QCD at nonzero chemical potential and the sign problem

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I: introduction

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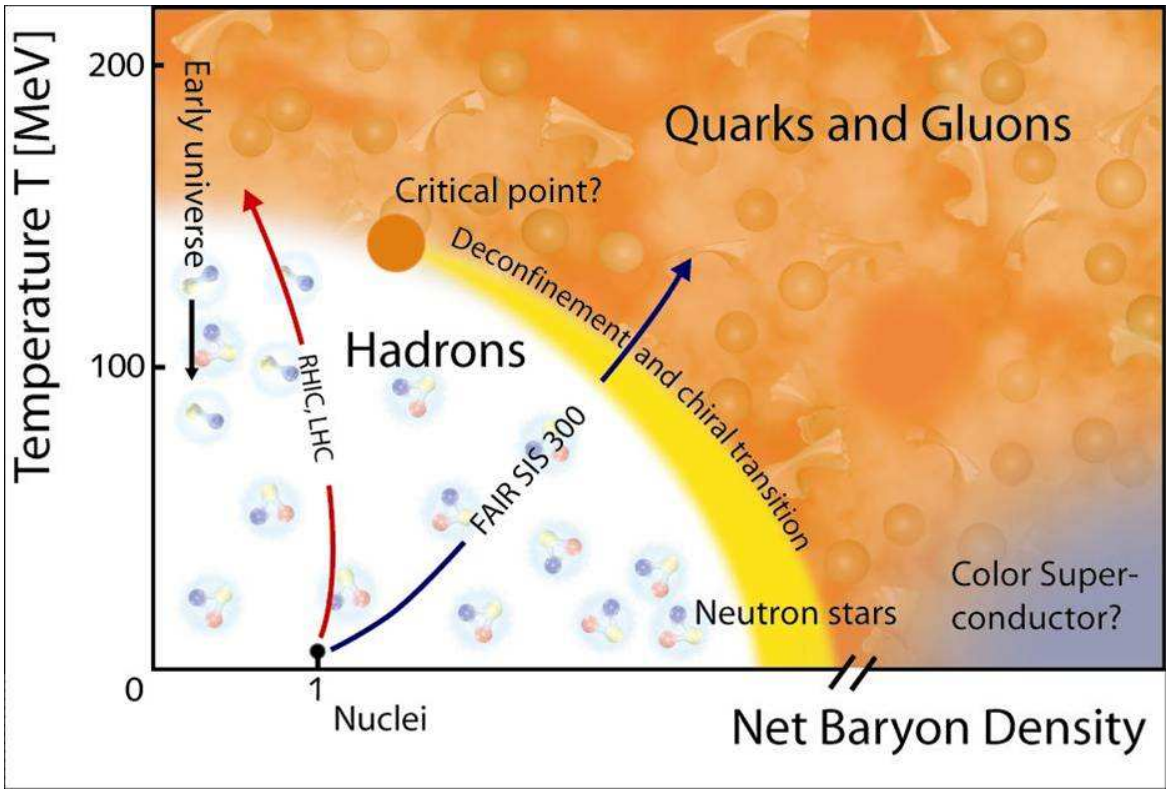
QCD phase diagram

extreme conditions: high temperature and/or density



early Universe

heavy-ion collisions

neutron stars

no first-principle determination at finite density :

lattice QCD and the sign problem

Lattice QCD at nonzero chemical potential

- fermion determinant is complex

$$[\det M(\mu)]^* = \det M(-\mu^*) \in \mathbb{C}$$

- no positive weight in path integral

$$Z = \int DU\, e^{-S_{\rm YM}} \det M(\mu)$$

- standard lattice methods based on importance sampling cannot be used

$$\Rightarrow \text{sign problem}$$

Outline

- chemical potential continuum/lattice
- remarks about sign/overlap/Silver Blaze problems
- standard approaches: reweighting, Taylor series, analytical continuation
- phase structure at imaginary chemical potential
- strong coupling
- complex Langevin dynamics

