Sign problem and diagrammatic representation of scalar vs. real QCD

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Heisenberg-Programm
Deutsche Forschungsgemeinschaft

Motivation

sign problem at nonzero chemical potential μ:
complex action = complex weight prevents importance sampling

- applies to many systems
- solved in sigma models (and in various other systems Gattringer et al.) through dual variables = diagrammatic representation FB et al. 15, 16

  sign problem is representation-dependent
- a similar diagrammatic representation of QCD does not solve the sign problem Rossi, Wolff 84

  a sign problem even at $\mu = 0$ Karsch, Mütter 89

$\Rightarrow$ shed light on QCD via gauge theories with scalar quarks

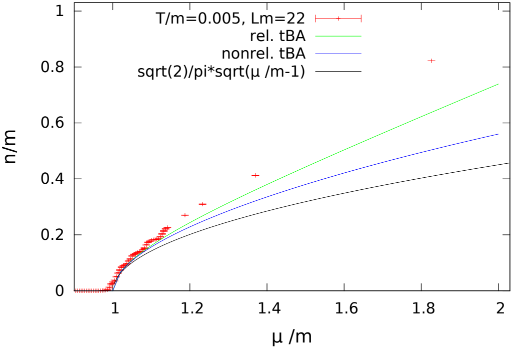
($\uparrow$ relevant beyond the Standard model!?)

- disentangle sign problems due to μ and due to quarks as fermions
- study more than one flavor
- goal: include gauge action = beyond strong coupling
- as the sign problem is solved indeed (see below) one could test other approaches to QCD at nonzero μ

Appetizer: 2dim. O(3) model through dual simulations

generation of particle number density at $\mu \geq m$ ‘Silver blaze’

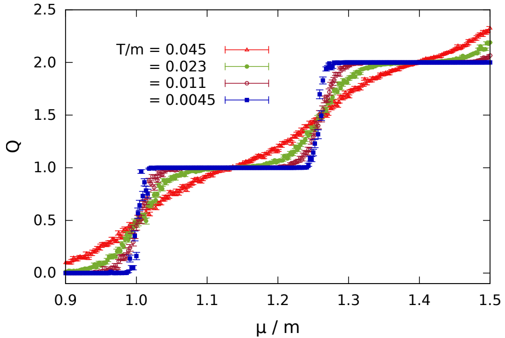
- where the mass m is dynamically generated as in QCD 2dim



- very low $T \Rightarrow$ quantum phase transition of second order
- dynamical critical exponent z consistent with 2 up to 6400×160

particle interactions

- from finite size L (and low T)



$Lm = 4.4$

sharp jumps in particle number

- $\mu_{\text{crit},1} = m \Rightarrow$ mass threshold as for large L above

  $\mu_{\text{crit},2} = E_{\text{min}}^{Q=2} \Rightarrow$ phase shifts δ a la Lüscher

  agree with analytical S-matrix and numerical spectroscopy

Common setting

- gauge fields and bosons $\leftarrow$ second derivative — not Grassmannians

$$S \sim -\sum_{x,\nu}\sum_f \Big[\phi_f^\dagger(x)U_\nu(x)\phi_f(x+\hat\nu)e^{-\mu_f\delta_{\nu,0}} + \underbrace{\phi_f(x)U_\nu^\dagger(x)\phi_f^\dagger(x+\hat\nu)e^{\mu_f\delta_{\nu,0}}}_{\text{not } c.c.\text{: compl. action}}\Big]$$

plus $(2d+(am)^2)|\phi|^2$: Gaussian

	CP(N-1) in 1+1d	scalar QCD in 3+1d
scalar ϕ_f flavors f gauge field U	complex number $\lvert\phi\rvert = 1^\sharp$ N U(1) (auxiliary)	color vector N_f SU(3)$^\flat$
	$^\sharp$ asympt. freedom, dyn. mass generation etc.	$^\flat$ no plaquette yet strong coupling

Idea

integrate out original lattice fields introducing new 'dual' variables

$$Z(\mu) = \int_{\{\phi,U\}} \underbrace{e^{-S[\phi,U;\mu]}}_{\in\mathbb{C} \text{ or } \mathbb{R}} \quad \Rightarrow \quad Z \quad = \sum_{\{k_\nu\}} \underbrace{w[k_\nu]}$$

= exact partition function (and observables)

see first half of dualizing the 2d Ising model: Kramers, Wannier 41

diagrammatic representation:

- dual variables are nonnegative integers k_ν on lattice bonds

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diagrammatic representation:

