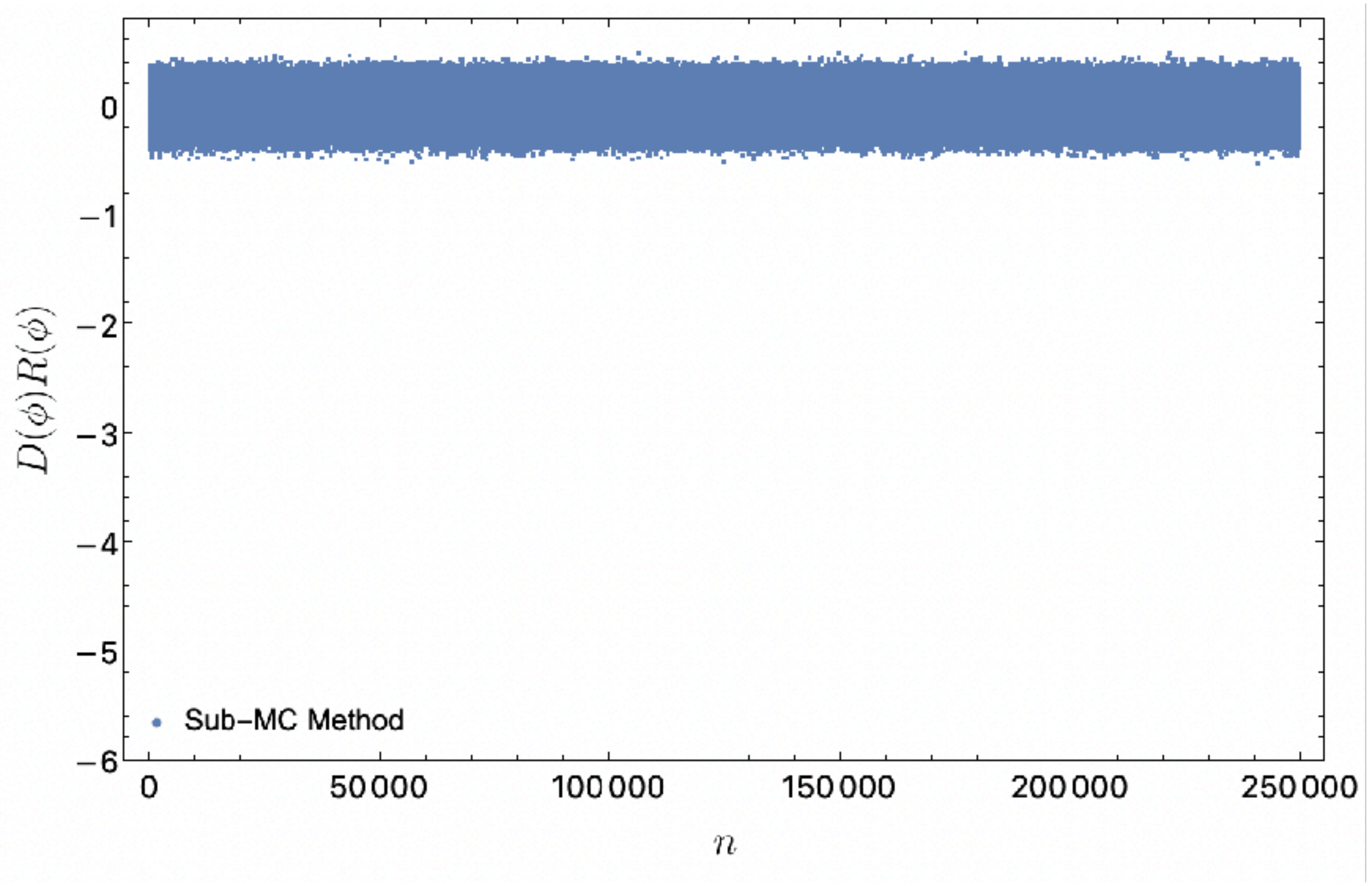
Finite Variance

- Exceptional configurations are reweighted well





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