QCD, random matrix theory and the sign problem

Jacques Bloch

University of Regensburg

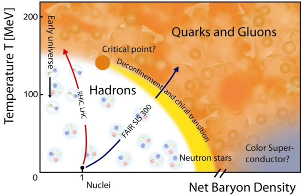
Berlin, May 23, 2011

Outline

1. QCD, quark chemical potential and sign problem
2. Lattice QCD and chiral random matrix theory
3. Spectral features of RMT and sign problem
4. Subset solution to sign problem in dynamical RMT simulations

Introduction

- QCD at nonzero temperature and density → phase diagram



- Dynamical simulations of QCD at nonzero chemical potential μ: complex fermion determinant → sign problem in MC simulations
- Universality properties of the Dirac operator to leading order in the ε-regime of QCD → investigate using random matrix theory
- Dynamical simulations of random matrices (DRMT) at nonzero μ also suffer from sign problem → playground for algorithmic developments
- Subset method: avoids the sign problem in DRMT case

Confinement and chiral symmetry

Properties of QCD:

- Confinement: no free quarks, only bound states
- massless quarks: action invariant under independent transformations of left-handed and right-handed fermions → chiral symmetry

$$SU(N_f)_L \times SU(N_f)_R \times U(1)_A \times U(1)_V$$

  - Adler-Bell-Jackiw anomaly: $U(1)_A$ broken by quantum corrections
  - chiral symmetry is spontaneously broken (nonperturbative):

$$SU(N_f)_L \times SU(N_f)_R \to SU(N_f)_V$$

    - light pions: pseudo-Goldstone bosons
    - light quarks but heavy hadrons: dynamically generated constituent quark mass
- phase transition: deconfinement and chiral symmetry restoration

QCD at nonzero quark chemical potential

- QCD Partition function (in Euclidean space):

$$Z_{\text{QCD}} = \int \mathcal{D}A_\mu \left[\prod_{f=1}^{N_f} \int \mathcal{D}\psi_f \mathcal{D}\bar{\psi}_f \right] e^{-(S_G + S_F)}$$

S_G: SU(3) gauge action, S_F: fermion action

$$S_F = \sum_{f=1}^{N_f} \int d^4x \, \overline{\psi}_f(x) D(x; m_f, \mu) \psi_f(x)$$

with Dirac operator $D(x; m, \mu) = m + \gamma_\mu \partial^\mu_{\text{cov}} + \mu\gamma_4$

- QCD at nonzero quark density → quark chemical potential μ couples to quark density $\psi^\dagger \psi = \overline{\psi}\gamma_4\psi$

The fermion determinant

- Integration over fermion fields:

$$Z_{\text{QCD}} = \int \mathcal{D}A_\mu \, e^{-S_G} \prod_{f=1}^{N_f} \det[D(x;m_f,\mu)]$$

- Expectation value of observable Y given by ensemble average:

$$\langle Y \rangle = \frac{1}{Z_{\text{QCD}}} \int \mathcal{D}A_\mu \, Y(A_\mu) \underbrace{e^{-S_G} \prod_{f=1}^{N_f} \det[D(x;m_f,\mu)]}_{\text{MCMC weight function P ?}}$$

- Fermion determinant:

$$\det[D(x;m_f,\mu)] \text{ is } \begin{cases} \text{real} & \text{for } \mu = 0 \\ \text{complex} & \text{for } \mu \neq 0 \end{cases}$$

Lattice QCD

- Simulate QCD on a discretized Euclidean space-time lattice
  $\longrightarrow$ partition function similar to statistical physics
- Approximate functional integral by Markov chain Monte-Carlo simulation with a finite number of relevant $SU(3)$ configurations
- Use importance sampling, e.g. Metropolis method
  $\longrightarrow$ configurations distributed according to the QCD action
- Sample average of Y using measurements on N_{MC} configurations:

$$\overline{Y} = \frac{1}{N_{\text{MC}}} \sum_{j}^{N_{\text{MC}}} Y_j$$

- Sign problem at $\mu \neq 0$: $\det[D(\mu)]$ becomes complex
  $\longrightarrow$ can no longer be interpreted as probabilistic weight for MCMC