Quantum statistical mechanics

system at finite temperature $T(=1/\beta)$

conserved charge N, spatial volume V

- partition function: $Z = \mathrm{Tr}\, e^{-(H-\mu N)/T} = e^{-F/T}$
- charge (density): $\langle N \rangle = T \frac{\partial}{\partial \mu} \ln Z \qquad \langle n \rangle = \frac{1}{V} \langle N \rangle$
- fluctuations: $\langle \chi \rangle = \frac{1}{V} \left[\langle N^2 \rangle - \langle N \rangle^2 \right] = \frac{\partial \langle n \rangle}{\partial \mu}$
- ...

compute partition function, free energy and other thermodynamic quantities

determine phase structure

Various conserved charges

Consider two flavours: up and down μ_u, μ_d

- quark (baryon) chemical potential $\mu_u = \mu_d = \mu_q$

  $\mu_B = 3\mu_q$

- quark number $\langle n \rangle = \langle n_u \rangle + \langle n_d \rangle$

- isospin $\mu_u = -\mu_d = \mu_{\rm iso}$ $\langle n_{\rm iso} \rangle = \langle n_u \rangle - \langle n_d \rangle$

- electrical charge $\mu_u = \frac{2}{3}\mu, \mu_d = -\frac{1}{3}\mu$

  $\langle q \rangle = \frac{2}{3}\langle n_u \rangle - \frac{1}{3}\langle n_d \rangle$

Chemical potential (continuum/fermions)

free fermions $\Rightarrow$ global symmetry $\Rightarrow$ Noether charge

$$S = \int_0^{\beta=1/T} d\tau \int d^3x\, \bar{\psi}\left[\gamma_\nu \partial_\nu + m\right]\psi$$

$$\psi \to e^{i\alpha}\psi \qquad\qquad \bar{\psi} \to \bar{\psi} e^{-i\alpha}$$

$$N = \int d^3x\, \bar{\psi}\gamma_4\psi = \int d^3x\, \psi^\dagger\psi \quad \Rightarrow \quad \partial_\tau N = 0$$

add $\quad \beta\mu N = \beta\mu \int d^3x\, \bar{\psi}\gamma_4\psi = \int_0^\beta d\tau \int d^3x\, \mu\bar{\psi}\gamma_4\psi$

Chemical potential (continuum/fermions)

- action (with abelian gauge field)

$$S = \int_0^\beta d\tau \int d^3x\, \bar{\psi}\left[\gamma_\nu(\partial_\nu + iA_\nu) + \mu\gamma_4 + m\right]\psi$$

$$= \int d^4x\, \bar{\psi} D \psi$$

- two observations:
  - μ appears as iA_4:
    imaginary component of abelian vector field
  - " complex action": no γ_5 hermiticity

$$\gamma_\nu^\dagger = \gamma_\nu \quad \gamma_5^\dagger = \gamma_5, \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \quad \{\gamma_\nu, \gamma_5\} = 0, \quad \gamma_5^2 = 1$$

Chemical potential (continuum/fermions)

- at $\mu = 0$: $\quad (\gamma_5 D)^\dagger = \gamma_5 D \quad$ or $\quad D^\dagger = \gamma_5 D \gamma_5$

$$\det D^\dagger = \det (\gamma_5 D \gamma_5) = \det D = (\det D)^*$$

$\Rightarrow$ real determinant

- no longer true when $\mu \neq 0$

- instead: $\quad D^\dagger(\mu) = \gamma_5 D(-\mu^*)\gamma_5$

note:

- real determinant for imaginary chemical potential

Chemical potential

- sign problem not specific for fermions

$\Rightarrow$ due to complexity of the weight/action/determinant

- not due to Grassman nature of fermions

  (after all, standard lattice simulations work well at zero chemical potential)

- also present in bosonic theories at nonzero density

$\Rightarrow$ complex action problem

Chemical potential (continuum/bosons)

