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A simple idea for Lattice QCD at finite density

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We pursue the idea of adding the naıve μN term, where μ is the quark chemical potential and N is the conserved quark number, to the lattice QCD action. While computations of higher order susceptibilities, required for estimating the location of the QCD critical point, need a lot fewer number of quark propagators at any order as a result, it has its problem. We discuss a solution, and examine if it works.

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1. Introduction

QCD at finite density is one of the most fascinating topics of research currently because of the tantalizing experimental possibility of exploring the the possible region of QCD critical point in the T-μ phase diagram. The challenges of the conceptual difficulties, such as the complex fermion determinant and getting the physics of axial anomaly correct on the lattice make it further attractive. A lot of progress has been made in recent years [1] making it thus a very active field of research. In the early years of lattice QCD, one of the important problem was how to incorporate a finite chemical potential, μ, in the local Dirac operator on the lattice. Naively introducing μ as a Lagrange multiplier of the local point-split conserved charge $\bar{\psi}_x\gamma_4\psi_{x+\hat{0}} + \bar{\psi}_{x+\hat{0}}\gamma_4\psi_x$ led to μ-dependent divergences in the free energy of quarks in the continuum limit. Arguing that since μ enters in the continuum like a fourth component of a static gauge field, the chemical potential should enter on the lattice as $e^{\pm\mu a}$ factors, multiplying the forward and backward temporal gauge links respectively [2]. It did eliminate the undesired divergences mentioned above. However, this proposal is not unique though: weights $(1 \pm a\mu)/\sqrt{(}1 - a^2\mu^2)$ to the temporal links also lead to finite results for the free energy [3]. In fact the most general weights $f(\mu a), g(\mu a)$ should follow $f(a\mu)\cdot g(a\mu) = 1$ with $f(0) = f'(0) = 1$ in order to cure the divergences on the lattice [4]. The analytical proof of absence of divergences in all these cases above was for free quarks. Indeed, further numerical computations in quenched QCD showed it to work for the interacting case as well [5], while a similar check in the full theory is still lacking.

We revisit the problem of introduction of chemical potential on the lattice again with a view to develop a simpler alternative. We foresee two important applications in which the alternative we pursue here may be of practical relevance in the coming years. Heavy ion collision experiments at RHIC at Brookhaven National Laboratory and at FAIR, GSI may likely produce strongly interacting systems at finite density. An important theoretical input for modeling of the evolution of these systems is the QCD equation of state(EoS). In order to calculate the EoS as a function of μ one needs higher order quark number susceptibilities. The latter are also important measurables on the lattice which relate directly to the fluctuations of net baryon number [6] that are being measured in the heavy ion collision experiments. Furthermore, these are also important in estimating the location of the critical point in the QCD phase diagram. The critical point is governed by the singularity of the Taylor expansion of the baryon number susceptibility in μ_B/T. Its location can be determined by the radius of convergence of this Taylor expansion. It, in turn, depends on the ratios of the higher order quark number susceptibilities. Therefore, their accurate and efficient measurement on the lattice is necessary although a rather challenging problem. Having a Dirac operator with a linear μN term, simplifies the problem quite a lot. For example, the number of the inversions of the Dirac operator needed to calculate the eighth order quark number susceptibility with the naive staggered quarks reduces from 20 to 8 [7]. For other improved Dirac operators and even higher order QNS, the gain is even more which leads to a significant reduction of the computational time.

Since the study of QCD critical point would be a major problem of interest in the coming years both from experimental and theory perspective, it is also important to consider how crucial is the role of exact chiral fermions at finite density for the lattice studies. The presence of the critical end-point depends crucially on the number of light quark flavours. Model-based consid-

erations favour its presence for QCD with only two light quarks [8]. In addition, it needs the anomalous $U_A(1)$ symmetry-restoration to take place at sufficiently high temperatures [8]. A moderately heavy strange quark may affect the location of the QCD critical end-point quantitatively but not its existence. Majority of the calculations on QCD at finite density on the lattice employ staggered fermions and its improved versions. However, the continuum flavour and spin symmetries are intermingled for the staggered quarks and the flavour singlet $U_A(1)$ anomaly is recovered only in the continuum limit. As is well-known, the overlap [9] and/or domain wall fermions [10] are much more preferable from the chiral symmetry perspective. They have both the correct chiral and flavour symmetry on lattice as well as an index theorem on the lattice [11, 12]. These are likely to be crucial for investigations of the QCD critical point. At present the computations with chiral fermions are prohibitively expensive.

