Complex Langevin simulations of a finite density matrix model for QCD

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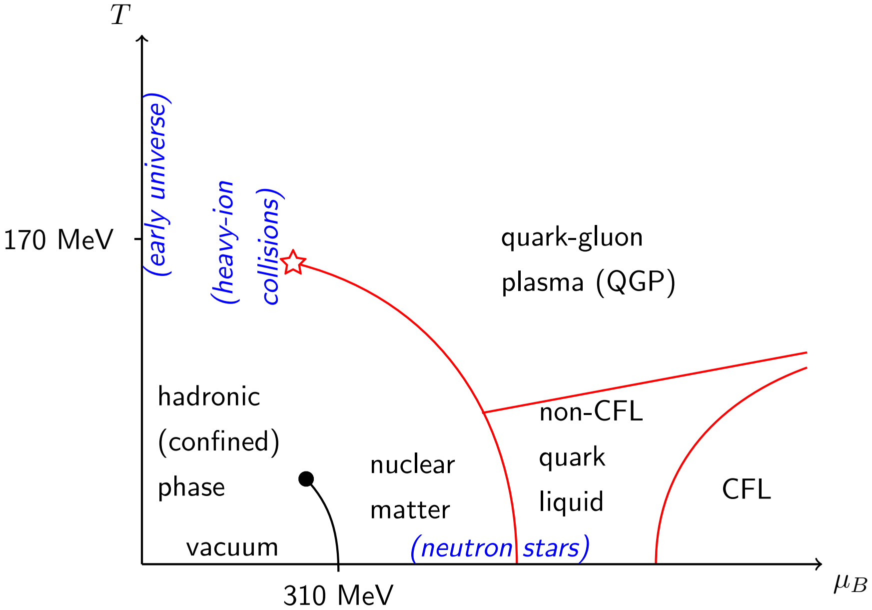
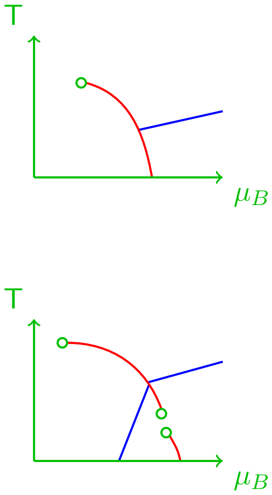
Phase diagram from a theorist's viewpoint

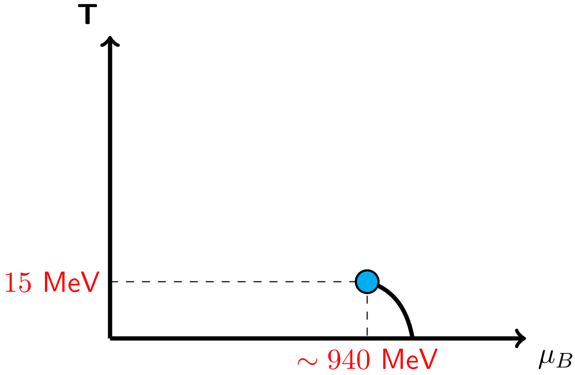


Less conservative viewpoints

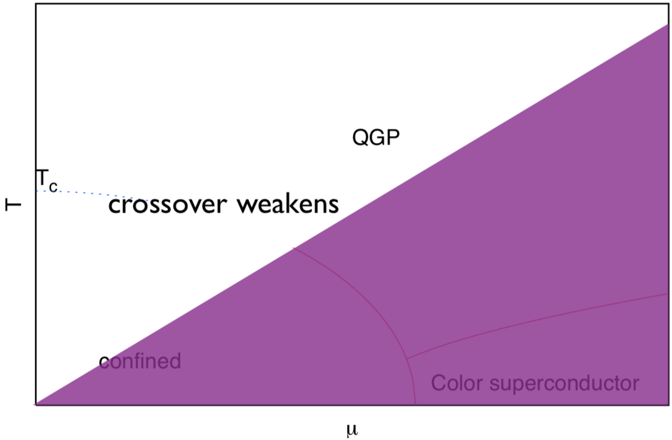


NJL with vector interactions Zhang, Kunihiro, Fukushima 2009, Ginzburg-Landau approach Baym et al 2006, beyond mean field Ferroni, Koch, Pinto 2010

The experimentalist's viewpoint



Calculable from first principles



(Courtesy of Owe Philipsen-)
Numerical simulations not feasible when $\mu/T > 1$ or when $\mu > m_\pi/2$.

No evidence for a critical endpoint in the controllable region.

