Lattice QCD at Large Isospin Density: 6144 Pions in a Box

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Outline

1. Background & Motivation
2. Methodology
3. Results
4. Current and Future Work
QCD Phase Diagram

Figure: A. Steidl, CRC-TR-211
Neutron Star Equation of State

Equation of State \[ \text{Mass-Radius Relation, ...} \]

Ideally, would compute EOS directly; however, \( \mu_B \neq 0 \implies \text{sign problem} \)
Isospin & Isospin Chemical Potential

- No sign problem for isospin chemical potential
  - → amenable to Monte-Carlo calculations
- Phase Diagram (Son and Stephanov 2000):

\[
\langle d\gamma_5 u \rangle = 0
\]

\[\langle \pi^+ \rangle \neq 0\]

\[\langle d\gamma_5 u \rangle \neq 0\]
Lattice QCD

- Discretize space and time
- Evaluate with Monte Carlo

\[
\langle \mathcal{O}(U) \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{O}(U) e^{-S(U)}
\]

\[
\approx \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} \mathcal{O}(U_i),
\]

\[U_i \sim e^{-S(U)}\]

- Generate ensemble \(\{U_i \sim e^{-S(U_i)}\}\), evaluate many observables \(\mathcal{O}(U_i)\)
## Canonical vs Grand Canonical Ensemble

### Grand Canonical

\[
Z = \sum_s e^{-\beta(E_s - \mu N_s)}
\]

- Fix chemical potential \(\mu\)
- More experimentally relevant
- Can simulate directly \((S \mapsto S + \mu N)\)
  - [Brandt et al 2212.14016]
- Separate ensemble for each \(\mu\)

### Canonical

\[
Z_N = \sum_s \delta_{N_s, N} e^{-\beta E_s}
\]

- Fix particle number \(N\)
- Requires all energies \(E_s\)
- Multiple \(\mu\) on same ensemble
- Convert via relation

\[
\mu = \frac{dE_N}{dN}
\]
Multipion Correlation Functions

- Goal: extract $l = l_z = n$ energies for $n = 1, \ldots, N$
- $\implies$ need to compute $n$-$\pi^+$ correlator $C_n$ for $n = 1, \ldots, N$

$$C_n(t) = \sum_{\{y_i\}} \left\langle \left( \sum_x \pi^-(x, t) \right)^n \pi^+(y_1, 0) \ldots \pi^+(y_n, 0) \right\rangle$$

$$= (\pi^+)^n \sim e^{-E_n t} + \ldots$$

- Naive Wick contractions: $O(n!)$, works for $n \lesssim 10$
- Previous work: up to $n = 72$ (Detmold et al. 2012)
The Pion Block

**Definition:**

\[ \Pi_{ij}(x, y; t) = \sum_z S_{ik}(x, 0; z, t) S_{kj}^+(z, t; y, 0) \]

**Numerically:** \( N \times N \) matrix, \( N = N_{\text{site}} N_{\text{spin}} N_{\text{color}} = \max \# \text{ of pions} \)

\begin{align*}
\text{S} &= \text{up/down quark propagator} \\
\Pi_{ij}(x, y; t) &= \sum_z S_{ik}(x, 0; z, t) S_{kj}^+(z, t; y, 0) \\
&= S = \text{up/down quark propagator}
\end{align*}
Pion Correlators from Pion blocks

- Using $\Pi$, can compute $C_n$ for $n \leq N$:

  - $\text{Tr}(\Pi)^3$
  - $\text{Tr}(\Pi^2) \text{Tr}(\Pi)$
  - $\text{Tr}(\Pi^3)$

- Including symmetry/sign factors:

  $$C_3 = \text{Tr}(\Pi)^3 - 3 \text{Tr}(\Pi^2) \text{Tr}(\Pi) + 2 \text{Tr}(\Pi^3)$$

- Combining with recursive relations (+ other methods) $\implies n = 72$
Description of the Algorithm