Quark chemical potential on the lattice

Discretized version of fermion action:

$$S_F = \sum_{x,y} \bar{\psi}_y D_{yx} \psi_x$$

Wilson Dirac-operator with chemical potential :

$$(D_W)_{yx}(\mu) = \delta_{yx} - \kappa \sum_{i=1}^{3} \left[(1+\gamma_i) U_i(x) \delta_{y,x+\hat{\imath}} + (1-\gamma_i) U_i^\dagger(x) \delta_{y,x-\hat{\imath}} \right]$$
$$- \kappa \left[e^{\mu} (1+\gamma_4) U_4(x) \delta_{y,x+\hat{4}} + e^{-\mu} (1-\gamma_4) U_4^\dagger(x) \delta_{y,x-\hat{4}} \right]$$

(Hasenfratz-Karsch, Kogut et al. 1983)

- removes fermion doubling
- breaks chiral symmetry

- Color matrices U_i
- Dirac matrices γ_i
- Hopping parameter: $\kappa = (2am + 8)^{-1}$

Chiral symmetry on the lattice

- chiral symmetry on the lattice – Ginsparg-Wilson relation:

$$\{D, \gamma_5\} = aD\gamma_5 D$$

- massless overlap Dirac-operator (Neuberger-Narayanan)

$$D_{\text{ov}} = \mathbb{1} + \gamma_5 \,\text{sgn}(\gamma_5 D_W)$$

where D_W is Wilson-Dirac operator:

$$(D_W)_{yx} = \delta_{yx} - \kappa \sum_{i=1}^{4} (T_i^+ + T_i^-)$$

with $\quad (T_\nu^\pm)_{yx} = (1 \pm \gamma_\nu) U_{x,\pm\nu} \delta_{y,x\pm\hat{\nu}}$

- D_{ov} has exact zero modes with definite chirality $\langle\gamma_5\rangle = \pm 1$ reflecting topological charge of gauge configuration (Atiyah-Singer index theorem)

Quark chemical potential and chiral symmetry on the lattice

Generalize overlap Dirac operator to nonzero quark chemical potential

- Overlap operator at $\mu \neq 0$ (JB, Wettig PRL97(012003) 2006):

$$D_{\text{ov}}(\mu) = \mathbb{1} + \gamma_5 \, \text{sgn}(\gamma_5 D_W(\mu))$$

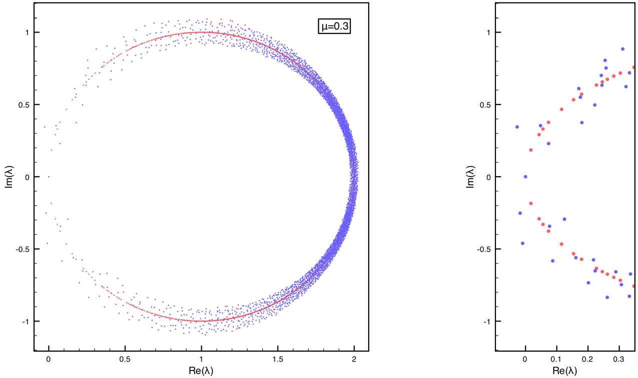
where $D_W(\mu)$ is Wilson-Dirac operator at $\mu \neq 0$: (Hasenfratz-Karsch 1983, Kogut et al. 1983)

$$D_W(\mu) = 1 - \kappa \sum_{i=1}^{3} (T_i^+ + T_i^-) - \kappa (e^{\mu} T_4^+ + e^{-\mu} T_4^-)$$

- Sign problem at $\mu \neq 0$: $\det[D_{\text{ov}}(\mu)]$ is complex $\longrightarrow$ can no longer be incorporated in probability distribution for MCMC

Typical spectrum ($V = 4^4, \beta = 5.1, m_W = -2$)

$\mu = 0.3$



- $D_{\text{ov}}(\mu)$ satisfies Ginsparg-Wilson relation $\longrightarrow$ lattice chiral symmetry
- exact zero modes with definite chirality
- naturally violates γ_5-Hermiticity $\longrightarrow$ spectrum no longer on circle

