The QCD phase diagram from the lattice

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Motivation

What happens to matter when it is heated and/or compressed?
Water changes its state when heated or compressed.

What happens to quarks and gluons when heated or compressed?
QCD under extreme conditions

Confinement: quarks are bound in color-neutral hadrons: $qqq$ baryons & $q\bar{q}$ mesons

Compress or heat baryons: hadrons overlap $\rightarrow$ confinement “lost”
$\Rightarrow$ expect interesting/unusual behaviour

Temperature $T$

Pressure, chemical potential $\mu$

Thermal excitation of mesons (pions)

Increased baryon density
The wonderland phase diagram of QCD from Wikipedia

- **Quark-gluon plasma (QGP)**
- **Hadronic (confined) phase**
- **Vacuum**

**Caveat:** everything in red is a conjecture

For $T$ or $\mu \to \infty$:
- Interaction weak (asymptotic freedom)

- Crystal phase(s)
- Quarkyonic phase
- Strangelets

Also:

$$\mu_{\text{quark}} = \frac{1}{3} \mu_{\text{Baryon}}$$
May or may not exist

No gauge-invariant order parameter: no phase transition required
“Small” deformation of two-flavor massless case:
OK IF u,d quarks are “light”.
No info on location of critical point

\[ N_f = 2, \, m_u = m_d = 0 \]

\[ \langle \bar{\psi}\psi \rangle = 0 \]

\[ \langle \bar{\psi}\psi \rangle \neq 0 \]
Finite $\mu$: what is known?

Mineral, possible phase diagram

QGP

confined

$T_c$

crossover (lattice)

Nuclear liquid-gas transition (exp.)

Color superconductor

$\mu$
Heavy-ion collisions

Knobs to turn:
- atomic number of ions
- collision energy $\sqrt{s}$

So far, no sign of QCD critical point
(esp. RHIC beam energy scan)

"critical opalescence"?

non-Gaussian fluctuations (Stephanov)
Finite $\mu$: what is known?

**Lattice:** Sign problem *as soon as $\mu \neq 0$*

- **Minimal, possible phase diagram**
  - Nuclear liquid-gas transition (exp.)
  - Color superconductor
  - Confined
  - QGP
  - Crossover (lattice)
Lattice QCD: Euclidean path integral

space + imag. time $\rightarrow 4d$ hypercubic grid:

$$Z = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_E[\{U,\bar{\psi},\psi\}]}$$

- Discretized action $S_E$:
  
  - $\bar{\psi}(x)U_{\mu}(x)\psi(x + \hat{\mu}) + h.c.$,
  
  - $\beta \text{ReTr} U_P$, $U_P$ plaquette matrix

  $$a \rightarrow 0 \Leftrightarrow \beta = \frac{6}{g_0^2} \rightarrow \infty$$

- Monte Carlo: with Grassmann variables $\psi(x)\psi(y) = -\psi(y)\psi(x)$ ??
  Integrate out analytically (Gaussian) $\rightarrow$ determinant non-local

$$\text{Prob(config}\{U\}) \propto \det^2 \mathcal{D}(\{U\}) e^{\beta \sum_P \text{ReTr} U_P}$$

real non-negative when $\mu = 0$
Why are we stuck at $\mu = 0$? The “sign problem”

- quarks anti-commute $\rightarrow$ integrate analytically: $\det(D(U) + m + \mu \gamma_0)$
  
  $\gamma_5 (i\phi + m + \mu \gamma_0)\gamma_5 = (-i\phi + m - \mu \gamma_0) = (i\phi + m - \mu^* \gamma_0)^\dagger$

  
  \[
  \begin{align*}
  \det D(\mu) &= \det^* D(-\mu^*)
  
  \text{det real only if } \mu = 0 \text{ (or } i\mu), \text{ otherwise can/will be complex}
  \end{align*}
  \]
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$$\det \mathcal{D}(\mu) = \det^* \mathcal{D}(-\mu^*)$$

- Measure $d\varpi \sim \det \mathcal{D}$ must be complex to get correct physics:

$$\langle \text{Tr Polyakov} \rangle = \exp(-\frac{1}{T} F_q) = \int \text{Re Pol} \times \text{Re} \; d\varpi - \text{Im Pol} \times \text{Im} \; d\varpi$$

$$\langle \text{Tr Polyakov}^* \rangle = \exp(-\frac{1}{T} F_{\bar{q}}) = \int \text{Re Pol} \times \text{Re} \; d\varpi + \text{Im Pol} \times \text{Im} \; d\varpi$$

