Improving Monte Carlo Integration by Symmetrizations

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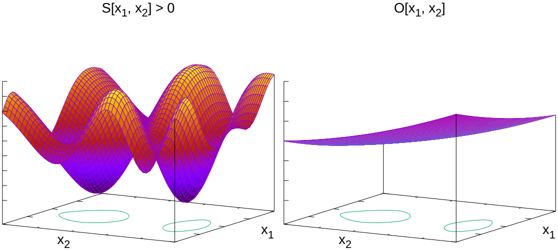
Monte Carlo importance sampling

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x \, O[x] \, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x \, \mathrm{e}^{-S[x]}},$$

Monte Carlo importance sampling

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x \, O[x] \, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x \; \mathrm{e}^{-S[x]}}, \qquad \text{prob. density} \quad p(x) = \frac{\mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x \; \mathrm{e}^{-S[x]}}$$



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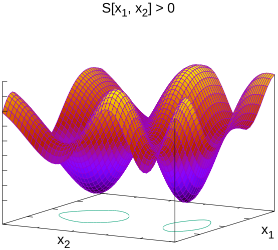
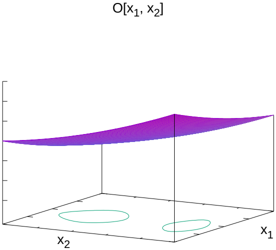
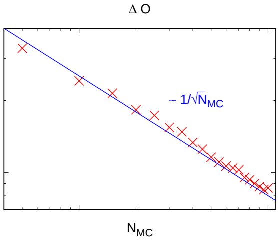
$$N_{MC}\; [x]_i \qquad \langle O \rangle = \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} O_p[x]_i$$





$\xrightarrow{N_{MC}}$



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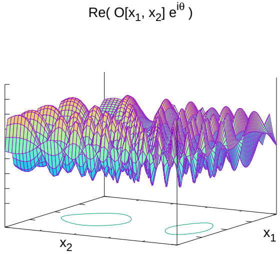
$N_{MC}\ [x]_i \qquad \langle O \rangle = \dfrac{1}{N_{MC}} \displaystyle\sum_{i=1}^{N_{MC}} O_p[x]_i$

$S \in \mathbb{C}$

$$\frac{\int_{D^d} \mathrm{d}x\, O[x]\, \mathrm{e}^{i\theta[x]}\, \mathrm{e}^{-\Re(S[x])}}{\int_{D^d} \mathrm{d}x\ \mathrm{e}^{i\theta[x]}\, \mathrm{e}^{-\Re(S[x])}}$$



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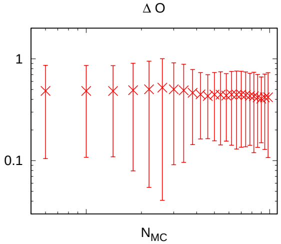
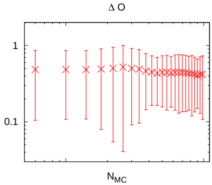
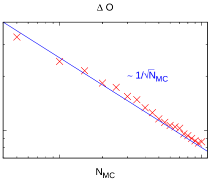


Possible Solution

$S \in \mathbb{C}$



$S > 0$



Symmetrized Configurations

Possible Solution

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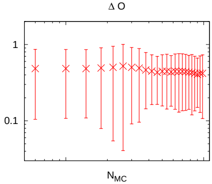

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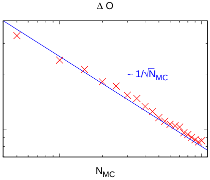


Symmetrized Configurations

1 Dimension 1d-QCD

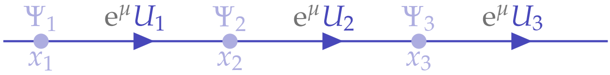
2 Dimensions 2d $\mathcal{U}(1)$-gauge theory

1 Dimension

1D-QCD

Ψ : mass m

1D-QCD



Ψ : mass m

$$S[U, \overline{\Psi}, \Psi] = \sum_i m \overline{\Psi}_i \Psi_i + e^{\mu} \overline{\Psi}_i U_i \Psi_{i+1} + e^{-\mu} \overline{\Psi}_{i-1} U_i^* \Psi_i$$

