QCD at Finite Density and the Sign Problem

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Contents

I. Motivation

Questions

QCD and |QCD|

QCD Phase Diagram

Issues and Questions

- QCD at nonzero chemical potential has a sign problem and an overlap problem.
- Can we quantify the sign problem and overlap problem, and determine its dependence on the parameters of the phase diagram?
- Are there regions of phase space or observables for which these problems become manageable?
- Will it ever be possible to access interesting physics related to the existence of a Fermi surface by lattice QCD methods?
- Is the sign problem a fundamental problem rather than a technical problem that can be evaded?

QCD Partition Function

The QCD partition at temperature $1/\beta$ and quark chemical potential μ is given by

$$Z_{\rm QCD}(\mu,\beta) \quad = \quad \sum_k e^{-\beta(E_k-\mu N_k)},$$

where the sum is over all states with energy E_k and quark number N_k .

- Because of charge conjugation symmetry, $Z_{\rm QCD}(\mu,\beta)$ is an even function of μ .
- $Z_{\rm QCD}(\mu,\beta)$ is expected to have a well-defined high-temperature expansion in powers of μ^2/T^2 .
- Interesting effects related to the formation of a Fermi-sphere cannot be obtained from this expansion.
- This partition function can be rewritten as a Euclidean quantum field theory

$$Z_{\rm QCD} \quad = \quad \langle \prod_k^{N_f} \det(D + m_k + \mu_k\gamma_0)\rangle_{\rm YM}.$$

Dirac operator

quark mass matrix

imaginary vector potential

|QCD|

We will compare the QCD partition function and the QCD partition function where the fermion determinant has been replaced by its absolute value (the phase quenched QCD partition function)

$$Z_{|\mathrm{QCD}|} = \langle |\det(D+m+\mu\gamma_0)|^2\rangle = \langle \det(D+m+\mu\gamma_0)\det(D+m-\mu\gamma_0)\rangle.$$

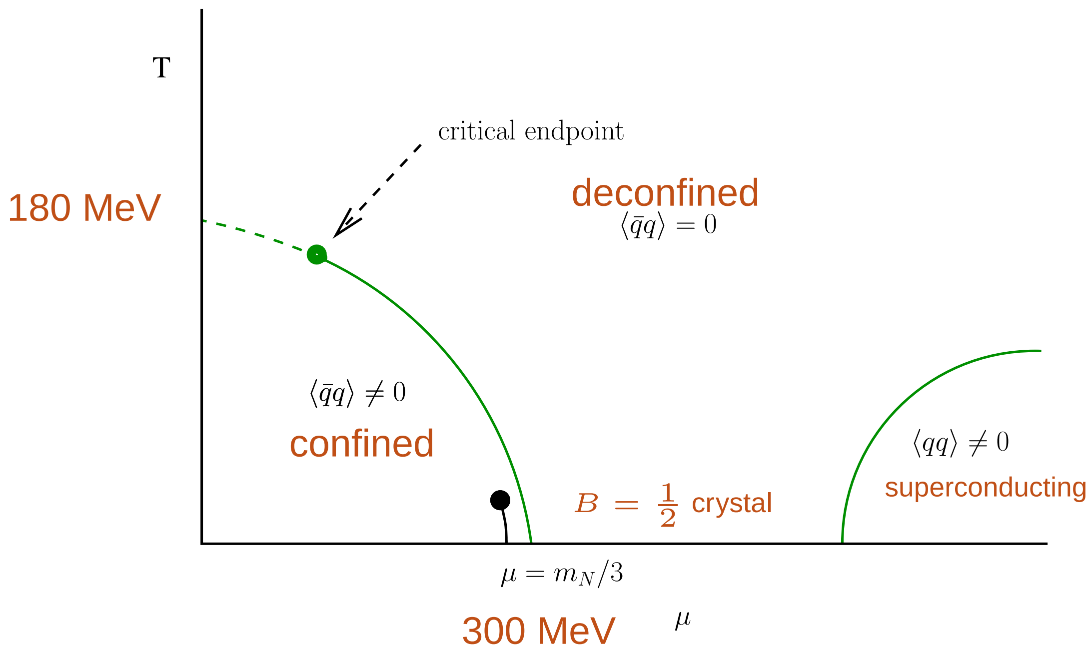
Therefore, μ can be interpreted as an isospin chemical potential. Goldstone bosons made out of quarks and conjugate anti-quarks are charged with respect to the chemical potential. Alford-Kapustin-Wilczek-1999

The mass of the Goldstone bosons is given by $M_k - 2\mu q_k$ with q_k the charge of the Goldstone bosons.

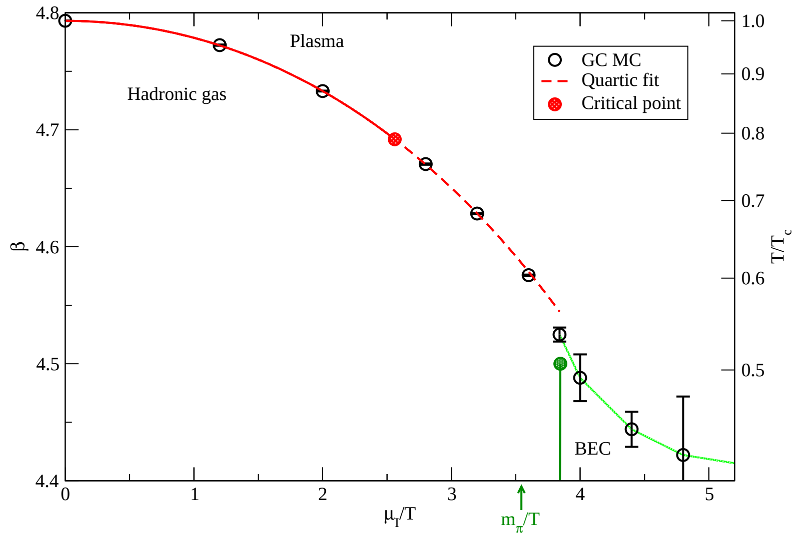
A phase transition to a Bose condensed phase takes place at $\mu = m_\pi/2$.

KSTVZ-2000, Toublan-JV-2000, Son-Stephanov-2000

Phase Diagram QCD and |QCD|



Schematic QCD phase diagram.



Phase diagram of phase quenched QCD (de Forcrand-Stephanov-Wenger-2007). Agrees with earlier work by Kogut and Sinclair.