Adding μ

- adding to the continuum Euclidean Dirac operator D the quark number operator $\mu\psi^\dagger\psi$
- $D + \mu\gamma_0$
- jeopardizes γ_5-Hermiticity which ensures reality of $\det(D)$
- remember that the probability weight is given by $\det(D)^{N_\mathrm{f}} e^{-S_g}$
- when $\mu = 0 \rightarrow D^\dagger = \gamma_5 D \gamma_5$
- $\gamma_5(D + m + \mu\gamma_0)\gamma_5 = D^\dagger + m - \mu\gamma_0 = (D + m - \mu^*\gamma_0)^\dagger$
- $\det(D + m + \mu\gamma_0) = \det(D + m - \mu^*\gamma_0)^*$ which is real when $\mu = 0$
- possible ways out: study QCD with imaginary μ or at finite isospin chemical potential

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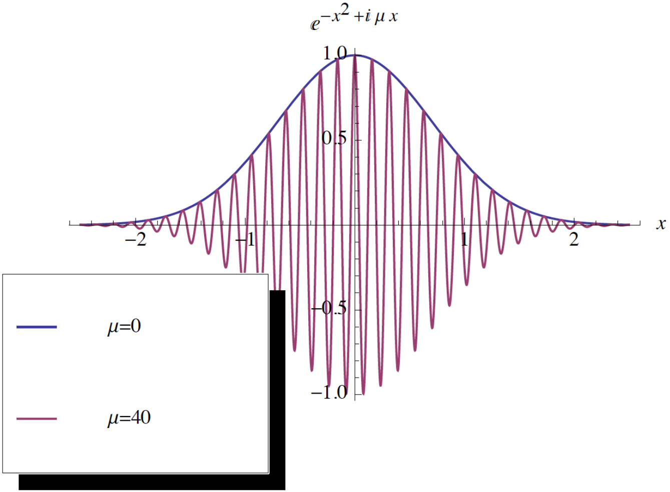
The sign problem



Many approaches

- Conventional/Monte Carlo based methods
  - Reweighting
  - Taylor expansion
  - Imaginary μ
  - Strong Coupling Expansion
  - Mean Field analyses
- Alternative methods
  - Stochastic Quantization-Complex Langevin
  - Lefschetz Thimble
  - Canonical ensembles
  - Dual variables
  - Density of States

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Stochastic quantization as an alternative

- consider the trivial "QFT" given by the partition function
- $\mathcal{Z} = \int e^{-S(x)} dx$
- in the real Langevin formulation
- $x(t + \delta t) = x(t) - \partial_x S(x(t))\delta t + \delta\xi$
- stochastic variable $\delta\xi$ with zero mean and variance given by $2\delta t$
- generalization to complex actions Parisi (1983), Klauder (1983)
- $x \to z = x + iy$
- $z(t + \delta t) = z(t) - \partial_z S(z(t))\delta t + \delta\xi$
- one can study gauge theories with complex actions Aarts, James, Seiler, Sexty, Stamatescu, ...

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Is this "the" solution to the sign problem?

- proof relating Langevin dynamics to the path integral quantization-no longer holds
- simulations are not guaranteed to converge to "the correct solution"
- criteria of convergence not fulfilled in practical simulations (at least for some range of the parameters)

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Validity criteria

- action S and observables $\mathcal{O}$ should be holomorphic in the complexified variables (up to singularities)
- the probability distribution of the complexified variables z along the CL trajectories should be suppressed close to the singularities of the drift term and of the observable
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RMT

- focus on a much simpler theory than QCD. Random Matrix Theory
- same flavor symmetries with QCD which uniquely determine (in the ϵ-regime)
  - mass dependence of the chiral condensate $\langle \bar{\eta}\eta \rangle = \partial_m \log Z$
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The Stephanov Model

- $\mathcal{Z} = \int DW e^{-n\Sigma^2 \mathrm{Tr} WW^\dagger} det^{N_f} \begin{pmatrix} m & iW+\mu \\ iW^\dagger+\mu & m \end{pmatrix}$

  Stephanov (1996) and Halasz, Jackson, Verbaarschot(1997)

- solve via bosonization
- $\mathcal{Z}^{N_f=1}(m,\mu) = \pi e^{-nm^2} \int_0^\infty du (u-\mu^2)^n I_0(2mn\sqrt{u}) e^{-nu}$