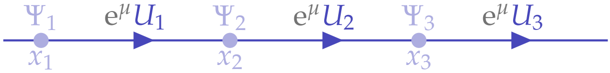
1D-QCD

Ψ : mass m

$$S[U,\overline{\Psi},\Psi] = \sum_i m\overline{\Psi}_i\Psi_i + e^{\mu}\overline{\Psi}_i U_i \Psi_{i+1} + e^{-\mu}\overline{\Psi}_{i-1}U_i^*\Psi_i$$

$$= \overline{\Psi}\,\mathfrak{D}[U]\,\Psi, \qquad U_i \in \mathcal{G}, \text{ e.g. } \mathcal{U}(N), \mathcal{SU}(N)$$

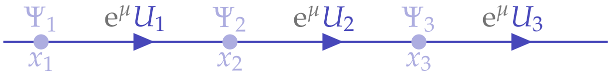
Partition Function



Ψ : mass m

$$Z[U] = \int_{\mathcal{G}} \mathrm{d}U_1 \int_{\mathcal{G}} \mathrm{d}U_2 \int_{\mathcal{G}} \mathrm{d}U_3 \int \mathrm{d}\overline{\Psi} \int \mathrm{d}\Psi \; \mathrm{e}^{-S[U,\overline{\Psi},\Psi]}$$

Partition Function



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$$= \int_{\mathcal{G}^3} \mathrm{d}^3 U \qquad \det \mathfrak{D}[U]$$

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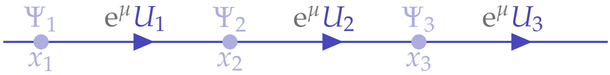

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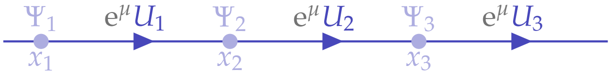
$$= \int_{\mathcal{G}^3} \mathrm{d}^3 U \qquad \det \mathfrak{D}[U]$$

$$= \int_{\mathcal{G}^3} \mathrm{d}^3 U \left(c(m) + \qquad 2^{-3}\, \mathrm{e}^{-3\mu} \left(\prod_{j=1}^{3} U_j \right)^* \right.$$

$$\left. + (-1)^3\, 2^{-3}\, \mathrm{e}^{\,3\mu} \left(\prod_{j=1}^{3} U_j \right) \right)$$

Gauge invariance



Ψ : mass m

Physics unchanged

$$U_j \to G_j^* U_j G_{j+1}, \qquad G_j \in G, \qquad U_j \in G$$

partition function

$$Z[U] = \int_{\mathcal{G}^3} \mathrm{d}^3 U \left(c(m) + 2^{-3}\, \mathrm{e}^{-3\mu} \left(\prod_{j=1}^{3} U_j \right)^* + (-1)^3\, 2^{-3}\, \mathrm{e}^{\,3\mu} \left(\prod_{j=1}^{3} U_j \right) \right)$$

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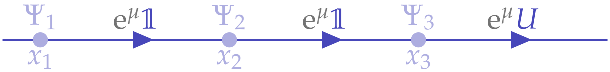

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Why difficult for MC?

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Why difficult for MC?

$$Z[U] = \int_{\mathcal{U}(1)} \mathrm{d}U \qquad \Big(c(m) + 2^{-3}\,\mathrm{e}^{-3\mu}\, U^* + \underline{(-1)^3 2^{-3}\,\mathrm{e}^{3\mu}\, U} \Big)$$

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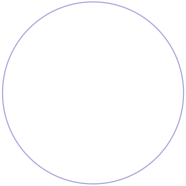
$$\int_{\mathcal{U}(1)} \mathrm{d}U\, U$$



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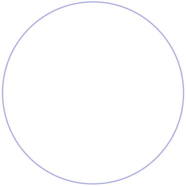
$$\int_{\mathcal{U}(1)} \mathrm{d}U\, U = \int_0^{2\pi} \mathrm{d}\theta\ \mathrm{e}^{i\theta} = 0$$