The high temperature expansion of the free energy can be obtained by a Taylor expansion (Allton-et-al-2003, Gavai-Gupta-2003), reweighting (Fodor-Katz-2002) or from an extrapolation from imaginary μ (Lombardo-2000, de Forcrand-Philipsen-2002, D'Elia-Lombardo-2002).

II. Sign Problem

Average Phase Factor

Phase Factor and Dirac Spectra

Distribution of the Phase

Can we Evade the Sign Problem

Sign Problem for $\mu \neq 0$

Because the Dirac operator at nonzero μ is nonhermitean, the fermion determinant is complex

$$\det(D + \mu\gamma_0 + m) = e^{i\theta} |\det(D + \mu\gamma_0 + m)|.$$

The $fundamental$ problem is that the average phase factor may vanish in the thermodynamic limit, so that Monte-Carlo simulations are not possible (sign problem).

The severity of the sign problem can be measured by the ratio

$$\langle e^{2i\theta} \rangle_{1+1^*} \equiv \frac{\langle \det^2(D + m + \mu\gamma_0) \rangle}{\langle |\det(D + m + \mu\gamma_0)|^2 \rangle} \sim e^{-V(F_{N_f=2} - F_{pq})}.$$

full QCD
partition function

phase quenched
partition function

The phase of the quark determinant wipes out the pion condensation phase.

The difference in free energy between the phase quenched theory and the full theory (at low temperatures) is determined by pion physics.

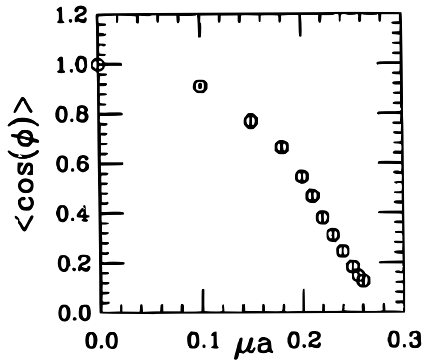
Splittorff-JV-2006

Phase Factor and Dirac Eigenvalues

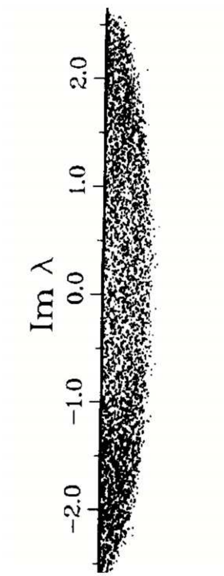
$$\det(D + m + \mu\gamma_0) = e^{i\theta} |\det(D + m + \mu\gamma_0)|$$

$$\prod_k (\lambda_k + m)$$

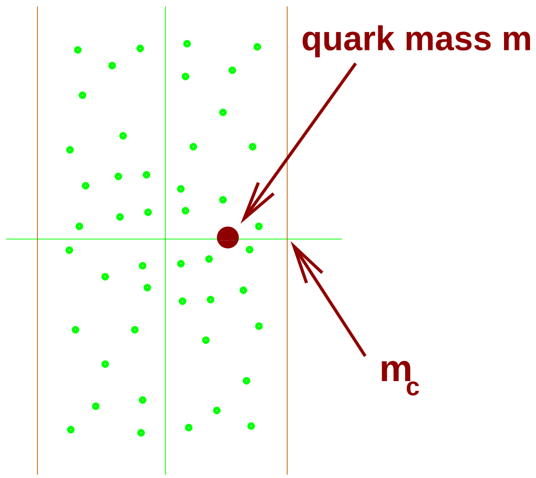
phase factor



Toussaint-1990



Barbour et al. 1986



Scatter plot of Dirac eigenvalues

$$m < m_c \qquad \text{then} \qquad \langle e^{i\theta} \rangle \sim 0$$

The Distribution of Phase

The distribution of the phase is given by

$$\langle \delta(\theta - \theta') \rangle_{1+1} \equiv \langle \delta(\theta - \theta') \mathrm{det}^2(D + m + \mu\gamma_0) \rangle = e^{2i\theta} \langle \delta(\theta - \theta') |\det(D + m + \mu\gamma_0)|^2 \rangle$$

The distribution of the phase angle for the phase quenched theory is a Gaussian. We thus find

$$\langle \delta(\theta - \theta') \rangle_{1+1} = e^{2i\theta - \theta^2/\Delta G} \quad \sim \quad e^{-(\theta - i\Delta G)^2/\Delta G}.$$

The distribution is peaked in the complex plane.

If we could use θ as integration variable this would be fine, but there are correlations between the phase and observables.

Using the Gaussian distribution we obtain

$$\langle e^{2i\theta} \rangle_{1+1^*} = \int d\theta e^{-\theta^2/\Delta G} e^{2i\theta} \sim e^{-\Delta G}, \qquad \text{but also,} \quad \langle e^{2i\theta} \rangle_{1+1^*} \sim e^{-V(F_{N_f=2} - F_{pq})}$$

So ΔG is the difference of free energy of the phase quenched theory and the two flavor theory. It can be approximated by one-loop chiral perturbation theory in the appropriate domain. Lombardo-Splittorff-JV-2009

The Distribution of Phase

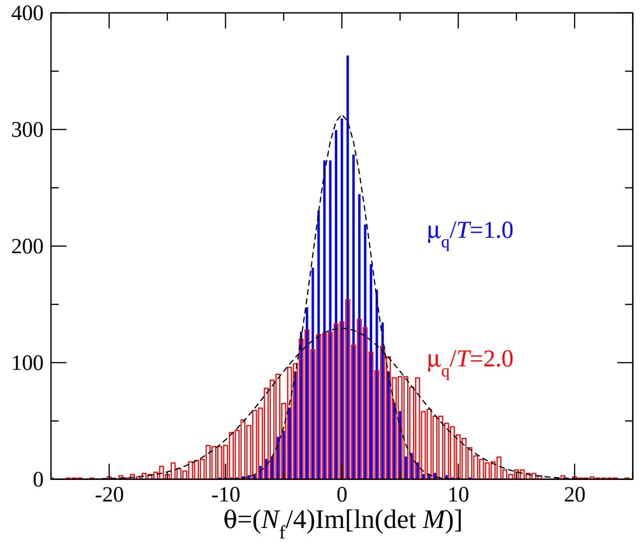
Both within one-loop chiral perturbation theory and in one-dimensional QCD we find for the distribution of the phase:

- ✓ $\mu < m_\pi/2$: $\rho(\theta)$ is a periodicized Gaussian

$$\langle \rho(\theta) \rangle_{1+1} = \frac{1}{\sqrt{2\pi \Delta G_0}} e^{-\frac{(\theta - i\Delta G)^2}{\Delta G}}.$$

one-loop chPT integral

- ✓ $\mu > m_\pi/2$: $\rho(\theta)$ is a periodicized Lorentzian Lombardo-Splittorff-JV-2009



Quenched distribution, Ejiri-2009. See also Nakagawa-etal-2012.