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The phase transition

- there is a phase transition separating a phase with zero and non-zero baryon density
- in the chiral limit $\mu_c = 0.527$ for $\mu \in \mathbb{R}$
- we can compute $\Sigma(m, \mu)$ and $n_B(m, \mu)$ and compare it with the Complex Langevin simulation
- first attempts in the Osborn model

$$\mathcal{Z} = \int D[W, W'] e^{-n\Sigma^2 \mathrm{Tr}(WW^\dagger + W'W'^\dagger)} det^{N_f} \begin{pmatrix} m & iW + \mu W' \\ iW^\dagger + \mu W' & m \end{pmatrix}$$

Mollgaard and Splittorff(2013-2014), Nagata, Nishimura, Shimasaki (2015-2016)

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- $A_{ij}(t + \delta t) = A_{ij}(t) - \partial_{A_{ij}} S(x(t))\delta t + \delta\xi_{ij}$
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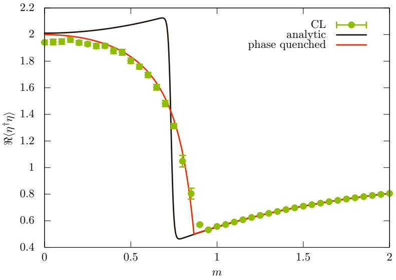
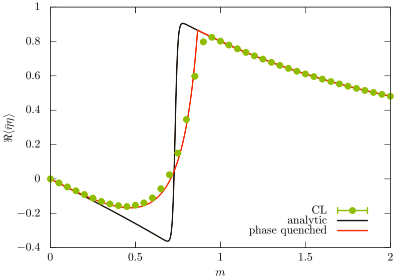
m-scan for $\mu = 1$



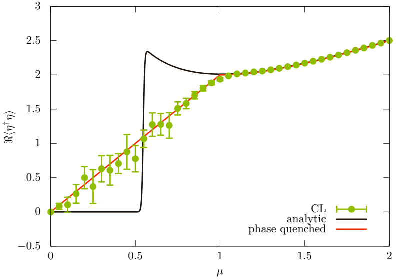
$\langle\eta^\dagger\eta\rangle$ for $\mu = 1$



$\langle\bar{\eta}\eta\rangle$ for $\mu = 1$

analytical pq results by Glesaaen, Verbaarschot and SZ (2016)

μ-scan for $m = 0$



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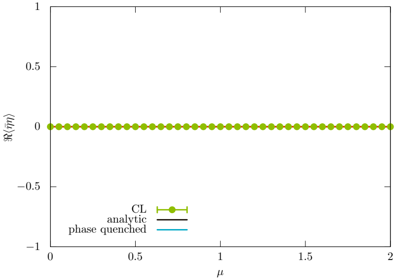

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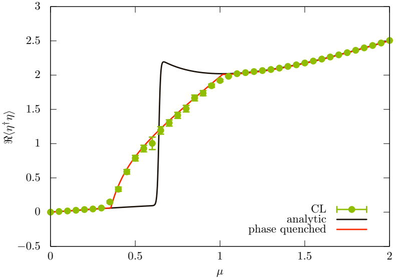
μ-scan for $m = 0.2$



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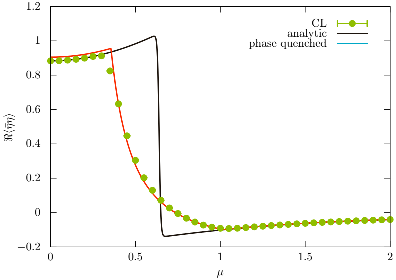

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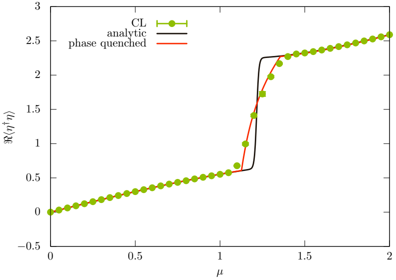

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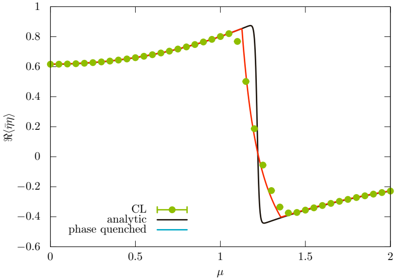

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Gauge Cooling

Originally suggested for QCD by Seiler, Sexty and Stamatescu(2012)

implemented for RMT by Nagata, Nishimura, Shimasaki (2015) in the Osborn model

- complexified action invariant under an enhanced gauge trafo
- steer the evolution in Langevin time towards more physical solutions
- successful application to the Osborn model
- complexified action is invariant $\mathrm{GL}(N, \mathbb{C})$
- $A' = \frac{1}{2}\Big(hAh^{-1} + (hA^T h^{-1})^T + i\big(hBh^{-1} - (hB^T h^{-1})^T\big)\Big)$
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The Cooling norms