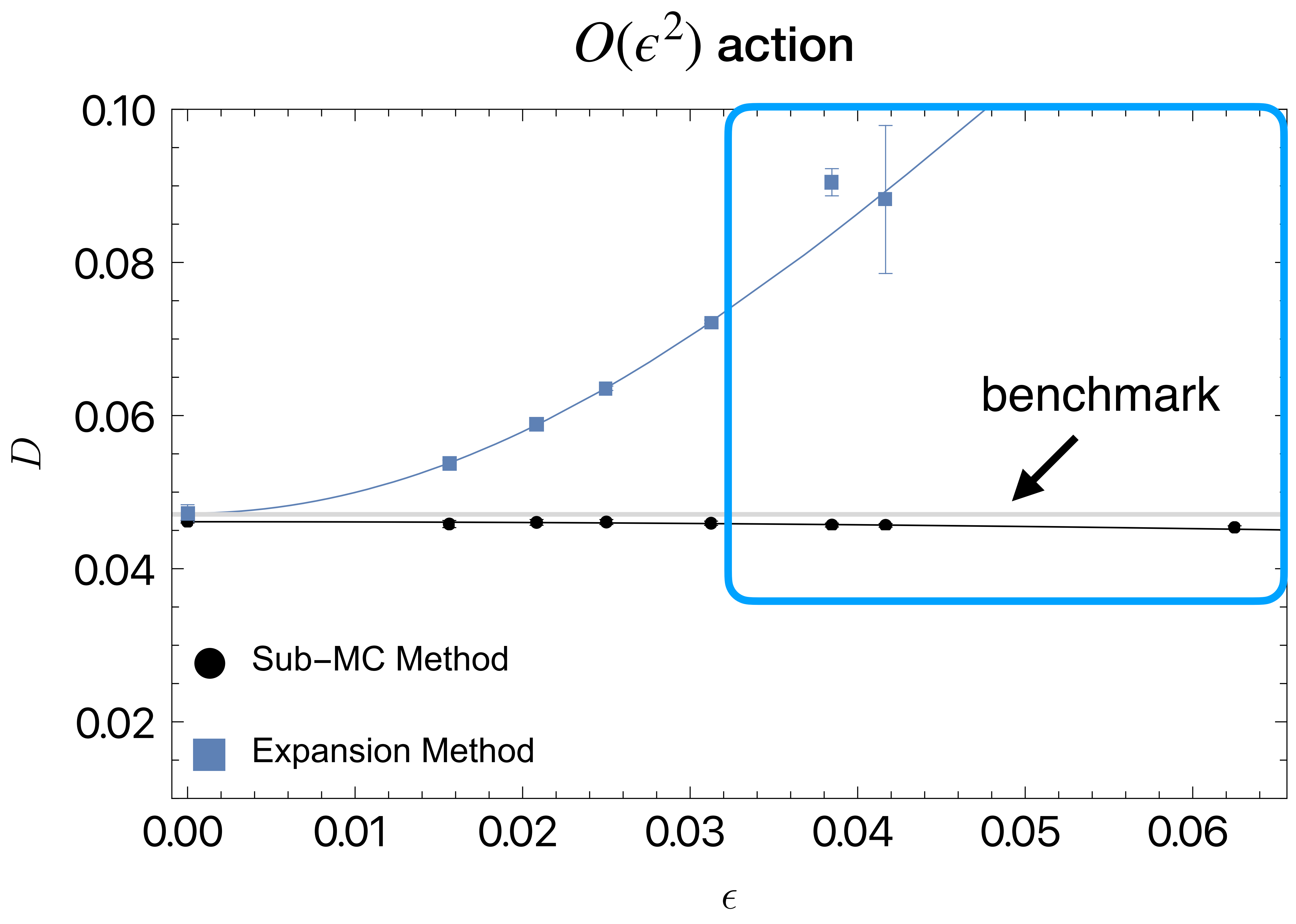
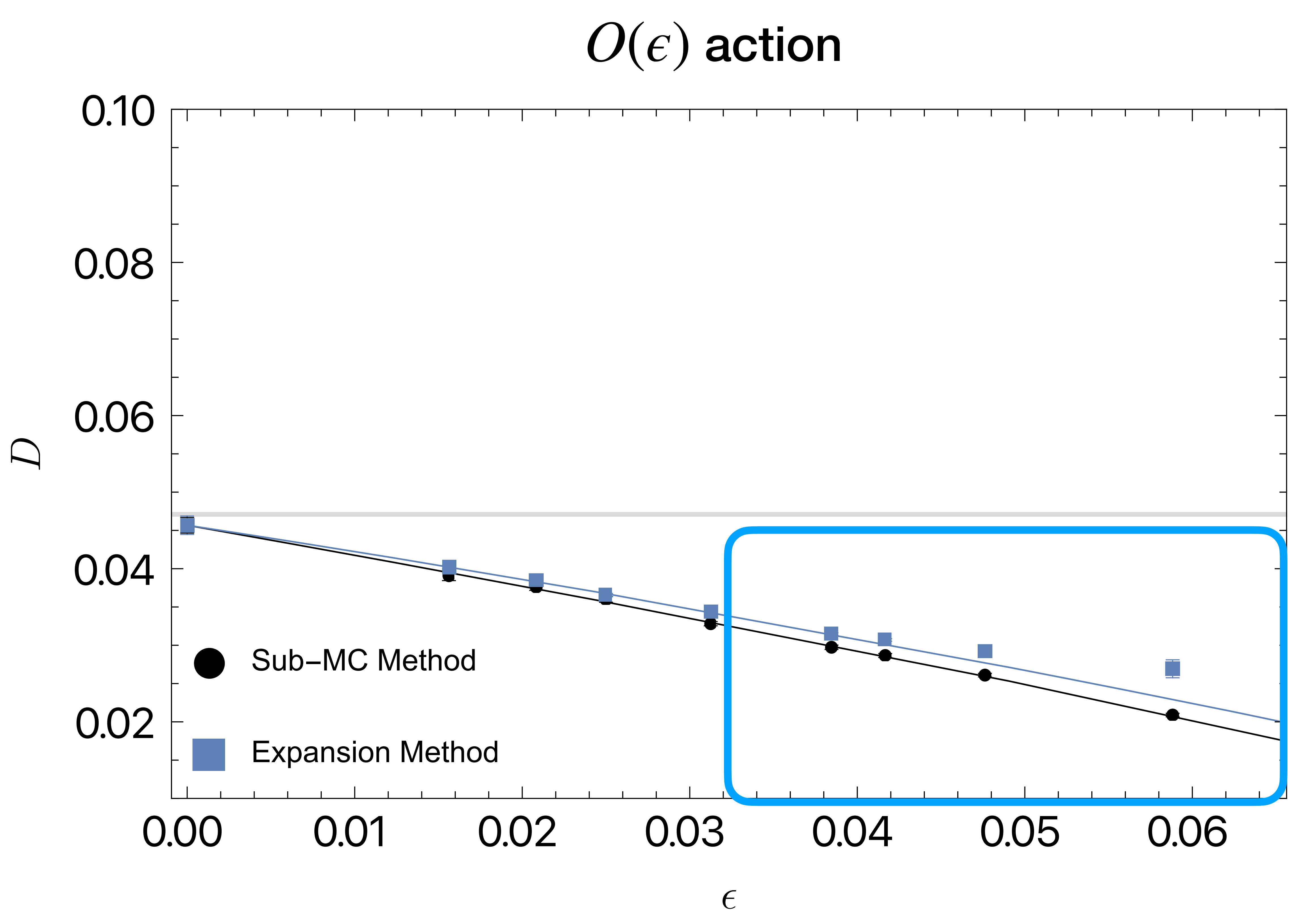
Comparison between Two Methods