Random matrix theory

- Chiral perturbation theory: to leading order (in ε-regime) the spectral properties of Dirac operator in QCD are universal and can be described by chiral random matrix theory (RMT).
- Two-matrix model (Osborn) for Dirac operator:

$$D_{\mu,m}(\phi_1,\phi_2) = \begin{pmatrix} m & i\phi_1 + \mu\phi_2 \\ i\phi_1^\dagger + \mu\phi_2^\dagger & m \end{pmatrix}$$

  with ϕ_1, ϕ_2 complex $(N+\nu)\times N$ matrices distributed according to partition function (ν zero modes)

$$Z = \int d\phi_1 d\phi_2 w(\phi_1) w(\phi_2) \det{}^{N_f} D_{\mu,m}(\phi_1,\phi_2)$$

  with Gaussian weights $w(\phi) = (N/\pi)^{N(N+\nu)} \exp(-N \operatorname{tr} \phi^\dagger \phi)$.
- $D_{\mu,m}$ is non-Hermitian $\longrightarrow$ complex determinant

Quenched RMT partition function – $N_f = 0$

- After diagonalization the partition function is:

$$Z_\nu(\mu^2, m) = \int_{\mathbb{C}} \prod_{k=1}^{N} d^2 z_k \, w^\nu(z_k, z_k^*; \mu^2) \, |\Delta_N(\{z^2\})|^2$$

  with weight function:

$$w^\nu(z, z^*; \mu^2) = |z|^{2\nu+2} \exp\left[-\frac{N(1-\mu^2)}{4\mu^2}(z^2 + z^{*2})\right] K_\nu \left[\frac{N(1+\mu^2)}{2\mu^2}|z|^2\right]$$

  and Vandermonde determinant: $\Delta_N(\{z^2\}) \equiv \prod_{i>j=1}^{N}(z_i^2 - z_j^2)$

- Using orthogonal polynomials wrt $w^\nu(z, z^*; \mu^2)$ – analytic computation of:
  - spectral density
  - individual eigenvalue distributions
  - average phase factor

Microscopic spectral density: LQCD versus chRMT

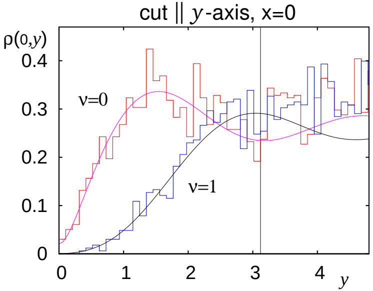
- Relating RMT to QCD – microscopic limit:
  take $N \to \infty$ while keeping $\hat{\mu}^2 = 2N\mu^2$, $\hat{m} = 2Nm$ fixed
- RMT: quenched microscopic spectral density

$$\rho_\nu(z) = \frac{|z|^2}{2\pi\hat{\mu}^2} e^{-\frac{z^2+z^{*2}}{8\hat{\mu}^2}} K_\nu\left(\frac{|z|^2}{4\hat{\mu}^2}\right) \int_0^1 dt\, t e^{-2\hat{\mu}^2 t^2} |I_\nu(tz)|^2$$

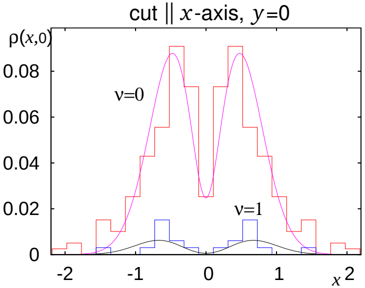
Akemann, Osborn, Splittorff, Verbaarschot 2004-2005

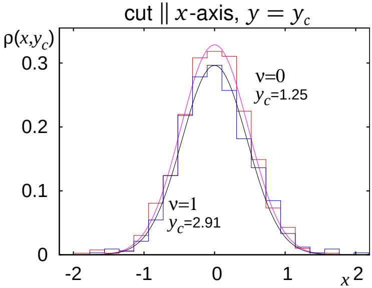
- Correspondence RMT $\longleftrightarrow$ LQCD: $z = \lambda V \Sigma$ and $\mu^2 = \mu^2_{\text{phys}} f_\pi^2 V$
- Low Energy Constants Σ and F of chiral perturbation theory can be extracted by fitting LQCD data to chRMT
- LQCD: overlap fermions have exact zero modes $\longrightarrow$ test RMT predictions for non-trivial topology $(\nu \neq 0)$

Spectral density, $V = 4^4$, $\mu = 0.1$, 8703 config.