- Key idea: change into eigenbasis of $\Pi$ and use symmetry
- Eigenvalues of $\Pi$: $x_1, \ldots, x_N$
- Expand via

$$\text{Tr}(\Pi^k) = \sum_{i=1}^{N} x_i^k$$
Example with $N = 4$:

$$C_3 = \text{Tr}(\Pi)^3 - 3 \text{Tr}(\Pi^2) \text{Tr}(\Pi) + 2 \text{Tr}(\Pi^3)$$

$$\quad = (x_1 + x_2 + x_3 + x_4)^3$$

$$\quad - 3(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1 + x_2 + x_3 + x_4)$$

$$\quad + 2(x_1^3 + x_2^3 + x_3^3 + x_4^3)$$
Example

Example with $N = 4$:

\[ C_3 = \text{Tr}(\Pi)^3 - 3 \text{Tr}(\Pi^2) \text{Tr}(\Pi) + 2 \text{Tr}(\Pi^3) \]

\[ = (x_1 + x_2 + x_3 + x_4)^3 \]
\[ - 3(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1 + x_2 + x_3 + x_4) \]
\[ + 2(x_1^3 + x_2^3 + x_3^3 + x_4^3) \]
\[ = 6(x_1x_2x_3 + x_1x_2x_4 + x_1x_3x_4 + x_2x_3x_4) \]
Description of the Algorithm

- General formula, first noted in [Detmold, 1408.6919]:
  \[ C_n = n!E_n(x_1, \ldots, x_N) = n! \sum_{i_1 < i_2 < \cdots < i_n} x_{i_1} \cdots x_{i_n} \]

- Problem: \( \binom{N}{n} \) terms – too many
- Solution: simplify using
  \[ E_n(x_1, \ldots, x_k) = E_n(x_1, \ldots x_{k-1}) + x_k E_{n-1}(x_1, \ldots, x_{k-1}) \]

- Need values for \( 1 \leq n, k \leq N \implies O(N^2) \) work for all correlators
  - Computing eigenvalues \( x_i \) is \( O(N^3) \)
- Computational effort: Propagators \( \gg \) Eigenvalues \( \gg \) Correlators
Results
Lattice Details

- Four ensembles, generated by NPLQCD/JLab/W&M/LANL
- Wilson Clover fermions
- Two lattice spacings \( a = 0.09 \text{ fm} \) & \( a = 0.07 \text{ fm} \)
- \( M_\pi \sim 170 \text{ MeV} \) and \( M_\pi \sim 130 \text{ MeV} \)
- \( 8^3 \) grid of smeared + sparsened point-source propagators
  - Maximum \# of pions: \( N = 12 \times 8^3 = 6144 \)
- Pion block \( \Pi = SS^\dagger \) ill-conditioned \( \implies \) use SVD on \( S \)
  - Same result, more numerically stable

<table>
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<th>Label</th>
<th>( a ) (fm)</th>
<th>( M_\pi ) (MeV)</th>
<th>( \beta )</th>
<th>( C_{SW} )</th>
<th>( am_{ud} )</th>
<th>( am_s )</th>
<th>( L^3 \times T )</th>
<th>( M_\pi L )</th>
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</thead>
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<tr>
<td>A</td>
<td>0.091(1)</td>
<td>166(2)</td>
<td>6.3</td>
<td>1.20536588</td>
<td>-0.2416</td>
<td>-0.2050</td>
<td>48(^3\times96)</td>
<td>3.7</td>
</tr>
<tr>
<td>B</td>
<td>0.091(1)</td>
<td>172(6)</td>
<td>6.3</td>
<td>1.20536588</td>
<td>-0.2416</td>
<td>-0.2050</td>
<td>64(^3\times128)</td>
<td>5.08</td>
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<tr>
<td>C</td>
<td>0.070(1)</td>
<td>166(2)</td>
<td>6.5</td>
<td>1.170082</td>
<td>-0.2091</td>
<td>-0.1778</td>
<td>72(^3\times192)</td>
<td>4.33</td>
</tr>
<tr>
<td>D</td>
<td>0.070(1)</td>
<td>128(2)</td>
<td>6.5</td>
<td>1.170082</td>
<td>-0.2095</td>
<td>-0.1793</td>
<td>96(^3\times192)</td>
<td>4.40</td>
</tr>
</tbody>
</table>
Results

Pion Correlator

\[ \log C_n(t) \times 10^4 \]

- \( n = 6144 \)
- \( n = 4000 \)
- \( n = 2000 \)
- \( n = 1000 \)
Log Normality

- Correlators vary dramatically, even on same timeslice
  - $\Rightarrow$ central limit theorem does not hold
- Solution: data exhibits log-normality $\log C_n[U] \sim \mathcal{N}(\mu, \sigma^2)$
- Equivalently: use cumulant expansion
  $$\log \langle e^X \rangle = \langle X \rangle + \frac{1}{2}(\langle X^2 \rangle - \langle X \rangle^2) + \ldots,$$
  with $X = \log C_n$
Effective Mass

\[ E_{\text{eff}}(t) = \log \frac{C_n(t)}{C_n(t-1)} \]
Effective Chemical Potential

\[ \mu^{(n)}_I(t) = \frac{dE^{(n)}_{\text{eff}}}{dn} \]