$\mu \neq 0 \Rightarrow F_q \neq F_{\bar{q}} \Rightarrow \text{Im}d\varpi \neq 0$
Why are we stuck at $\mu = 0$? The “sign problem”

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- Measure $d\omega \sim \det \mathcal{D}$ must be complex to get correct physics:

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  $\mu \neq 0 \Rightarrow F_q \neq F_{\bar{q}} \Rightarrow \text{Im} d\omega \neq 0$

- Origin: $\mu \neq 0$ breaks charge conj. symm., ie. usually complex conj.

Complex determinant $\rightarrow$ no probabilistic interpretation $\rightarrow$ Monte Carlo ??
Sampling oscillatory integrands

- Example: \( Z(\lambda) = \int dx \exp(-x^2 + i\lambda x) = \int dx \exp(-x^2) \cos(\lambda x) \)

- \( Z(\lambda)/Z(0) = \exp(-\lambda^2/4) \): exponential cancellations
  \( \rightarrow \) truncating deep in the tail at \( x \sim \lambda \) gives \( O(100\%) \) error
  “Every \( x \) is important” \( \iff \) How to sample?
Computational complexity of the sign pb

How to study: \( Z_\rho \equiv \int dx \rho(x) , \quad \rho(x) \in \mathbb{R} , \text{ with } \rho(x) \text{ sometimes negative} \)?

Reweighting: sample with \(|\rho(x)|\), and “put the sign in the observable”:

\[
\langle W \rangle \equiv \frac{\int dx \ W(x)\rho(x)}{\int dx \ \rho(x)} = \frac{\int dx \left[ W(x)\text{sign}(\rho(x)) \right] |\rho(x)|}{\int dx \ \text{sign}(\rho(x)) \ |\rho(x)|} = \frac{\langle W\text{sign}(\rho) \rangle_{|\rho|}}{\langle \text{sign}(\rho) \rangle_{|\rho|}}
\]
Computational complexity of the sign pb

• How to study: \( Z_\rho \equiv \int dx \, \rho(x), \quad \rho(x) \in \mathbb{R}, \) with \( \rho(x) \) sometimes negative?

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\]

\[
\langle \text{sign}(\rho) \rangle_{|\rho|} = \frac{\int dx \, \text{sign}(\rho(x)) |\rho(x)|}{\int dx \, |\rho(x)|} = \frac{Z_\rho}{Z_{|\rho|}} = \exp (- \frac{V}{T} \Delta f(\mu^2, T)), \text{ exponentially small diff. free energy dens.}
\]

Each meas. of \( \text{sign}(\rho) \) gives value \( \pm 1 \) \( \implies \) statistical error \( \approx \frac{1}{\sqrt{\# \text{ meas.}}} \)

Constant relative accuracy \( \implies \) need statistics \( \propto \exp(+2\frac{V}{T}\Delta f) \)

Large \( V \), low \( T \) inaccessible: signal/noise ratio degrades exponentially

“Figure of merit” \( \Delta f \): measures severity of sign pb.
**Frogs and birds**

- **Frogs**: *acknowledge* the sign problem
  - explore region of small $\mu/T$ where sign pb is mild enough
  - find tricks to enlarge this region
    
    Taylor expansion, imaginary $\mu$, strong coupling expansion,…

- **Birds**: *solve* the sign pb
  - solve QCD ?
  - find “QCD-ersatz” which can be made sign-pb free

Complex Langevin, Lefschetz thimble – fermion bags, $QC_2D$, isospin $\mu$,…

- **Think different**: build an analog QCD simulator with cold atoms
  
  $\longrightarrow$ ”Sign problem” conferences…
First frog steps: $\frac{\mu}{T} \lesssim 1$

Approximate $\langle W \rangle(\frac{\mu}{T})$ by truncated Taylor expansion:

$$\sum_{k=0}^{n} c_k(T) \left( \frac{\mu}{T} \right)^k$$

- Measure $c_k, k = 0, \ldots, n$ in a **sign-pb-free $\mu = 0$ simulation**
- Cheaper variant: fit $c_k, k = 0, \ldots, n$ to results of *imaginary* $\mu$ simulations