Can we Evade the Sign Problem?

Let is consider an observable $\mathcal{O}$. At nonzero chemical potential this operator is not necessarily Hermitian. For example $\mathcal{O}$ could be the baryon number

$$\mathcal{O} = \mathrm{Tr}\frac{\gamma_0}{D + m + \mu\gamma_0}.$$

We can decompose $\mathcal{O}$ as

$$\mathcal{O} = \mathrm{Re}[\mathcal{O}] + i\mathrm{Im}[\mathcal{O}]$$

Since $\mathcal{O}$ is a physical observable, its expectation value should be real. However, at nonzero chemical potential, the expectation value of the real and imaginary parts of the chemical potential is generally not real,

$$\langle \mathrm{Re}[\mathcal{O}] \det(D + m + \mu\gamma_0) \rangle \in \mathbb{C},$$

$$\langle \mathrm{Im}[\mathcal{O}] \det(D + m + \mu\gamma_0) \rangle \in \mathbb{C}.$$

Complex Gauge Fields

Can the complex weight be absorbed into trajectories of complex fields?

This makes sense if the integrand is peaks somewhere in the plane of complex gauge field.

A simple example is the Gaussian integral

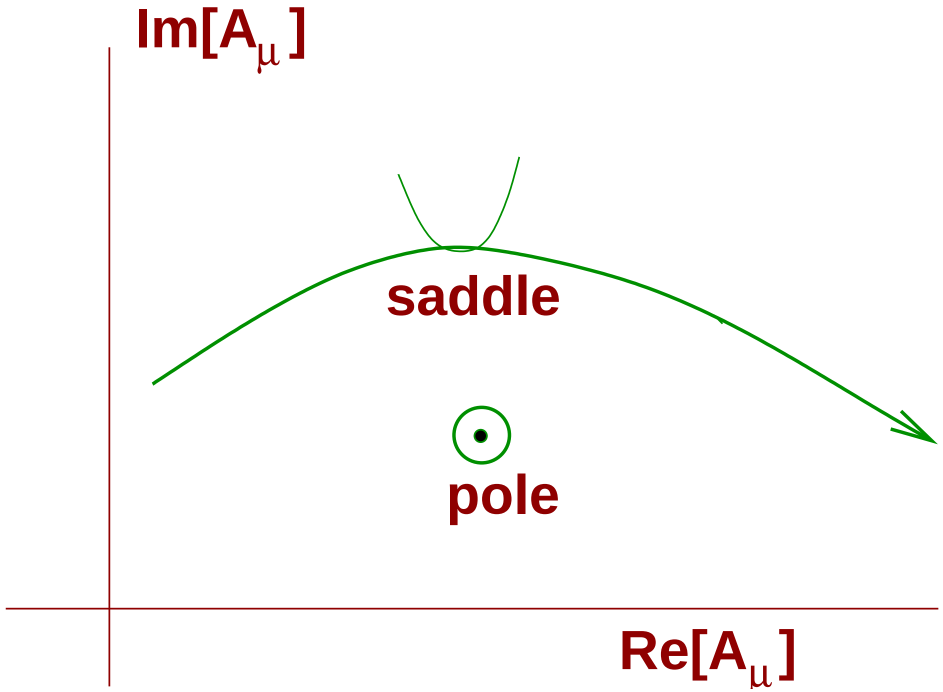
$$\int dx e^{-(x-ia)^2} = \int dx e^{-x^2+a^2+2iax}.$$

Integrating over the real axis, we have large phase fluctuations, but after shifting the integration contour by ia we get a well behaved Gaussian integral.

de Forcrand-2010, Lombardo-Splittorff-JV-2010

Poles and Saddles

Generally, observables have poles and when we change to complex trajectories we also need to take into account the pole contributions.



Deforming the integration contour over the saddle leads to a large reduction of the phase oscillations. However, we still have to take into account the pole contribution.

Integration trajectories close to the pole lead to large phase fluctuations. Pole contributions are better behaved if we stay away from the pole.

III. Distribution of the Baryon Number

Distribution of the Baryon Number Density

Overlap Problem

The Baryon Number Density

$$n_B = \frac{1}{V}\mathrm{Tr}\frac{1}{\gamma_0(D+m)+\mu}.$$

It satisfies the charge conjugation relation

$$n_B^*(\mu) = -n_B(-\mu).$$

Therefore n_B generally has a nonzero real and imaginary part.

$$\begin{aligned}\mathrm{Re}(n_B) &= \frac{1}{2}[n_B(\mu) - n_B(-\mu)] = \lim_{n\to 0}\frac{1}{2nV}\frac{d}{d\mu}\det{}^n(\gamma_0(D+m)+\mu)\det{}^n(\gamma_0(D+m)-\mu),\\ \mathrm{Im}(n_B) &= \frac{1}{2i}[n_B(\mu) + n_B(-\mu)] = \lim_{n\to 0}\frac{1}{2inV}\frac{d}{d\mu}\frac{\det^n(\gamma_0(D+m)+\mu)}{\det^n(\gamma_0(D+m)-\mu)}.\end{aligned}$$

Therefore, the real and imaginary part of the baryon number are determined by pion physics.

Since $\langle \mathrm{Im}(n_B)\rangle = \langle d\theta/d\mu\rangle$ so that $\langle \mathrm{Im}(n_B)\rangle_{1+1^*} = 0$ and $\langle \mathrm{Im}(n_B)\rangle_{1+1} = i(n_I - n_B)$