- $\mathcal{N}_H = \frac{1}{N}\mathrm{tr}\left[\left(X - Y^\dagger\right)^\dagger\left(X - Y^\dagger\right)\right]$ (N.B. $X(0) = W$ and $Y(0) = W^\dagger$ $X = A + iB$ and $Y = A^T - B^T$ when A, B are complexified)
- $\mathcal{N}_{AH} = \frac{1}{N}\mathrm{tr}\left[\left(\left(\phi + \psi^\dagger\right)^\dagger\left(\phi + \psi^\dagger\right)\right)^2\right]$
- ψ and ϕ are the off-diagonal elements of D: $\psi = iX + \mu$, $\phi = iY + \mu$
- $\mathcal{N}_{\mathrm{ev}} = \sum_{i=1}^{n_{\mathrm{ev}}} e^{-\xi\gamma_i}$
- $\mathcal{N}_{\mathrm{agg}} = (1-s)N_{AH/\mathrm{ev}} + sN_H, \quad$ where $s \in [0,1]$

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- $\mathcal{N}_{AH} = \frac{1}{N}\mathrm{tr}\left[\left(\left(\phi + \psi^\dagger\right)^\dagger \left(\phi + \psi^\dagger\right)\right)^2\right]$
- ψ and ϕ are the off-diagonal elements of D: $\psi = iX + \mu$, $\phi = iY + \mu$
- $\mathcal{N}_{\mathrm{ev}} = \sum_{i=1}^{n_{\mathrm{ev}}} e^{-\xi\gamma_i}$
- $\mathcal{N}_{\mathrm{agg}} = (1-s)N_{AH/\mathrm{ev}} + sN_H$, where $s \in [0,1]$

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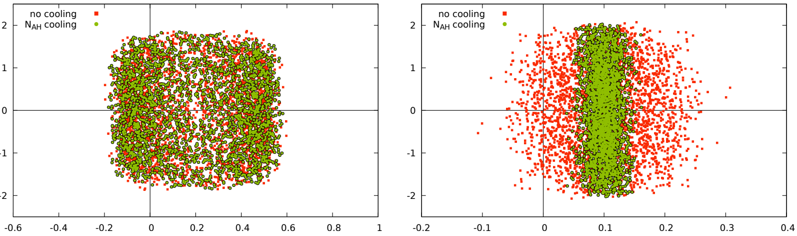
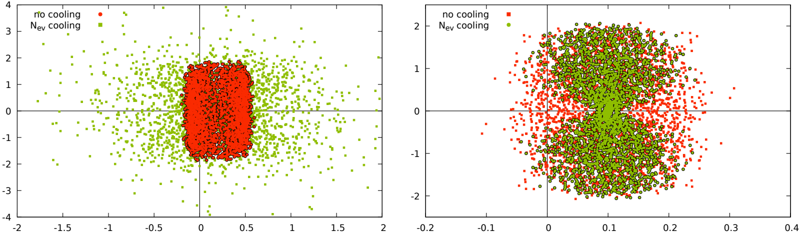
Cooling and the Dirac Spectrum



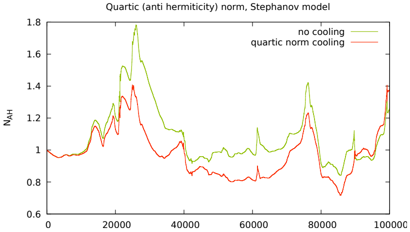
Scatter plots of the eigenvalues of the fermion matrix for a standard CL run together with the ones from a run cooled with the $\mathcal{N}_{AH}$ cooling norm. The plots show the eigenvalues from the last 60 trajectories, separated by 100 updates. The left hand plot shows the Stephanov model, while the Osborn model is shown to the right.

