QCD at Finite Density and the Sign Problem

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Darmstadt, November 2010

Acknowledgments

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Maria-Paula Lombarda (Frascati)

Financial Support: Stony Brook University
US Department of Energy

References

K. Splittorff and J. J. M. Verbaarschot, Phase of the fermion determinant at nonzero chemical potential, Phys. Rev. Lett. **98**, 031601 (2007) [arXiv:hep-lat/0609076].

L. Ravagli and J. J. M. Verbaarschot, QCD in One Dimension at Nonzero Chemical Potential, Phys. Rev. D **76**, 054506 (2007) [arXiv:0704.1111 [hep-th]].

J.C. Osborn, K. Splittorff and J.J.M. Verbaarschot, Phase Diagram of the Dirac Spectrum at Nonzero Chemical Potential, Phys. Rev. D **78**, 105006 (2008) [arXiv:0807.4584 [hep-lat]].

M.-P. Lombardo, K. Splittorff and J.J.M. Verbaarschot, Distributions of the Phase Angle of the Fermion Determinant in QCD, Phys. Rev. D **80**, 054509 (2009) [arXiv:0904.2122 [hep-lat]].

M.-P. Lombardo, K. Splittorff and J.J.M. Verbaarschot, The Fluctuations of the Quark Number and the Chiral Condensate, Phys. Rev. D **81**, 045012 (2010) [arXiv:0910.5482 [hep-lat]].

M.-P. Lombardo, K. Splittorff and J.J.M. Verbaarschot, Teflon Plated Observables (2010).

Contents

I. Motivation

II. The Sign Problem

III. Overlap Problem

IV. Teflon Plated Observables

V. Ergodicity

VI. Spectral Representations

VII. Conclusions

I. Motivation

Questions

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 it 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? ‘

QCD Partition Function

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

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

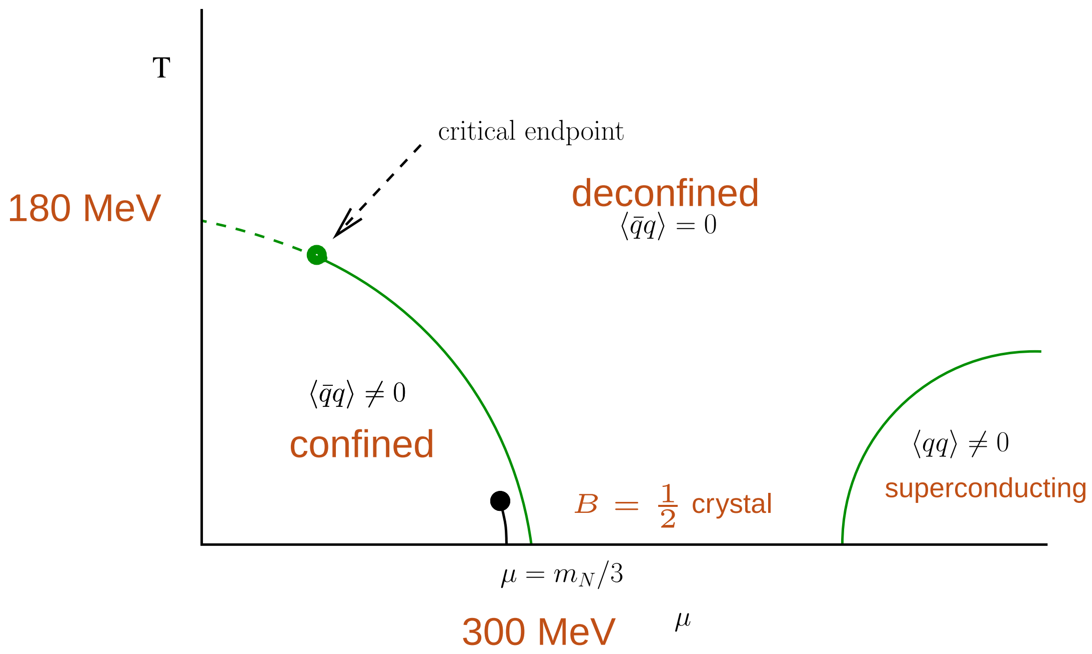
where the sum is over all states with energy E_k and quark number N_k .

- √ 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

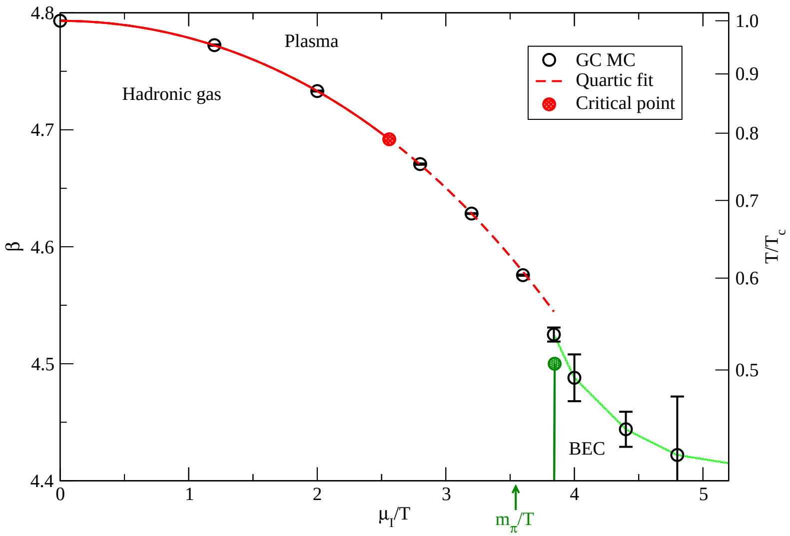
$$Z_{\rm QCD} \quad = \quad \langle \prod_k^{N_f} \det(D + m_k + \mu_k\gamma_0)\rangle_{\rm YM}.$$

Dirac operator — quark mass matrix — imaginary vector potential

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).