For QCD with, say with $N_f = 2$, we know that at low temperatures

$$\langle n_B\rangle_{1+1} = 0 \qquad \text{for} \quad \mu < m_N/3.$$

Expectation values of n_B for $\mu < m_\pi/2$

To one loop order in chiral perturbation theory we find

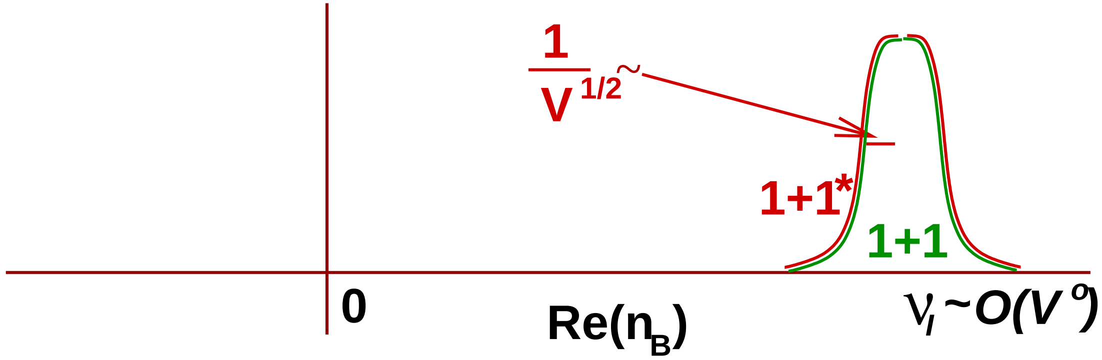
$$\begin{aligned} \langle \mathrm{Re}\, n_B \rangle_{1+1^*} &= \nu_I\,, \\ \langle \mathrm{Re}\, n_B \rangle_{1+1} &= \nu_I\,, \end{aligned}$$

$$\begin{aligned} \langle \mathrm{Im}\, n_B \rangle_{1+1^*} &= 0, \\ \langle \mathrm{Im}\, n_B \rangle_{1+1} &= i\nu_I\,. \end{aligned}$$

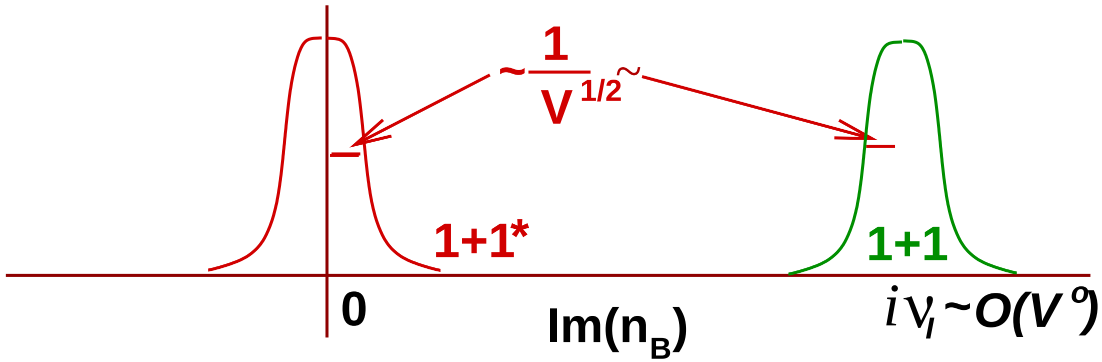
It it possible to evaluate all moments of both the real and the imaginary parts of the baryon density. Their distribution is a Gaussian with a width given by the sum and difference of the isospin number and the baryon number susceptibility, respectively.

Lombardo-Splittorff-JV-2009

Distribution of n_B for $\mu < m_\pi/2$



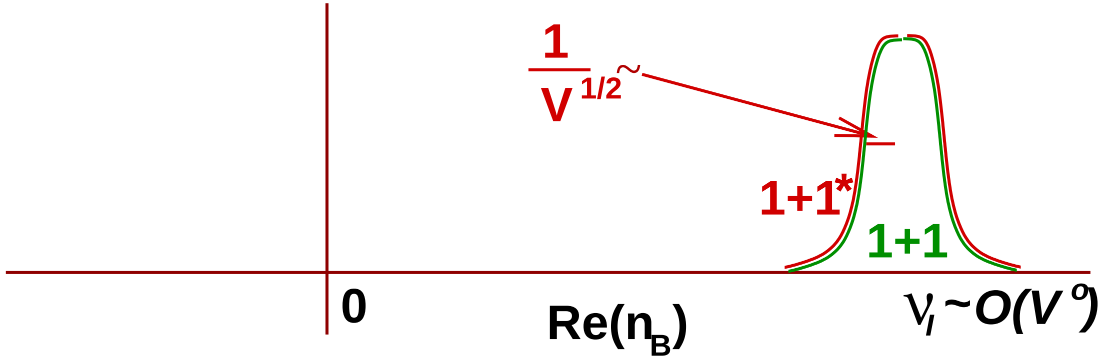
Distribution of the real part of the baryon number density for two dynamical fermions for full QCD (green) and phase quenched QCD (red).



Distribution of the imaginary part of the baryon density.

$$\nu_I = \frac{m_\pi^2 T}{\pi^2} \sum_{n=1}^{\infty} \frac{K_2(\frac{m_\pi n}{T})}{n} \sinh \frac{2\mu n}{T}.$$

Distribution of n_B for $\mu < m_\pi/2$



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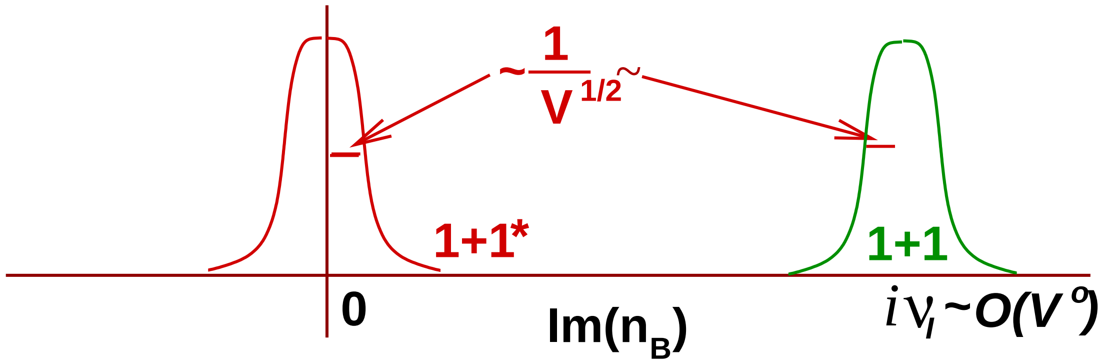
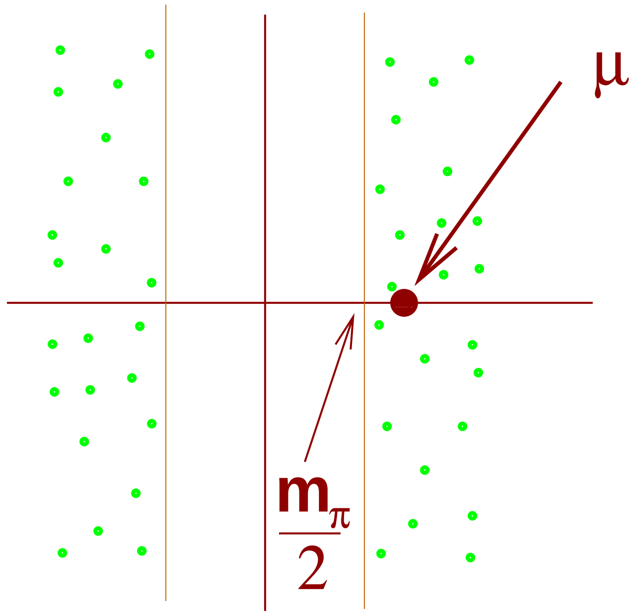