- Consistent behavior at large $\epsilon = \beta/N$





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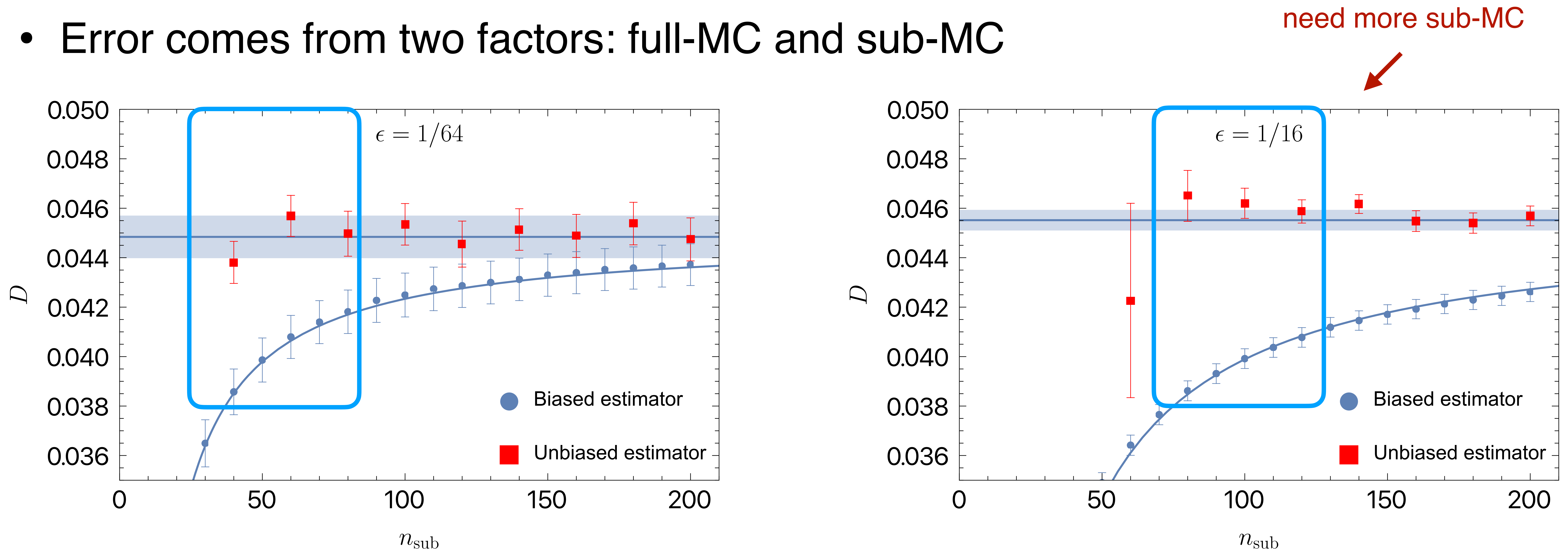
Unbiased Estimator

- One can use less samples
- Error comes from two factors: full-MC and sub-MC



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Conclusion

- Summary

1. Discussed the infinite variance problem of fermion on the lattice using its determinant
2. Suggested a way to solve the diverging variance problem:

- Extra time slice with sub-Monte Carlo method
- Unbiased estimation of reweighting factor $\propto 1/F(\phi)$ using sub-MC

3. Showed that the new method has a better behavior at large ϵ

- Future study

1. Extra time slice method with Hybrid Monte Carlo
2. Infinite variance problem with the sign problem

Backup

Path Integral Formulation

- BSS formula:

$$\det \begin{bmatrix} \mathbf{1} & 0 & \cdots & B_N \\ B_1 & \mathbf{1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & B_{N-1} & \mathbf{1} \end{bmatrix} = \det\left(\mathbf{1} - (-1)^N B_N \cdots B_1\right)$$

- Conventional action:

$$B_a(\phi_t)_{x,y} = (Z_a - 1 - \varepsilon_a i \sin\phi_{t,x})\delta_{x,y} - \epsilon\kappa\delta_{\langle x,y\rangle}$$

- Improved action:

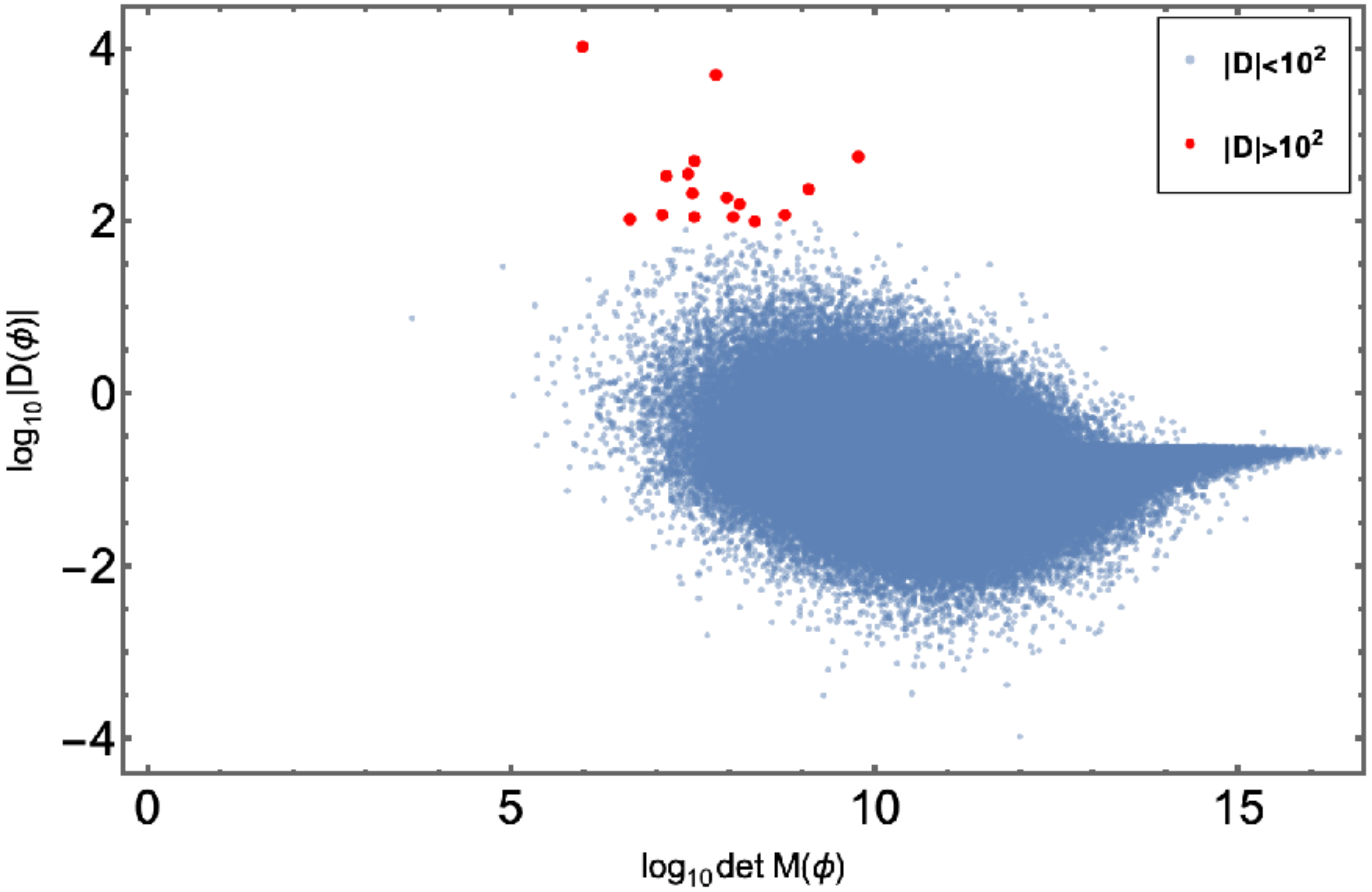
$$B^a(\phi_t)_{x,y} = \mathrm{e}^{-\tilde{H}_2^a}\mathrm{e}^{-\tilde{H}_4^a(\phi_t)}$$