Colliding Skyrmions

J.J.M. Verbaarschot, et al. / Scattering of skyrmions 613

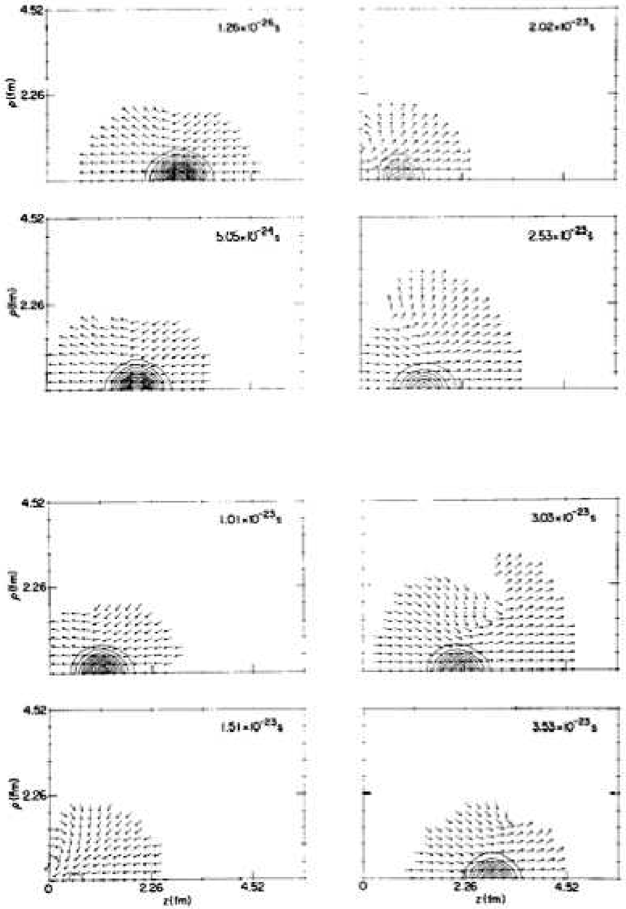


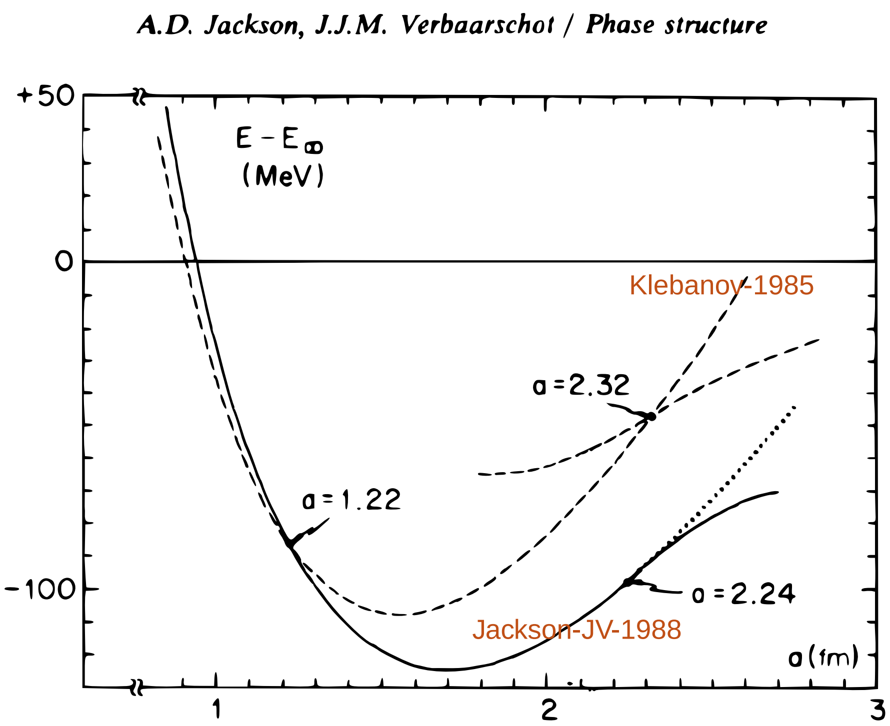
Fig. 3b. Contour plots of the kinetic energy density and vector plots of the direction of the momentum density for the scattering of two skyrmion configurations in which the χ_3 component in the initial configuration of the right-moving skyrmion has been multiplied by a factor −1 with respect to the spherically symmetric configuration ($\chi_2(-z) = -\chi_2(z)$, $\chi_3(-z) = -\chi_3(z)$, see eqs. (3)–(4)). The time evolution is displayed in intervals of $5.04 \cdot 10^{-24}$ s (400 timesteps) and the initial velocity is 0.6c. For further explanation see the caption of fig. 3a.

