Towards QCD Thermodynamics using Exact Chiral Symmetry on Lattice

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T. I. F. R., Mumbai

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Introduction
GW relation and $\mu \neq 0$
Our Results
Summary

Introduction

♦ A fundamental aspect of QCD – Critical Point in $T-\mu_B$ plane;
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♠ A fundamental aspect of QCD – Critical Point in $T$-$\mu_B$ plane; Based on symmetries and models, Expected QCD Phase Diagram

From Rajagopal-Wilczek Review
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... but could, however, be ... McLerran-Pisarski 2007

From Rajagopal-Wilczek Review
GW relation and $\mu \neq 0$

♠ Exact chiral invariance for a lattice fermion operator $D$ is assured if it satisfies the Ginsparg-Wilson relation: $\{\gamma_5, D\} = aD\gamma_5 D$. 
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♠ Exact chiral invariance for a lattice fermion operator $D$ is assured if it satisfies the Ginsparg-Wilson relation: $\{\gamma_5, D\} = a D \gamma_5 D$.

♠ In particular, the chiral transformations (Lüscher, PLB 1999) $\delta \psi = \alpha \gamma_5 (1 - \frac{a}{2} D) \psi$ and $\delta \bar{\psi} = \alpha \bar{\psi} (1 - \frac{a}{2} D) \gamma_5$, leave the action $S = \sum \bar{\psi} D \psi$ invariant:

$$\delta S = \alpha \sum_{x,y} \bar{\psi}_x \left[ \gamma_5 D + D \gamma_5 - \frac{a}{2} D \gamma_5 D - \frac{a}{2} D \gamma_5 D \right]_{xy} \psi_y = 0 \quad (1)$$
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♠ Overlap fermions, and Domain Wall fermions in the limit of large fifth dimension satisfy this relation.
Domain Wall Fermions

Proposed by Kaplan (PLB 1992), a convenient form for Domain Wall fermion action (Shamir, NPB, 1993) is:

\[ S_F = \sum_{s,s'=1}^{N_5} \sum_{x,x'} \bar{\psi}(x, s)D_{dw}(x, s; x', s')\psi(x', s') , \]  

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where \( D_{dw} \) is defined in terms of \( D_{w} \) as

\[ D_{dw}(x, s; x', s') = [a_5 D_{w} + 1] \delta_{s,s'} - [P_- \delta_{s,s'-1} + P_+ \delta_{s,s+1'}], \] (3)

with boundary conditions \( P_+ \psi(x, 0) = -am \ P_+ \psi(x, N_5) \) and \( P_- \psi(x, N_5 + 1) = -am \ P_- \psi(x, 1). \)
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♠ Only light modes attached to the wall(s) are physical. Divide out heavy modes by having the \( D_{dw}(am)/D_{dw}(am = 1) \) as the effective Domain Wall operator in \( \mathbb{Z} \).
As outlined in Edwards & Heller (PRD 63, 2001), one can integrate out the fermionic fields in the fifth direction to rewrite the above ratio as

\[ [(1 + am) - (1 - am)\gamma_5\tanh\left(\frac{N_5}{2} \ln |T|\right)] , \quad (4) \]

with

\[ T = (1 + a_5\gamma_5 D_w P_+)^{-1}(1 - a_5\gamma_5 D_w P_-). \]
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with \( T = (1 + a_5\gamma_5 D_w P_+)^{-1}(1 - a_5\gamma_5 D_w P_-) \).

Taking the limit \( N_5 \to \infty \) for \( a_5 = 1 \), one obtains sign function of \( \ln |T| \), proving that the DWF satisfy the Ginsparg-Wilson relation in this limit.

Taking the limit \( a_5 \to 0 \) such that \( L_5 = a_5 N_5 = \text{constant} \), one can show \( N_5 \ln T \to L_5 \gamma_5 D_{dw} \). Further, for \( L_5 \to \infty \), DWF reduce to the overlap fermions.

We use this form in our numerical work.
Introducing Chemical Potential

• Ideally, one should construct the conserved charge as a first step.