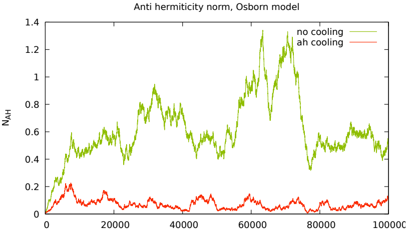
Cooling and the Dirac Spectrum



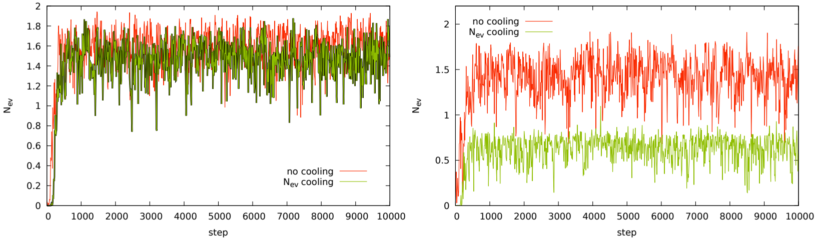
Scatter plots of the eigenvalues of the fermion matrix for a standard CL run together with the ones from a gauge cooled run. We chose the parameters $\{\xi = 100, n_{\rm ev} = 2\}$ for $\mathcal{N}_{\rm ev}$. The plots show the eigenvalues from the last 60 trajectories, separated by 100 updates. The left hand plot shows the Stephanov model, while the Osborn model is shown to the right

The anti-hermiticity norm





The eigenvalue norm



Value of $\mathcal{N}_{\mathrm{ev}}$ as a function of Langevin time. Stephanov model to the left, Osborn model to the right

The shifted representation

- shift μ away from the fermionic term by a COV
- initially $D = \begin{pmatrix} m & iA - B + \mu \\ iA^T + B^T + \mu & m \end{pmatrix}$
- Absorb μ into A with a COV $A' = A - i\mu$. The action in terms of A' and B is
  $S = N\mathrm{tr}\left(A'^T A' - 2i\mu A' + \mu^2 + B^T B\right) - N_f \mathrm{tr}\,\log\left(m^2 + X'Y'\right)$
  $X' = A' + iB$ and $Y' = A'^T - iB^T$. Now, the μ dependence has shifted from the fermionic to the bosonic term.
- Computing again the CL force term ...
- Advantage of the shifted representation is that it starts in an anti-Hermitian state, and since CL in non-deterministic, the configurations could evolve to a different minimum.

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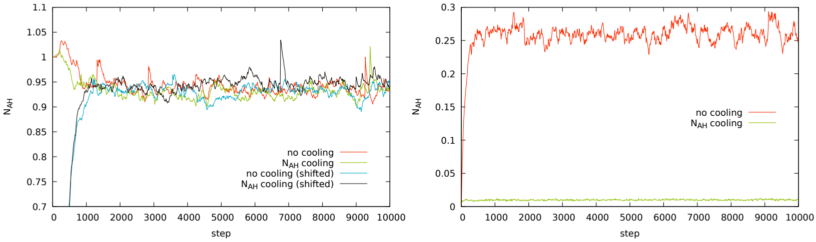
Shifted representation and cooling



$\mathcal{N}_{AH}$ as a function of Langevin time. Stephanov model (RHS), Osborn model (LHS). The Stephanov plot also includes the values from the shifted representation. These start at 0 for $t = 0$, but quickly shoot up to meet the unshifted curves. Although A and A' start out very different, they coincide after thermalization. This means that $\langle A' \rangle_{\mathrm{CL,shifted}} = \langle A \rangle_{\mathrm{CL,standard}} - i\mu$, and thus they converge to the same solution. The advantage of the shifted representation is that it starts in an anti-Hermitian state, and due to the fact that CL in non-deterministic, the configurations could evolve to a different minimum.

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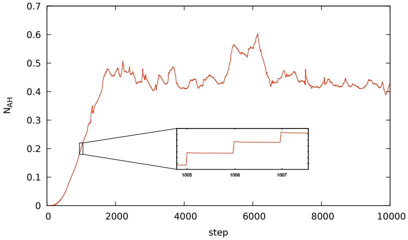

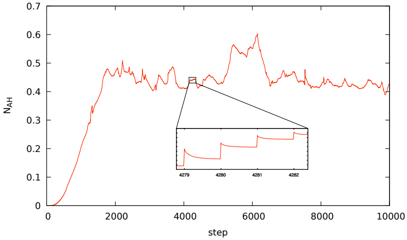

$\mathcal{N}_{AH}$ for the shifted representation of the Stephanov model as a function of Langevin time for 8×8 block matrices. The zoomed in plots show the evolution of $\mathcal{N}_{AH}$ with the application of the cooling step. There are 50 gauge cooling transformations between each Langevin step.

The deformation technique

- another idea Ito and Nishimura (2017) is to deform the Dirac operator, to "move" its smallest eigenvalues and then extrapolate to zero deformation parameter at the end of the calculation.
- deformation is achieved by a finite temperature term given by the two lowest Matsubara frequencies $\pm\pi T$

$$Z(m,\mu;\alpha) = \int \mathrm{D}[X,Y] \det \begin{pmatrix} m & X+\mu+i\Theta(\alpha) \\ Y+\mu+i\Theta(\alpha) & m \end{pmatrix}$$

where $\mathrm{D}[X,Y] = \mathrm{d}[X,Y]P(X,Y)$ and $\Theta(\alpha)$ is itself a block-matrix

$$\Theta(\alpha) = \begin{pmatrix} \alpha & 0 \\ 0 & -\alpha \end{pmatrix}$$

where α can be thought as the lowest Matsubara frequency.