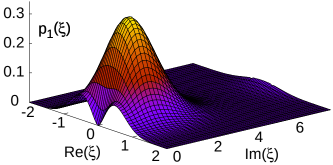
Σa^3	$f_\pi a$	χ^2/dof
0.0812(11)	0.261(6)	0.67





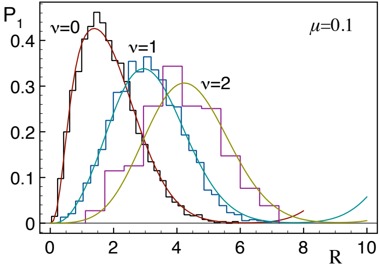
Individual eigenvalue distributions

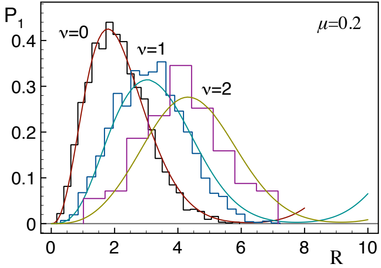
Distribution of first peak in RMT:



Integrated eigenvalue distribution – RMT vs LQCD:

$$P_1(R) = \int d\theta R\, p_1(R,\theta)$$





Phase factor of fermion determinant in chRMT

- Determinant of massive Dirac operator:

$$\det[D_{\mu,m}] \equiv R e^{i\theta}$$

- Average phase factor $\langle e^{2i\theta} \rangle$ reflects fluctuations of fermion determinant
  $\longrightarrow$ characterizes strength of sign problem in dynamical simulations
- Phase factor of the two-fermion determinant is:

$$e^{2i\theta} = \frac{\det(D(\mu)+m)}{\det(D^\dagger(\mu)+m)} = \prod_{k=1}^{N} \frac{m^2 - z_k^2}{m^2 - z_k^{*2}}$$

- Unquenched ensemble average ($\alpha = \mu^2$):

$$\langle e^{2i\theta} \rangle_{N_f} = \left\langle \frac{\det(D(\mu)+m)}{\det(D^\dagger(\mu)+m)} \right\rangle_{N_f} = \frac{Z_\nu^{N_f+1|1^*}(\alpha, m, m_f)}{Z_\nu^{N_f}(\alpha, m_f)}$$

$$= \frac{1}{Z_\nu^{N_f}} \int_{\mathbb{C}} \prod_{k=1}^{N} d^2 z_k \, w^\nu(z_k, z_k^*; \alpha) \, |\Delta_N(\{z^2\})|^2 \frac{m^2 - z_k^2}{m^2 - z_k^{*2}} \prod_{f=1}^{N_f} (m_f^2 - z_k^2) \,,$$

Average phase factor

- Zero topology: Splittorff & Verbaarschot, PRD 75 (2007) 116003
  General topol.: JB & Wettig, JHEP 03 (2009) 100, JHEP 05 (2011) 048
- Computable with complex Cauchy transform (Akemann, Pottier & Bergère (2004)):
- Microscopic limit of average phase factor with N_f equal mass fermions:

$$\langle e_s^{2i\theta} \rangle_{N_f} = \frac{1}{(2\hat{m})^{N_f} N_f!} \frac{\begin{vmatrix} \mathcal{H}^s_{\nu,0}(\hat{\alpha},\hat{m}) & \cdots & \mathcal{H}^s_{\nu,N_f+1}(\hat{\alpha},\hat{m}) \\ I^{(0)}_{\nu,0}(\hat{m}) & \cdots & I^{(0)}_{\nu,N_f+1}(\hat{m}) \\ \vdots & \vdots & \vdots \\ I^{(N_f)}_{\nu,0}(\hat{m}) & \cdots & I^{(N_f)}_{\nu,N_f+1}(\hat{m}) \end{vmatrix}}{\begin{vmatrix} I^{(0)}_{\nu,0}(\hat{m}) & \cdots & I^{(0)}_{\nu,N_f-1}(\hat{m}) \\ \vdots & \vdots & \vdots \\ I^{(N_f-1)}_{\nu,0}(\hat{m}) & \cdots & I^{(N_f-1)}_{\nu,N_f-1}(\hat{m}) \end{vmatrix}}$$

with $I_{\nu,k}(z) = z^k I_{\nu+k}(z)$, $I_k(z)$: modified Bessel function

Complex Cauchy transform (microscopic limit)