State of the art: Fodor et al, 1507.07510

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Crossover temp. versus chem. pot.
Steve Weinberg’s
Third Law of Progress in Theoretical Physics

You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you’ll be sorry

in “Asymptotic realms of physics”, 1983
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Optimal choice: Monte Carlo on physical states (no sign pb)

★ Integrate out quarks, then Monte Carlo on gluons: Not good (sign pb)

★ Integrate out gluons, then Monte Carlo on color singlets: Much better

Easy at strong coupling $\beta = \frac{6}{g_0^2} = 0$: 4-link interaction $\beta \Re \text{Tr} U_P$ drops out
Strong coupling limit at finite density (staggered quarks)

Chandrasekharan, Wenger, PdF, Unger, Wolff, ...

- Integrate over $U$'s, \textbf{then} over quarks: \textit{exact} rewriting of $Z(\beta = 0)$

New, discrete "\textit{dual}" degrees of freedom: meson & baryon \textit{worldlines}

Constraint at every site:
3 \textit{blue} symbols ($\bullet \bar{\psi} \psi$, meson hop)
or a \textit{baryon} loop

Update with \textit{worm algorithm}: "\textit{diagrammatic}" Monte Carlo
Integrate over $U$’s, then over quarks: *exact* rewriting of $Z(\beta = 0)$

New, discrete "*dual*" degrees of freedom: meson & baryon worldlines

Constraint at every site:
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Update with worm algorithm: "*diagrammatic*" Monte Carlo

The dense (crystalline) phase:
1 baryon per site; no space left
$\rightarrow \langle \bar{\psi}\psi \rangle = 0$
Results $\beta \approx 0$ w/ Unger, Langelage, Philipsen

- Sign pb almost gone: accessible volumes multiplied by $10^4$
- Phase diagram ($m_q = 0$): chiral phase transition

\[ \langle -\bar{\psi}\psi \rangle = 0 \]
\[ \langle -\bar{\psi}\psi \rangle \neq 0 \]

\[ \beta = 0 \]

\[ \mathcal{O}(\beta) \] corrections

cf. Wikipedia: $(m_q \neq 0)$
Conclusions

- QCD phase diagram: possibly rich -- or not

- QCD critical point: *not at small chem. pot.*

- Sign problem: hot, interdisciplinary topic

Remember: Corfu is home of Princess Nausicaa, one of the few women with whom Odysseus did *not* reach a critical point...
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in “Asymptotic realms of physics”, 1983

• Second Law: do not trust arguments based on lowest-order perturbation theory

• First Law: you will get nowhere by just churning equations
Basic properties of QCD

- QCD describes properties of *quarks* (cf. electrons – fermions) interacting by exchanging *gluons* (cf. photons – bosons)

- QCD is *asymptotically free*: weaker interaction at higher energy
The flip side of asymptotic freedom: “infrared slavery”

- Strong coupling at low energy → non-perturbative

- Quarks are **confined** into color-neutral (color singlet) **bound-states** (**hadrons**):
  
  \[ qqq \text{ baryons: proton & neutron (ordinary matter), ...} \]
  
  \[ q\bar{q} \text{ mesons: pion (lightest), kaon, rho, ...} \]
  
  \[ \textit{Exotics: glueballs, tetraquarks }qq\bar{q}\bar{q}, \text{ pentaquarks }qqqq\bar{q}, \text{ etc...} \]

In principle, all calculable by **Lattice QCD simulations**
Scope of lattice QCD simulations: Physics of color singlets

* “One-body” physics: confinement
  hadron masses
  form factors, etc.
Example: hadron masses

<table>
<thead>
<tr>
<th>BMW collaboration</th>
<th>PACS-CS collaboration</th>
</tr>
</thead>
</table>

Follow-up: neutron-proton mass diff.

arXiv:1406.4088 → Science
Scope of lattice QCD simulations: Physics of color singlets

* “One-body” physics: confinement, hadron masses, form factors, etc..

** “Two-body” physics: nuclear interactions, pioneers Hatsuda et al, Savage et al

hard-core + pion exchange?
**Scope of lattice QCD simulations: Physics of color singlets**

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  hadron masses 
  form factors, etc..

** “Two-body” physics: nuclear interactions 
  pioneers Hatsuda et al, Savage et al 
  hard-core 
  + pion exchange?

*** Many-[composite]-body physics: nuclear matter 
  phase diagram vs (temperature $T$, density $\mu_B$)
Motivation: how to make the sign problem milder?