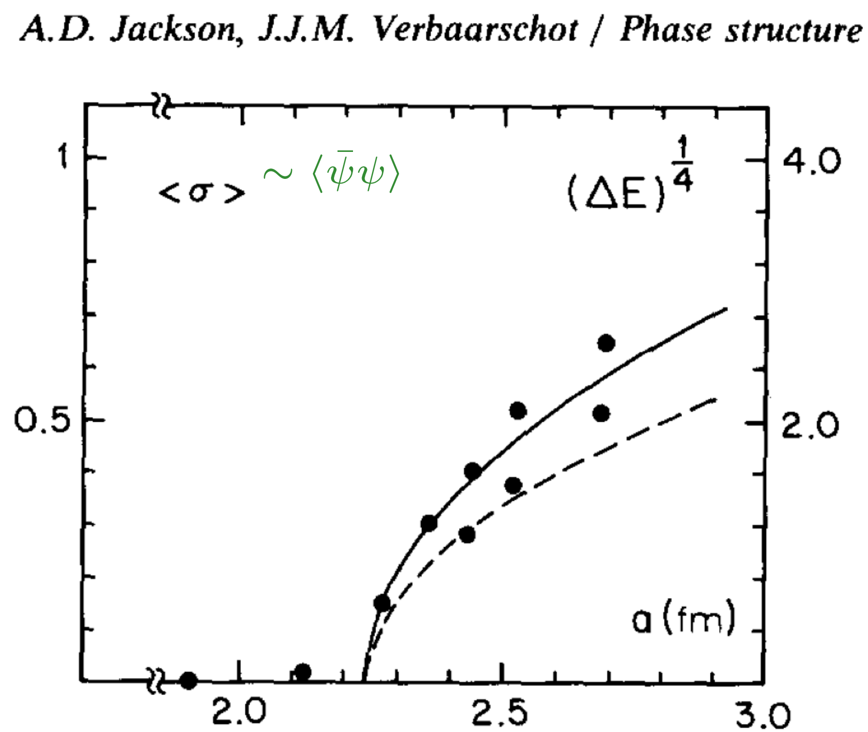
JV-Walhout-Wambach-Wyld-1987

Illinois 1985

Gordon Baym
John Bardeen
Frithjof Karsch
Shunzo Kumano
John Kogut
Vijay Pandharipande
Chris Pethick
David Pines
Jeff Ravenhall
Michael Stone
JV
Jochen Wambach
Bill Wyld

Skyrme Crystal





Chiral symmetry restoration in a Skyrme crystal.

Jackson-JV-1988

Quarkyonic phase. McLerran-Pisarski-2007

III. Sign Problem

Average Phase Factor

Distribution of the Phase

Phase Factor in 1d QCD

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 quenched QCD partition function can be written as

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

Because of this it can also be interpreted as QCD at isospin chemical potential $\mu_I = \mu$.
For low T a transition to a phase of condensed pions occurs at $\mu = m_\pi/2$.

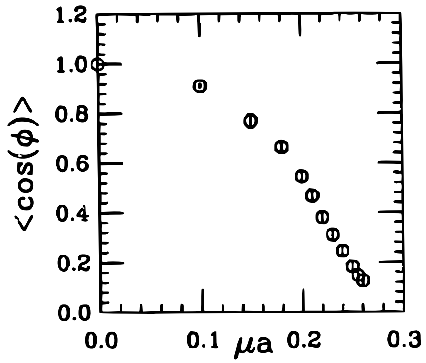
Alford-Kapustin-Wilczek-1999

Phase Factor and Dirac Eigenvalues

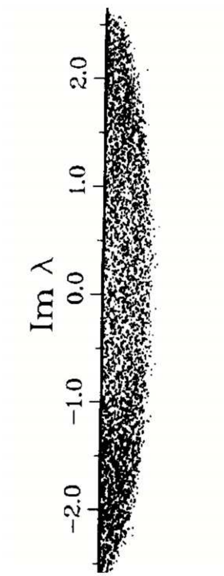
$$\det(D + m + \mu\gamma_0) = e^{i\theta}|\det(D + m + \mu\gamma_0)|$$

