Towards QCD Thermodynamics using Exact Chiral Symmetry on Lattice

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Introduction

GW relation and $\mu \neq 0$

Our Results

Summary

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- The finite temperature transition in our world, i.e., QCD with \(2 + 1\) flavours of dynamical quarks, is widely accepted to be governed by chiral symmetry.

- Staggered fermions have dominated the area of nonzero temperatures and densities.
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- Obtained from the long-distance behaviour of the correlator

$$\langle C_{AB}(z) \rangle = \langle \bar{A}(z) \bar{B}(0) \rangle - \langle \bar{A}(0) \rangle \langle \bar{B}(0) \rangle \sim \exp(-\mu(T)z), \text{ as } z \to \infty.$$ Here

$$\bar{A}(z) = \sum_{x,y,t} A(x, y, z, t)/N_s^2 N_t$$ is a local meson or baryon operator.
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  Here \( \bar{A}(z) = \sum_{x,y,t} A(x, y, z, t)/N_s^2 N_t \) is a local meson or baryon operator.

• Overlap fermions appear to do better.
Local masses \[ \sim \ln(C(r)/C(r + 1)) \] show nice plateau behaviour for pi & rho for Overlap (left) unlike staggered (right) fermions.

Gavai, Gupta, Lacaze PRD 2008

Gavai, Gupta PRD 2002
The pionic screening length shows significant $a^2$ corrections for staggered (left) unlike Overlap (right) fermions.

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QCD Phase diagram

♠ A fundamental aspect of QCD – Critical Point in $T-\mu_B$ plane;
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McLerran-Pisarski 2007
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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♦ 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:

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\delta S = \alpha \sum_{x,y} \bar{\psi}_x \left[ \gamma_5D + D\gamma_5 - \frac{a}{2}D\gamma_5D - \frac{a}{2}D\gamma_5D \right]_{xy} \psi_y = 0 \tag{1}
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♠ Overlap fermions, and Domain Wall fermions in the limit of large fifth dimension satisfy this relation.
Neuberger (PLB 1998) proposed the overlap-Dirac operator:

\[ aD = 1 + A(A^\dagger A)^{-1/2} = 1 + \gamma_5 \text{sign}(\gamma_5 A) \quad \text{with} \quad A = aD_w, \quad (2) \]
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♠ Here \( D_w \) is the Wilson-Dirac Operator given by,

\[ aD_w = \frac{1}{2} \{ \gamma_\mu (\partial_\mu^* + \partial_\mu) - a\partial_\mu^* \partial_\mu \} + M, \quad (3) \]

with \(-2 < M < 0\) and \(\partial_\mu\) and \(\partial_\mu^*\) as forward and backward gauge-invariant difference operators. An extra \(a/a_4\) factor for \(\mu = 4\) at \(T \neq 0\).
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♠ quark with a mass: \( D(ma) = ma + (1 - ma/2)D \)
Domain Wall Fermions

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

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

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

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

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

(5)

with boundary conditions \( P+ \psi(x,0) = -am P+ \psi(x,N_5) \) and \( P- \psi(x,N_5+1) = -am P- \psi(x,1) \).

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

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

with

\[T = (1 + a_5\gamma_5 D_w P_+)^{-1}(1 - a_5\gamma_5 D_w P_-).\]
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with \( T = (1 + a_5\gamma_5D_wP_+)^{-1}(1 - a_5\gamma_5D_wP_-) \).

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

Taking the limit \( a_5 \to 0 \) such that \( L_5 = a_5N_5 = \text{constant} \), one can show \( N_5 \ln T \to L_5\gamma_5D_{dw} \). 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).
• 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).

• We claim that chiral invariance is lost for nonzero \( \mu \). Note that

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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]_{xy} \psi_y ,
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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 \( \delta S = 0 \). True for both Overlap and Domain Wall fermions and any \( K,L \).
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.

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- 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 . . .

♠ the chiral transformations were $\delta \psi = \alpha \gamma_5 (1 - \frac{a}{2} D(a\mu)) \psi$ and $\delta \bar{\psi} = \alpha \bar{\psi} (1 - \frac{a}{2} D(a\mu)) \gamma_5$?
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• Symmetry transformations should not depend on “external” parameter $\mu$. Chemical potential is introduced for charges $N_i$ with $[H, N_i] = 0$. At least the symmetry should not change as $\mu$ does.
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• Symmetry transformations should not depend on “external” parameter $\mu$. Chemical potential is introduced for charges $N_i$ with $[H, N_i] = 0$. At least the symmetry should not change as $\mu$ does.

• 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 $\mu = 0$ $\implies \langle \bar{\psi} \psi \rangle(am = 0, T)$ is an order parameter for the chiral transition.
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 $Z$:

$$\lambda_{\pm} = 1 - [\text{sgn} \left( \sqrt{h^2 + h_5^2} \right) h_5 \pm i\sqrt{h^2}] / \sqrt{h^2 + h_5^2},$$

with

$$h_i = -\sin a p_i, \quad i = 1, 2 \text{ and } 3, \quad h_4 = -a \sin(a_4 p_4)/a_4 \text{ and}$$

$$h_5 = M - \sum_{i=1}^{3} [1 - \cos(a p_i)] - a[1 - \cos(a_4 p_4)]/a_4.$$
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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

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

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

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where $\omega_n$ are the Matsubara frequencies.
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• Can be evaluated using the standard contour technique or numerically.
Analytic Evaluation: $\mu = 0$. 

\[
\begin{align*}
\text{Im} \omega &= 0 \\
\text{i} \cosh^{-1} \frac{d}{2g} &= \\
\text{i} \sinh^{-1} \sqrt{f} &= \\
\text{i} \sinh^{-1} \sqrt{f} &= \\
-\text{i} \cosh^{-1} \frac{d}{2g} &= \\
\end{align*}
\]
Analytic Evaluation: \( \mu = 0 \).