- dual variables are nonnegative integers k_ν on lattice bonds
- hopefully: new weight is positive
- ▶ μ couples to a U(1) charge = difference of occupation numbers of particles minus antiparticles: still positive
- explicit conservation of the U(1) current: $\partial_\nu^{\text{discrete}} m_\nu = 0$ via Kronecker-δ constraints

worm algorithms

Dual variables at work in CP(N-1)

- polar coordinates: $\phi = r\, e^{i\varphi}$ (for all flavors)
  U(1) fields: $U_\nu = e^{i A_\nu}$
- action contains the forward and backward terms

$$r(x)r(x+\hat{\nu})\, \underbrace{e^{\mp i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}}_{\text{not real}}\, e^{\mp\mu\delta_{\nu,0}}$$

(0) expand the 'problematic' weight for all bonds and flavors $.._{\nu,f}(x)$

$$e^{(..)_+ + (..)_-} = \sum_{k^\pm=0}^{\infty} \frac{(..)_+^{k^+}(..)_-^{k^-}}{k^+!k^-!}$$

action terms to integer powers, original fields factorize

$$\text{weight} \sim \left(r(x)r(x+\hat{\nu})e^{i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{\mu\delta_{\nu,0}}\right)^{k_\nu^+(x)}$$
$$\times \left(r(x)r(x+\hat{\nu})e^{-i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{-\mu\delta_{\nu,0}}\right)^{k_\nu^-(x)}$$

(1) integrate out the phases ⇒ Lagrange multipliers

$$\int_0^{2\pi} d\varphi(x)\, e^{-i\varphi(x)\sum_\nu [k_\nu^+(x)-k_\nu^-(x)-x\leftrightarrow(x+\hat{\nu})]}$$

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$$\int_0^{2\pi} d\varphi(x)\, e^{-i\varphi(x)\sum_\nu [k_\nu^+(x)-k_\nu^-(x)-x\leftrightarrow(x+\hat{\nu})]} = \delta_{\text{Kronecker}}(\nabla_\nu \overbrace{m_\nu}^{k_\nu^+ - k_\nu^-})\ \forall x$$

either 1 = positive (✓) or 0 = ignored (analytic cancellations!)

current conservation for m ⇒ closed loops

$$\text{weight} \sim \left(r(x)r(x+\hat{\nu})e^{i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{\mu\delta_{\nu,0}}\right)^{k^+_\nu(x)}$$
$$\times \left(r(x)r(x+\hat{\nu})e^{-i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{-\mu\delta_{\nu,0}}\right)^{k^-_\nu(x)}$$

(1) integrate out the phases $\Rightarrow$ Lagrange multipliers

$$\int_0^{2\pi} d\varphi(x)\, e^{-i\varphi(x)\sum_\nu[k^+_\nu(x)-k^-_\nu(x)-x\leftrightarrow(x+\hat{\nu})]} = \delta_{\text{Kronecker}}(\nabla_\nu \overbrace{m_\nu}^{k^+_\nu - k^-_\nu})\ \forall x$$

either 1 = positive (✓) or 0 = ignored (analytic cancellations!)

current conservation for $m \Rightarrow$ closed loops

(2) μ enters with the same dual variable $m = k^+ - k^-$

$$e^{-\mu\sum_x m_0(x)} = e^{-\mu N_t \sum_{\vec{x}} m_0(x_0,\vec{x})} = e^{-\mu\beta Q}$$

as in the energy (defining) rep. of the grand canonical ensemble

net charge/particle number Q: flux through any time slice x_0
or temporal winding number of the m-loops

movie

$$\text{weight} \sim \Big(r(x)r(x+\hat{\nu})e^{i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{\mu\delta_{\nu,0}}\Big)^{k_\nu^+(x)} \times \Big(r(x)r(x+\hat{\nu})e^{-i(\varphi(x)-\varphi(x+\hat{\nu})+A_\nu(x))}e^{-\mu\delta_{\nu,0}}\Big)^{k_\nu^-(x)}$$

(3) integrate out the radii
(with Gaussian part) $\Rightarrow$ positive weight

ratio of gamma functions

(4) flavor-diagonal U(1) is gauged:

$$\int_0^{2\pi} dA_\nu(x) e^{iA_\nu(x)\sum_f m_\nu^f(x)} = \delta\Big(\sum_f m_{\nu,f}(x)\Big)$$

total charge over all flavors vanishes explicitly

Dual variables at work in scalar QCD

FB, Wellnhofer 17

- action again, for simplicity same μ for all flavors:

$$S = -\beta \sum_{x,\nu} \mathrm{tr}\Big[\overbrace{\sum_f \phi_f(x+\hat{\nu})\phi_f(x)^\dagger}^{J_\nu(x)\ \text{(matrix)}} U_\nu(x)\, e^{-\mu\delta_{\nu,0}} + J_\nu(x)^\dagger U_\nu(x)^\dagger e^{\mu\delta_{\nu,0}}\Big]$$