- complex scalar field, global symmetry: $\phi \to e^{i\alpha}\phi$
- action: $S = \int d^4x \, \left(|\partial_\nu \phi|^2 + m^2 |\phi|^2 + \lambda |\phi|^4 \right)$
- conserved charge: $N = \int d^3x \, i \left(\phi^* \partial_4 \phi - (\partial_4 \phi^*) \phi \right)$

back to partition function $Z = \mathrm{Tr}\, e^{-(H-\mu N)/T}$

hamiltonian $\Rightarrow$ canonical momenta $\Rightarrow$

integrate out momenta $\Rightarrow$ euclidean path integral

Chemical potential (continuum/bosons)

rederive path integral:

- write $\phi = (\phi_1 + i\phi_2)/\sqrt{2}$
- canonical momenta $\pi_1 = \partial_4 \phi_1, \pi_2 = \partial_4 \phi_2$

$$N = \int d^3x \, (\phi_2 \pi_1 - \phi_1 \pi_2)$$

- partition function:

$$Z = \mathrm{Tr}\, e^{-(H-\mu N)/T}$$
$$= \int D\phi_1 D\phi_2 \int D\pi_1 D\pi_2 \exp \int d^4x \Big[i\pi_1 \partial_4 \phi_1 + i\pi_2 \partial_4 \phi_2 - \mathcal{H} + \mu(\phi_2 \pi_1 - \phi_1 \pi_2) \Big].$$

- integrate out momenta

when all the dust settles:

Chemical potential (continuum/bosons)

- chemical potential appears as imaginary vector potential

$$S = \int d^4x \left[(\partial_4 + \mu)\phi^*(\partial_4 - \mu)\phi + |\partial_i \phi|^2 + m^2|\phi|^2 + \lambda|\phi|^4 \right]$$

or

$$S = \int d^4x \left[|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu(\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda|\phi|^4 \right]$$

- linear term is purely imaginary: complex action
- quadratic term from integrating out momenta

same symmetry: $S^*(\mu) = S(-\mu^*)$

Towards the Silver Blaze problem

consider massive particle with mass m at low temperature:

- μ is the change in free energy when a particle carrying the corresponding quantum number is added

  i.e. energy cost for adding one particle

- if $\mu < m$: not enough energy to create a particle $\Rightarrow$ no change in groundstate

- if $\mu > m$: plenty of energy available $\Rightarrow$ nonzero density

onset at $\mu = \mu_c (= m)$ at zero temperature

generic principle of statistical mechanics

$\Rightarrow$ demonstrate for free fermions

Free fermions: onset at low temperature

standard thermal field theory: free fermion gas

$$\ln Z = 2V \int \frac{d^3p}{(2\pi)^3} \left[\beta\omega_{\mathbf{p}} + \ln\left(1 + e^{-\beta(\omega_{\mathbf{p}} - \mu)}\right) + \ln\left(1 + e^{-\beta(\omega_{\mathbf{p}} + \mu)}\right) \right]$$

- density: $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}$

$$\langle n \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial \mu} = 2 \int_{\mathbf{p}} \left[\frac{1}{e^{\beta(\omega_{\mathbf{p}} - \mu)} + 1} - \frac{1}{e^{\beta(\omega_{\mathbf{p}} + \mu)} + 1} \right]$$

- low-temperature limit: $T \to 0, \beta \to \infty$

  case 1:

$$\mu < m \ : \quad \langle n \rangle \sim 2 \int_{\mathbf{p}} \left[e^{-\beta(\omega_{\mathbf{p}} - \mu)} - e^{-\beta(\omega_{\mathbf{p}} + \mu)} \right] \to 0$$

