Dualizing lattice field theories at nonzero chemical potential

1+1d CP(N-1), 3+1d scalar QCD

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The setting

- thermodynamic partition function of bosons

$$Z = \mathrm{tr}\exp\left(-\beta\hat{H}[\phi]\right)$$

as a field theory path integral

$$Z = \int D\phi\,\exp\left(-\int d\vec{x}\int_0^\beta d\tau\,\mathcal{L}_{\text{Eucl.}}(\phi^{(*)},\partial_\tau\phi^{(*)},\partial_{\vec{x}}\phi^{(*)})\right)$$

and corresponding lattice formulations = hoppings

$$\phi(x)^*\phi(x+\hat{\nu}) + c.c.$$

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as a field theory path integral — angle $\partial_\tau \varphi + i\mu$

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and corresponding lattice formulations = hoppings

$$\phi(x)^*\phi(x+\hat{\nu})e^{-\mu} + c.c.e^{\mu} \quad \text{for temporal } \hat{\nu}$$

- ϕ complex and action invariant under U(1) phase rotations

  conserved charge to which a chemical potential μ can be coupled

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  ↑ not *c.c.* anymore

- ϕ complex and action invariant under U(1) phase rotations

  conserved charge to which a chemical potential μ can be coupled

  $\Rightarrow$ generically a sign problem (in the second repr. only) no θ

The models

relativistic bosons

coupling β, lattice spacing set to 1

- CP(N-1) models in 1+1d:

$$S = \beta \sum_{x,\nu} \sum_{f=1}^{N} \Big[\phi_f^*(x) U_\nu(x) \phi_f(x+\hat{\nu}) e^{-\mu_f \delta_{\nu,0}} + \underbrace{\phi_f(x) U_\nu^*(x) \phi_f^*(x+\hat{\nu}) e^{\mu_f \delta_{\nu,0}}}_{\text{not } c.c.}\Big]$$

$|\phi|^2 = 1$ nontrivial: dynamical mass gap, instantons, top. freezing

$U_\nu(x) \in U(1)$: no Maxwell term $\Rightarrow$ auxiliary

integrate out $\Rightarrow$ action quartic in ϕ

global ‘flavor’ symmetry $U(N) \ni U(1)^N$: conserved charges $\Rightarrow \mu_f$

local (gauge) symmetry $U(1)$: total charge vanishes

- O(N) models similar: invariant under $O(N) \ni SO(2)$’s $\cong U(1)$’s

- QCD in 3+1d with scalar quarks:

$$S = \beta \sum_{x,\nu} \sum_{f=1}^{N} \left[\phi_f^\dagger(x) U_\nu(x) \phi_f(x+\hat{\nu}) e^{-\mu_f \delta_{\nu,0}} + \phi_f(x) U_\nu^\dagger(x) \phi_f^\dagger(x+\hat{\nu}) e^{\mu_f \delta_{\nu,0}} \right]$$

  ϕ integrated with mass term = gaussian measure

  $U_\nu(x) \in SU(3)$: 'gluons' $\rightsquigarrow$ confinement, dynamical mass gap
  no kinetic term yet = strong coupling

  each $\phi_f(x) \in \mathbb{C}^3$: colored

  again global flavor symmetry $U(N)$
  local (gauge) symmetry $SU(3)$

- other models where dual variables solved sign problems

C. Gattringer and his group, 11-17

Idea of dual variables

(ii) integrate out original fields

especially the U(1) angles to which μ couples

(i) at the expense of expanding the weights e^{-S} first

expansion variables = dual variables/occup. numbers: integers

- exact mapping (up to interchanging integrals and infinite sums)
- with some luck: new weight positive $\rightsquigarrow$ num. simulations

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- indeed solves the sign problem in CP(N-1) and O(N) models
  almost obvious from O(2) model — but other dualizations in the literature
- not so for the *fermionic* sign problem in QCD at strong coupling:
  mild sign problem even at $\mu = 0$ — Rossi, Wolff 84; Karsch, Mütter 89

Dualizing CP(N-1)