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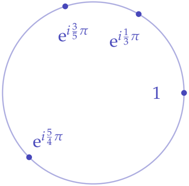

$$\overset{\mathrm{MC}}{\approx} \frac{1}{4}\left(1 + \mathrm{e}^{i\frac{1}{3}\pi} + \mathrm{e}^{i\frac{3}{5}\pi} + \mathrm{e}^{i\frac{5}{4}\pi}\right) \approx 0.48 + 1.11i$$

$$\xrightarrow{N_{MC}\to\infty} 0$$

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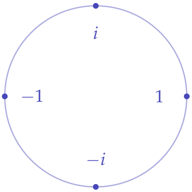

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$$\xrightarrow{N_{MC}\to\infty} 0$$

$$\overset{\text{sym}}{\approx} \frac{1}{4}\left(1 + i + (-i) + (-1)\right) = 0$$

Problem of the chemical potential

$$Z[U] = \int_{\mathcal{U}(1)} \mathrm{d}U \; \left(c(m) + 2^{-3}\, \mathrm{e}^{-3\mu}\, U^* + \underline{(-1)^3 2^{-3}\, \mathrm{e}^{3\mu}\, U} \right)$$

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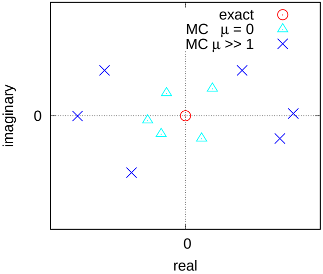

Symmetrize configurations - Idea

[Bloch 2013] 1d-QCD with $\mathcal{SU}(3)$-links

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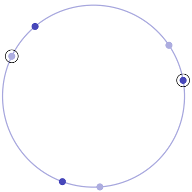

$$U \in \mathcal{SU}(3) \to \{e^{\frac{2\pi i k}{3}} U, \quad k \in \mathbb{Z}_{N_3}\}$$

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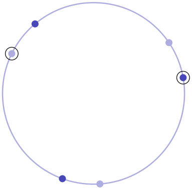

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$$\int_{\mathcal{SU}(3)} \mathrm{d}h\, f(U) \approx \qquad \left(\frac{1}{3}\sum_{k=1}^{3} f(e^{\frac{2\pi i k}{3}} U_j)\right)$$

Symmetrize configurations - Idea

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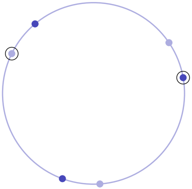

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$$\int_{\mathcal{SU}(3)} \mathrm{d}h\, f(U) \approx \frac{1}{N_{MC}} \sum_{j=1}^{N_{MC}} \left(\frac{1}{3} \sum_{k=1}^{3} f(\mathrm{e}^{\frac{2\pi i k}{3}}\, U_j) \right)$$

Complete Symmetrization

$\mathcal{U}(1)$ for $f \in P_{N_{sym}-1}$ polynomial exact

$$\int_{U(1)} \mathrm{d}h\, f(U) \approx \frac{1}{N_{sym}} \sum_{k=1}^{N_{sym}} f(\mathrm{e}^{\frac{2\pi i k}{N_{sym}}}\, U)$$

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$N > 1$ for $f \in P_{2m+1}$ polynomial exact

$$\int_{G} \mathrm{d}h\, f(U) \approx \frac{1}{\#Q_G} \sum_{V \in Q_G(m)} w_V f(VU)$$

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Q_G $G = S^n$ [Genz 2003, Sylvester 1970]

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Q_G $G = S^n$ [Genz 2003, Sylvester 1970]
$S^3 \simeq SU(2), \quad SU(N) \simeq \times_{j=1}^{N} S^{2j-1}, \quad U(N) \simeq \times_{j=2}^{N} S^{2j-1}$

Application to the Partition Function

$$Z[U] = \int_{\mathcal{G}} \mathrm{d}U \ \det \mathfrak{D}[U], \qquad \mathcal{G} = \mathcal{U}(N) \text{ or } \mathcal{SU}(N)$$

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MCMC

$$Z \approx \frac{1}{N_{MC}} \sum_{k=1}^{N_{MC}} \det \mathfrak{D}(U_k), \qquad U_k \in G \text{ random}$$