• Non-locality makes it difficult, even non-unique (Mandula, 2007).
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- Simpler alternative: $D_w \rightarrow D_w(a\mu)$ by $K(a\mu) = \exp(a\mu)$ and $L(a\mu) = \exp(-a\mu)$ in positive/negative time direction respectively. (Bloch and Wettig, PRL 2006; PRD 2007).
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- Note $\gamma_5 D_w(a\mu)$ is no longer Hermitian, requiring an extension of the sign function. B & W proposal: For complex $\lambda = (x + iy)$, $\text{sign}(\lambda) = \text{sign} (x)$. 
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• Gattringer-Liptak, PRD 2007, showed for \( M = 1 \) numerically that no \( \mu^2 \) divergences exist for the free case (\( U = 1 \)).
We show this to be true analytically and for all $M$ as well. Furthermore, this holds for all functions such that $K(a\mu) \cdot L(a\mu) = 1$ for Overlap (Banerjee, Gavai, Sharma, PRD 2008) and Domain Wall Fermions (Gavai, Sharma 2008).
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• We claim that chiral invariance is lost for nonzero $\mu$. Note that

$$\delta S = \alpha \sum_{x,y} \bar{\psi}_x \left[ \gamma_5 D(a\mu) + D(a\mu)\gamma_5 - \frac{a}{2} D(0)\gamma_5 D(a\mu) - \frac{a}{2} D(a\mu)\gamma_5 D(0) \right]_{xy} \psi_y ,$$

under Lüscher’s chiral transformations.  

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• However, the sign function definition above merely ensures

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which is not sufficient to make \( \delta S = 0 \).
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$$\delta S = \alpha \sum_{x,y} \bar{\psi}_x \left[ \gamma_5 D(a\mu) + D(a\mu) \gamma_5 - \frac{a}{2} D(0) \gamma_5 D(a\mu) - \frac{a}{2} D(a\mu) \gamma_5 D(0) \right] \psi_y,$$

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$$\gamma_5 D(a\mu) + D(a\mu) \gamma_5 - a D(a\mu) \gamma_5 D(a\mu) = 0,$$

(6)

which is not sufficient to make $\delta S = 0$. True for both Overlap and Domain Wall fermions and any $K, L$. 

Extreme QCD 2008, North Carolina State University, Raleigh, USA, July 21, 2008
Our Results

• We investigated thermodynamics of free overlap and domain wall fermions with an aim to examine the continuum limit analytically and numerically.

• Analytically, we prove the absence of $\mu^2$-divergences for general $K$ and $L$. Our numerical results were for tuning the irrelevant parameter $M$ to obtain small deviations from continuum limit on coarse lattices.
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- Energy density and pressure can be obtained from $\ln Z = \ln \det D_{ov}$ by taking $T$ and $V$, or equivalently $a_4$ and $a$, partial derivatives.
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• Energy density and pressure can be obtained from $\ln Z = \ln |\det D_{ov}|$ by taking $T$ and $V$, or equivalently $a_4$ and $a$, partial derivatives.

• Dirac operator is diagonal in momentum space. Use its eigenvalues to compute $Z$:
  \[
  \lambda_{\pm} = 1 - \left[ \text{sgn} \left( \sqrt{h^2 + h_5^2} \right) h_5 \pm i\sqrt{h^2} \right] / \sqrt{h^2 + h_5^2}, \quad \text{with}
  \]
  \[
  h_i = -\sin a p_i, \quad i = 1, 2 \text{ and } 3, \quad h_4 = -a \sin(a_4 p_4) / a_4 \quad \text{and}
  \]
  \[
  h_5 = M - \sum_{i=1}^{3} \left[ 1 - \cos(a p_i) \right] - a [1 - \cos(a_4 p_4)] / a_4.
  \]
• Easy to show that $\epsilon = 3P$ for all $a$ and $a_4$. 
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• I will show results for $\epsilon/\epsilon_{SB}$ which is also $P/P_{SB}$.
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• Hiding $p_i$-dependence in terms of known functions $g$, $d$ and $f$, the energy density on an $N^3 \times N_T$ lattice is found to be

$$\epsilon a^4 = \frac{2}{N^3 N_T} \sum_{p_i, n} F(\omega_n) = \frac{2}{N^3 N_T} \sum_{p_i, n} \left[ (g + \cos \omega_n) + \sqrt{d + 2g \cos \omega_n} \right]$$

$$\times \left[ \frac{(1 - \cos \omega_n)}{d + 2g \cos \omega_n} + \frac{\sin^2 \omega_n (g + \cos \omega_n)}{(d + 2g \cos \omega_n)(f + \sin^2 \omega_n)} \right]$$

(7)

where $\omega_n$ are the Matsubara frequencies.
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where $\omega_n$ are the Matsubara frequencies.

