Lessons from the 3d $U(1)$ Gross-Neveu Model

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The effectiveness of the Glasgow algorithm is explored via implementation in the 3d $U(1)$ Gross-Neveu model and the realisation of the Goldstone mechanism in this model is compared and contrasted with its realisation in QCD.

1. Introduction

In QCD the fermion determinant is complex for chemical potential, $\mu$ non-zero, therefore generating an ensemble at $\mu \neq 0$ is impracticable. The fermion number density, $J_0$, measures the excess of quarks relative to anti-quarks and is expected to start to rise from zero at some value, $\mu_o$. The onset, $\mu_o$ corresponds to the point where the phase of nuclear matter is more energetically favourable than the vacuum state (for which $J_0 = 0$). Chiral symmetry restoration occurs at $\mu_c$ and we expect [2] that $\mu_o \lesssim \mu_c \simeq m_p/3$, where $m_p$ is the proton mass. Quenched simulations, on the other hand, predict $\mu_c \simeq m_{\pi}/2$ suggesting that in the limit where the bare quark mass, $m_q \to 0$ chiral symmetry is restored for any $\mu \neq 0$. This result is unphysical because the pion should not couple to the baryon chemical potential.

First attempts to simulate full QCD using the Glasgow method [3] also produced perplexing results [4]. On an $8^4$ lattice with bare quark mass $m_q = 0.01$ at $\beta = 5.1$ we found $\mu_o \simeq 0.1$ which differs considerably from the strong coupling analysis [3] prediction $\mu_c \simeq 0.65$ for $\beta = 5.0$. Furthermore the scaling of $\mu_o$ with $m_q$ was consistent with a Goldstone boson controlling the onset.

This result has motivated an assessment of the effectiveness of the Glasgow method via its implementation in a simpler model. The method involves expansion of the Grand Canonical Partition Function (GCPF) as a polynomial in the fugacity variable ($e^{\mu/T}$).

Consider the conventional expression for the GCPF in lattice QCD

$$Z \sim \int [dU] \det (M(U, \mu_{\text{meas}}, m_q)) e^{-S_g(U)}$$

The GCPF (for fixed $m_q$) can be rescaled and expressed as an ensemble average of $\det M$ at $\mu = 0$:

$$Z(\mu) = \frac{\int [dU] \det M(\mu_{\text{meas}})}{\int [dU] \det M(\mu_{\text{upd}} = 0)} \frac{\det M(\mu_{\text{upd}} = 0)}{\det M(\mu_{\text{meas}})} e^{-S_g(U)}$$

$$= \left\langle \frac{\det M(\mu_{\text{meas}})}{\det M(\mu_{\text{upd}} = 0)} \right\rangle_{\mu_{\text{upd}} = 0}$$

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where $\mu_{\text{upd}}$ is the chemical potential at which the statistical ensemble is updated and is distinct from $\mu_{\text{meas}}$ which appears in the functional measure for the exact hybrid Monte Carlo (HMC) simulations and in $R_{rw}$ below. Note that generating the ensemble at $\mu_{\text{upd}} = 0$ allows us to circumvent the problem of the complex action in the HMC algorithm. For optimum efficiency of the Glasgow method we require a large overlap between the ensemble generated using $\det M(\mu_{\text{upd}})$ and the exact ensemble generated using $\det M(\mu_{\text{meas}})$. Let us define a reweighting factor $R_{rw} \equiv \frac{\det M(\mu_{\text{meas}}, m)}{\det M(\mu_{\text{upd}}, m)}$. The relative magnitude of the factor $R_{rw}$ configuration by configuration gives a measure of the overlap. If there is poor overlap between the simulated ensemble and the true ensemble it is conceivable that only a small fraction of the configurations will contribute significantly to $Z$ (those where $R_{rw}$ is large in magnitude) in which case very high statistics would be required to extract realistic observables.

The relevant features of the 3d Gross-Neveu (GN) model for $\mu \neq 0$ studies are that it has a chiral transition with a massless pion in the broken phase and it can be formulated such that the fermion determinant is positive definite for $\mu \neq 0$.