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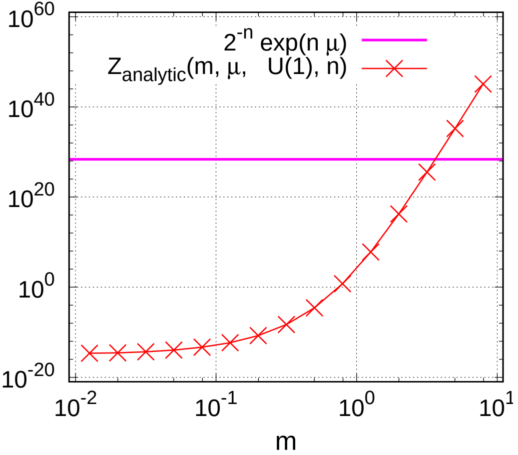
poly. exact

$$Z \approx \frac{1}{\# Q_G} \sum_{V \in Q_G} w_V \det \mathfrak{D}(VU) \qquad U \in G \text{ random}$$

Analytic Result Partition Function

$$Z[U] = \int_{\mathcal{U}(1)} \mathrm{d}U \ \left(c(m) + 2^{-n}\,\mathrm{e}^{-n\mu}\,U^* + (-1)^n 2^{-n}\,\mathrm{e}^{n\mu}\,U\right)$$

- $\mathcal{G} = \mathcal{U}(1)$
- double prec
- $\mu = 2$
- $n = 50$ points



Result Partition Function

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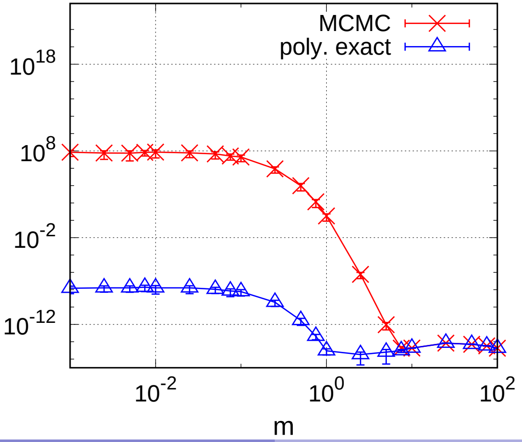
$$\frac{\langle Z\rangle_{\text{quadrature}} - \langle Z\rangle_{\text{analytic}}}{\langle Z\rangle_{\text{analytic}}}$$

- $\mathcal{G} = \mathcal{U}(1)$
- double prec
- $\mu = 1$
- $n = 20$ points
- 50 repetitions

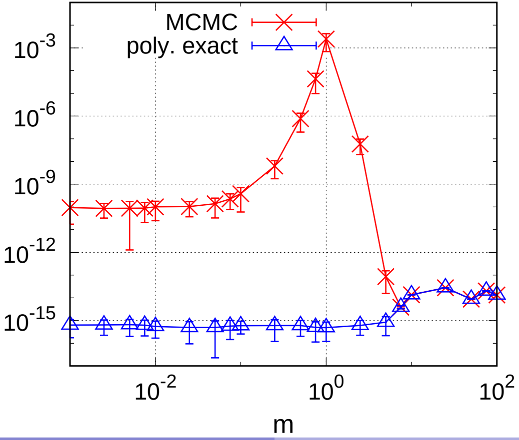


Result Partition Function

$$Z[U] = \int_{\mathcal{SU}(3)} \mathrm{d}U \, \det\left(c(m) + 2^{-n}\, \mathrm{e}^{-n\mu}\, U^* + (-1)^n 2^{-n}\, \mathrm{e}^{n\mu}\, U\right)$$

$$\frac{\langle Z\rangle_{\text{quadrature}} - \langle Z\rangle_{\text{analytic}}}{\langle Z\rangle_{\text{analytic}}}$$

- $\mathcal{G} = \mathcal{SU}(3)$
- double prec
- $\mu = 1$
- $n = 20$ points
- 50 repetitions