Large error cancellation!
\[ \sigma(aE_{\text{eff}}) \sim \mathcal{O}(100) \]
\[ \sigma(a\mu_I) \sim \mathcal{O}(0.1) \]
Multipion Energies

\[ E_n (\text{TeV}) \]

- LQCD A
- LQCD B
- LQCD C
- \( nm_\pi \)

\[ 48^3 \times 96 \]
\[ 72^3 \times 192 \]
\[ 64^3 \times 128 \]
Chemical Potential

SB = Stefan Boltzmann (noninteracting Fermi Gas)
\( \chi_{PT} = \) chiral perturbation theory
Energy Density

SB = Stefan Boltzmann (noninteracting Fermi Gas)
χPT = chiral perturbation theory
pQCD = perturbative QCD

LQCD A = 48^3 \times 96
LQCD B = 64^3 \times 128
LQCD C = 72^3 \times 192
**Speed of Sound**

\[ c_s^2 \leq \frac{1}{3} \]

\[ c_s^2 = \frac{dp}{d\epsilon} = \frac{n}{dE/dn} \frac{d^2E}{dn^2} \]

LQCD A = 48^3 \times 96  
LQCD B = 64^3 \times 128  
LQCD C = 72^3 \times 192
Current and Future Work
Baryons, Isospin, and Sign Problems

- Baryon-density path integral w/ quark chemical potential $\mu = \mu_B/3$:

$$Z_B(\mu_B) = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S[U]-\int \bar{\psi} M[U;\mu] \psi}$$

$$= \int \mathcal{D}U e^{-S_g[U]} \text{Re} \left( \det M[U; \mu_B/3] \right)^2$$

- Fermionic determinant $\det M[U, \mu]$ not positive for $\mu \neq 0$:

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

- $\implies$ path integral measure is not positive for $\mu_B \neq 0$:
- However, measure is positive for $\mu_I \neq 0$:

$$Z_I(\mu_I) = \int \mathcal{D}U e^{-S[U]} \det M[U; \mu_I/2] \det M[U; -\mu_I/2] \left| \det M[U; \mu_I/2] \right|^2$$
QCD Inequalities

- Inequality arising from *phase quenching* \((\text{Re}(z) \leq |z|)\)

\[
Z_B(\mu_B) = \int \mathcal{D}U e^{-S[U]} \text{Re} \left( \det M[U; \mu_B/3] \right)^2 \\
\leq \int \mathcal{D}U e^{-S[U]} |\det M[U; \mu_B/3]|^2 \\
= Z_I(\mu_I = 2\mu_B/3)
\]

- Becomes \(PV = T \log Z\)

\[
P_B(\mu_B) \leq P_I(\mu_I = 2\mu_B/3)
\]

- Saturated up to \(O(\alpha_s^3)\) in perturbative QCD (!)
Baryonic EOS Bounds

Constraints from nuclear matter + pQCD and relations

\[ P = \int d\mu \, n; \quad \epsilon = -P + \mu \, n; \quad \frac{d \log n}{d \log \mu} = \frac{1}{c_s^2} \geq 1 \]
BCS Gap and Pressure

- Condensate $\langle u \gamma^5 \bar{d} \rangle \sim \Delta$ contributes to pressure

$$P(\Delta) - P(\Delta = 0) = \frac{N_c}{8\pi^2} \Delta^2 \mu_I^2 (1 + O(g_s))$$

- Exponentially larger for $\mu_I$ vs. $\mu_B$

$$\Delta(\mu_B) = b\mu_B \exp \left( -\frac{3\pi^2}{\sqrt{2}g_s} \right)$$

$$\Delta(\mu_I) = b'\mu_I \exp \left( -\frac{3\pi^2}{2g_s} \right)$$

Constant (known)

[Ref: Fujimoto, 2312.11443]
Extracting BCS Gap

\[ \Delta^2 \propto \frac{P_{\text{lat}} - P_{\text{pQCD}}}{\mu^2} \]

\[ \Delta^2 \] vs. \[ \mu_I \] (MeV)
Pion Stars

- Proposed class of compact stars: pion stars
  - See [Brandt et al 1802.06685]
  - Note: also need to include weak interactions

![Graph showing the relationship between mass and radius for Pion Stars and Black holes](chart)

- Mass $M$ in $M_\odot$
- Radius $R$ in km
New method allows probing of high $\mu_I$ potential at $T = 0$