- Severity of sign pb. is \textit{representation dependent}:

  Generically: \[ Z = \text{Tr} \exp^{-\beta H} = \text{Tr} \left[ \exp^{-\frac{\beta}{N} H} \left( \sum |\psi\rangle \langle \psi| \right) \exp^{-\frac{\beta}{N} H} \left( \sum |\psi\rangle \langle \psi| \right) \cdots \right] \]

  Any complete set \( \{|\psi\rangle\} \) will do

  If \( \{|\psi\rangle\} \) form an \textit{eigenbasis} of \( H \), then \[ \langle \psi_k | \exp^{-\frac{\beta}{N} H} | \psi_l \rangle = \exp^{-\frac{\beta}{N} E_k} \delta_{kl} \geq 0 \rightarrow \text{no sign pb} \]
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QCD physical states are color singlets \( \rightarrow \) Monte Carlo on colored gluon links is bad idea

Usual: • integrate over quarks analytically \( \rightarrow \) \( \det(\{U\}) \)

• Monte Carlo over gluon fields \( \{U\} \)

Reverse order: • integrate over gluons \( \{U\} \) analytically

• Monte Carlo over quark color singlets (hadrons)

• Caveat: must turn off 4-link coupling \( \beta \sum_P \text{ReTr} U_P \) by setting \( \beta = 0 \)

\( \beta = \frac{6}{g_0^2} = 0: \) strong-coupling limit \( \leftrightarrow \) continuum limit (\( \beta \rightarrow \infty \))
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\[ Z(\beta = 0) = \int \prod_x d\bar{\psi} d\psi \prod_{x,\nu} \left( \int dU_{x,\nu} e^{-\{\bar{\psi}_x U_{x,\nu} \psi_{x+\nu} - h.c.\}} \right) \]
  Product of 1-link integrals performed analytically
More difficulties: the overlap problem

- Further danger: **insufficient overlap** between sampled and reweighted ensembles

**Very large weight** carried by very rarely sampled states

→ **WRONG** estimates in reweighted ensemble for finite statistics

- Example: sample \( \exp\left( -\frac{x^2}{2} \right) \), reweight to \( \exp\left( -\frac{(x-x_0)^2}{2} \right) \) → \( \langle x \rangle = x_0 \)?

- Estimated \( \langle x \rangle \) saturates at largest sampled \( x \)-value
- Error estimate too small

**Insufficient overlap** \((x_0 = 5)\)

**Very non-Gaussian distribution** of reweighting factor

Log-normal \( \text{Kaplan et al.} \)

**Solution:** Need stats \( \propto \exp(\Delta S) \)
The CPU effort grows exponentially with $L^3/T$

CPU effort to study matter at nuclear density in a box of given size
Give or take a few powers of 10...

Crudely based on: • 1 sec on 1GF laptop for $2^4$ lattice, $a = 0.1$ fm
• effort $\propto \exp\left(2\frac{V}{T} \rho_{\text{nucl.}} (m_B - 3/2m_\pi)\right)$
Severity of sign problem? Monitor $\Delta f = -\frac{1}{V} \log \langle \text{sign} \rangle$

\[ \langle \text{sign} \rangle = \frac{Z}{Z_{||}} \sim \exp\left(-\frac{V}{T} \Delta f(\mu^2)\right) \] as expected

- Determinant method $\rightarrow \Delta f \sim \mathcal{O}(1)$. Here, \textbf{Gain $\mathcal{O}(10^4)$ in the exponent!}
  - heuristic argument correct: color singlets closer to eigenbasis
  - negative sign? product of \textit{local} neg. signs caused by spatial baryon hopping:
    - no baryon $\rightarrow$ no sign pb (no silver blaze pb.)
    - saturated with baryons $\rightarrow$ no sign pb
Can compare masses of differently shaped “isotopes”

\[ am(A) \sim a\mu_B^{\text{crit}} A + (36\pi)^{1/3}\sigma a^2 A^{2/3}, \text{ ie. (bulk + surface tension)} \]

empirical mass formula, parameter-free \((\mu_B^{\text{crit}} \text{ and } \sigma \text{ measured separately})\)

“Magic numbers” with increased stability: \(A = 4, 8, 12\) (reduced area)