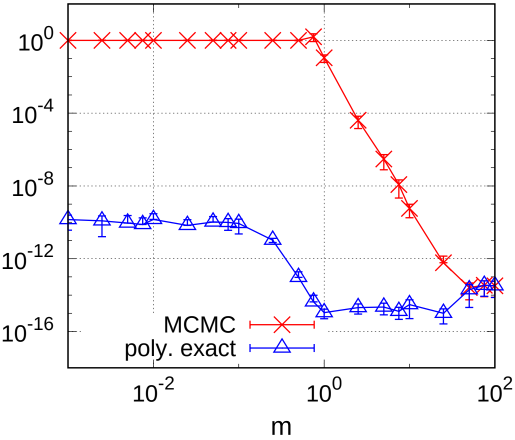


Result Chiral Condensate

$$\langle \overline{\Psi}\Psi \rangle = \partial_m \ln Z = \frac{\int_{\mathcal{G}} \mathrm{d}h_{\mathcal{G}}\, \partial_m \det \mathfrak{D}}{\int_{\mathcal{G}} \mathrm{d}h_{\mathcal{G}}\, \det \mathfrak{D}}$$

$$\frac{\langle \overline{\Psi}\Psi \rangle_{\text{quadrature}} - \langle \overline{\Psi}\Psi \rangle_{\text{analytic}}}{\langle \overline{\Psi}\Psi \rangle_{\text{analytic}}}$$

- $\mathcal{G} = \mathcal{U}(2)$
- double prec
- $\mu = 1$
- 8 lattice points
- 50 repetitions



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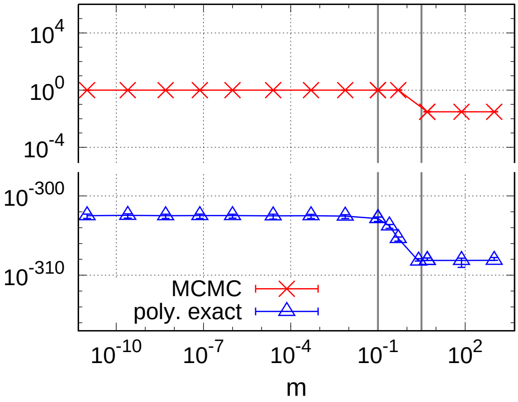
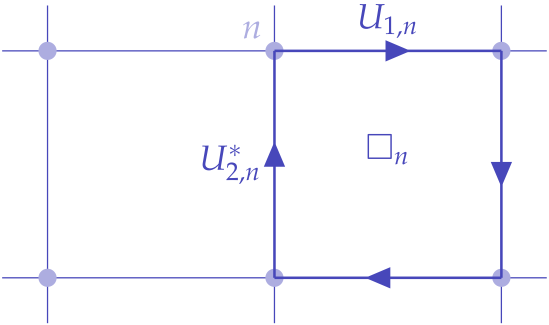


2 Dimensions

2D-GAUGE $U(1)$ THEORY



$$S[U] = \beta \sum_n \Re(\square_n)$$

Applying Symmetrizations

1dQCD $U \in \mathcal{U}(1)$

$$Z \approx \frac{1}{N_{sym}} \sum_{k=1}^{N_{sym}} \det \mathfrak{D}(e^{\frac{2\pi ik}{N_{sym}}} U), \qquad N_{sym} = 4$$

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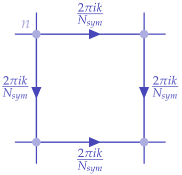
2d-gauge theory $U = \{U_{\mu,n}, \mu \in \{1,2\}, n \in \{1,...,V_{lat}\}\}$

$$\underbrace{\frac{1}{N_{sym}} \sum_{k=1}^{N_{sym}} O[e^{\frac{2\pi ik}{N_{sym}}} U]}_{?}$$

How to sum

$$\underbrace{\sum_{k=1}^{N_{sym}} O[e^{\frac{2\pi i k}{N_{sym}}} U]}_{?} \to \sum_{k=1}^{N_{sym}} O[$$



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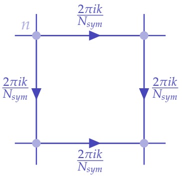
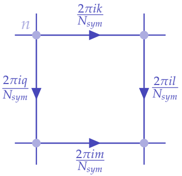


$]$

$$\to \sum_{..,k,l,m,q,..} O[$$



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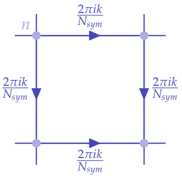

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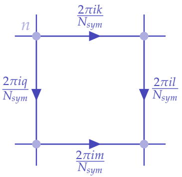

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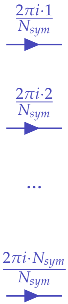