• Can be evaluated using the standard contour technique or numerically.
Analytic Evaluation: \( \mu = 0. \)
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- Poles at $\omega = \pm i \sinh^{-1} \sqrt{f}$ and Poles (branch points) at $\pm i \cosh^{-1} \frac{d}{2g}$.
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- Evaluating integrals, \( \epsilon a^4 = 4N^{-3} \sum_{p_j} \left[ \sqrt{f/1+f} \right] [\exp(N_T \sinh^{-1} \sqrt{f}) + 1]^{-1} + \epsilon_3 + \epsilon_4 \), where \( f = \sum_i \sin^2(\alpha p_i) \).
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- Can be seen to go to $\epsilon_{SB}$ as $a \to 0$ for all $M$. 

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More Details: \( T = 0, \mu \neq 0 \)

- Defining \( K(\mu) + L(\mu) = 2R \cosh \theta \) and \( K(\mu) - L(\mu) = 2R \sinh \theta \), the same treatment as above goes through by substituting \( \sin \omega_n \rightarrow R \sin(\omega_n - i\theta) \) and \( \cos \omega_n \rightarrow R \cos(\omega_n - i\theta) \).
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- Energy density is also functionally the same with \( F(1, \omega_n) \to F(R, \omega_n - i\theta) \).

- Additional observable, number density: Has the same pole structure so similar computation.
Divergence Cancellation at $T = 0, \mu \neq 0$

- Doing the contour integral, the energy density turns out to be:

\[
\epsilon a^4 = (\pi N^3)^{-1} \sum_{p_j} \left[ 2\pi \text{Res} \ F(R, \omega) \Theta (K(a\mu) - L(a\mu) - 2\sqrt{f}) \\
+ \int_{-\pi}^{\pi} F(R, \omega) d\omega - \int_{-\pi}^{\pi} F(1, \omega) d\omega \right].
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  + \int_{-\pi}^{\pi} F(R, \omega) d\omega - \int_{-\pi}^{\pi} F(1, \omega) d\omega \right].
  \]

- $R = K(a\mu) \cdot L(a\mu) = 1$ ensures cancellation of the last two terms and the canonical result in the continuum limit $a \to 0$.

- If $R \neq 1$, one has a $\mu^2$ divergence in the continuum limit as well as violation of Fermi surface since $\epsilon \neq 0$ for any $\mu$. 
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- $K$ and $L$ should be such that $K(a\mu) - L(a\mu) = 2a\mu + O(a^3)$ with $K(0) = 1 = L(0)$. 
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- $K$ and $L$ should be such that $K(a\mu) - L(a\mu) = 2a \mu + \mathcal{O}(a^3)$ with $K(0) = 1 = L(0)$.

- Generalization to $T \neq 0$ and $\mu \neq 0$ case straightforward. One merely needs two different contours depending on pole locations and value of $\theta$. 
Numerical Evaluation

♣ Zero temperature contribution: as $N_T \to \infty$, $\omega$ sum becomes integral which we estimated numerically.
♣ Continuum limit by holding $\zeta = N/N_T = LT$ fixed and increasing $N_T$. 
Numerical Evaluation

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![Graph showing the relationship between $e/e_{SB}$ and $N_T$ for different values of $\zeta$.]
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![Graphs showing the relationship between $\varepsilon/\varepsilon_{SB}$ and $N_T$ for different values of $\zeta$ and $M$.]
Approach to SB-Limit

\[ \frac{e}{e_{SB}} \]

\[ \frac{1}{N_T^2} \]

\[ \zeta = 5 \]
Approach to SB-Limit

\[ \frac{\epsilon}{\epsilon_{SB}} = 5 \]

\[ \frac{p}{p_{SB}} \]

1-link actions
Wilson
staggered
overlap
O(1/N^2_t)

Banerjee, Gavai & Sharma, arXiv:0803.3925
Hegde, Karsch, Laermann & Shcheredin, arXiv:0801.4883

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Results for $M = 1$ agree with Hegde et al. (free energy); Smaller corrections than for Staggered or Wilson fermions.
Approach to SB-Limit

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\[ \zeta = 5 \]

\[ p/p_{SB} = (\pi/N_T)^2 \]

\[ N_T \]

\[ 1\text{-link actions} \]

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\( \heartsuit \) Results for \( M = 1 \) agree with Hegde et al. (free energy); Smaller corrections than for Staggered or Wilson fermions.

\( \heartsuit \) \( 1.50 \leq M \leq 1.60 \) seems optimal, with 2-3 % deviations already for \( N_T = 12 \).
Domain Wall Fermions ($a_5 \to 0$)

Rajiv V. Gavai and Sayantan Sharma, in preparation.
-domain Wall Fermions $(a_5 \to 0)$

$\frac{\varepsilon}{\varepsilon_{SB}}$ vs $\frac{1}{N_T^2}$ for $M = 1.55, \zeta = 4$

$\frac{\varepsilon}{\varepsilon_{SB}}$ vs $\frac{1}{N_T^2}$ for $L_5 = 14, \zeta = 4$

Rajiv V. Gavai and Sayantan Sharma, in preparation.