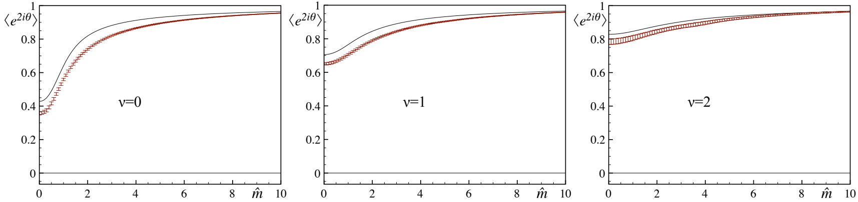
$$\mathcal{H}^s_{\nu,k}(\hat{\alpha},\hat{m}) = -\frac{e^{-2\hat{\alpha}}}{4\pi\hat{\alpha}\hat{m}^\nu}\int_{\mathbb{C}}\frac{d^2z}{z^2-\hat{m}^2}\frac{|z|^{2(\nu+1)}}{z^{*\nu}}e^{-\frac{z^2+z^{*2}}{8\hat{\alpha}}}K_\nu\left(\frac{|z|^2}{4\hat{\alpha}}\right)I_{\nu,k}(z^*)$$

- Integrand of $\mathcal{H}_{\nu,k}(\alpha,m)$ strongly oscillates in $\mathrm{Im}\, z$ direction
- Numerical solution too inaccurate
- Semi-analytic solution using complex analysis and properties of orthogonal polynomials

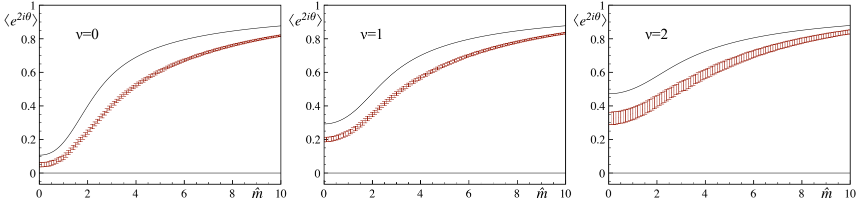
$$\mathcal{H}^s_{\nu,k}(\hat{\alpha},\hat{m}) = \frac{e^{-2\hat{\alpha}-\frac{\hat{m}^2}{8\hat{\alpha}}}}{4\hat{\alpha}}\int_0^{\hat{m}} du\, u^{k+1}K_\nu\left(\frac{\hat{m}u}{4\hat{\alpha}}\right)e^{-\frac{u^2}{8\hat{\alpha}}}I_{\nu+k}(u)$$
$$+\frac{(4\hat{\alpha})^{\nu+k}}{2\hat{m}^\nu}\int_1^\infty ds\, e^{-\frac{\hat{m}^2}{8\hat{\alpha}s}-2\hat{\alpha}s}(1-s)^k s^{\nu-1}$$

Compare chRMT versus quenched LQCD

$\mu = 0.1\ (\hat{\alpha} = 0.175)$



$\mu = 0.2\ (\hat{\alpha} = 0.615)$

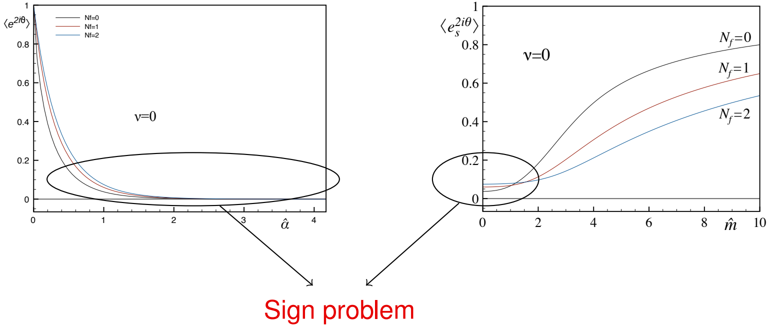


- Agreement only qualitative → not enough EV's in universality region

- Average phase factor $\langle e^{2i\theta} \rangle$ reflects fluctuations of fermion determinant
  $\longrightarrow$ characterizes strength of sign problem

Analytic RMT results for $\langle e^{2i\theta} \rangle$

$\langle e^{2i\theta} \rangle$ vs $\hat{\alpha} = 2N\mu^2$ $(\hat{m} = 0)$ $\qquad$ $\langle e^{2i\theta} \rangle$ vs $\hat{m} = 2Nm$ $(\hat{\alpha} = 1)$