$\prod_k(\lambda_k + m)$

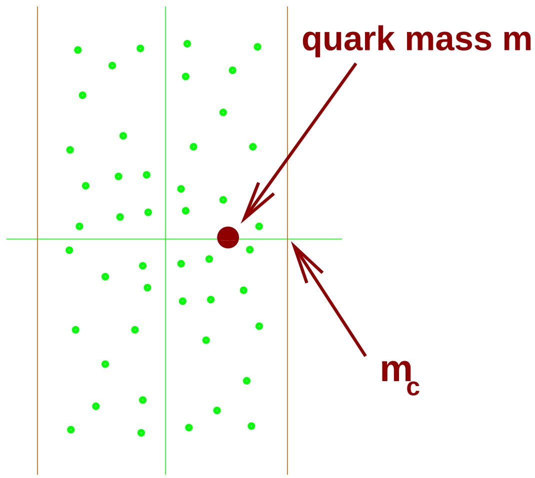
phase factor



Toussaint-1990



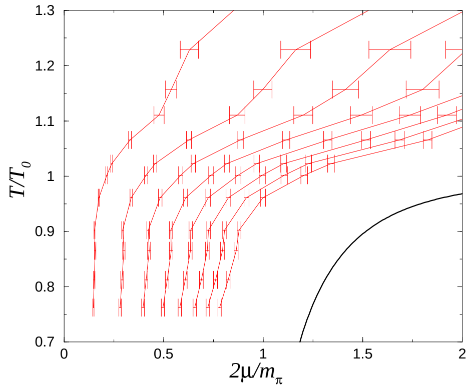
Barbour et al. 1986



Scatter plot of Dirac eigenvalues

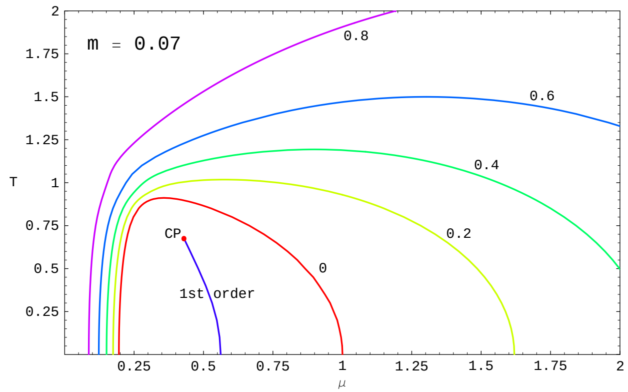
$$m < m_c \qquad \text{then} \qquad \langle e^{i\theta}\rangle \sim 0$$

Phase Diagram and Average Phase Factor



Lattice results showing contour lines with equal variance of the phase of the fermion determinant.

Allton-et al-2005, Splittorff-2006



Analytical random matrix result for phase diagram of average phase factor. Curves show contours of equal average phase factor. Han-Stephanov-2008, Ravagli-JV-2008

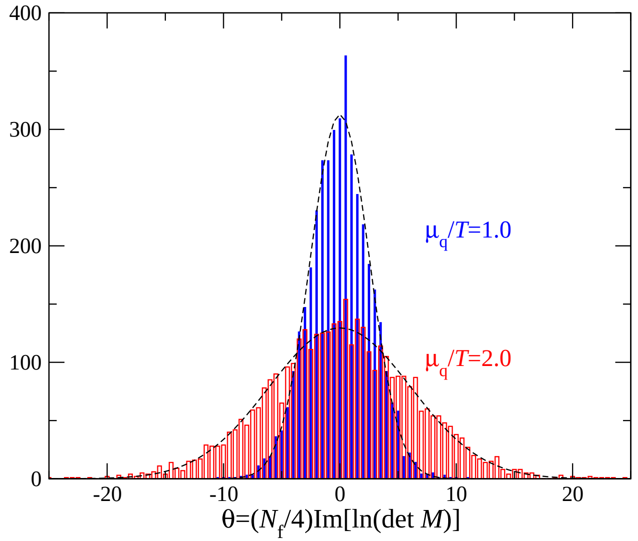
The Distribution of Phase

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



Quenched distribution, Ejiri-2009

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

Lombardo-Splittorff-JV-2009

III. Overlap Problem

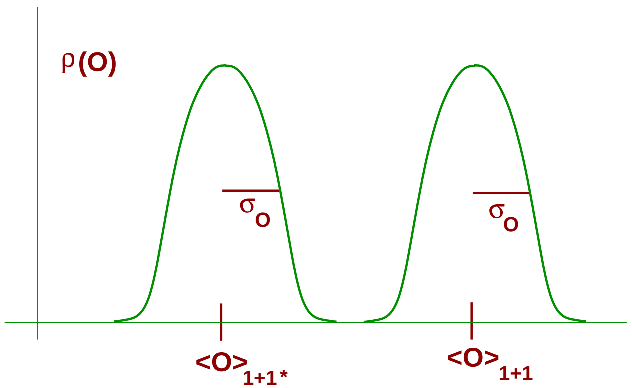
Overlap Problem

Distribution of the Baryon Number Density

Overlap Problem

It is possible to put the phase factor in the observable and use gauge field configurations generated by $Z_{|QCD|}$ (known as reweighting).

This may introduce the overlap problem, namely that observables for the ensemble that is generated seem to converge to the wrong value. For example this could happen when the average is dominated by rare fluctuations.



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

The severity of the overlap problem is determined by the ratio

$$R = \frac{|\langle O\rangle_{1+1^*} - \langle O\rangle_{1+1}|}{\sigma_O^{1+1} + \sigma_O^{1+1^*}}.$$

A quantitative estimate of this ratio can be obtained by evaluating it to one loop chiral perturbation theory.