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- Beyond a critical value of α the eigenvalue spectrum opens up and at this point chiral symmetry is restored. We can thus extrapolate from higher values in α for which there are no eigenvalues at the origin. In our studies we will see a gap opening at $\alpha \approx 1.0$
- But let's see this in practice...

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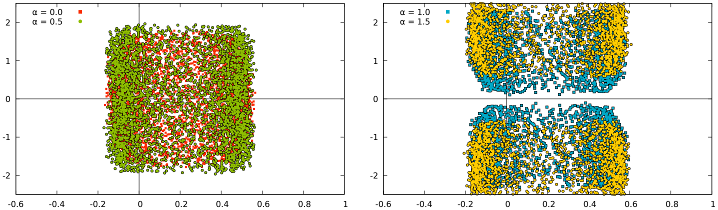
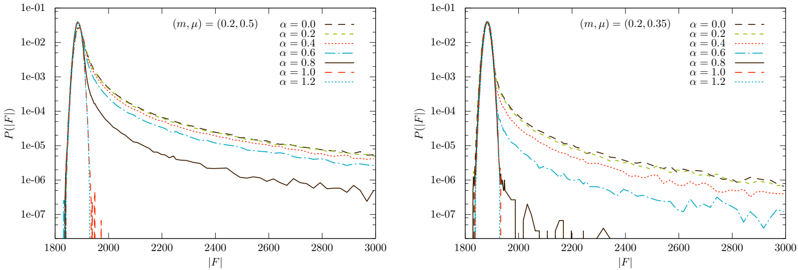


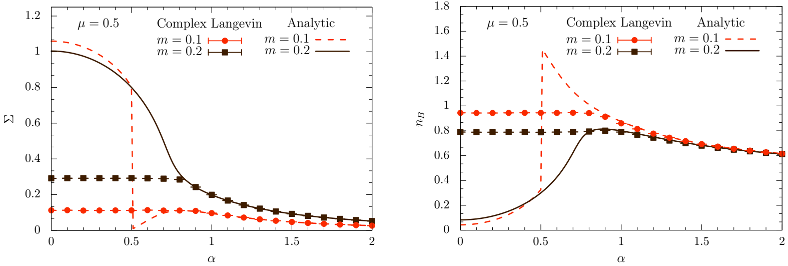
Scatter plots of eigenvalues from simulating with $N = 48$, $\mathrm{d}t = 5 \times 10^{-5}$, $t_{\text{end}} = 5.0$, measured every 400 steps after thermalization. Both plots show $m = 0.2$ and $\mu = 0.5$ for varying values of the "temperature" α.

The deformation technique



The density of the CL forces for $\mu = 0.5$ (LHS) and $\mu = 0.35$ (RHS). Data gathered with a $t_{\text{final}} = 100$ run using $\mathrm{d}t = 5 \times 10^{-5}$. If the decay fall is exponential (or faster) the CL will give the correct result but not if it decays as power law (or slower). Define α_c as the first α value that gives power law decay.

The deformation technique



Physical observables as a function of the parameter α. Analytic solutions (lines) for various values of the mass in addition to values from a simulation at $N = 24$ and $(m, \mu) = (0.2, 0.5)$. The parameters of the simulation correspond to the solid analytic line. Chiral condensate (LHS), baryon number density (RHS).

Natural questions to ask: Which points do you include in your extrapolation and which fitting ansatz do you use and what about the phase transition for small masses?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Reweighted Complex Langevin

- generate a CL trajectory for parameter values where complex Langevin is correct
- perform a reweighting of the trajectory to compute observables in an extended range of the parameters where CL used to fail

Reweighting

- target ensemble with parameters $\xi = (m, \mu, \beta)$ (for the general QCD case-drop β for RMT)
- auxiliary ensemble with parameters $\xi_0 = (m_0, \mu_0, \beta_0)$
- Reweighting from auxiliary to target

$$\langle O \rangle_\xi = \frac{\int dx w(x;\xi)\mathcal{O}(x;\xi)}{\int dx w(x;\xi)} = \frac{\int dx w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\right]}{\int dx w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\right]}$$

$$= \frac{\langle \frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\rangle_{\xi_0}}{\langle \frac{w(x;\xi)}{w(x;\xi_0)}\rangle_{\xi_0}}$$

- but now we have a complex weight $w(x;\xi_0) = e^{-S(x;\xi_0)}$ so we need CL for this too!