  (anti)particles thermally excited but Boltzmann suppressed

Free fermions: onset at low temperature

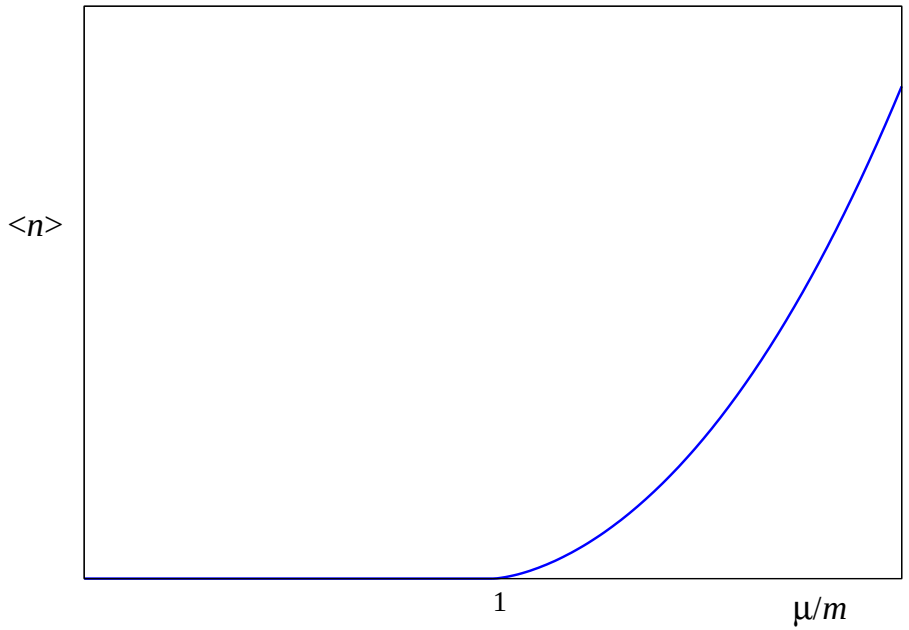
- case 2: $\mu > m$

  Fermi-Dirac distribution become step function at $T = 0$

$$\mu > m \ : \quad \langle n \rangle \sim 2 \int_{\mathbf{p}} \Theta(\mu - \omega_{\mathbf{p}}) = \frac{\left(\mu^2 - m^2\right)^{3/2}}{3\pi^2} \Theta(\mu - m)$$

filled Fermi sphere:

nonzero density



- onset at $\mu = \mu_c = m$
- no μ dependence below onset

Free bosons: onset at low temperature

- same is true for Bose gas: Bose-Einstein condensation
- need interaction term for stabilization
- massless particle at onset (Goldstone boson)

$$S = \int d^4x \left[|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu(\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda |\phi|^4 \right]$$

important: at $T = 0$

- thermodynamic quantities ($\ln Z, p, f, \langle n \rangle, \chi, \ldots$) are independent of μ as long as μ is below the mass of the lightest particle in channel with appropriate quantum numbers
- relevant for Silver Blaze problem Cohen 04

Chemical potential on the lattice

- naively adding $\mu\bar{\psi}\gamma_4\psi$ leads to unexpected (i.e. μ dependent) UV divergences
- instead:
  - couple to conserved charge on the lattice
  - should appear as iA_4
- lattice action: $S \sim \bar{\psi}_x U_{\nu x}\gamma_\nu\psi_{x+\nu} - \bar{\psi}_{x+\nu}U^\dagger_{\nu x}\gamma_\nu\psi_x$
- conserved current: $j_\nu \sim \bar{\psi}_x U_{\nu x}\gamma_\nu\psi_{x+\nu} + \bar{\psi}_{x+\nu}U^\dagger_{\nu x}\gamma_\nu\psi_x$ (point-split)

modify temporal hopping terms:

- forward hopping: $U_{4x} = e^{iA_{4x}} \Rightarrow e^{\mu}$
- backward hopping: $U^\dagger_{4x} = e^{-iA_{4x}} \Rightarrow e^{-\mu}$

Chemical potential on the lattice

- correct naive continuum limit
- couples to exactly conserved charge on the lattice
- no new UV divergences

Hasenfratz & Karsch 83, Kogut et al 83

non-unique: Gavai & Bilic 84

(different prescriptions should agree in continuum limit)

note:

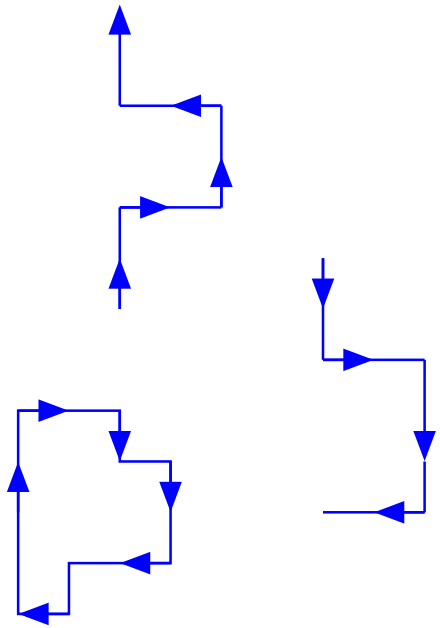
- use lattice units: $\mu \equiv a\mu$
- always clear what is meant: appears in combination

(lattice) $\mu N_\tau = \mu/T$ (continuum)

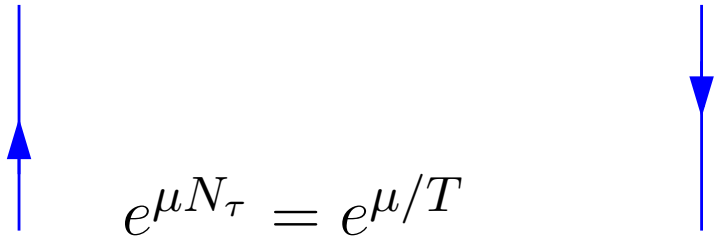
Chemical potential on the lattice

chemical potential introduces an imbalance between forward and backward hopping

- forward hopping (quark)
  $\Rightarrow$ favoured as $e^{\mu n_\tau}$
- backward hopping (anti-quark)
  $\Rightarrow$ disfavoured as $e^{-\mu n_\tau}$
- closed worldline
  $\Rightarrow$ μ dependence cancels exactly



μ dependence only remains when worldline wraps around time direction



$e^{\mu N_\tau} = e^{\mu/T}$ $\qquad$ $e^{-\mu N_\tau} = e^{-\mu/T}$

Chemical potential on the lattice

suggestion:

- μ is effectively a boundary condition

make explicit:

- field redefinition $\psi_x = e^{-\mu\tau}\psi'_x \qquad \bar{\psi}_x = e^{\mu\tau}\bar{\psi}'_x$
- μ dependence drops from all terms $\bar{\psi}_x e^{\mu}\psi_{x+4}$ etc (and also from spatial terms)
- but appears as a boundary condition

$$\psi_{N_\tau} = -\psi_0 \quad \Rightarrow \quad \psi'_{N_\tau} = -e^{\mu N_\tau}\psi'_0$$

wrapping around the temporal direction

Bose gas on the lattice

- add $e^{\pm\mu}$ in temporal hopping terms

$$S = \sum_x \Bigg[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda (\phi_x^* \phi_x)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu\delta_{\nu,4}} \phi_{x+\nu} + \phi_{x+\nu}^* e^{\mu\delta_{\nu,4}} \phi_x \right) \Bigg]$$

- continuum limit:
  - second derivatives ok
  - first derivatives $+\mu$ ok
  - no derivatives $-\mu^2$ ok

How hard is the sign problem?

partition function: $Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_B} \det M$

complex weight due to complex determinant

$$[\det M(\mu)]^* = \det M(-\mu^*)$$

write $\det M = |\det M| e^{i\varphi}$ and absorb phase in observable

$$\langle O \rangle_{\text{full}} = \frac{\int DU\, e^{-S_B} \det M\, O}{\int DU\, e^{-S_B} \det M} = \frac{\int DU\, e^{-S_B} |\det M|\, e^{i\varphi} O}{\int DU\, e^{-S_B} |\det M|\, e^{i\varphi}}$$

$$= \frac{\langle e^{i\varphi} O \rangle_{\text{pq}}}{\langle e^{i\varphi} \rangle_{\text{pq}}}$$

expectation values are taken wrt phase-quenched weight

well-defined in principle ...