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, $\langle \mathrm{Im}(n_B)\rangle = \langle\theta\rangle$ so that $\langle \mathrm{Im}(n_B)\rangle_{1+1^*} = 0$ and $\langle \mathrm{Im}(n_B)\rangle_{1+1^*} = i\nu_I$

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

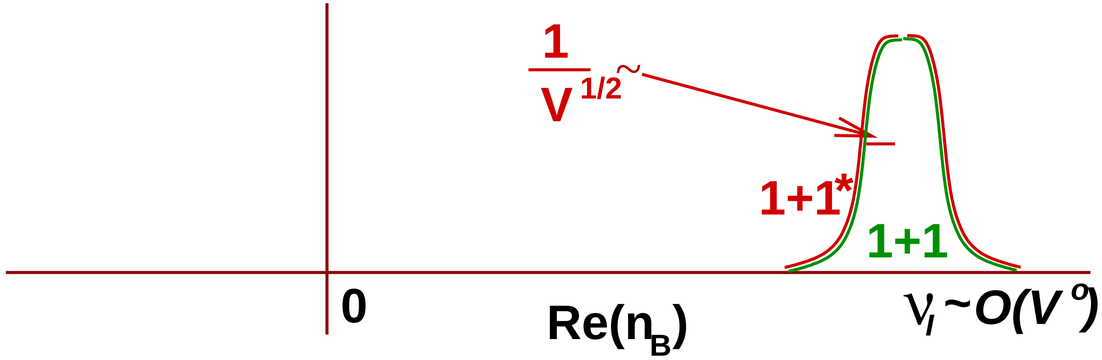
$$
\begin{aligned}
\langle \mathrm{Re}\, n_B \rangle_{1+1^*} &= \nu_I\,, \\
\langle \mathrm{Re}\, n_B \rangle_{1+1} &= \nu_I\,,
\end{aligned}
$$

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

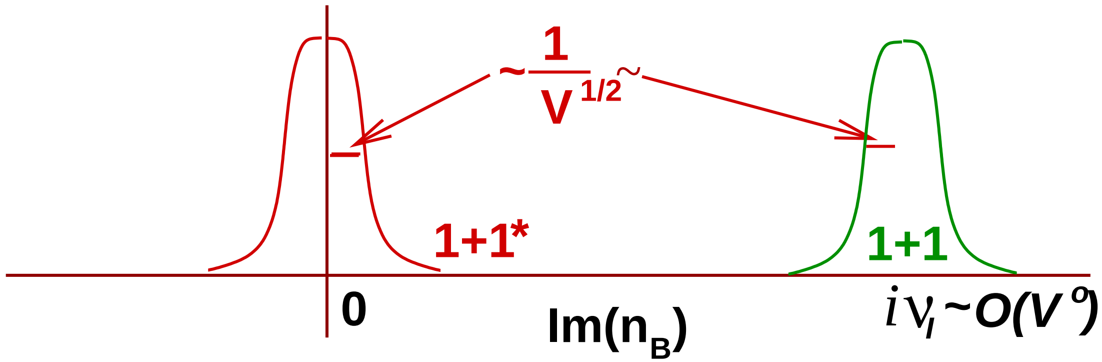
It it possible to evaluate all moments of both the real and the imaginary parts of the baryon density. Their distribution is a Gaussian with a width given by the sum and difference of the isospin number and the baryon number susceptibility, respectively.

Lombardo-Splittorff-JV-2009

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



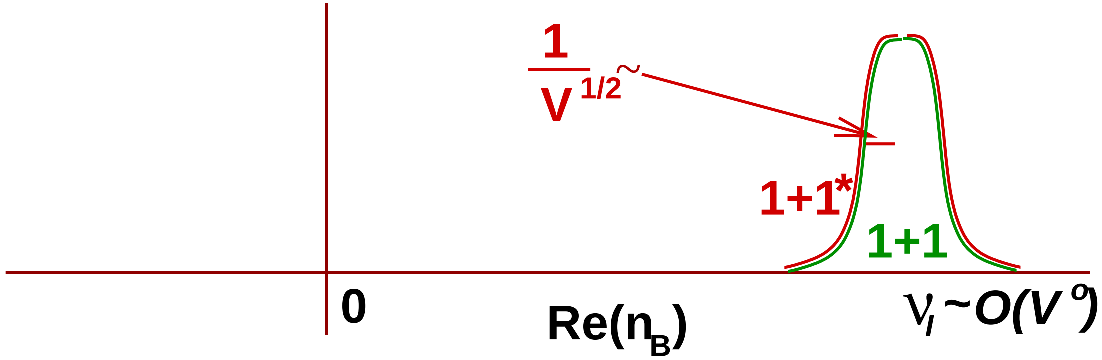
Distribution of the real part of the baryon number density for two dynamical fermions for full QCD (green) and phase quenched QCD (red).