Unquenching the beast

Examine sign problem using
dynamical simulations
of chiral random matrix theory

Dynamical simulations with complex weights

- Ensemble average of y in ensemble with weight w:

$$\langle y \rangle_w = \frac{\int dx\, w(x) y(x)}{\int dx\, w(x)}$$

- Reweighting: Introduce auxiliary ensemble with weight w_{aux}:

$$\langle y \rangle_w = \frac{\int dx\, w_{\text{aux}}(x) \frac{w(x)}{w_{\text{aux}}(x)} y(x)}{\int dx\, w_{\text{aux}}(x) \frac{w(x)}{w_{\text{aux}}(x)}} = \frac{\left\langle \frac{w}{w_{\text{aux}}} y \right\rangle_{w_{\text{aux}}}}{\left\langle \frac{w}{w_{\text{aux}}} \right\rangle_{w_{\text{aux}}}}$$

  Ensemble w_{aux} can be sampled using importance sampling methods.
  Typical examples for w_{aux}: quenched, phase quenched, sign quenched

- Problem: Work needed to make reliable measurements on the statistical ensemble grows exponentially with volume and μ
  Reason: computation of exponentially small reweighting factors from a statistical sampling of largely canceling contributions

Subset method for dynamical RMT simulations

Principle: rewrite partition function as integral over subsets Ω:

$$Z = \int d\Omega \, W(\Omega) \, \sigma_{\mu,m}(\Omega)$$

with subsets

$$\Omega(\phi) = \left\{ \psi(\phi;\theta_n) : \theta_n = \frac{\pi n}{N_s} \wedge n = 0, \ldots, N_s - 1 \right\},$$

containing N_s orthogonal rotations of a given $\phi = (\phi_1, \phi_2)$:

$$\begin{cases} \psi_1(\phi;\theta) = \cos\theta \ \phi_1 + \sin\theta \ \phi_2 \\ \psi_2(\phi;\theta) = \cos\theta \ \phi_2 - \sin\theta \ \phi_1 \end{cases}$$

- Gaussian weights $w(\psi_1)w(\psi_2)$ are independent of $\theta \to W(\Omega)$
- Fermionic subset weights:

$$\sigma_{\mu,m}(\Omega) = \sum_{n=0}^{N_s-1} \det{}^{N_f} D_{\mu,m}(\psi(\phi;\theta_n))$$

Subset method – Equivalence

- For each configuration $\phi = (\phi_1, \phi_2)$ of original partition function
  $\longrightarrow$ subset $\Omega(\phi)$
- Set of all subsets forms an N_s-fold covering of the RMT ensemble
  $\longrightarrow$ equivalent partition function

Subset method – Positivity theorem

Subset method is based on the following *positivity theorem:*

> For any such subset Ω the fermionic subset weight $\sigma_{\mu,m}(\Omega)$ is *real* and *positive* if $N_s > NN_f$ (for arbitrary m and $\mu < 1$)

More specifically:

- For any μ and $m = 0$:

$$\sigma_{\mu,0}(\Omega) = (1-\mu^2)^{NN_f}\,\sigma_{0,0}(\Omega)$$

  - $\sigma_{0,0}$ is real and positive $\rightarrow$ $\sigma_{\mu,0}$ also real and positive for $\mu < 1$
  - For $\mu = 1$ the sum of determinants is exactly zero

- For $m \neq 0$: $\sigma_{\mu,m}$ is real and $\sigma_{\mu,m}(\Omega) > (1-\mu^2)^{NN_f}\,\sigma_{0,m}(\Omega)$ for $\mu < 1$ $\rightarrow$ $\sigma_{\mu,m}$ is positive

Subset method – Simulations

- Use weights $W(\Omega)\sigma_{\mu,m}(\Omega)$ to generate subsets of random matrices using a Metropolis algorithm
- In practice: set subset size N_s to its minimum value, i.e., $N_s = NN_f + 1$
- Successive subsets in the Markov chain are generated as follows:
  - randomly choose configuration in current subset
  - generate new configuration by making random step
  - construct subset corresponding to new configuration
  - apply accept-reject step to proposed subset

  $\longrightarrow$ satisfies detailed balance
- Sample average $\overline{O}$ of observable O over sample of N_{MC} subsets Ω_k:

$$\overline{O}_{\mu,m} = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} \sum_{n=0}^{N_s-1} \frac{\det^{N_f} D_{\mu,m}(\psi^{kn})}{\sigma_{\mu,m}(\Omega_k)} O_{\mu,m}(\psi^{kn}),$$

where $\psi^{kn} \in \Omega_k$.