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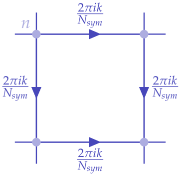

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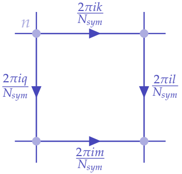

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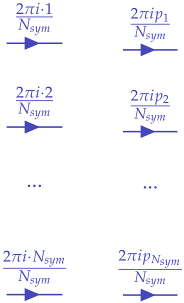

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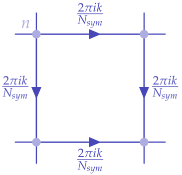

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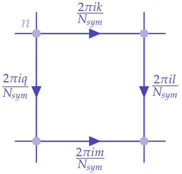
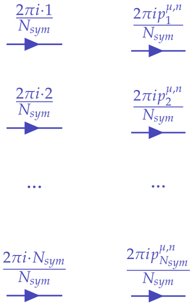
$$\to \sum_{..,k,l,m,q,..} O[$$



$]$



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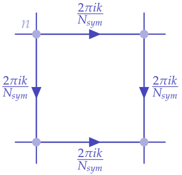
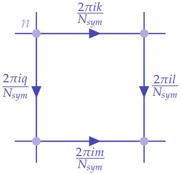


$$]$$

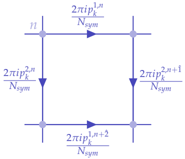
$$\rightarrow \sum_{..,k,l,m,q,..} O[$$



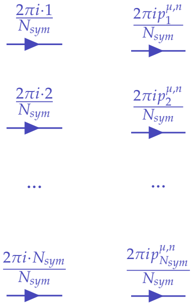
$$]$$

[Kuo 2006]

$$\rightarrow \sum_{k=1}^{N_{sym}} O[$$



$$]$$



Plaquette

$$\langle \Box \rangle = \frac{\int \mathrm{d}U \, \Box[U] \, \mathrm{e}^{-S[U]}}{\int \mathrm{d}U \; \mathrm{e}^{-S[U]}}$$

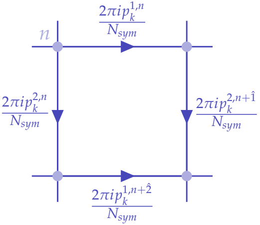
Thermalization Heatbath $\rightarrow [U]$

Plaquette

$$\langle \Box \rangle = \frac{\int \mathrm{d}U \, \Box[U] \, \mathrm{e}^{-S[U]}}{\int \mathrm{d}U \; \mathrm{e}^{-S[U]}}$$

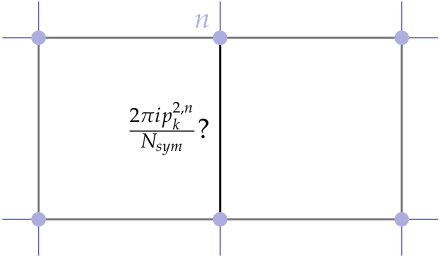
Thermalization Heatbath $\rightarrow [U]$

$$\langle \Box \rangle \approx \frac{1}{N_{sym}} \sum_{k=1}^{N_{sym}} O[\quad \cdots \quad]$$



"Symmetrized Configurations"

Metropolis Step



Proposal

$$U'_{2,n} = \mathrm{e}^{\frac{2\pi i p_k^{2,n}}{N_{sym}}} U_{2,n}$$

Accept/Reject

$$\mathrm{e}^{-(S_{loc}(U')-S_{loc}(U))}$$

Algorithm

Thermalization $\rightarrow [U]$

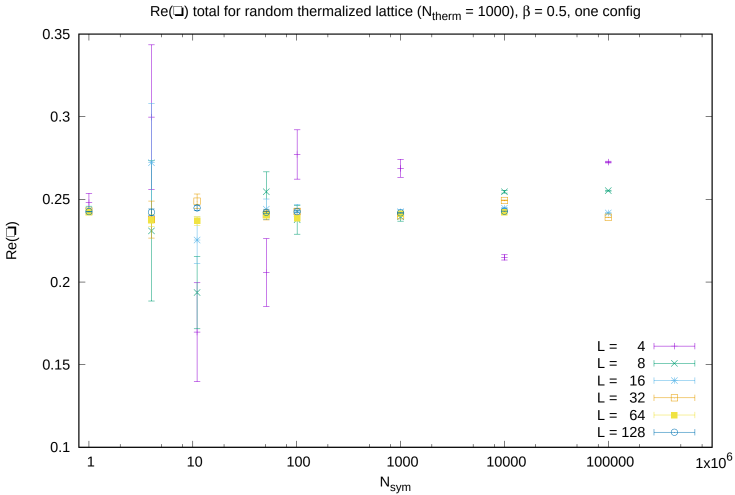
Create Symmetrization Stacks $\rightarrow (p_k)^{\mu,n}$