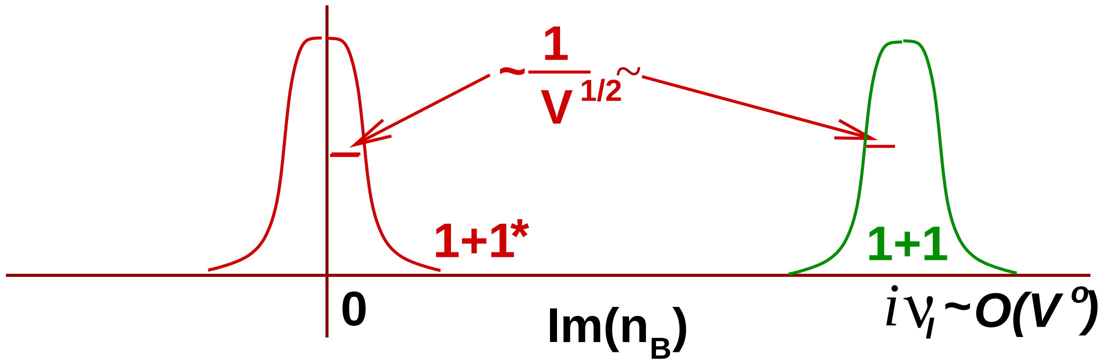
Distribution of the imaginary part of the baryon density.

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

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



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

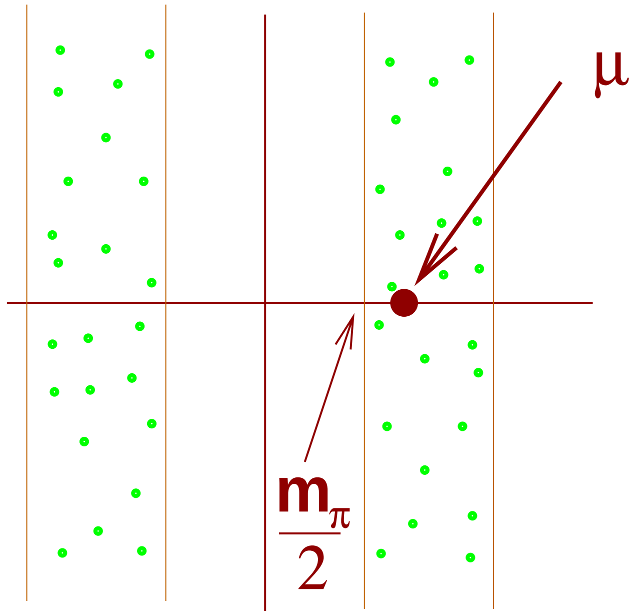


Distribution of the imaginary part of the baryon density.

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

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

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

VI. Teflon Plated Observables

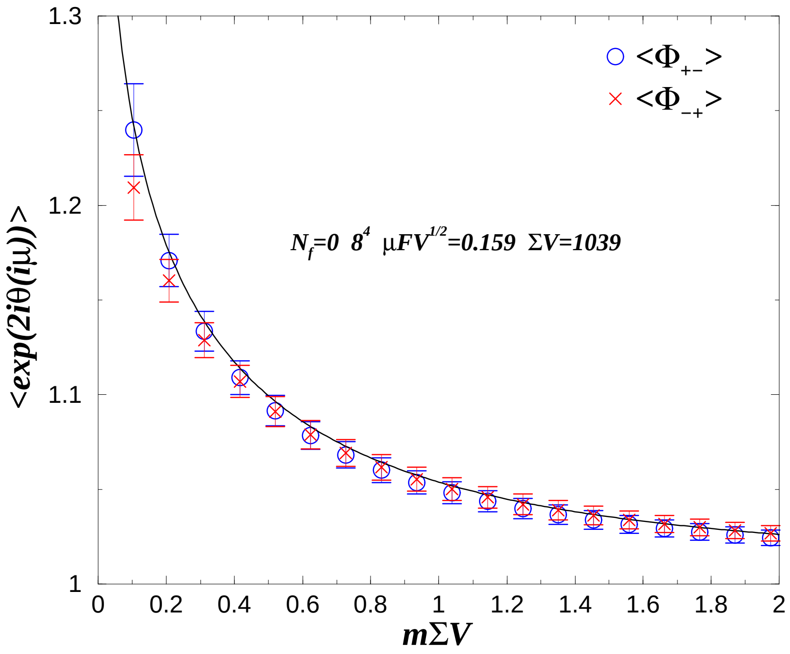
Infrared Dominance of the Phase Factor

Correlations with Phase Factor

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.

Teflon Plated Observables

- √ Observables that are not sensitive to the infrared part of the Dirac spectrum can be measured in QCD at nonzero chemical potential.

More generally, these are observables that have no correlations with the phase factor,

$$\underbrace{\langle \mathcal{O} e^{2i\theta} \rangle_{|QCD|}} = \langle \mathcal{O} \rangle_{|QCD|} \underbrace{\langle e^{2i\theta} \rangle_{|QCD|}}.$$

Then

$$\langle \mathcal{O} \rangle_{QCD} = \langle \mathcal{O} \rangle_{|QCD|}.$$

Examples:

- √ Chiral condensate for $\mu < m_\pi/2$ and very low temperatures.
- √ Baryon density for $T \gtrsim T_{\rm co}$.
- √ $T_{\rm co}(\mu)$ Allton-et al-2002

There is no sign problem or overlap problem but do we learn anything about QCD at nonzero chemical potential?

Correlators in Chiral Perturbation Theory

Correlators between operator such as n_q , n_I , $\langle\bar{\psi}\psi\rangle$ and the phase factor can be calculated in chiral perturbation theory.