◊ $L_5 \geq 14$ seems to be large enough to get $L_5$-independent results.
\[ \text{Domain Wall Fermions } (a_5 \rightarrow 0) \]

\[ \frac{\varepsilon}{\varepsilon_{SB}} \text{ vs } \frac{1}{N_T^2} \]

\[ L_5 \geq 14 \text{ seems to be large enough to get } L_5\text{-independent results.} \]

\[ \text{Optimal range again seems to be } 1.50 \leq M \leq 1.60. \]

Rajiv V. Gavai and Sayantan Sharma, in preparation.
Domain Wall Fermions \((a_5 = 1)\)

Rajiv V. Gavai and Sayantan Sharma, in preparation.
Domain Wall Fermions \( (\alpha_5 = 1) \)

\[ \frac{e}{e_{SB}} \text{ vs } N_T \]

\[ \frac{BS}{e_{SB}} \text{ vs } \frac{1}{N_T^2} \]

Rajiv V. Gavai and Sayantan Sharma, in preparation.

◊ \( \zeta \geq 4 \) seems to be large enough to get thermodynamic limit.
◊ Optimal range now seems to be \( 1.40 \leq M \leq 1.50 \); \( M = 1.9 \) used by Chen et al. (PRD 2001) in their study of order parameters of FTQCD.
Numerical Evaluation

Two Observables: \( \Delta \epsilon(\mu, T) = \epsilon(\mu, T) - \epsilon(0, T) \) and Susceptibility,
\( \sim \partial^2 \ln Z / \partial \mu^2 \).
Numerical Evaluation

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◊ For odd \( N_T \) and large enough \( \mu \) the sign function is undefined as an eigenvalue becomes pure imaginary.
Numerical Evaluation

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♦ Former computed for two $r = \mu/T = 0.5$ and 0.8 while latter for $\mu = 0$. 

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Susceptibility too behaves the same way as the energy density.
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Domain Wall Fermions ($a_5 = 1$)

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Domain Wall Fermions \((a_5 = 1)\)

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♥ Again \(1.40 \leq M \leq 1.50\) seems optimal, with small deviations already \(N_T = 12\).
Summary

- Exact chiral symmetry without violation of flavour symmetry important for many studies on lattice, especially for the critical point and the QCD phase diagram in $\mu$–$T$ plane.

- Overlap and Domain wall fermions lose their chiral invariance on introduction of chemical potential in the Bloch-Wettig method and its generalizations.
Summary

- Exact chiral symmetry without violation of flavour symmetry important for many studies on lattice, especially for the critical point and the QCD phase diagram in $\mu$–$T$ plane.

- Overlap and Domain wall fermions lose their chiral invariance on introduction of chemical potential in the Bloch-Wettig method and its generalizations.

- However, any $\mu^2$-divergence in the continuum limit is avoided for it and an associated general class of functions $K(\mu)$ and $L(\mu)$ with $K(\mu) \cdot L(\mu) = 1$.

- For the choice of $1.5 \leq M \leq 1.6$ ($1.4 \leq M \leq 1.5$), both the energy density and the quark number susceptibility at $\mu = 0$ exhibited the smallest deviations from the ideal gas limit for $N_T \geq 12$ for Overlap (Domain Wall) Fermions.
Consequences

- Exact Chiral Symmetry on lattice lost for any $\mu \neq 0$: Real or Imaginary! Note $D_w(a\mu)$ is Hermitian for the latter case.

- $\mu$-dependent mass for even massless quarks.
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• $\mu$-dependent mass for even massless quarks.

• Only smooth chiral condensates: No (clear) chiral transition for any (large) $\mu$ possible. How small $a$, or large $N_T$ may suffice?

• All coefficients of a Taylor expansion in $\mu$ do have the chiral invariance but the series will be smooth and should always converge.
What if . . .

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- Moreover, symmetry groups different at each \( \mu \). Recall we wish to investigate \( \langle \bar{\psi} \psi \rangle(a\mu) \) to explore if chiral symmetry is restored.

- The symmetry group remains same at each \( T \) with \( \mu = 0 \)
  \( \Rightarrow \langle \bar{\psi} \psi \rangle(\mu = 0, T) \) is an order parameter for the chiral transition.