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$$\begin{aligned}\langle O\rangle_{\xi} &= \frac{\int dx w(x;\xi)\mathcal{O}(x;\xi)}{\int dx w(x;\xi)} = \frac{\int dx w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\right]}{\int dx w(x;\xi_0)\left[\frac{w(x;\xi)}{w(x;\xi_0)}\right]} \\ &= \frac{\langle \frac{w(x;\xi)}{w(x;\xi_0)}\mathcal{O}(x;\xi)\rangle_{\xi_0}}{\langle \frac{w(x;\xi)}{w(x;\xi_0)}\rangle_{\xi_0}}\end{aligned}$$

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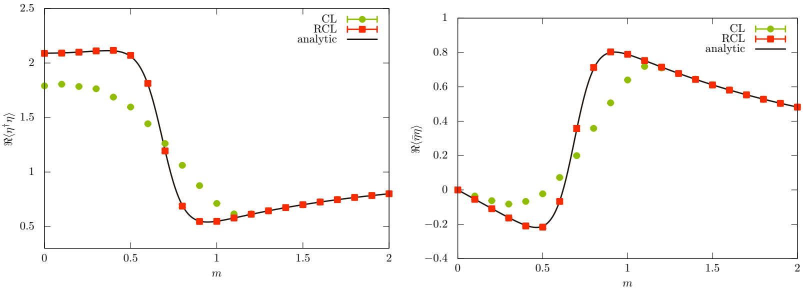
m-scan for $\mu = 1$

reweighted from an auxiliary ensemble with $m_0 = 4$ and $\mu_0 = 1$ using $\mathcal{O}(15000)$ confs

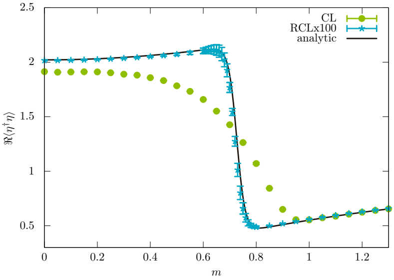


$\langle\eta^\dagger\eta\rangle$ for $\mu = 1$ and $n = 6$

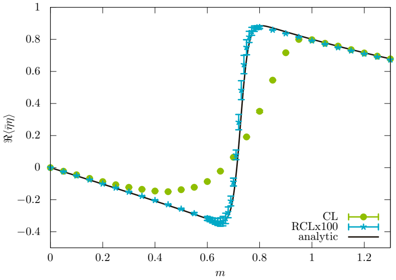
$\langle\bar{\eta}\eta\rangle$ for $\mu = 1$ and $n = 6$

m-scan for $\mu = 1$

Auxiliary ensemble $m_0 = 1.3, \mu_0 = \mu = 1.0$ using $\mathcal{O}(560000)$ confs



$\langle\eta^\dagger\eta\rangle$ for $\mu = 1$ and $n = 24$

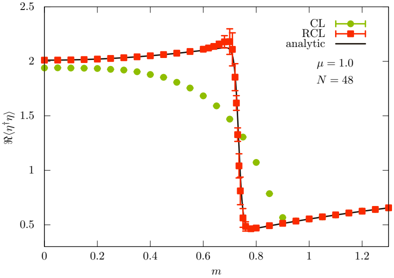


$\langle\bar{\eta}\eta\rangle$ for $\mu = 1$ and $n = 24$

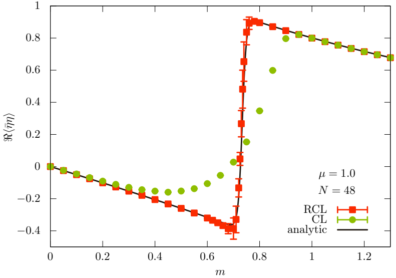
The number of confs needed, builds up very rapidly. So one has to "just" to generate an auxiliary trajectory long enough to overcome the sign problem.

m-scan for $\mu = 1$

Auxiliary ensemble $m_0 = 1.3, \mu_0 = \mu = 1.0$ using $\mathcal{O}(122000000)$ confs



$\langle\eta^\dagger\eta\rangle$ for $\mu = 1$ and $n = 48$



$\langle\bar{\eta}\eta\rangle$ for $\mu = 1$ and $n = 48$

if you (or the computer) work(s) hard enough you can also deal with the matrices of the original size that we were dealing with $n = 48$

Conclusions and outlook

- studied the CL algorithm for an RMT model for QCD/ comparing numerical with exact analytical results for all the range of parameters (m, μ)
- compared to previous similar studies this model possesses a phase transition to a phase with non-zero baryon density
- fails to converge to QCD and it converges to $|QCD|$
- partial attempt to fix the issues via RCL procedure $\rightarrow$ correct results, even when CL does not work for the target ensemble
- gauge cooling or the deformation technique seem unable to overcome the pathologies of this model

Thanks a lot for your attention!!!