- $U_\nu(x) \in SU(3)$: group integrals not so simple

  fortunately a closed expression exists: Eriksson et al. 81

$$\int dU \exp\left(\mathrm{tr}\left[JUe^{-\mu} + J^\dagger U^\dagger e^{-\mu}\right]\right) = \sum_{a,b,c,k,\bar{k}=0}^{\infty} \frac{\text{positive}(a,b,c,k,\bar{k})}{a!b!c!k!\bar{k}!}$$

$$\times\, (\mathrm{tr} JJ^\dagger)^a \times \mathcal{O}((JJ^\dagger)^2)^b \times (\det JJ^\dagger)^c \times (\det J\, e^{-\mu})^k \times (\det J^\dagger e^{\mu})^{\bar{k}}$$

  dual variables/occup. numbers $(a,b,c,k,\bar{k})$: again on bonds $.._\nu(x)$

Interpreting dualized scalar QCD

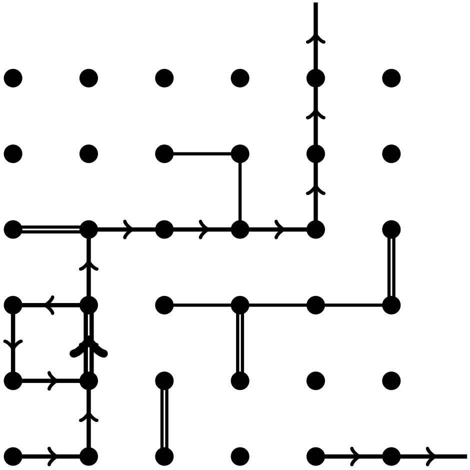
weight $\sim (\mathrm{tr} JJ^\dagger)^a \mathcal{O}((JJ^\dagger)^2)^b (\det JJ^\dagger)^c \times e^{-\mu(k-\bar{k})_{\nu=0}} \times (\det J)^k (\det J^\dagger)^{\bar{k}}$

- first three terms μ-indep.: quarks hop with antiquarks = 'mesons'
  pos. functions of positive operator $JJ^\dagger$
- next term: μ couples to the charge of the current $k - \bar{k} = m$
  positive ✓
- conserved? yes, by the remaining integral over ϕ-integral:

  $$\int_{\mathbb{C}} d\phi\, e^{-\mathrm{mass}^2|\phi|^2}\, \phi^A \phi^{*B} \neq 0 \quad \text{iff } A = B \qquad \text{(phase integration!)}$$

  constrains the last two terms exactly such that m conserved
- last two terms: 'baryons' and 'antibaryons'
  positive?

- example configuration



- bosonic occupation numbers from 0 (empty sites admissible) to ∞
  here mostly 0 and 1

Sign problem in scalar QCD

depends crucially on the number of flavors:

- $N = 1, 2$: μ-independent

  no (anti)baryons: $\det J = \det_{3\times 3} \left(\phi^{\text{shifted}}_{f=1} \otimes \phi^{\dagger}_{f=1} + \phi^{\text{shifted}}_{f=2} \otimes \phi^{\dagger}_{f=2}\right) = 0$

  at most two indep. rows/columns

  no sign problem

- $N = 3$: μ-dependent

  scalar baryon needs 3 flavors (to compensate color antisymmetry)

  sign problem solved

$$\det J = \det_{3\times 3} \Big(\sum_{f=1}^{3} \phi_f(x + \hat{\nu}) \otimes \phi_f(x)^{\dagger} \Big) = \det \big(\phi_1|\phi_2|\phi_3\big)_{x+\hat{\nu}} \det \big(\phi_1|\phi_2|\phi_3\big)^{*}_{x}$$

along a loop $\det(\ldots)^{*}_{x}$ meets $\det(\ldots)_{x}$ from the next (anti)baryon

- $N \geq 4$: μ-dependent
  sign problem unsolved
  a similar det-formula exists, but positive?
  a few simple example graphs are indeed positive
  finer constraints needed: conservation of each flavor number