Distribution of the imaginary part of the baryon density.

$$\nu_I = \frac{m_\pi^2 T}{\pi^2} \sum_{n=1}^{\infty} \frac{K_2(\frac{m_\pi n}{T})}{n} \sinh \frac{2\mu n}{T}.$$

$$\langle n_B \rangle_{1+1} = \langle \mathrm{Re}(n_B) \rangle_{1+1} + i \langle \mathrm{Im}(n_B) \rangle_{1+1} = \nu_I + i i \nu_I = 0.$$

Distribution of n_B for $\mu > m_\pi/2$



Spectrum of $\gamma_0(D+m)$

For $\mu > m_\pi/2$ moments of the baryon number diverge due to eigenvalues close to μ .
For the p -th moment we obtain after excluding a disc around μ with radius ϵ ,

$$\langle |n|^{2p} \rangle_{1+1^*} \sim \epsilon^{2p-4}.$$

Therefore the distribution of $|n|$ has a power tail ($1/|n|^5$ in this case).

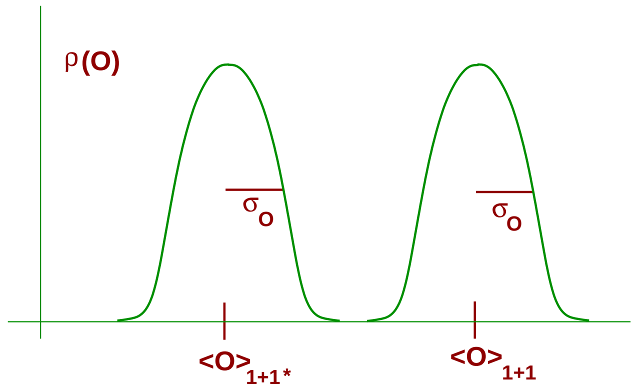
It becomes virtually impossible to sample the baryon number.

Lombardo-Splittorff-JV-2009

Overlap Problem

Therefore if we put the phase factor in the observable and use gauge field configurations generated by $Z_{|QCD|}$ (known as reweighting) we will generate an incorrect distribution for the imaginary part of the baryon number density.

This gives the overlap problem: the observable seems to converge to the the incorrect value and the correct value can only be obtained because of very rare fluctuations.



Distribution of an operator for the phase quenched ensemble and the full theory.

A quantitative estimate of the overlap probelm can be obtained by evaluating the distribution of the observables to one loop order in chiral perturbation theory.

Overlap problems also may result because of distributions with heavy tails of the distributions.

Endres-Kaplan-Lee-Nicholson-2011

IV. Sign Problem in the ϵ Domain

Infrared Dominance of the Phase Factor

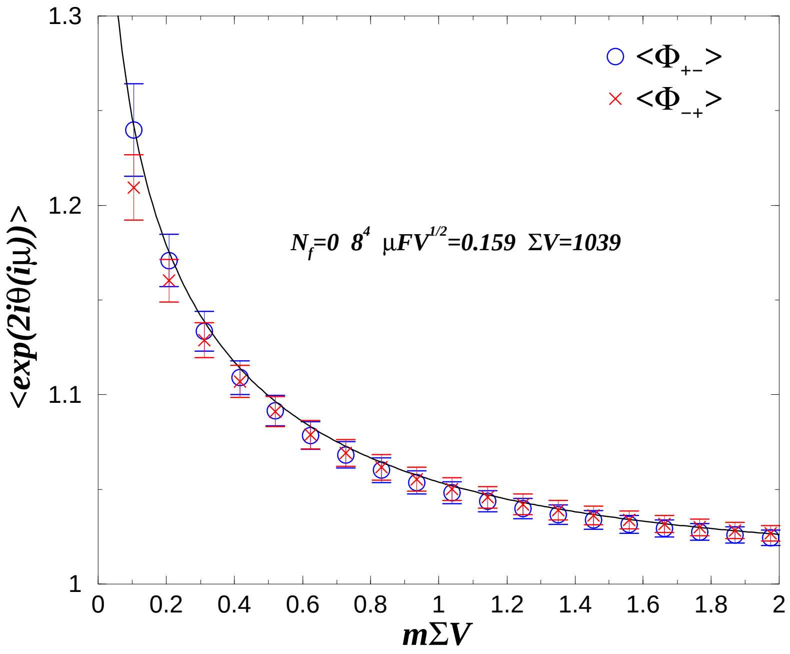
Spectral Representations

Alternative to Banks-Casher Formula

Infrared Dominance of the Phase Factor

Both in the ϵ and p domain the mass and chemical potential dependence of QCD and QCD like partition functions can be obtained from chiral perturbation theory.

Therefore the average phase factor in this domain is determined by chPT, or in QCD, by the infrared part of the Dirac spectrum. Notice that the chemical potential can be gauged to the boundary.



"Phase" of the fermion determinant for imaginary chemical potential.

Splittorff-Svetitsky-2007

Analytical continuation of average phase factor:

$$\left\langle \frac{\det(D+i\mu)}{\det(D-i\mu)} \right\rangle = 1 - 4\hat{\mu}^2 I_0(\hat{m}) K_0(\hat{m}).$$

Here, $\hat{m} = mV\Sigma$ and $\hat{\mu}^2 = \mu^2 F_\pi^2 V$. The analytical result has been obtained in the microscopic domain

Damgaard-Splittorff-2006, Splittorff-JV 2007.