Sign and overlap problems

- what is average phase factor $\langle e^{i\varphi} \rangle_{\rm pq}$?

$$\langle e^{i\varphi} \rangle_{\rm pq} = \frac{\int DU\, e^{-S_B} |\det M|\, e^{i\varphi}}{\int DU\, e^{-S_B} |\det M|} = \frac{Z_{\rm full}}{Z_{\rm pq}} = e^{-\Omega \Delta f} \to 0$$

- ratio of two partition functions! note: $Z_{\rm full} \leq Z_{\rm pq}$

$$Z = e^{-F/T} = e^{-\Omega f} \qquad \Omega = N_\tau N_s^3$$

- average phase factor $\to 0$ in thermodynamic limit!
  (unless $f = f_{\rm pq}$)

this is the overlap problem: sampling with the 'wrong' weight

exponentially hard

Origin of overlap problem

phase-quenched physics is different!

consider two flavours: $[\det D(\mu)]^2$ vs $|\det D(\mu)|^2$

- recall $D^\dagger(\mu) = \gamma_5 D(-\mu^*)\gamma_5$
- then $|\det D(\mu)|^2 = \det D(-\mu) \det D(\mu)$

$\Rightarrow$ isospin chemical potential! up/down quark: $\pm\mu$

- lightest particle with nonzero isospin: pion
- lightest particle with nonzero baryon number: nucleon

Onset, phase-quenching and Silver Blaze

full QCD with quark chemical potential:

- onset when μ equals [lightest baryon mass (nucleon) - binding energy]/3
  nuclear matter

phase-quenched QCD with isospin chemical potential:

- onset when μ equals [pion mass]/2 (nonzero isospin)
  pion condensation

$0 < \mu < m_\pi/2$ full $=$ phase-quenched at $T = 0$

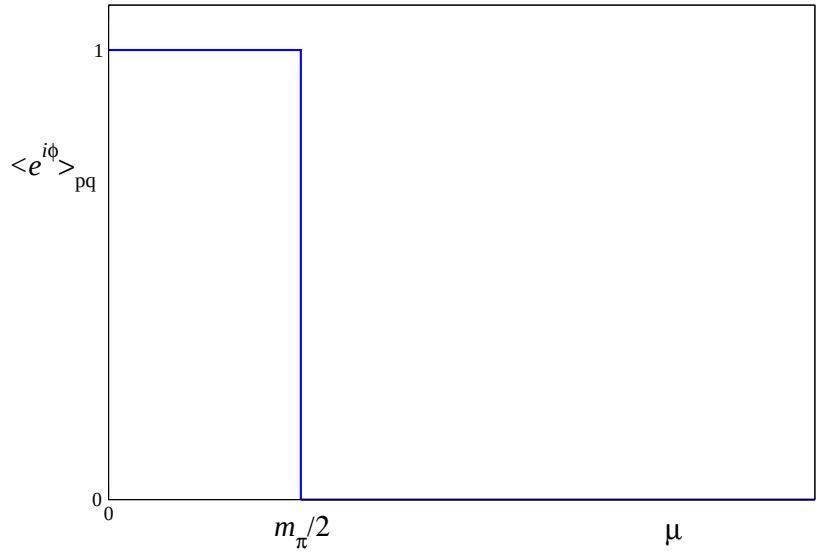
no severe sign problem, but no interesting physics

$m_\pi/2 < \mu \lesssim m_B/3$ severe sign problem

strong cancelations required to cancel μ dependence of phase-quenched theory

Onset, phase-quenching and Silver Blaze

average phase factor at $T = 0$



- perform lattice simulations in phase-quenched theory
- extract full QCD results

$\Rightarrow$ requires severe cancelations of the μ dependence in region $m_\pi/2 < \mu \lesssim m_B/3$

most straightforward numerical methods will fail this test!