Subset method – Simulations

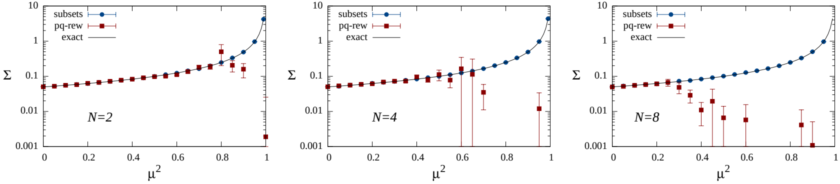
- Apply the subset method to compute the chiral condensate

$$\Sigma = \frac{1}{2N} \operatorname{tr} D^{-1}$$

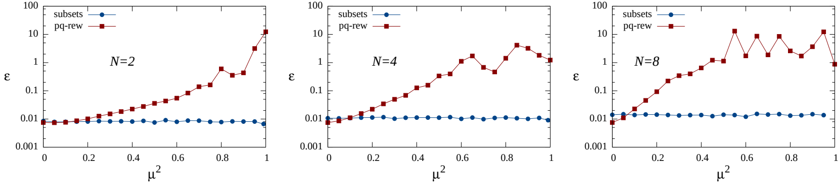
- In each Markov chain we generate N_{MC}=100,000 subsets.
- Successive subsets in Markov chains are correlated with integrated autocorrelation time τ. Number of independent subsets: $N_{MC}/2\tau$.
- Statistical errors: standard error formula corrected for autocorrelations
- Compare with standard reweighting methods (quenched, phase quenched and sign quenched). Generate $(NN_f + 1) \times N_{MC}$ random matrices to get same total number of matrices as in subset method.
- Simulations for $N = 2, \ldots, 34$ with $N_f = 1$ and $m = 0.1/2N$ (mass is small w.r.t. magnitude of smallest eigenvalue)

Subset method vs phase-quenched reweighting
Chiral condensate Σ vs μ^2 for $N = 2, 4, 8$

(Full line: exact analytical result)



relative statistical error ε



Results

Σ versus μ^2

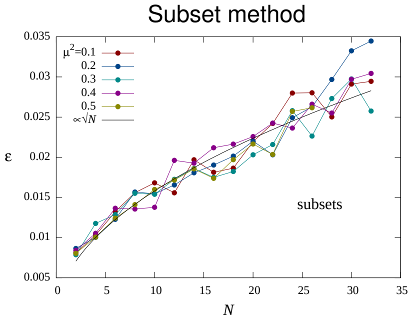
Phase quenched reweighting:

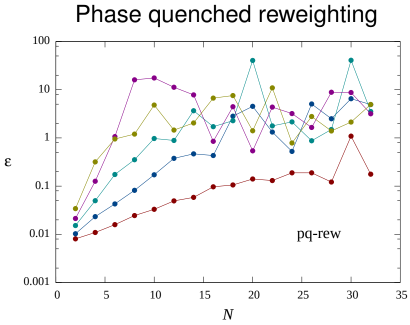
- As matrix size increases: reweighting method fails for smaller and smaller μ^2 due to sign and overlap problem
- Error grows exponentially with μ, until method fails when set of sampled matrices no longer overlaps with relevant configurations

Subset method:

- results reliable up to much larger values of μ^2 and agree with the analytical predictions.
- Error independent of the chemical potential

Relative error ε on the chiral condensate versus matrix size N





(semi-log plot)

Results

Σ versus N

Phase quenched reweighting:

- Work grows exponentially with N and μ

Subset method:

- Error independent of μ
- Error proportional to
  - $\sqrt{N}$ for fixed number of sampled subsets
  - N for fixed number of sampled matrices
- For constant error: number of sampled matrices should grow as N^2

Comparison:

- cancellations no longer happen through statistical sampling, but occur deterministically inside subsets of size O(n).

Summary & Outlook

- Chiral RMT gives spectral information about Dirac operator of QCD
- Average phase factor characterizes sign problem and can be computed in RMT
- Sign problem of QCD is also present in dynamical RMT simulations
- Subset method solves the sign problem for Osborn model

- Open question: is subset method applicable to physically relevant systems?