Phase Quenched QCD

- ignore the complex phase of the fermion determinant
- $\mathcal{Z}_{pq} = \mathcal{Z}_{iso} = \int dA |\det(D(\mu))|^2 e^{-S_g}$
- $|\det(D(\mu))|^2 = \det D(\mu)(\det(D(\mu)))^* = \det D(\mu) \det D(-\mu)$
- since $\gamma_5(\gamma_\mu D^\mu + m - \mu\gamma_0)\gamma_5 = (\gamma_\mu D^\mu + m + \mu\gamma_0)^\dagger$
- $\langle O \rangle_{pq} = \frac{1}{\mathcal{Z}_{pq}} \int dAO |\det D(\mu)|^2 e^{-S_g}$
- this theory has a different phase diagram and different properties than QCD
- for $T <<$ and $\mu >> \rightarrow$ Bose condensation of charged pions

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The analytical solution

Halasz, Jackson, Verbaarschot(1997)

$$\int \mathcal{D}[\ldots] \exp \left[-i \sum_{k=1}^{N_f} \psi^{k\,*} \begin{pmatrix} m & iW + \mu \\ iW^\dagger + \mu & m \end{pmatrix} \psi^k \right] e^{-n\Sigma^2 \mathrm{Tr} W W^\dagger}$$

perform the W integration

$$\int \mathcal{D}[\ldots] e^{\left[-\frac{1}{n\Sigma^2} \psi^{f\,*}_{L\,k} \psi^{f}_{R\,i} \psi^{g\,*}_{R\,i} \psi^{g}_{L\,k} + m \left(\psi^{f\,*}_{R\,i} \psi^{f}_{R\,i} + \psi^{f\,*}_{L\,k} \psi^{g}_{L\,k} \right) + \mu \left(\psi^{f\,*}_{R\,i} \psi^{f}_{L\,i} + \psi^{f\,*}_{L\,k} \psi^{f}_{R\,k} \right) \right]}$$

write the four-fermion term as a difference of two squares and linearize via a Hubbard-Stratonovich trafo

$$\exp(-AQ^2) \sim \int d\sigma \exp\left(-\frac{\sigma^2}{4A} - iQ\sigma\right)$$

The analytical solution

then one carries out the Grassmann integrals

$$Z(m,\mu) = \int \mathcal{D}\sigma \exp[-n\Sigma^2 \mathrm{Tr}\sigma\sigma^\dagger] \det{}^n \begin{pmatrix} \sigma + m & \mu \\ \mu & \sigma^\dagger + m \end{pmatrix}$$

which for one-flavor and $\Sigma = 1$ becomes

$$\mathcal{Z}^{N_f=1}(m,\mu) = \int d\sigma d\sigma^* e^{-n\sigma^2} (\sigma\sigma^* + m(\sigma+\sigma^*) + m^2 - \mu^2)^n$$

The analytical solution

in polar coordinates after the angular integration
$\mathcal{Z}^{N_f=1}(m,\mu) = \pi e^{-nm^2} \int_0^\infty du(u-\mu^2)^n I_0(2mn\sqrt{u})e^{-nu}$ in the thermodynamic limit one can perform a saddle point analysis
$I_0(z) \sim e^z/\sqrt{2\pi z}$
and the saddle point equation takes the form
$\frac{1}{u-\mu^2} = 1 - \frac{m}{\sqrt{u}}$

The analytical solution

A 1st order phase transition takes place at the points where $|Z_{u=u_b}| = |Z_{u=u_r}|$, with u_b and u_r two different solutions of the saddle-point equation give the same free-energy. This condition can be rewritten as $|(u_b - \mu^2)e^{2m\sqrt{u}_b - u_b}| = |(\mu^2 - u_r)e^{2m\sqrt{u}_r - u_r}|$. A general solution is quite cumbersome, but for $m \to 0$ we find that $u_r = 0$ and $u_b = 1 + \mu^2$. This leads to the critical curve

$$\mathrm{Re}\left[1 + \mu^2 + \log \mu^2\right] = 0$$

which for real μ, $\mu_c = 0.527\ldots$