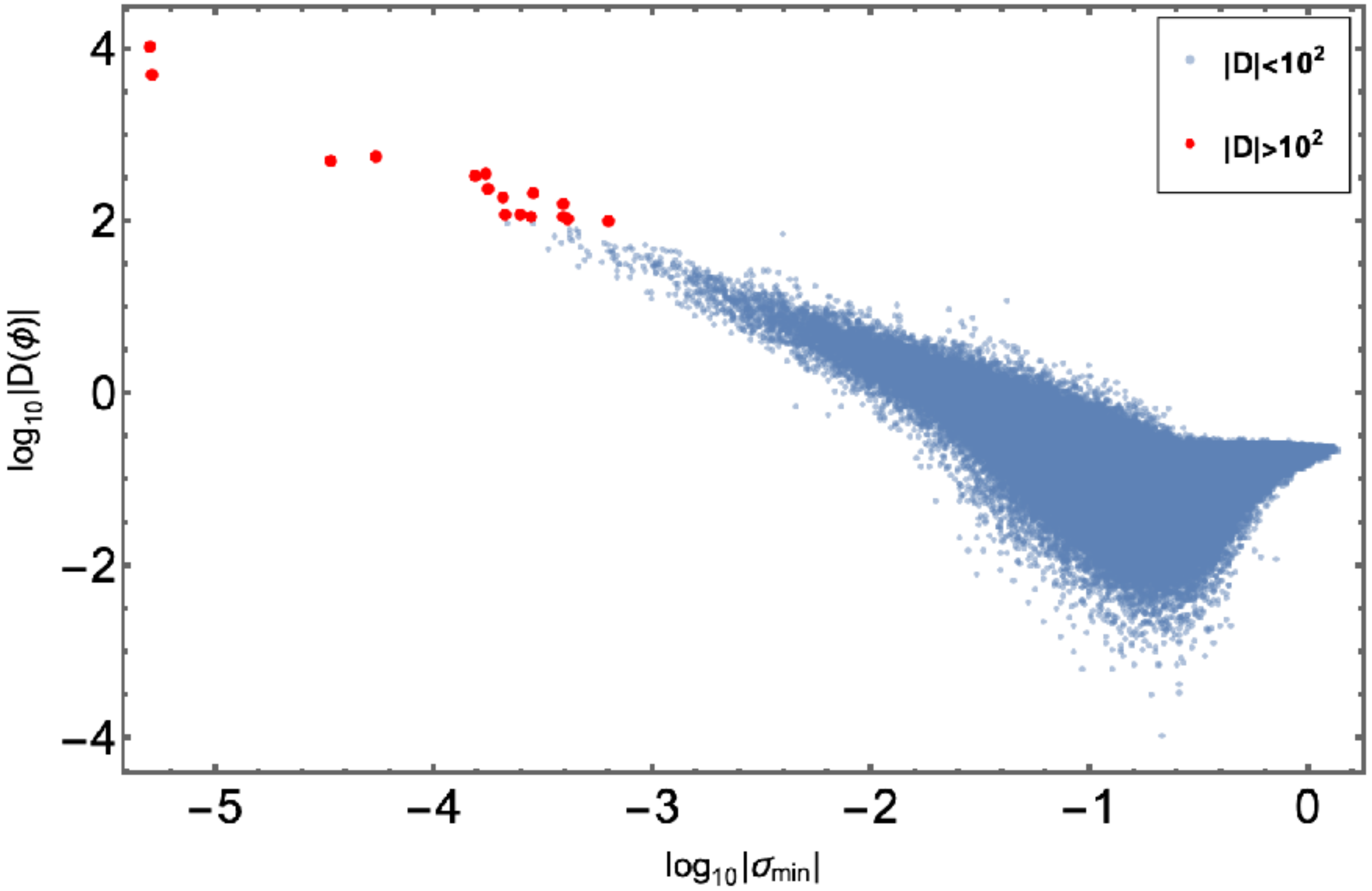
with

$$(\tilde{H}_2^a)_{x,y} = \kappa\epsilon\delta_{\langle x,y\rangle} + \varepsilon_a\epsilon\mu\delta_{x,y}$$

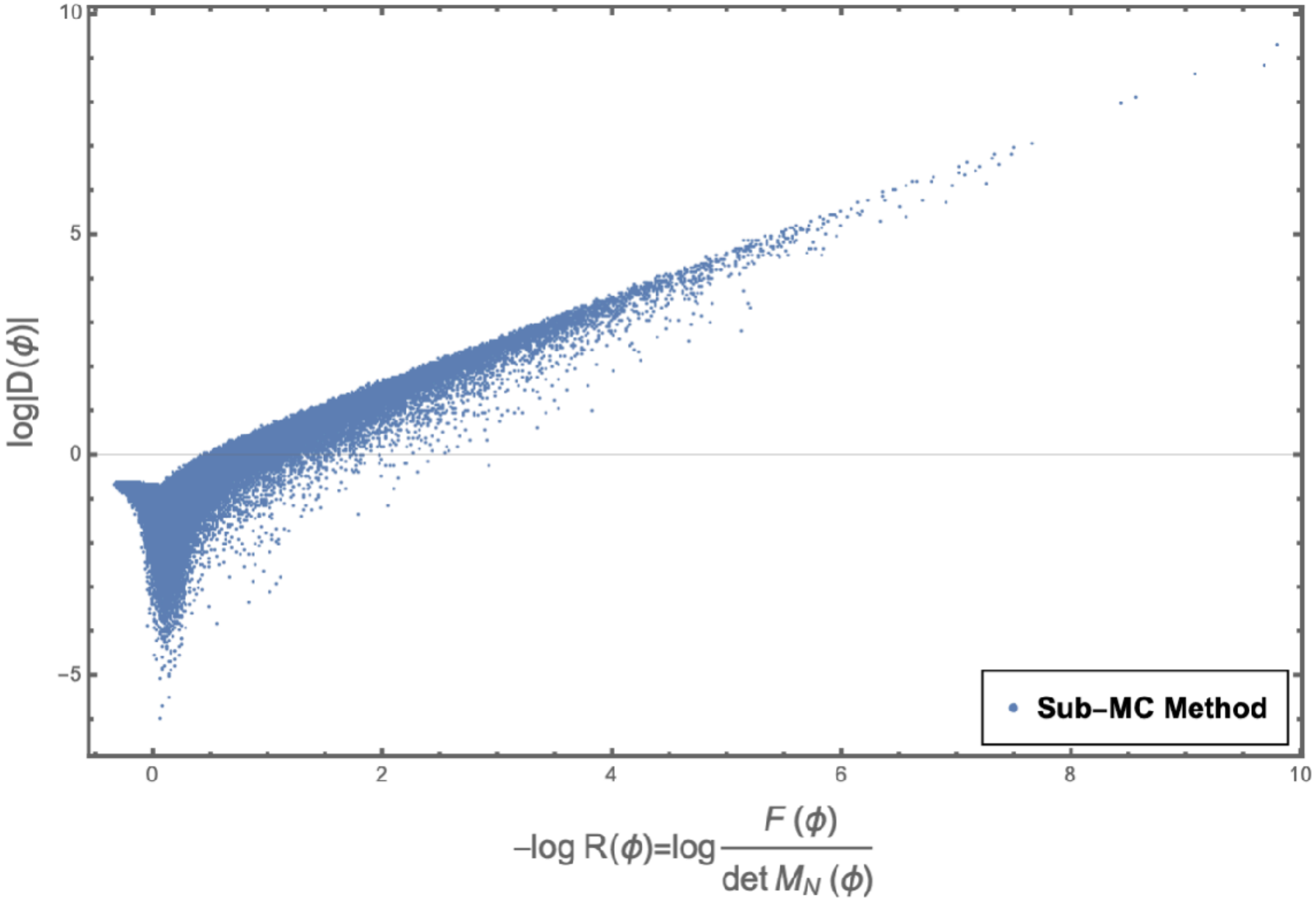
$$\tilde{H}_4^a(\phi_t)_{x,y} = -\, i\varepsilon_a \sin\phi_{t,x}\delta_{x,y}$$