Mirroring the Glasgow reweighting technique implemented in full QCD ($\mu \neq 0$) simulations we performed an expansion of the Grand Canonical partition function (GCPF) for the 3d GN action in the fugacity variable $e^{\mu/T}$.

The full lattice action for the bosonized GN model with U(1) chiral symmetry is given in [6,7]. The functional measure used in the HMC algorithm is $\det(M^\dagger M)$. The Dirac fermion matrices, $M$ and $M^\dagger$, can be conveniently expressed in terms of matrices $G$ and $V$ where $G$ contains all the spacelike links while $V$ ($V^\dagger$) contains the forward(backward) timelike links

$$2iM_{xy}(\mu) = Y_{xy} + G_{xy} + V_{xy}e^\mu + V_{xy}^\dagger e^{-\mu}; \quad -2iM_{xy}^\dagger(\mu) = Y_{xy}^\dagger + G_{xy} + V_{xy}e^\mu + V_{xy}^\dagger e^{-\mu}$$

and the term describing the Yukawa couplings of scalars to fermions is given (in terms of the auxiliary fields $\sigma$ and $\pi$ on dual lattice sites $\tilde{x}$) by

$$Y_{xy} = 2i(m_q + \frac{1}{8} \sum_{<x,\tilde{x}>} (\sigma(\tilde{x}) + i\epsilon\pi(\tilde{x})))\delta_{xy}. \quad (3)$$

The determinants of these fermion matrices are related to that of the propagator matrix $P$ (following Gibbs [1]):

$$P = \begin{pmatrix} -GV - YV & V \\ -V & 0 \end{pmatrix}$$

by

$$\det(2iM) = e^{\mu n_s n_t} \det(P - e^{-\mu}) \quad \det(2iM^\dagger) = e^{\mu n_s n_t} \det((P^{-1})^\dagger - e^{-\mu}) \quad (5)$$

Since $\det M$ has been expressed in terms of the determinant of a matrix which is diagonal in $e^{-\mu}$ we can expand $\det M$ as a polynomial in $e^\mu$. We can measure the averaged characteristic polynomial over the ensemble generated at $\mu = 0$ and provided that the coefficients are sufficiently well determined, we can use this to provide an analytic continuation to any non-zero $\mu$. Consider a lattice with $n_s$ spatial and $n_t$ temporal dimensions.
Determination of the eigenvalues of $P^n_t$ allows us to construct the complete fugacity expansion for the GCPF:

$$Z = \sum_{n=-2n_s^2}^{2n_s^2} \langle b_{\{n\}} \rangle e^{n\mu t} = \sum_{n=-2n_s^2}^{2n_s^2} e^{(\epsilon_n-n\mu)/T}. \quad (6)$$

The expansion coefficients $\langle b_{\{n\}} \rangle$ are evaluated in the simulation and thermodynamic observables can be obtained from derivatives of $\ln Z$.

The simulated 3d GN $U(1)$ model has a positive definite functional measure so we can choose $\mu_{\text{upd}} \neq 0$ to investigate the influence of this choice on the observables. Exact hybrid Monte Carlo (HMC) simulations showed a clear separation of the scales $m_\pi/2$ and $\mu_c$ indicating that the existence of a Goldstone mode in the spectrum of a theory need not precipitate chiral symmetry restoration for $\mu \ll m_p/3$ in QCD.

Does the poor overlap in the Glasgow algorithm prevent us from seeing the discontinuity in the number density at $\mu_c \gg m_\pi/2$?

We will compare exact HMC and Glasgow method simulations on a $16^3$ lattice at a four-fermi coupling of $1/g^2 = 0.5$ and $m = 0.01$. We simulated the $N_f = 12$ ($N = 3$ staggered) model. In the exact simulations for this parameter set there was a clear discontinuity (at $\mu_c = 0.725(25)$) in fermion number density as a function of the chemical potential. There was no evidence of an onset in the number density at $\mu \simeq m_\pi/2 = 0.18(1)$. In fact $\mu_o \lesssim \mu_c$ for the exact HMC simulation.