Future/ongoing work:
- Other mesons (e.g. $K^+$ for $\mu_s \neq 0$), mixed systems of mesons
- Finite temperature $T \neq 0$
- Probing BCS state
Conclusion/Outlook

- New method allows probing of high $\mu_I$ potential at $T = 0$
- Future/ongoing work:
  - Other mesons (e.g. $K^+$ for $\mu_s \neq 0$), mixed systems of mesons
  - Finite temperature $T \neq 0$
  - Probing BCS state

Thanks for listening! Questions?
Backup
Correlators & Energies

Extracting energies from correlators:

\[
\langle \mathcal{O}^\dagger(0) \mathcal{O}(t) \rangle = \langle \Omega | \mathcal{O}^\dagger e^{-Ht} \mathcal{O} | \Omega \rangle = \sum_{X,Y} \langle \Omega | \mathcal{O}^\dagger | X \rangle \langle X | e^{-Ht} | Y \rangle \langle Y | \mathcal{O} | \Omega \rangle \\
= \sum_{X} | \langle \Omega | \mathcal{O}^\dagger | X \rangle |^2 e^{-E_X t}
\]

What we can compute (Wick contractions)

What we want (extract from fit)

Schematically:

\[
O^\dagger(0) \sim \sum A_X e^{-E_X t}
\]
Eigenvalues

- Distribution of $n$th largest eigenvalue $x_n$ across time:

- Looks like a correlation function ($x_n(t) \sim e^{-Et}$)

- $n = 6000$
- $n = 4000$
- $n = 2000$
- $n = 1000$
Eigenvalues

- Assume exponential decay

\[ x_i(t) = A_n e^{-\alpha_i t} \]

- Derive \( n \)-pion correlator

\[
C_n(t) = \sum_{i_1<\ldots<i_n} x_{i_1} \ldots x_{i_n} = \sum_{i_1<\ldots<i_n} A_{i_1} \ldots A_{i_n} e^{-(\alpha_{i_1}+\ldots+\alpha_{i_n}) t}
\]

- Energies \( E \sim \alpha_{i_1} + \ldots + \alpha_{i_n}, \alpha_i \sim \text{single particle energies} \)
- Eigenvectors \( \sim \text{single particle wavefunctions} \)
- Caveat: \( x_i \) are single-configuration quantities, shouldn’t over-interpret
Polystropic Index & Trace Anomaly

\[ \gamma = \frac{d \log P}{d \log \epsilon} ; P \sim \epsilon^\gamma \]

\[ \Delta = \frac{\epsilon - 3p}{3\epsilon} \]

LQCD A = 48^3 \times 96
LQCD B = 64^3 \times 128
LQCD C = 72^3 \times 192
Formulae for isospin density

- Relativistic Gas:
  \[ \mu_I = (6\pi^2 \rho_I)^{1/3} \]  

- ChiPT (Son and Stephanov, 2000)
  - (conventions from Detmold et al, 2008)
  \[ \rho_I = \frac{1}{2} f_{\pi}^2 \mu_I \left( 1 - \frac{m_{\pi}^4}{\mu_I^4} \right) \]
Needed configurations

- If $\log X \sim \mathcal{N}(\mu, \sigma^2)$, central limit theorem needs at least
  \[ N_{\text{conf}}^{(\text{min})} = e^{\sigma^2} - 1 \]
- Estimate of $N_{\text{conf}}^{(\text{min})}$:

![Graph showing logarithmic relationship between $N_{\text{conf}}^{(\text{min})}$ and $n$.]
Proof of Correlator Formula (Sketch)

\[
P_{(\lambda_1, \ldots, \lambda_n)}(x) = x_1^{\lambda_1} \cdots x_n^{\lambda_n}
\]

\[
C_n = \sum_{\sigma \in S_n} \epsilon(\sigma) P_{\lambda(\sigma)}(x)
\]

\[
= \sum_{\sigma \in S_n} \sum_{\lambda'} \epsilon(\sigma) \chi_{\lambda'}(\sigma) S_{\lambda'}(x)
\]

\[
= \sum_{\lambda'} S_{\lambda'}(x) \sum_{\sigma \in S_n} \epsilon(\sigma) \chi_{\lambda'}(\sigma)
\]

\[
= n! S_{(1, \ldots, 1)}(x)
\]

\[
= n! E_n(x)
\]
Log Normality

$p$-value

$t/a = 10$
$t/a = 15$
$t/a = 20$
Effective Mass

Effective mass for $n = 1$

- $m_{eff}(t)$ vs. $t$
Cumulants

\[
\log C_{6000} \times 10^4
\]

\[
\begin{align*}
N_\kappa &= 1 \\
N_\kappa &= 2 \\
N_\kappa &= 3
\end{align*}
\]

\[
0 \quad 20 \quad 40 \quad 60 \quad 80
\]

\[
t/a
\]

\[
-30 \quad -25 \quad -20 \quad -15 \quad -10 \quad -5
\]