- this case would be interesting for going beyond strong coupling via
  bosons in 'induced QCD' — Budczies, Zirnbauer 03
  Brandt, Lohmayer, Wettig 16
  or Hubbard-Stratonovich bosons — Vairinhos, de Forcrand 14

  incorporate the plaquette with terms linear and factorizing in *U*'s
  $\Rightarrow$ just a few more bosons to dualize

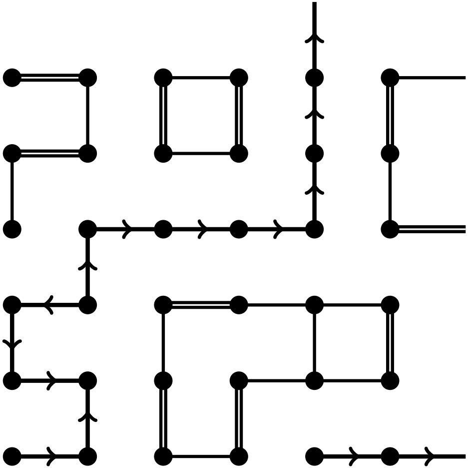
Revisit fermionic QCD

- action to be dualized

$$S=\beta\sum_{x,\nu}\eta_\nu(x)\,\mathrm{tr}\Big[\overbrace{\sum_f\psi_f(x+\hat{\nu})\psi_f(x)^\dagger}^{J_\nu(x)}\,U_\nu(x)\,e^{-\mu\delta_{\nu,0}}-\ldots e^{\mu\delta_{\nu,0}}\Big]$$

- can use the U-integration again (fermion bilinears J commutative) to arrive at meson and baryon occupation numbers
- different constraints at sites due to Grassmann nature:
  Grassmannians never twice (Pauli principle)
  final integration: each Grassmann component must appear once at each site

- example configuration (massless quarks)



- baryons self- and meson-avoiding (but closed)
- all sites visited three times

Sign problem in fermionic QCD

$$S = \beta \sum_{x,\nu} \eta_\nu(x)\,\mathrm{tr}\Big[\sum_f \psi_f(x+\hat\nu)\psi_f(x)^\dagger U_\nu(x)\, e^{-\mu\delta_{\nu,0}} - \ldots e^{\mu\delta_{\nu,0}}\Big]$$

sources of minus signs:

- staggered fermion factors: $\eta_\nu(x) \in \{-1, 1\}$
- minus in front of second term: Dirac operator is first order
- reordering Grassmannians for final integration: -1 per quark loop
- antiperiodic boundary conditions: -1 per winding quark loop

$\Rightarrow \exists$ configurations with negative weights, at $\mu = 0$ already (!)

observation:

- all sources of signs absent for scalar quarks
  and indeed the sign problem disappears as well

Summary

- dualization of 'problematic' action terms:
  expanding the weight e^{-S} and integrating out angles $\Rightarrow$ explicit current conservation

  $$\text{weight} \sim e^{-\mu \sum_{\vec{x}} m_0(x)} = e^{-\mu\,\text{charge}}$$

  $\Rightarrow$ no sign problem

- CP(N-1) ✓
  physics at $\mu \geq m$

- scalar QCD at strong coupling for $N_f \leq 3$ ✓
  $\Rightarrow$ more flavors for gauge action
  $\Rightarrow$ test of other approaches in phase diagram

- real QCD
  source of the sign problem in dual formulation: fermion nature

Outlook: coherent state path integrals

- conventional path integrals in QM:

$$\mathrm{tr}\, e^{-\beta\hat{H}} \overset{|p\rangle,|q\rangle}{=} \int \prod_{k=1}^{N\to\infty} dp_k dq_k\, e^{-S_{\mathrm{disc}}[p,q]} \approx \int Dp(t)Dq(t)\, e^{\int dt\left[ip\dot{q}-\frac{p^2}{2m}-V(q)\right]}$$

- recall coherent states:

$$|z\rangle := e^{z\hat{a}^\dagger}|0\rangle \text{ with } z\in\mathbb{C}, \quad a|z\rangle = z|z\rangle$$

coherent state path integrals:

$$\mathrm{tr}\, e^{-\beta\hat{H}} \overset{|z\rangle}{=} \int \prod_{k=1}^{N\to\infty} dz_k\, e^{-S_{\mathrm{disc}}[z^*,z]} \approx \int Dz(t)\, e^{\int dt\left[\overbrace{i \arg z\, |\dot{z}|^2}^{\in\mathbb{C}}-H(z^*,z)\right]}$$

- too naive transition "≈" to continuous paths yields wrong results even for simple bosonic and spin systems (!) Galitski, Wilson 11 [PRL]

resolution: treat arg z (Lagrange multipliers) exactly with dual variables