However, recently domain wall fermions have been used to measure the chiral crossover transition temperature on the lattice [13]. This gives us a hope that with the increase in computational resources and smarter algorithms, use of chiral fermions would be more realistic in the coming years. Non-locality of the overlap fermions makes the introduction of the chemical potential non-trivial. Bloch and Wettig [14] proposed to use the same exponential prescription as above for the timelike links of the Wilson-Dirac kernel $D_W(a\mu)$ to define the corresponding overlap Dirac matrix at nonzero density. The free energy from this overlap fermion action has no a^{-2} divergences [15, 16] in the free case. Unfortunately, however, it has no chiral invariance for nonzero μ either [16]. Using the definition of the chiral projectors for overlap fermions, we [17] proposed a chirally invariant Overlap action for nonzero μ :

$$\begin{aligned} S^F &= \sum_n [\bar{\psi}_{n,L}(aD_{ov} + a\mu\gamma^4)\psi_{n,L} + \bar{\psi}_{n,R}(aD_{ov} + a\mu\gamma^4)\psi_{n,R}] \\ &= \sum_n \bar{\psi}_n [aD_{ov} + a\mu\gamma^4(1 - aD_{ov}/2)]\psi_n \ . \end{aligned}$$

It was shown that the fermion action is invariant under the Luescher transformation [12] and the corresponding order parameter, the chiral condensate in unique for all values of $a\mu$ [17]. Moreover the anomaly is μ-independent on the lattice as is expected from the continuum [18]. It, however, has the same μ-dependent a^{-2} divergences in the number density and the energy density as the linear μ-case for naive/staggered fermions [18]. Furthermore, unlike that case, these cannot be removed by exponentiation of the μ-term [18]. So either one has exact chiral invariance on the lattice or have to deal with the divergences in the continuum limit of $a \to 0$. One needs to understand the origin of these μ-dependent divergences better. In quantum field theories, removal of divergences from physical quantum theories has lead to extensive studies of the different regulators and their suitability for different physical problems. We aim to have an understanding of the nature of the divergences at finite density, and look for methods to remove them in alternate, perhaps simplifying, ways.

2. The divergences at finite density : Why and how to remove them

2.1 Non-interacting fermions at finite chemical potential

As a first step we examined carefully the free dense quark gas in continuum. We found that contrary to the common belief, these divergences are *not* due to lattice artifacts. Indeed, the μ-

dependent divergences exist in the continuum theory as well when appropriate care is taken in manipulating divergent integrals. The lattice regulator simply makes it easy to spot them. Using a Pauli-Villars cut-off Λ in the continuum theory, one can also show the presence of $\mu\Lambda^2$ terms in the number density easily [20]. We will sketch the argument here briefly, referring the reader to [20] for more details. Let us recall that QCD partition function can be written in the path integral formalism as,

$$\mathscr{Z} = \int \mathscr{D}A_\mu \mathscr{D}\bar{\psi}\mathscr{D}\psi e^{\int_0^{1/T} d\tau \int d^3x \left[-1/2\mathrm{Tr}(F^2_{\mu,\nu}) - \bar{\psi}(\gamma_\mu(\partial_\mu - igA_\mu) + m)\psi\right]} \tag{2.1}$$

where $(\bar{\psi})\ \psi$ and A_μ represents the (anti-)fermion and the gluon fields respectively. One introduces a chemical potential μ_i for each conserved charge $\mathscr{N}_i = \int d^3x \bar{\psi}_i \gamma_4 \psi_i$, leading to the additional term $\mu_i \mathscr{N}_i$ in the action above. Canonical definitions consisting of first and second derivative of $\mathscr{Z}$ with respect to $\mu_q = \mu$ yield quark number density and susceptibility,

$$n = -\frac{T}{V}\frac{\partial \ln \mathscr{Z}(\mu)}{\partial \mu}|_{T=fixed} \quad ; \qquad \chi = -\frac{T}{V}\frac{\partial^2 \ln \mathscr{Z}(\mu)}{\partial \mu^2}|_{T=fixed} \tag{2.2}$$