- Poles at \( \omega = \pm i \sinh^{-1} \sqrt{f} \) and Poles (branch points) at \( \pm i \cosh^{-1} \frac{d}{2g} \).
Analytic Evaluation: $\mu = 0$.

- Poles at $\omega = \pm i \sinh^{-1}\sqrt{f}$ and Poles (branch points) at $\pm i \cosh^{-1}\frac{d}{2g}$.

- 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 $f = \sum_i \sin^2(ap_i)$. 

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- Can be seen to go to $\epsilon_{SB}$ as $a \to 0$ for all M.
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 \( F(1, \omega_n) \rightarrow F(R, \omega_n - i\theta) \).

- 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:

$$\epsilon a^4 = (\pi N^3)^{-1} \sum_{p_j} \left[2\pi \text{Res} \ F(R, \omega) \Theta \left(K(a\mu) - L(a\mu) - 2\sqrt{f}\right) + \int_{-\pi}^{\pi} F(R, \omega) d\omega - \int_{-\pi}^{\pi} F(1, \omega) d\omega \right].$$
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- $R = K(a\mu) \cdot L(a\mu) = 1$ 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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  + \int_{-\pi}^{\pi} F(R, \omega) d\omega - \int_{-\pi}^{\pi} F(1, \omega) d\omega \right].
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- $K$ and $L$ should be such that $K(a\mu) - L(a\mu) = 2a \mu + \mathcal{O}(a^3)$ with $K(0) = 1 = L(0)$. 
**Divergence Cancellation at** $T = 0, \mu \neq 0$

- Doing the contour integral, the energy density turns out to be :
  \[\epsilon a^4 = (\pi N^3)^{-1} \sum_{p_j} \left[ 2\pi \text{Res} \ F(R, \omega) \Theta (K(a\mu) - L(a\mu) - 2\sqrt{f}) \right. \]
  \[\left. + \int_{-\pi}^{\pi} F(R, \omega) d\omega - \int_{-\pi}^{\pi} F(1, \omega) d\omega \right].\]

- $R = K(a\mu) \cdot L(a\mu) = 1$ 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 $\mu$.

- $K$ and $L$ should be such that $K(a\mu) - L(a\mu) = 2a \mu + O(a^3)$ 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 \( N_T \).
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![Graph showing numerical evaluation results](image)


R. V. Gavai  Top  19
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![Graph 1](image1.png)

![Graph 2](image2.png)
Approach to SB-Limit

\[ \frac{\varepsilon}{\varepsilon_{SB}} \]

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

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

\[ \epsilon / \epsilon_{SB} \]

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

\[ N_{\tau} \]

\[ (\pi / N_{\tau})^2 \]

\[ \zeta = 5 \]

Banerjee, Gavai & Sharma, PRD78, 2008

Hegde, Karsch, Laermann & Shcheredin, arXiv:0801.4883
Approach to SB-Limit

Results for $M = 1$ agree with Hegde et al. (free energy); Smaller corrections than for Staggered or Wilson fermions.
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$\heartsuit 1.50 \leq M \leq 1.60$ seems optimal, with 2-3 % deviations already for $N_T = 12$. 
Domain Wall Fermions \((a_5 \rightarrow 0)\)

Rajiv V. Gavai and Sayantan Sharma, in preparation.
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\(L_5 \geq 14\) seems to be large enough to get \(L_5\)-independent results.
Domain Wall Fermions \( (a_5 \rightarrow 0) \)

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

\[ \frac{\beta_{SB}}{\varepsilon} \] vs \( \frac{1}{N_T^2} \)

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\( L_5 \geq 14 \) seems to be large enough to get \( L_5 \)-independent results.

\( \diamond \) Optimal range again seems to be \( 1.50 \leq M \leq 1.60 \).
Domain Wall Fermions \((a_5 = 1)\)

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Domain Wall Fermions \((\alpha_5 = 1)\)

\[ \begin{array}{c}
\begin{array}{c}
\text{M}=1.50 \\
\zeta=2 \\
\zeta=3 \\
\zeta=4 \\
\zeta=5
\end{array}
\end{array} \]

\[ \begin{array}{c}
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\text{M}=1.0 \\
\text{M}=1.40 \\
\text{M}=1.45 \\
\text{M}=1.50 \\
\text{M}=1.55 \\
\text{M}=1.60
\end{array}
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Rajiv V. Gavai and Sayantan Sharma, in preparation.

\[\begin{array}{c}
\diamond \zeta \geq 4 \text{ seems to be large enough to get thermodynamic limit.} \\
\diamond \text{Optimal range now seems to be } 1.40 \leq M \leq 1.50; \ M = 1.9 \text{ used by Chen et al. (PRD 2001) in their study of order parameters of FTQCD.}
\end{array}\]
Numerical Evaluation

◊ Two Observables: $\Delta \epsilon(\mu, T) = \epsilon(\mu, T) - \epsilon(0, T)$ and Susceptibility, $\sim \partial^2 \ln Z / \partial \mu^2$. 
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Again $1.50 \leq M \leq 1.60$ seems optimal, with 2-3 % deviations already for $N_T = 12$. 
Domain Wall Fermions \((a_5 = 1)\)

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Domain Wall Fermions ($a_5 = 1$)

♥ Again Susceptibility behaves the same way as the energy density.

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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.