Determinant & Singular Value



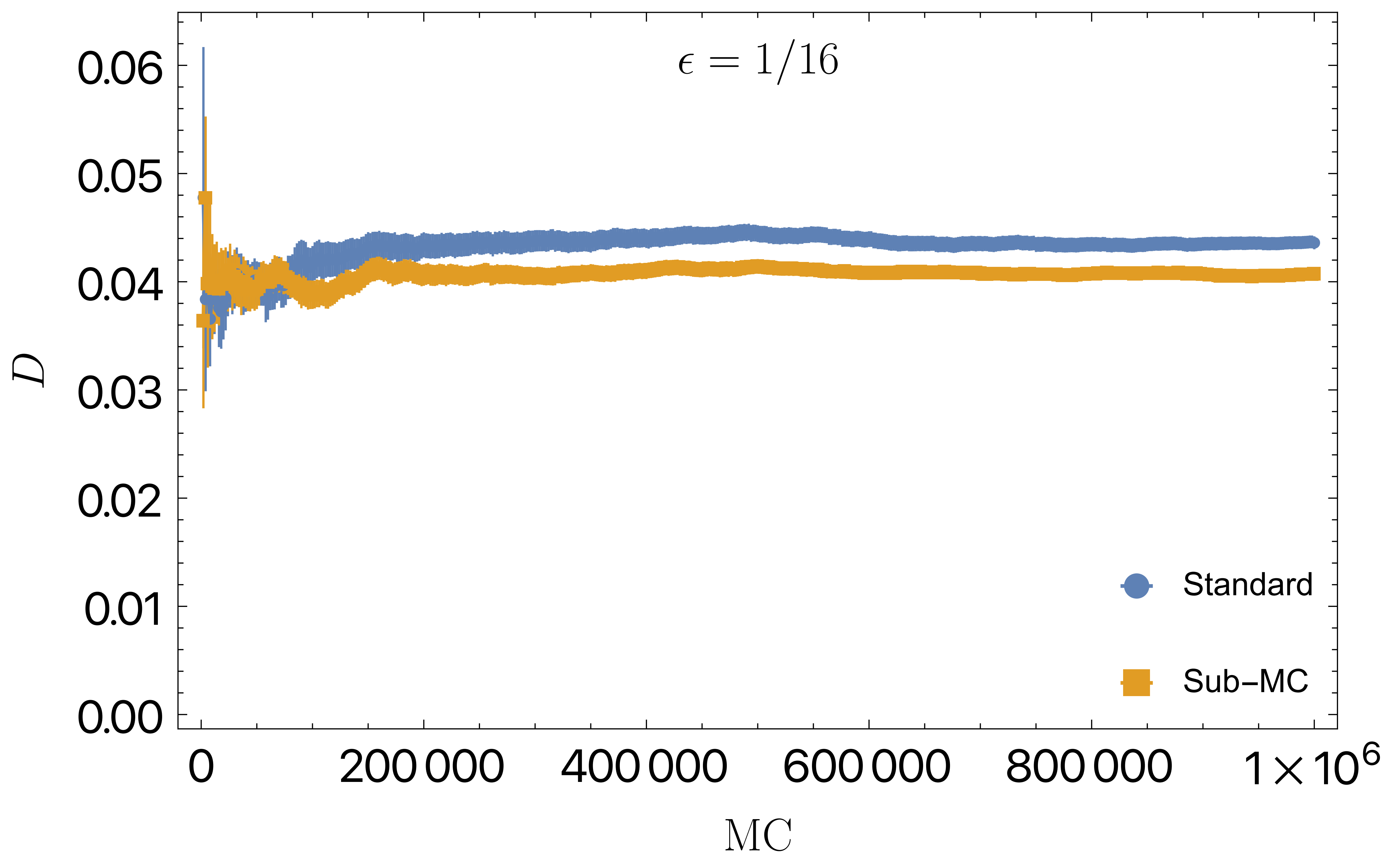


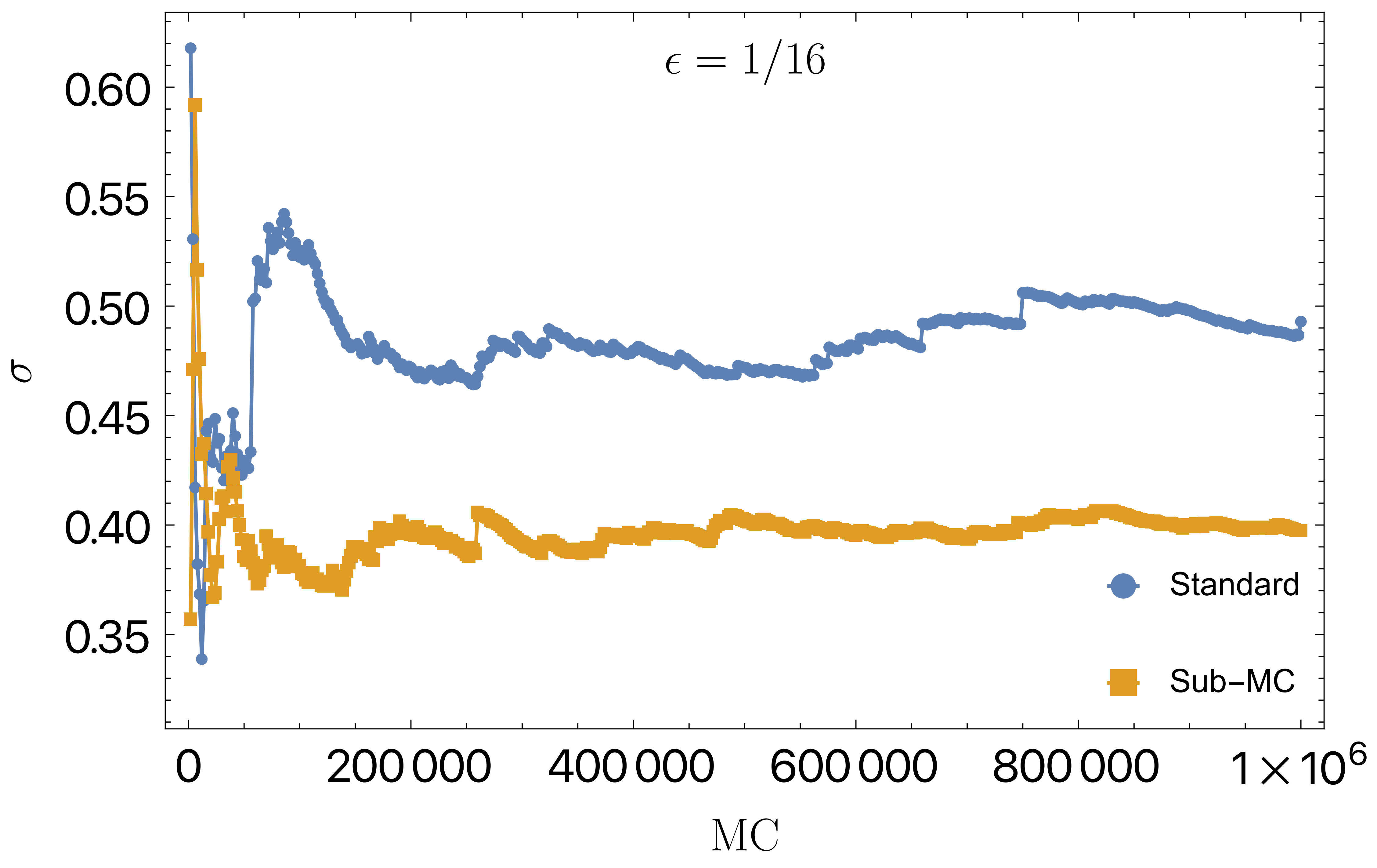
Reweighting