(i) expand each term in e^{-S} — neglecting $\dots_\nu^f(x)$

$$e^{\beta\,[\phi^* U\phi]e^{-\mu\delta_{\nu,0}}}\, e^{\beta\,[\phi U^*\phi^*]e^{\mu\delta_{\nu,0}}} = \sum_{k,\bar{k}=0}^{\infty} \frac{\beta^{\,k+\bar{k}}}{k!\bar{k}!} \underbrace{[\phi^* U\phi]^k[\phi U^*\phi^*]^{\bar{k}}}_{r^{\,k+\bar{k}+\text{shifted}}\, e^{\,i\varphi(k-\bar{k}-\text{shifted})}\, e^{\,iA(k-\bar{k})}} e^{-\mu(k-\bar{k})_{\nu=0}}$$

used $\phi = re^{i\varphi}$ and $U = e^{iA}$

(ii) integrate out original fields

- radii: doable $\Rightarrow$ positive weight — ratio of gamma functions
- angles: $\int_0^{2\pi} d\varphi\, e^{i\varphi X} = 2\pi\delta_{\text{Kronecker}}(X)$

  with $X = \sum_\nu [m_\nu^f(x) - m_\nu^f(x-\hat{\nu})] = \nabla_\nu m_\nu^f(x)$ and $m = k - \bar{k}$

  explicit conservation of symmetry currents m^f $\Rightarrow$ world lines

- μ's couple to the conserved charges: $e^{-\mu\sum_x m_0(x)} = e^{-\beta\mu\sum_{\vec{x}} m_0(\vec{x})}$

  as in the energy representation of the grand canonical ensemble

  conserved charge is the net number of *m*-loops winding in time

- μ's do not cause minus signs in the weight unless μ imaginary

  $\Rightarrow$ sign problem solved if there was none at vanishing μ

  cancellations in $\int_0^{2\pi} d\varphi\, e^{i\varphi X} \sim \delta(X)$: either positive or zero
  $\uparrow$ neglect

- gauge fields:

  $$\int_0^{2\pi} dA_\nu(x) e^{iA_\nu(x)\sum_f m^f_\nu(x)} = \delta\big(\sum_f m^f_\nu(x)\big)$$

  total charge (over all flavors) vanishes

Simulation algorithm

how to simulate a system with constraints?

- between two config.s on the constraint surface, move away from it:

  importance sampling (detailed balance etc.) on general configs. with remaining weight when ignoring δ's

  more efficient then accept/reject step only at the end when the next admissible config. is obtained

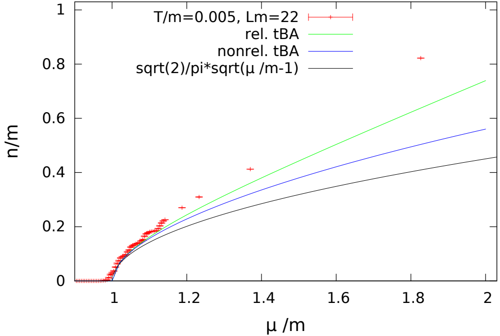
e.g. worm algorithm Prokof'ev, Svistunov 01

- violate the constraint at two sites*, called head and tail
- keep the tail fixed and let the head walk around changing bond variables (taking the weight into account)
- admissible configuration when the head bites the tail
- worms can wind: change the charge

* this algorithm computes two-point functions on the fly

Physics of the O(3)=CP(2) model at nonzero μ I

- low T: no particle/charge density until μ reaches the dyn. mass

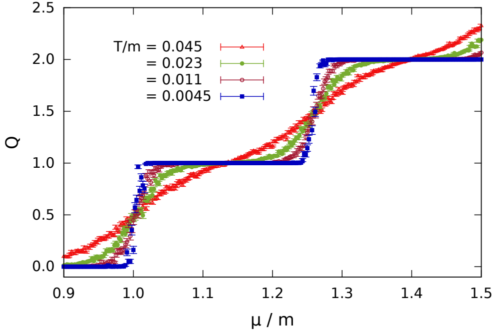


($T \to 0$ & thermod. limit need $N_t, N_s \to \infty$, up to 6400×160 or 320^2)

$\Rightarrow$ quantum phase transition at $\mu = m$, crossovers at $T > 0$

- $\mu \gtrsim m$: contact to Bethe ansätze for repulsive 1d bosons — Lieb-Liniger
  or even 1d fermions (nonrel., spinless) — Tonks-Girardeau
- dynamical critical exponent $z \approx 2$ consistent with these fermions

- low T and small sizes L (but $> 1/m$)