For example in a small chemical potential and small temperature expansion we obtain

$$\langle \mathrm{Re}(n_B)\, e^{2i\theta}\rangle_{1+1^*} - \langle \mathrm{Re}(n_B)\rangle_{1+1^*}\langle e^{2i\theta}\rangle_{1+1^*} = 0,$$

$$\frac{\langle \mathrm{Im}(n_B)\, e^{2i\theta}\rangle_{1+1^*} - \langle \mathrm{Im}(n_B)\rangle_{1+1^*}\langle e^{2i\theta}\rangle_{1+1^*}}{\langle \mathrm{Im}(n_B) e^{2i\theta}\rangle_{1+1^*}} = 1.$$

Lombardo-Splittorff-JV-2010

V. Ergodicity

Ergodicity (Self-Averaging)

- Ergodicity: Space-Time average of an observable is equal to the ensemble average.
- QCD at nonzero chemical potential is maximally nonergodic: space-time averaging gives the phase quenched result.
- Master configurations do not exist for QCD at nonzero chemical potential.
- One way out might be to complexify the fields so that cancellations can be achieved by spatial averaging.
- One method that may achieve this is the complex Langevin algorithm which has its own issues. de Forcrand-2009

Not being self-averaging is a fundamental problem for QCD at $\mu \neq 0$.

Notice that QCD at imaginary chemical potential is ergodic.

VI. Spectral Representations

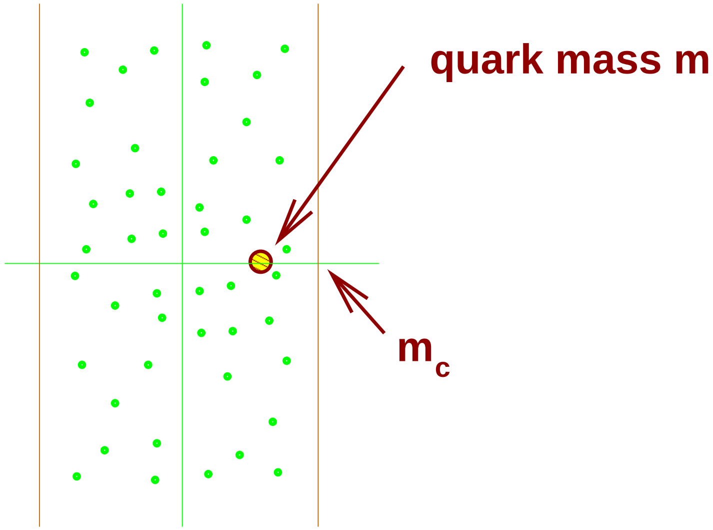
Dirac Spectra

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

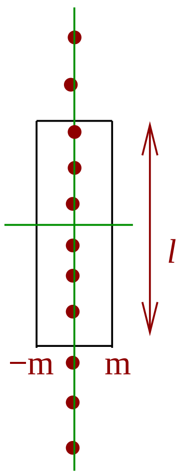
- √ The critical point is when the quark mass hits the cloud of eigenvalues.
- √ For phase quenched QCD this is the point when $\mu = m_\pi/2$.
- √ For Wilson fermions this is the onset of the Aoki phase.

- √ 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:

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



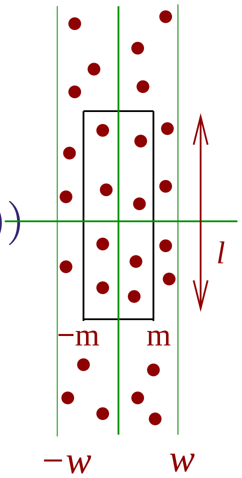
Hermitian Dirac operator

$$\oint ds \Sigma(s) = il(\Sigma(m) - \Sigma(-m)) = 2\pi i l \rho(0)$$

$$\Sigma(m) = \pi\rho(0).$$

Banks-Casher formula

Chiral condensate has a discontinuity in m



Nonhermitian Dirac operator

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

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

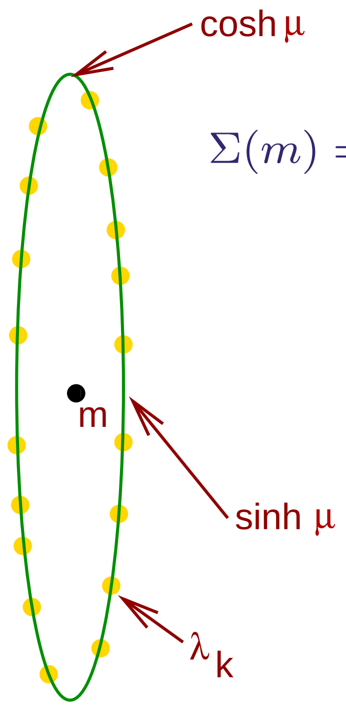
density of eigenvalues in the plane

Chiral condensate goes to zero linearly in m

Critical value of the quark mass: $w_c = m$.