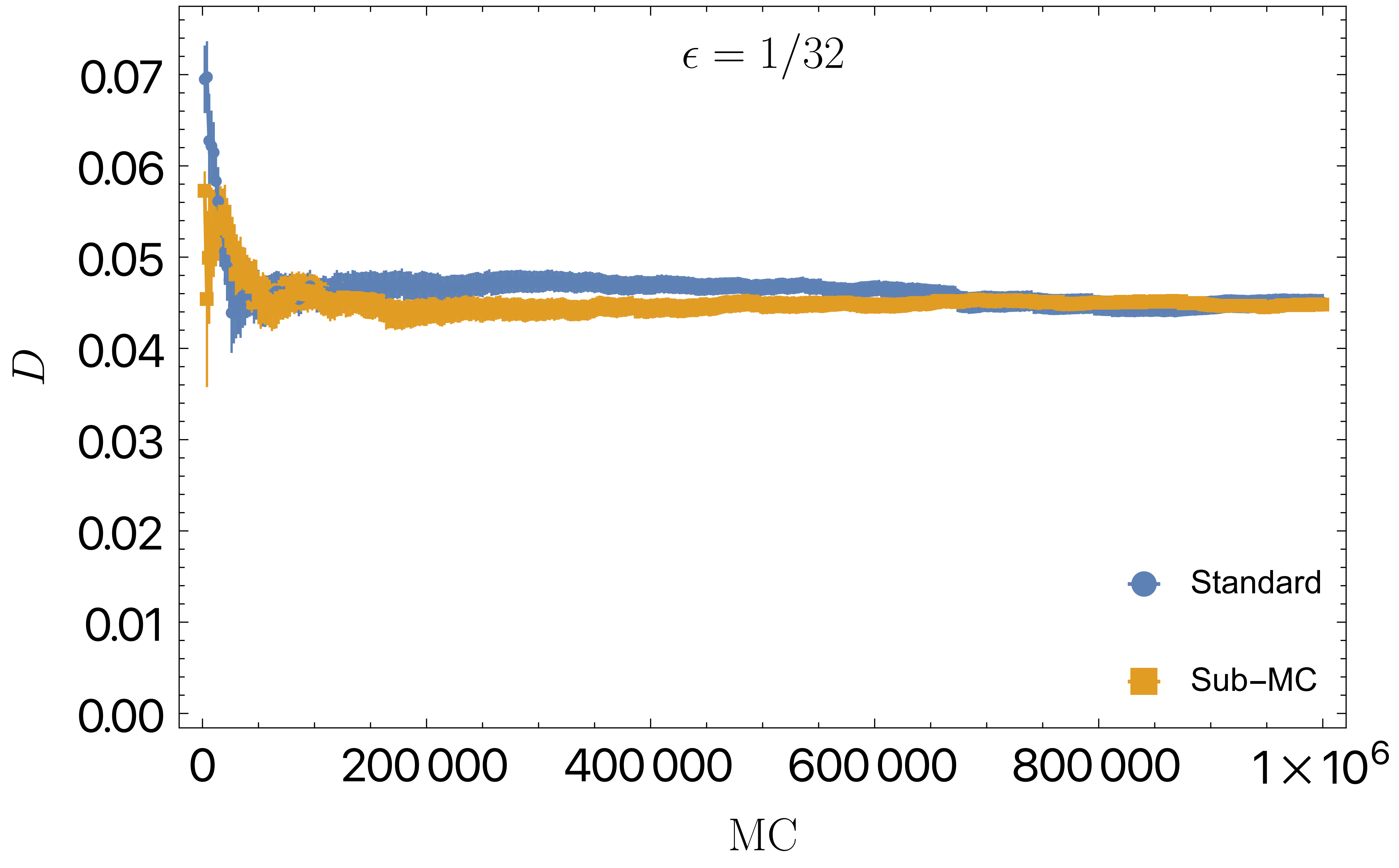
Diagonal Discretization

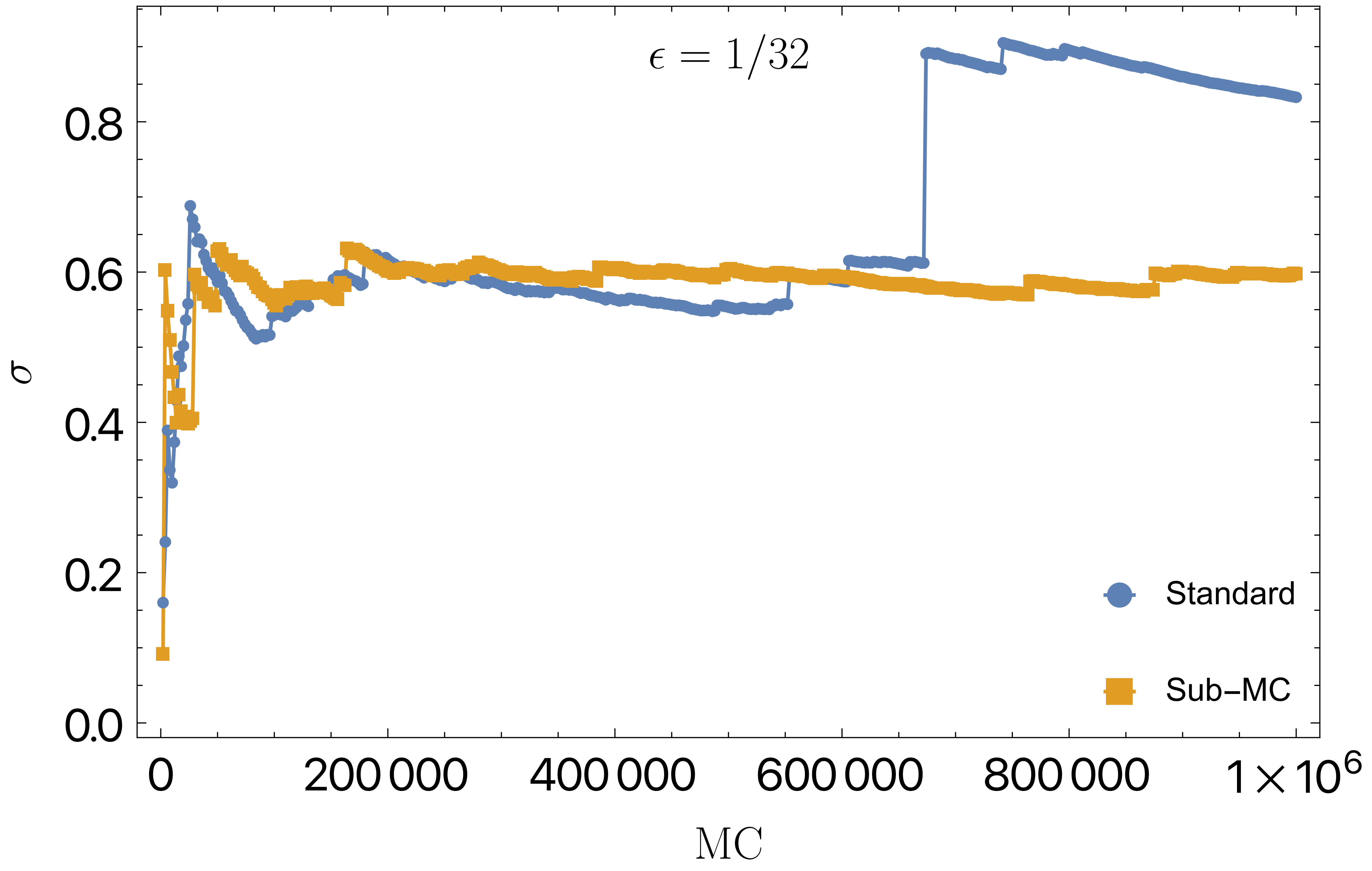
$$B^a(\phi_t)_{x,y} = -\,[\mathrm{e}^{h\delta_{\langle\,,\,\rangle}}]_{x,y} e^{i\phi_{x,t}}$$





Diagonal Discretization





J. Wynen, E. Berkowitz, C. Körber, T. Lähde, T. Luu, Phys. Rev. B **100**, 075141 (2019)