These can be calculated analytically when the gauge interactions are switched off. For simplicity we consider only massless fermions though this derivation can be easily extended to finite quark mass. The expression for the free quark number density is then

$$n = \frac{4iT}{V}\sum_n \int \frac{d^3p}{(2\pi)^3}\frac{(\omega_n + i\mu)}{p^2 + (\omega_n + i\mu)^2} \equiv \frac{4iT}{V}\sum_n \int \frac{d^3p}{(2\pi)^3}\sum_{\omega_n} F(\omega_n, \mu, \vec{p}), \tag{2.3}$$

where $p^2 = p_1^2 + p_2^2 + p_3^2$. All the gamma matrices are Hermitian in our convention. $T = 0$ and $\mu = 0$ corresponds to the vacuum contribution which can be removed by subtracting $n(T = 0, \mu = 0)$. Although this is identically zero for number density, the corresponding subtraction for the energy density is actually $\propto \Lambda^4$. Due to the Fermi-Dirac distribution functions, one does not expect any ultraviolet divergences at finite T. We therefore consider the $T = 0$ contribution of the above expression to examine the presence of divergences, if any. The sum over ω_n turns into a continuous ω integral and the explicit expression for the zero-T contribution to the number density is,

$$n = 4i\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\frac{d^3p}{(2\pi)^3}\frac{(\omega + i\mu)}{p^2 + (\omega + i\mu)^2}\ . \tag{2.4}$$

Under a variable transformation $\omega + i\mu = \omega'$, it can be recast as

$$n = 4i\int_{-\infty+i\mu}^{\infty+i\mu} \frac{d\omega'}{2\pi}\frac{d^3p}{(2\pi)^3}\frac{\omega'}{p^2 + \omega'^2}\ . \tag{2.5}$$

In calculating this expression one considers a suitable contour as shown in Figure 1 with a cut-off Λ for the ω integral in order to regulate the divergent terms, and identify them by powers of Λ. The expression in Eq. 2.5 can be seen to be the line integral 3 in Figure 1. By adding and subtracting the line integrals labelled as $1, 2, 4$, one obtains the result from the contour integral in terms of the residue of the quark propagator pole with the corresponding θ-function defining the Fermi surface and leading to the usual μ^3-term. Out of the subtracted terms, the line integral 1 is exactly zero due to CP symmetry. However, the contribution of the arms 2 and 4 in the Figure 1 clearly do not

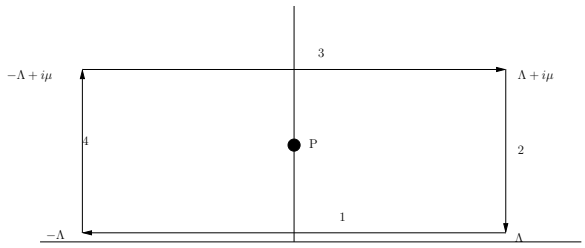

Figure 1: The contour integral used for calculating the zero temperature part of the number density.

cancel each other. The $\mu\Lambda^2$ terms can be shown to arise from the algebraic sum of these terms [20], being of the form $\log\left[\frac{p^2+(\Lambda+i\mu)^2}{p^2+(\Lambda-i\mu)^2}\right]$. In the limit $\Lambda \gg \mu$, and with the same cut-off Λ for momentum p, an expansion in μ/Λ shows that while the leading Λ^3 terms do cancel from the numerator and denominator, the $\mu\Lambda^2$ terms add, and survive. It is easy to see that a similar $\mu^2\Lambda^2$ divergent term persists in the energy density as well. It is amusing to note that the divergence is absent in the number density for nonzero isospin chemical potential with $\mu_B = 0$, since this amounts to putting two flavours of quarks in the Lagrangian with chemical potentials μ_I and $-\mu_I$. The divergent term then cancels explicitly between the two quark flavours since it comes with an equal and opposite sign. The corresponding energy density, however, does have the $\mu^2\Lambda^2$ divergent term. On the other hand, the divergence does exist for imaginary chemical potential for the number density as well, as we show below.

2.2 Non-interacting fermions in presence of imaginary μ

The expression for the number density for free fermions in presence of imaginary chemical potential at zero temperature is

$$n = -4i\int_{-\Lambda}^{\Lambda}\frac{d\omega}{2\pi}\frac{d^3p}{(2\pi)^3}\frac{(\omega-\mu)}{p^2+(\omega-\mu)^2}\ . \tag{2.6}$$

Performing the ω integral, which in this case is on real ω-axis only, one gets,

$$n = -4i\int\frac{d^3p}{(2\pi)^4}\ln\left(\frac{p^2+(\Lambda-\mu)^2}{p^2+(\Lambda+\mu)^2}\right)\ . \tag{2.7}$$

In the limit $\Lambda \gg \mu$, one can again expand the numerator and the denominator of the integrand. As above, we further assume the same cut-off Λ for the momentum integral.