Sign Problem in the ϵ Domain

- Because the sign problem is dominated by the infrared part of the Dirac spectrum, we will analyze it in the ϵ domain or microscopic domain of QCD.
- This is the domain where the pion Compton wave length remains much larger than the size of the box in the thermodynamic limit.
- In this domain QCD is equivalent to a random matrix theory with the global symmetries of QCD.
- This problem has been solved at nonzero chemical potential
  - ⋆ The joint eigenvalue distribution is known analytically Osborn-2004
  - ⋆ The eigenvalue density is know analytically for any number of flavors Osborn-2004, Akemann-Osborn-Splittorf-JV-2004
  - ⋆ The relation between the chiral condensate and the spectral density has been understood Osborn-Splittorff-JV-2005, 2008

VI. Spectral Representations

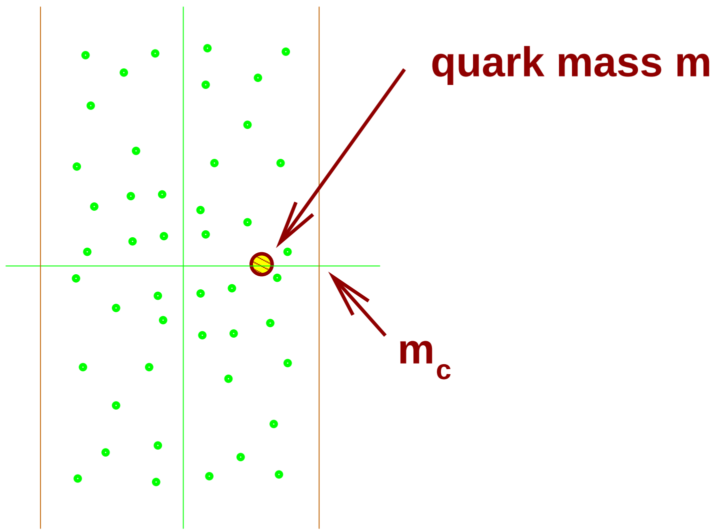
Dirac Spectra

Alternative to Banks-Casher Relations

QCD in 1d

Spectral Representations

Spectral representations of the Dirac operator have been extremely useful for nonhermitean theories.



Scatter plot of Dirac eigenvalues

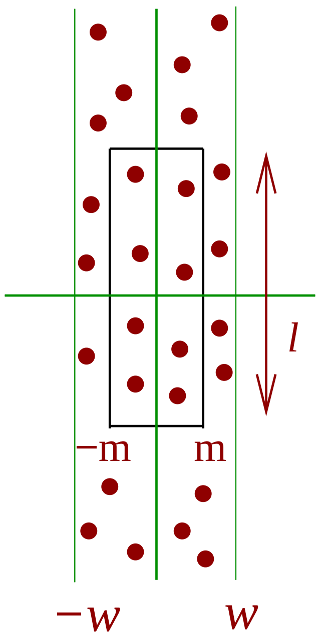
- The critical point is when the quark mass hits the cloud of eigenvalues.
- For phase quenched QCD this is the point when $\mu = m_\pi/2$.
  Gibbs-1986,Splittorff-JV-2006
- For Wilson fermions this is the onset of the Aoki phase.

- For nonhermitean theories theories with a complex determinant, the support of the Dirac spectrum does not depend on the complex phase of the determinant.
- Exponential cancellations can wipe out the critical point and reveal a completely different physical system. This is the case of QCD at nonzero baryon density.

Chiral Condensate and Banks-Casher Formula

Chiral condensate:

$$\Sigma(m) = \langle \bar{q} q \rangle = \frac{1}{V} \partial_m \log Z = \frac{1}{V} \sum_k \frac{1}{m + \lambda_k}.$$



Nonhermitian

Dirac operator

$$\oint ds \Sigma(s) = il(\Sigma(m) - \Sigma(-m))$$
$$= 2\pi i \rho_2(0) \frac{m}{w}$$

$$\Sigma(m) = \pi \rho_2(0) \frac{m}{w}$$

density of eigenvalues in the plane

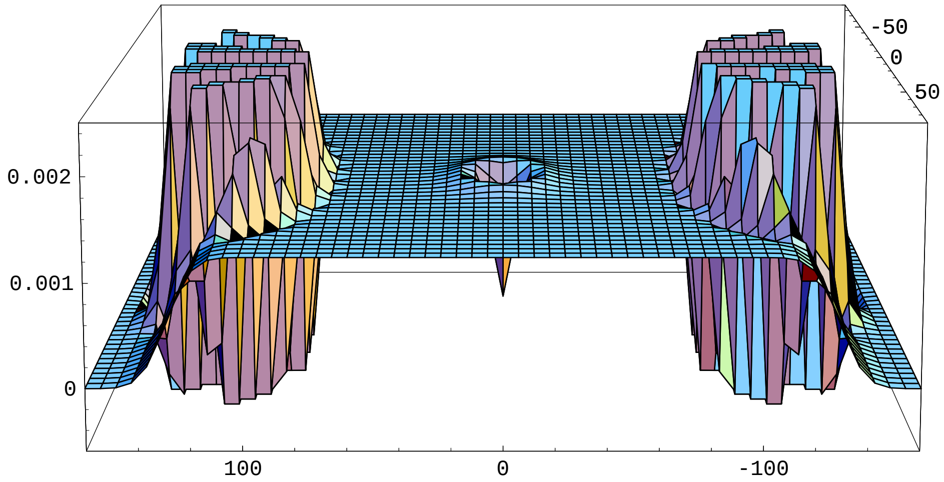
Chiral condensate goes to zero linearly in m

Critical value: $w_c = m$.

In physical terms this can be written as: $\mu_c = m_\pi/2$.

At low temperature the chiral condensate has to remain constant until $\mu = m_N/3$.

Eigenvalue Density for One Flavor QCD



Spectral density for QCD with one dynamical flavor.

Asymptotic form

$$\rho(x > 0, y) = \frac{1}{4\pi\mu^2} e^{-V\frac{(y+i(|x|+|m|-4\mu^2)^2}{8\mu^2} - V\frac{(x-2\mu^2)^2}{2\mu^2}}.$$

This has oscillations with a period of $O(1/V)$ and an amplitude that increases exponentilally with V.

It provides a generic mechanism to get a discontinuity of the chiral condensate without having a dense line of eigenvalues.

Osborn-Splittorf-JV-2005

Chiral Condensate for One Flavor QCD

Spectral density shows oscillations on the scale of $1/V$ with an amplitude that grows exponentially with the volume

$$\rho(x, y, \mu) = \rho_{\rm quenched}(x, y, \mu) + \rho_{\rm osc}(x, y, \mu).$$

Chiral condensate after integration over y

$$\Sigma_{\rm osc} = \int_{-2\mu^2}^{2\mu^2} dx \Sigma_{\rm osc}(x, \mu), \qquad \Sigma_{\rm osc}(x, \mu) \equiv \int dy \frac{1}{x + iy + m} \rho_{\rm osc}(x, y, \mu).$$

The integral can be performed by a saddle point approximation. For $|x| < 2\mu^2$ the saddle point contribution is exponentially suppressed with respect to the quenched result and only the contribution from the pole at $y = i(x + m)$ remains.