Onset, phase-quenching and Silver Blaze

same happens in Bose gas

phase-quenching:

- linear term ignored $+\mu\,(\phi^*\partial_4\phi - \partial_4\phi^*\phi)$
- quadratic term kept $(m^2-\mu^2)|\phi|^2$

$\Rightarrow$ theory with μ^2 dependent effective potential

- ordinary symmetry breaking as μ^2 is increased
- μ dependence immediate in phase-quenched theory

Silver Blaze region: $0 < \mu < m$

Dirac eigenvalues and Silver Blaze

original formulation of Silver Blaze problem:

- weight and therefore configurations and eigenvalues of Dirac operator depend on μ
- this μ dependence should cancel: sensitive test
- commonly demonstrated using spectrum of Dirac operator Cohen 04, Splittorff, Verbaarschot, Osborn 05

write $D + m$ with $D = \not{D} + \mu\gamma_4$

then $Z = \int DU \, \det(D+m) e^{-S_{\rm YM}} = \langle \det(D+m) \rangle_{\rm YM}$

write $\det(D+m) = \prod (\lambda_k + m)$ where $D\psi_k = \lambda_k \psi_k$

- since D is not γ_5 hermitian, eigenvalues not real or imaginary, instead $\lambda_k \in \mathbb{C}$

Dirac eigenvalues and Silver Blaze

- chiral condensate

$$\langle\bar{\psi}\psi\rangle = \frac{1}{\Omega}\frac{\partial \ln Z}{\partial m} = \left\langle \frac{1}{\Omega}\sum_k \frac{1}{\lambda_k + m}\prod_j (\lambda_j + m) \right\rangle_{\rm YM}$$

- introduce density of eigenvalues

$$\rho(z;\mu) = \frac{1}{Z}\int DU\ \det(D+m)e^{-S_{\rm YM}}\frac{1}{\Omega}\sum_k \delta^2(z-\lambda_k)$$

$$= \left\langle \det(D+m)\frac{1}{\Omega}\sum_k \delta^2(z-\lambda_k) \right\rangle_{\rm YM}$$

- then $$\langle\bar{\psi}\psi\rangle = \int d^2z\,\frac{\rho(z;\mu)}{z+m}$$

Dirac eigenvalues and Silver Blaze

$\rho(z;\mu)$ depends on μ since $D+m$ does

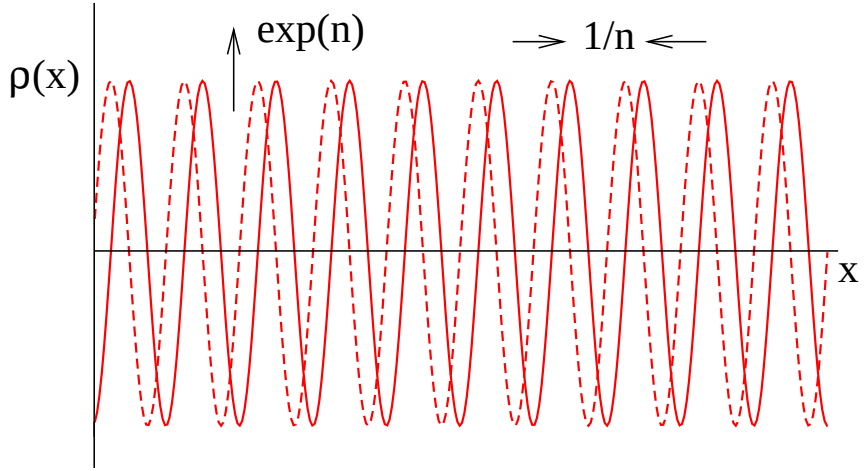
$$\langle\bar{\psi}\psi\rangle = \int d^2z\, \frac{\rho(z;\mu)}{z+m}$$

if $\mu \lesssim m_B/3$ (below onset), all μ dependence should cancel

achieved:

$\rho(z;\mu)$ is complex, oscillating with amplitude $e^{\Omega\mu}$ and period $1/\Omega$

only when all oscillations are correctly integrated, μ dependence will cancel



'solution to Silver Blaze problem'
from viewpoint of Dirac spectral density

Where are we?

complex weight:

- straightforward importance sampling not possible
- overlap problem
- extreme care is needed: Silver Blaze problem

various possibilities:

- preserve overlap as best as possible
- use approximate methods at small chemical potential
- do something radical:
  - rewrite partition function in other dof
  - explore field space in different way
  - . . .