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

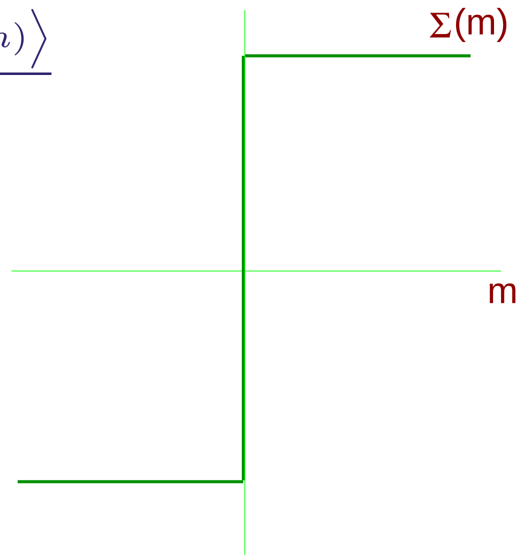
QCD in 1d



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



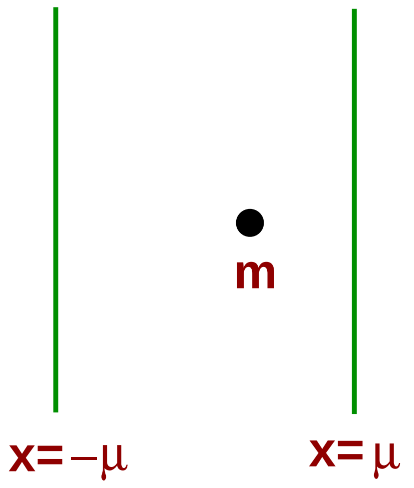
Ravagli-JV-2007

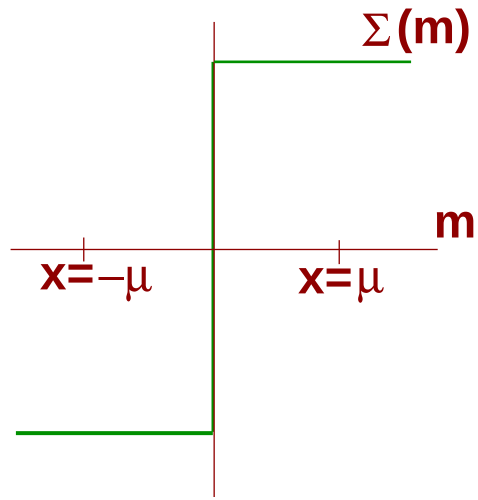
Eigenvalues are equally spaced on an ellipse with a random overall phase.

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

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

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

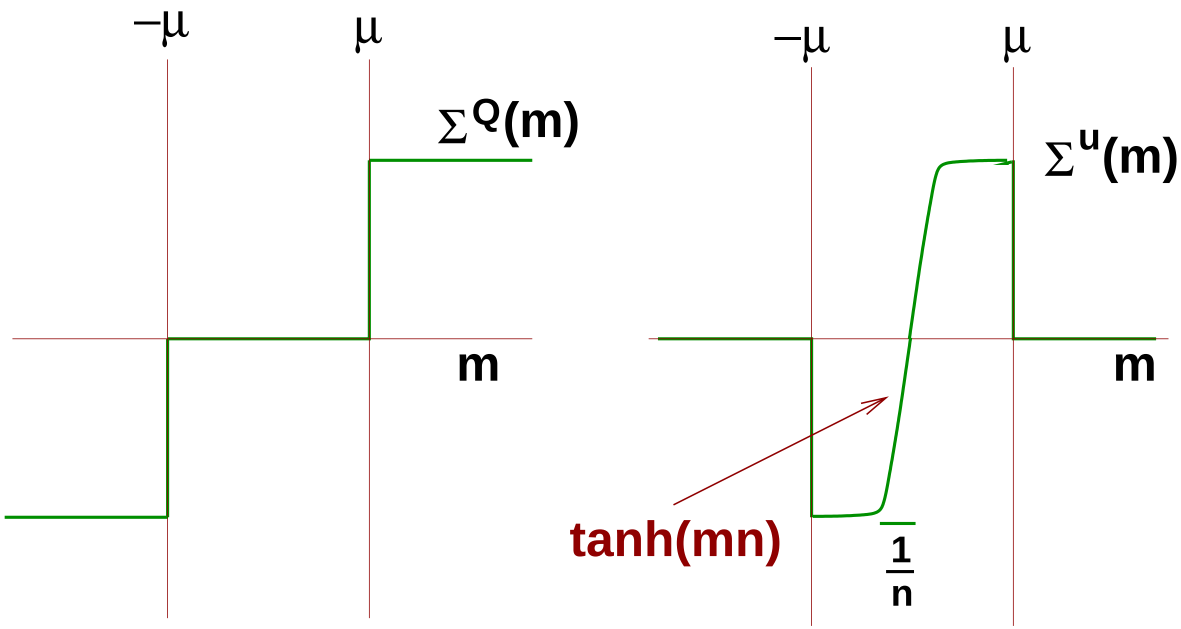
Chiral Condensate in 1d

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

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

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

$$\Sigma^u(m) = (\theta(m + mu) - \theta(m + \mu)) \tanh(mn).$$



The chiral condensate becomes discontinuous in the continuum limit.

Ravagli-JV-2007, Aarts-Splittorff-2010

Conclusions and Outlook

VII. Conclusions and Outlook

- √ The physics of QCD at finite baryon density is obscured by both the sign problem and the overlap problem.

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In Summary

Thanks, Jochen