The result is given by

$$\frac{1}{2\mu^2}[\theta(m)\theta(-x - m) - \theta(-m)\theta(x + m)].$$

For $m > 0$ the x -integral gives $1 - m/2\mu^2$. Adding the quenched result we obtain

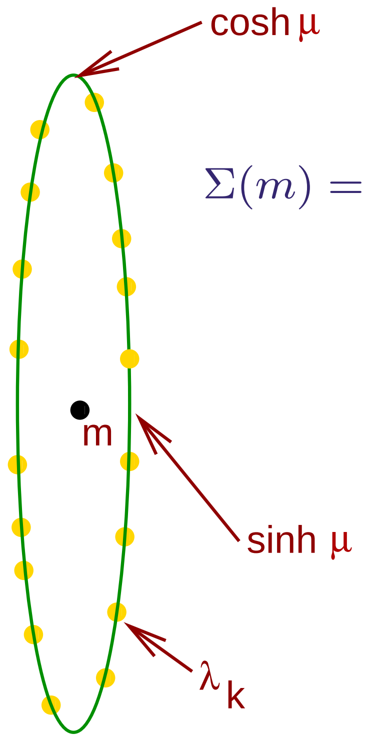
$$\frac{m}{2\mu^2} + [1 - \frac{m}{2\mu^2}] = 1.$$

IV. Sign Problem for One Dimensional QCD

Dirac Spectrum and Chiral Condensate

Langevin Equation

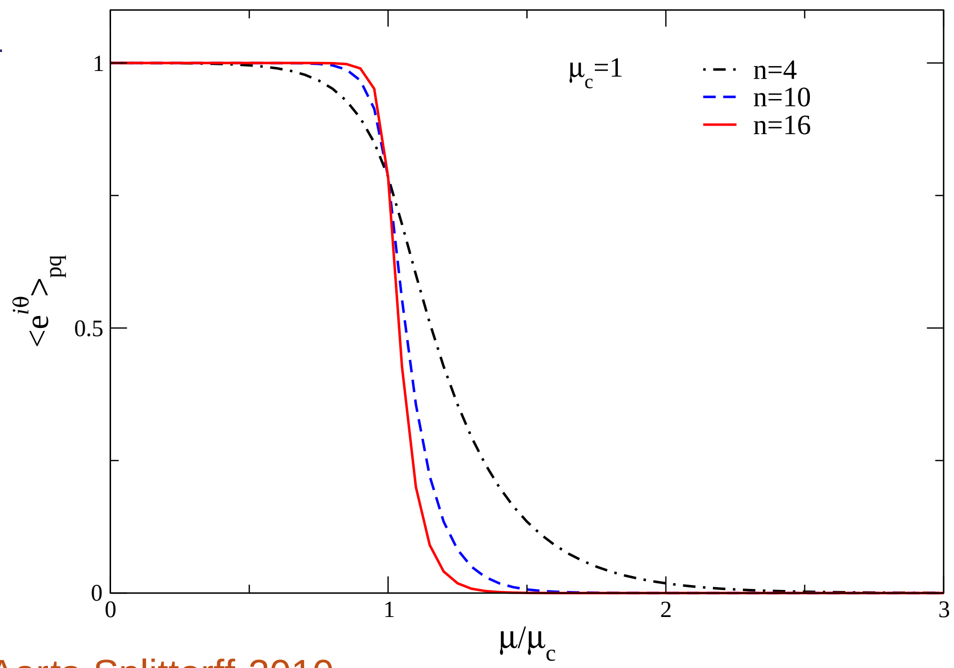
U(1) QCD in 1d



Dirac spectrum of 1d QCD

$$\Sigma(m) = \frac{\left\langle \sum_k \frac{1}{\lambda_k+m} \prod_k (\lambda_k+m) \right\rangle}{\left\langle \prod_k (\lambda_k+m) \right\rangle}$$

determinant with
a complex phase



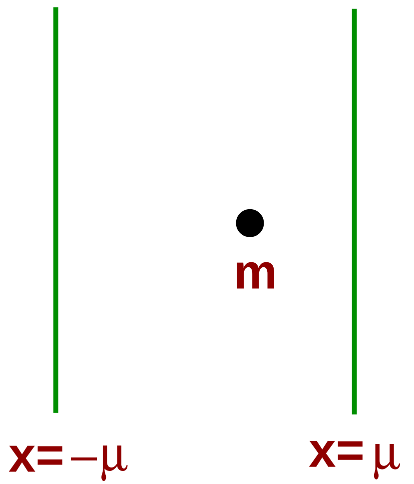
Ravagli-JV-2007, Aarts-Splittorff-2010

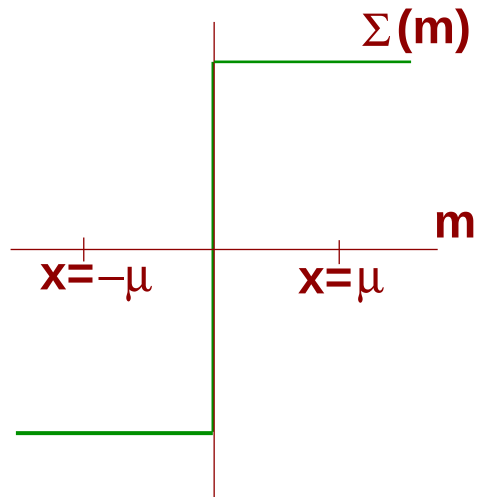
Eigenvalues are equally spaced on an ellipse with a random overall phase.

In the limit of a dense spectrum, $\Sigma(m)$ is discontinuous across the imaginary axis despite the fact that there are no eigenvalues for $\mu \neq 0$.

The chiral condensate is continuous across the ellipse where the eigenvalues are located.