$Lm = 4.4$

$\Rightarrow$ plateaus and sharp jumps in particle number as function of μ

- $\mu_{c,1} = m$: mass threshold as for large L above

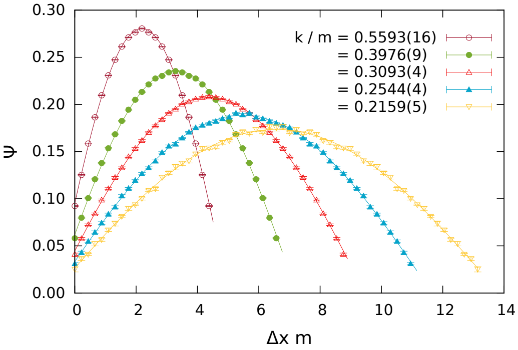
  $\mu_{c,2} = E_{\text{min}}^{Q=2} \Rightarrow$ particle interaction $\Rightarrow$ phase shifts δ a la Lüscher

- agrees with analytical S-matrix Zamolodchikov[2] 78

  and numerical spectroscopy Lüscher, Wolff 90

- on $Q = 2$ plateaus

distribution (histogram) of two unit m_0's $\leftarrow$ particle world lines = probability $|\psi(\Delta x_1)|^2$:



different L's

$\Rightarrow$ perfect standing waves, up to a cusp at the origin

$\Rightarrow$ two particle potential is Dirac-delta like $\Rightarrow$ phase shifts again

Dualizing scalar QCD

- 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

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

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

- upon integrating the link fields (step ii) we have expanded e^{-S} into a five-fold sum (step i) with dual variables/occup. numbers $(a, .., \bar{k})$

Interpreting dualized scalar QCD

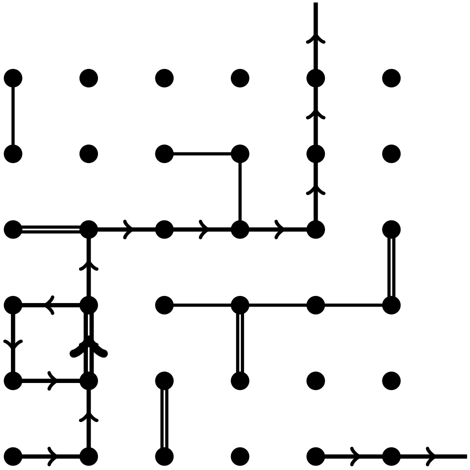
$$(\mathrm{tr} JJ^\dagger)^a \times \mathcal{O}((JJ^\dagger)^2)^b \times (\det JJ^\dagger)^c \times e^{-\mu(k-\bar{k})_{\nu=0}} \times (\det J)^k \times (\det J^\dagger)^{\bar{k}}$$

- first three terms μ-independent: 'mesons'
  positive functions of the positive operator $JJ^\dagger$
- next term: μ couples to the charge of the current $k - \bar{k} = m$
  conserved? yes, by the remaining integral over ϕ-integral, schematically:

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

  constrains the last two terms (since mesons $\mathcal{O}(JJ^\dagger)^\# = \mathcal{O}(\phi\phi^\dagger)^{2\#}$) exactly such that m conserved
- last two terms: 'baryons' and 'antibaryons'
  positive?

- example configuration



- differences to fermionic QCD:
  k, $\bar{k}$ from 0 to $\infty \leftarrow$ bosonic occup. numbers (empty sites possible)
  intersections of mesons and baryons possible

Sign problem in scalar QCD

depends crucially on the number of flavors:

- $N = 1, 2$: μ-independent

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

  matrix has at most two indep. rows/columns

  no sign problem

- $N = 3$: μ-dependent

  'scalar baryon needs 3 flavors'

  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 formula like the one above exists, but does not yield positivity in an obvious manner

- this case would be interesting for going beyond strong coupling incorporating the plaquette via:

  bosons in 'induced QCD' — Budczies, Zirnbauer 03; Brandt, Lohmayer, Wettig 16

  or Hubbard-Stratonovich bosons — Vairinhos, de Forcrand 14

Revisit fermionic QCD

action to be dualized

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

sources of minus signs:

- staggered fermion factors $\eta \in \{-1, 1\}$
- 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 (!)

all sources absent for scalar quarks

Summary and outlook

- dualization of angles (fields)

$$\int_0^{2\pi} d\varphi \, e^{i\varphi \sum_\nu [m_\nu(x) - m_\nu(x-\hat{\nu})]} \sim \delta(\nabla_\nu m_\nu)$$

  $\Rightarrow$ explicit current conservation

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

  $\Rightarrow$ no sign problem

- O(N) and CP(N-1) ✓
  physics at $\mu \geq m$
- scalar QCD ✓
  real QCD!?
- dualization of nonrelativistic bosons (and even spins) in coherent state path integrals