It is clear that the chemical potential $\mu_{\text{upd}}$ at which the statistical ensemble is generated has a strong influence on the thermodynamic observables of the simulation. Fig. 1 shows the number density for the exact HMC simulation (discussed above) and for three simulations with the Glasgow method: one for $\mu_{\text{upd}} = 0.0$ another for $\mu_{\text{upd}} = 0.7\ (< \mu_c)$ and finally with $\mu_{\text{upd}} = 0.8\ (> \mu_c)$ The discontinuity at $\mu_c$ associated with the fermion losing dynamical mass, which is clearly evident in the exact HMC data is not consistently
reproduced by the Glasgow algorithm. In fact the chiral transition is seen only when \( \mu_{\text{upd}} \lesssim \mu_c \). For \( \mu_{\text{upd}} > \mu_c \), \( J_0 \) reflects only the chirally symmetric phase (where \( m_f = m_q \)) of the exact HMC data while for \( \mu_{\text{upd}} = 0 \), \( J_0 \) reflects only the phase of broken chiral symmetry (where \( m_f \gg m_q \)). This suggests that there is insufficient overlap.

The Lee-Yang zeros \( [8] \) in the complex \( \mu \) plane are the zeros of Eqn. \( 6 \) and their distribution should reflect \( \mu_c \). We expect the zero with the smallest imaginary part to approach the real axis as the lattice volume is increased. A phase transition occurs whenever a root approaches the real axis in the infinite volume limit. The zeros for the \( \mu_{\text{upd}} = 0.0, 0.7 \) are plotted in Fig.\( 2 \). For \( \mu_{\text{upd}} = 0 \) notice the two zeros emerging from the body of the distribution. These two isolated zeros are located at a chemical potential \( \mu \simeq \mu_c \). There was no evidence for \( \mu_c \) in \( J_0 \) for \( \mu_{\text{upd}} = 0 \) so it is more likely these two zeros are associated with \( \mu_o \) rather than \( \mu_c \). For \( \mu_{\text{upd}} = 0.7 \) we did see a discontinuity in \( J_0 \) at \( \mu_c \) and in this case we see an arc of zeros forming which intersects the real \( \mu \)-axis at \( \mu \simeq \mu_c \).

How do we explain the fact that \( \mu_o \simeq \mu_c \) in simulations of this model but not in QCD? Consider the lattice Ward identity for the chiral condensate:

\[
\sum_y \langle \bar{\psi} \gamma_5 \psi(y) \bar{\psi} \gamma_5 \psi(x) \rangle = \sum_y \langle \text{tr}(G^\dagger_{-\mu}(x,y)G_{+\mu}(x,y)) \rangle - \langle \text{tr}\gamma_5 G(x,x) \rangle \langle \text{tr}\gamma_5 G(y,y) \rangle = -\langle \bar{\psi}(x)\psi(x) \rangle \frac{1}{m_q} \tag{7}\]

The pion susceptibility Eqn.(7) consists of a connected channel and a disconnected channel. In QCD the pion has a dominant connected contribution therefore we can identify the pion mass in QCD with a pole in the pseudoscalar propagator, \( G_{ps} \), defined by (with \( G = M^{-1} \)):

\[
G_{ps}(t) = \sum_\vec{x} G_{+\mu}(\vec{x},t)G^\dagger_{-\mu}(\vec{x},t) \simeq e^{-m_p t} \tag{8}\]
Figure 3. Measurements at $\mu = 0.0$ showing the disconnected and connected contributions to the pion susceptibility on a $16^3$ lattice with $1/g^2 = 0.5$ and $m = 0.01$.