Alternative to the Banks-Casher Relation





For large V and small μ the eigenvalues of the Dirac operator are located on two parallel lines $x \pm \mu$ resulting in the chiral condensate

$$\Sigma(m) = \int \frac{dxdy}{\pi} \frac{1}{m-x-iy} \underbrace{\delta(|x|-\mu)\left[1 - \frac{(e^{V(x+iy)} + e^{-V(x+iy)})}{e^{Vm}+e^{-Vm}}\right]}_{\rho(x,y) \quad \text{for} \quad N_f = 1} = \tanh(Vm).$$

In the thermodynamic limit $(V \to \infty)$ this results in a discontinuity across $m = 0$, but only after exponentially large cancellations. Osborn-Splittorff-JV-2005, Ravagli-JV-2008

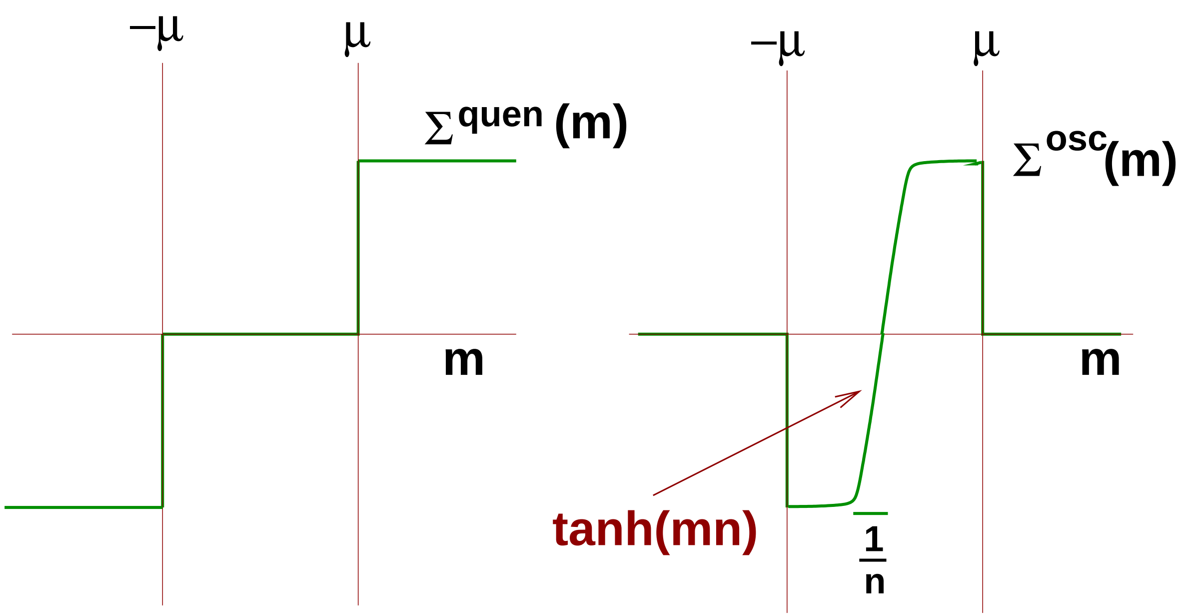
Chiral Condensate in 1d

The first term ($\sim \delta(|x| - \mu)$) gives the quenched contribution

$$\Sigma^{\text{quenched}}(m) = \text{sign}(m - \mu) + \text{sign}(-m + \mu).$$

This follows from electrostatic arguments with eigenvalues as charges. The second term is evaluated as

$$\Sigma^{\text{osc}}(m) = (\theta(m + \mu) - \theta(m - \mu)) \tanh(mn).$$



The chiral condensate becomes discontinuous in the continuum limit.

Ravagli-JV-2007

Complex Langevin for 1d QCD

Spectral density is given by

$$\rho(y) = 1 - \frac{\cosh(V(\mu + iy))}{\cosh(Vm)}.$$

Langevin equation

$$\frac{dy}{dt} = \frac{d\log\rho(y)}{dy} + \eta = \frac{iV\sinh V(\mu + iy)}{\rho(y)} + \eta$$

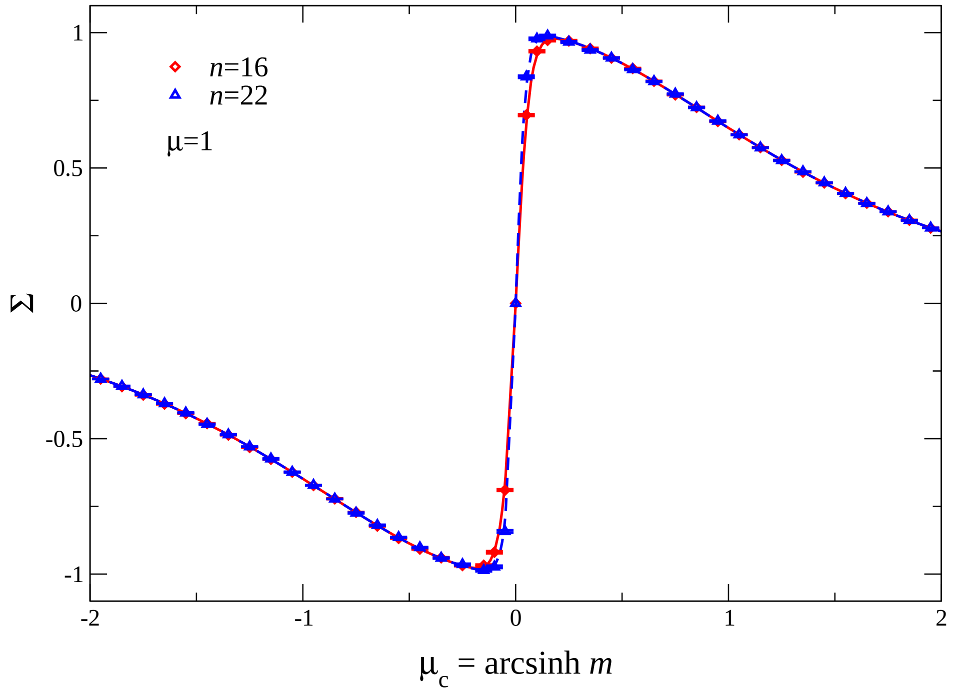
For complex Langevin $y = v + iw$ with $v, w \in \mathbb{R}$.

Solution:

$$\begin{aligned} w &= \mu, \\ \frac{dv}{dt} &= \frac{iV\sinh(V(iv))}{1 - \frac{\cosh(iVv))}{\cosh(Vm)}} + \eta. \end{aligned}$$

The equation for v is the Langevin equation for $\mu = 0$ and converges to the correct distribution. Aarts-Splittorff-2010

Complex Langevin in 1d QCD



Result for the chiral condensate of one-flavor 1d QCD from the complex Langevin equation compared to the exact analytical result.

Aarts-Splittorff-2010

Conclusions and Outlook

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- √ To make progress we have to rethink the problem for much simpler model systems.