for all k in $\{1, ..., N_{sym}\}$

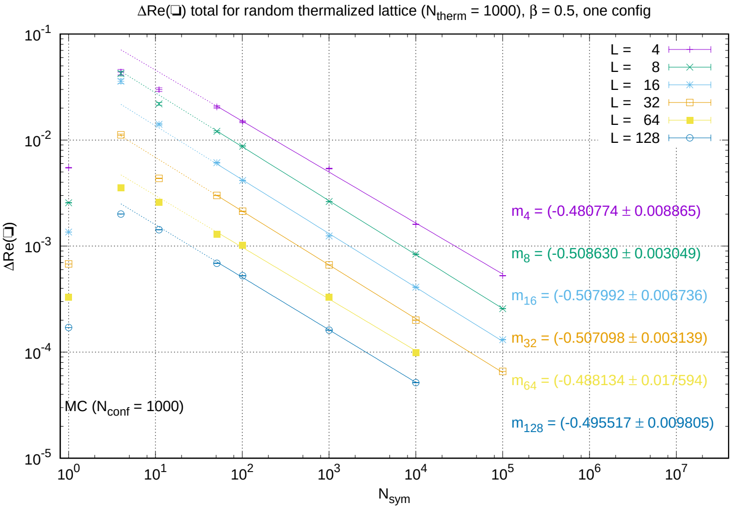
  Metropolis Step $\rightarrow [U]_k$

Compute Observable $\rightarrow \frac{1}{N_{sym}} \sum_{k=1}^{N_{sym}} O[U]_k$

First Results Plaquette



First Results Error



Acceptance: ~ 0.7

Adding a sign-Problem $S_\theta = S + i\theta Q$

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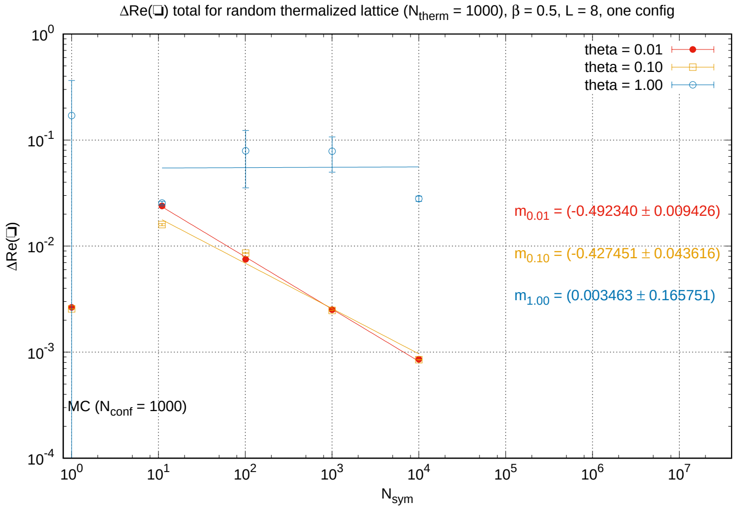
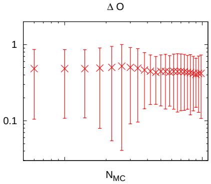