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More Correlator Trace Formulae

\[ C_4 = \text{Tr}(\Pi)^4 - 6 \text{Tr}(\Pi^2) \text{Tr}(\Pi)^2 + 3 \text{Tr}(\Pi^2)^2 + 8 \text{Tr}(\Pi^3) \text{Tr}(\Pi) - 6 \text{Tr}(\Pi^4) \]
\[ C_5 = \text{Tr}(\Pi)^5 - 10 \text{Tr}(\Pi^2) \text{Tr}(\Pi)^3 + 15 \text{Tr}(\Pi^2)^2 \text{Tr}(\Pi) + 20 \text{Tr}(\Pi^3) \text{Tr}(\Pi)^2 - 20 \text{Tr}(\Pi^3) \text{Tr}(\Pi^2) - 30 \text{Tr}(\Pi^4) \text{Tr}(\Pi) + 24 \text{Tr}(\Pi^5) \]
\[ C_6 = \text{Tr}(\Pi)^6 - 15 \text{Tr}(\Pi^2) \text{Tr}(\Pi)^4 + 45 \text{Tr}(\Pi^2)^2 \text{Tr}(\Pi)^2 - 15 \text{Tr}(\Pi^2)^3 + 40 \text{Tr}(\Pi^3) \text{Tr}(\Pi)^3 - 120 \text{Tr}(\Pi^3) \text{Tr}(\Pi^2) \text{Tr}(\Pi) + 40 \text{Tr}(\Pi^3)^2 - 90 \text{Tr}(\Pi^4) \text{Tr}(\Pi)^2 + 90 \text{Tr}(\Pi^4) \text{Tr}(\Pi^2) + 144 \text{Tr}(\Pi^5) \text{Tr}(\Pi) - 120 \text{Tr}(\Pi^6) \]
\[ C_7 = \text{Tr}(\Pi)^7 - 21 \text{Tr}(\Pi^2) \text{Tr}(\Pi)^5 + 105 \text{Tr}(\Pi^2)^2 \text{Tr}(\Pi)^3 \]
\[ - 105 \text{Tr}(\Pi^2)^3 \text{Tr}(\Pi) + 70 \text{Tr}(\Pi^3) \text{Tr}(\Pi)^4 - 420 \text{Tr}(\Pi^3) \text{Tr}(\Pi^2) \text{Tr}(\Pi)^2 \]
\[ + 210 \text{Tr}(\Pi^3) \text{Tr}(\Pi^2)^2 + 280 \text{Tr}(\Pi^3)^2 \text{Tr}(\Pi) - 210 \text{Tr}(\Pi^4) \text{Tr}(\Pi)^3 \]
\[ + 630 \text{Tr}(\Pi^4) \text{Tr}(\Pi^2) \text{Tr}(\Pi) - 420 \text{Tr}(\Pi^4) \text{Tr}(\Pi^3) + 504 \text{Tr}(\Pi^5) \text{Tr}(\Pi)^2 \]
\[ - 504 \text{Tr}(\Pi^5) \text{Tr}(\Pi^2) - 840 \text{Tr}(\Pi^6) \text{Tr}(\Pi) + 720 \text{Tr}(\Pi^7) \]
Aside: Sign Problems in General

Simple example:

\[ Z = \int \, dx \, f(x) = \int \, dx \, e^{-x^2} \cos(kx) \]

\[ \langle O \rangle = \frac{1}{Z} \int \, dx \, f(x) O(x) \]

Compute by via sampling \( x_1, \ldots, x_N \sim p(x) \); (\( p \) = arbitrary prob dist)

\[ \langle O \rangle \approx \frac{1}{N} \sum_i \, f(x_i) \frac{O(x_i)}{p(x_i)} \approx \frac{1}{N} \sum_i \, f(x_i) \frac{O(x_i)}{p(x_i)} e^{-k^2} \pm O\left(\frac{1}{\sqrt{N}}\right) \]

For large \( k \) need \( N \sim e^{k^2} \) to resolve denominator

For e.g. Baryon density, “\( k \)” \( \sim \mu_B V \)