Gibbs [1] derived a relation between the eigenvalues of $P$ and $m_\pi$ in QCD. If $\lambda_{ps}$ is an eigenvalue of $P$ associated with the mass pole in $G_{ps}$ and assuming the pion susceptibility has a dominant connected contribution it follows that $m_\pi = 2 \ln |\lambda_{ps}|$. Let us consider how the existence of this mass pole could affect $\mu_o$. Notice that $\det M$ can be simply expressed in terms of the eigenvalues of $P$ and $Z$ can be similarly expressed in terms of its zeros $\alpha_i$ in the $e^\mu$ plane:

$$\det M = e^{n_3 n_4 \mu} \prod_{i=1}^{4n_3 n_4} (e^\mu - \lambda_i) \quad ; \quad Z = e^{n_3 n_4 \mu} \prod_{i=1}^{4n_3 n_4} (e^\mu - \alpha_i).$$

(9)

Since $Z = \langle \det(M) \rangle$ we see that on a single configuration $\alpha_i = \lambda_i$. Note however that the ensemble averaged $\alpha_i$'s are not in general the same as the ensemble averages of the $\lambda_i$'s.

The number density on a single configuration $J_0 \sim \partial \ln \det M / \partial \mu$ whereas the ensemble average is given by $J_0 \sim \partial \ln \langle \det M \rangle / \partial \mu$. Presumably the unphysical singularity at $\mu_o \simeq m_\pi/2$ in $J_0$ associated with the pole in $G_{ps}$ at $m_\pi/2$ could disappear if we achieved the $\alpha_i$ appropriate to the correct statistical ensemble and we envisage that $\mu_o$ would cancel in the large ensemble limit. The mass pole at $m_\pi/2$ should disappear if we have a confining theory.

It will be shown that in the 3d GN $U(1)$ model the Goldstone pole forms in the disconnected channel therefore the state described by $G_{ps}$ no longer corresponds to the Goldstone pion. Instead we find:

$$G_{ps} \simeq e^{-2m_f(\mu=0)t}$$

(10)

Since $|\lambda_{ps}|$ will now correspond to the dynamical fermion mass $m_f$ rather than $m_\pi/2$ we have no reason to expect an early onset associated with the Goldstone pole in the 3d GN $U(1)$ model.

Fig. 3 shows the disconnected contribution to the Ward identity for a simulation at zero chemical potential. For this simulation we found $\langle \psi \bar{\psi} \rangle / m_q \simeq 40$, therefore we require
that the sum of the connected and disconnected diagrams be of similar order so that Eqn. 7 is satisfied. The connected contribution was stable at a value of around 0.5 therefore the dominant contribution must come from the disconnected diagram. We found that the disconnected contribution was very noisy with large downward peaks. The data suggests that considering the connected contribution alone will never be sufficient to satisfy Eqn. 4.

We repeated our measurements for a non-zero chemical potential. We chose \( \mu = 0.5 \) thus ensuring that we were still in the phase of broken chiral symmetry. The results were consistent with those at zero chemical potential as one would expect.

The disconnected contribution to the pion susceptibility gives a very noisy signal which suggests that a very long run would be required to equilibrate sufficiently to satisfy the lattice Ward identity.

The Glasgow algorithm is most effective at predicting \( \mu_c \) for \( \mu \lesssim \mu_c \) when the configurations of the statistical ensemble reflect the system close to criticality.

In QCD the pseudoscalar channel pole is formed from connected diagrams corresponding to \( G_{+\mu}(t)G_{-\mu}^*(t) \). A baryonic pion forms from a quark and a conjugate quark and condenses in this channel which explains why we find \( \mu_o = m_\pi/2 \) [9]. This induces the unphysical early onset of chiral symmetry restoration in the quenched theory and will persist in the Glasgow algorithm unless either large statistics or sufficient overlap is achieved so that the phase of the determinant eliminates the conjugate quarks.

In 3d GN \( U(1) \) the Goldstone mechanism is realised by a pseudoscalar channel pole formed from disconnected diagrams and the state \( G_{+\mu}(t)G_{-\mu}^*(t) \) yields a bound state of mass \( 2m_f(\mu = 0) \) which is considerably heavier than the pion. Even on individual configurations in this model we expect \( \mu_o \simeq \mu_c \gg m_\pi/2 \) because no baryonic pion condenses in the connected channel.

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