Acceptance: ~ 0.7

Conclusions

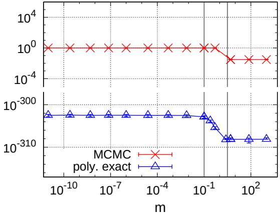
$S \in \mathbb{C}$



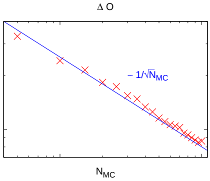
↑

1dQCD

↓



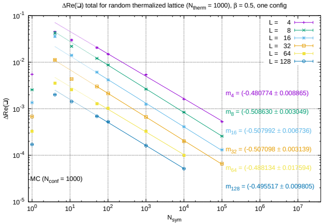
$S > 0$



↑

2d $\mathcal{U}(1)$ gauge theory

↓



Thank You

Quadrature Rule

$$\int_G \mathrm{d}h\, f(U) \approx \frac{1}{\#Q_G} \sum_{V \in Q_G(m)} w_V f(VU)$$

$$\int_a^b \mathrm{d}x\, f(x) \approx \int_a^b \mathrm{d}x\, L(x) = \int_a^b \mathrm{d}x \left(\sum_{i=1}^{n-1} f(x_i) l_i(x) \right)$$
$$= \sum_{i=1}^{n-1} f(x_i) \underbrace{\int_a^b \mathrm{d}x\, l_i(x)}_{w_i}$$

$$L^{(m,N-1)}(f, \mathbf{x}) = \sum_{|\mathbf{p}|=m} \underbrace{\prod_{i=1}^{N} \prod_{j=0}^{p_i-1} \frac{x_i^2 - t_j^2}{t_{p_j}^2 - t_j^2}}_{l} \{f(\mathbf{t_p})\}$$

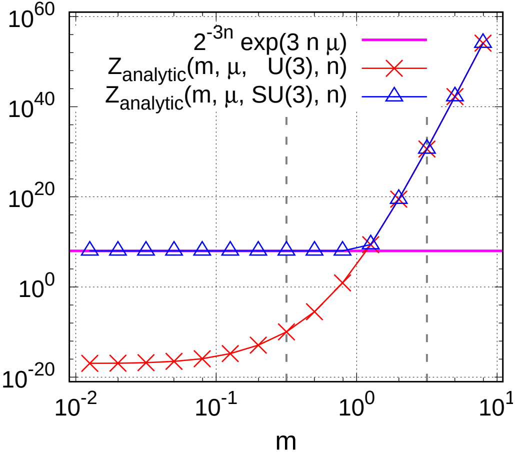
$$|\mathbf{t_p}| = t_{p_1} + ... t_{p_N} = 1, |\mathbf{p}| = p_1 + ... + p_N = m, \qquad t_i = \sqrt{\frac{i+1}{m+N}}$$

Analytic Result Partition Function $\mathcal{SU}(3)$

$$Z[U] = \int_{\mathcal{SU}(3)} \mathrm{d}U \, \det\left(c(m) + 2^{-3}\, \mathrm{e}^{-3\mu}\, U^* + (-1)^3 2^{-3}\, \mathrm{e}^{3\mu}\, U\right)$$

$$Z_{ana}^{\mathcal{SU}(N)} = Z_{ana}^{\mathcal{U}(N)} + 2^{1-Nn} \cosh(Nn\mu), \quad n \text{ even}$$

- $\mathcal{G} = \mathcal{SU}(3)$
- double prec
- $\mu = 1$
- 20 lattice points
- 50 repetitions



Result Partition Function $\mathcal{SU}(3)$

$$Z[U] = \int_{\mathcal{SU}(3)} \mathrm{d}U \, \det\left(c(m) + 2^{-3}\, \mathrm{e}^{-3\mu}\, U^* + (-1)^3 2^{-3}\, \mathrm{e}^{3\mu}\, U\right)$$

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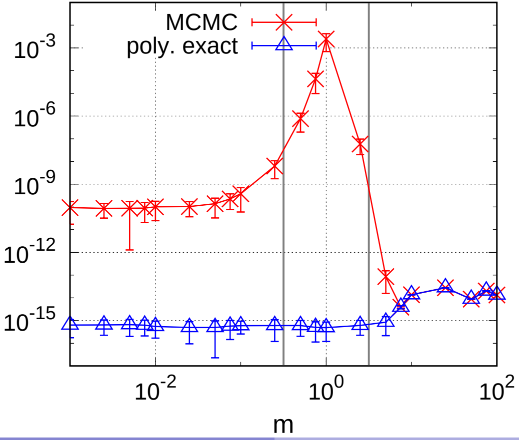

Poly. Exact. - Condensate with smaller m values