Keeping terms upto $1/\Lambda^3$, one obtains the number density as,

$$n = i\frac{\mu^3}{3\pi^2} + i\frac{\mu\Lambda^2}{4\pi^2}\ . \tag{2.8}$$

The imaginary nature of number density comes out, as expected. Indeed, one recovers the *same quadratic* divergence back if one perform analytic continuation to real μ. This is reassuring since it shows that the presence of divergence for nonzero μ is not due to the particular contour method we chose in Figure 1, as the integrals in this case are performed on the real ω-axis for imaginary chemical potential.

2.3 Free quark gas on the lattice

We have seen that for non-interacting fermions within a cut-off regulator scheme one obtains a $\mu\Lambda^2$ divergence. This explains the presence of a similar divergence in the lattice expression of number density for non-interacting fermions, since the lattice regulator is simply a cut-off regulator and the μ/a^2 term in the number density on a lattice is just a manifestation of the continuum divergence. This can be explicitly seen following the same computation as above. The expression of the number density on a $N^3 \times N_T$ lattice with linear μ and a conserved point-split charge is,

$$na^3 = \frac{i}{N^3 N_T} \sum_{\vec{p},n} \frac{(\sin\omega_n + i\mu a \cos\omega_n)\cos\omega_n}{f + (\sin\omega_n + i\mu a\cos\omega_n)^2} \ . \tag{2.9}$$

where $f = (ma)^2 + \sin^2(ap_1) + \sin^2(ap_2) + \sin^2(ap_3), p_j = 2n_j\pi/N,\ n_j \in Z$. At $T = 0$ one converts the sum over the Matsubara frequencies into an integral, and obtains a line integral in the complex ω plane analogous to the line integral marked 3 in Figure 1. It can be calculated using a contour as in Figure 1 but with $\tanh^{-1}(a\mu)$ in place of μ. Again the residue of the contour integral yields the Fermi surface on a finite lattice even in this method. The divergence now comes from the line integral equivalent to the one marked 1 in Figure 1. On the lattice one can perform the integral over ω to obtain the zero temperature part of the number density. Taking successive derivatives of this term with respect to μ gives the zero temperature artifacts in the linear μ method for the second and fourth order susceptibilities [19]:

$$\chi_{20}(T=0) = -\frac{1}{4N^3}\sum_{\vec{p}}\left(1 - \sqrt{\frac{f}{1+f}}\right) \ , \ \chi_{40}(T=0) = -\frac{3}{4N^3}\sum_{\vec{p}}\left(2 - \frac{3+2f}{1+f}\sqrt{\frac{f}{1+f}}\right) \ . \tag{2.10}$$

3. Testing the idea on the lattice

Having noted that the divergence on the lattice is no different that a Λ-cut-off in the continuum theory, we proposed, and demonstrated, earlier that a subtraction of the $T = 0$ ideal gas term for the quark number susceptibility on the same size N^3 lattice does eliminate the divergence in the continuum limit obtained by sending $N_T \to \infty$ for the free case [19]. Here we concern ourselves with the test of that idea for interacting theory. We calculated the susceptibilities(QNS) for two degenerate quark flavours on quenched lattices with the linear μ Dirac operator [20]. The pure $SU(3)$ gauge configurations were generated using the Cabibbo-Marinari pseudo-heatbath algorithm with three $SU(2)$ subgroup update per sweep using the Kennedy-Pendleton updating method. We generated $N_T = 4, 6, 8, 10$ and 12 lattices and 25-100 independent configurations each at two different temperatures given by $T/T_c = 1.25, 2$. To keep the finite volume effects under control we checked and used $N_s = 4N_T$. The second order QNS was calculated by inverting the Dirac operator on 400 and 500 Gaussian random vectors at $2, 1.25T_c$ respectively. The results obtained using this method contain unphysical μ^2/a^2 and μ^0 artifacts for second and fourth order QNS. For removing them we calculate the corresponding free theory QNS at zero temperature in Eq. (2.10) and perform the continuum extrapolation. The expressions for these $T = 0$ values and the corresponding numerical values are displayed in Table 1. Performing the subtraction, the physical values of the second

N_T	T(MeV)	m/T_c	$\chi_{20}(T=0)$	$\chi_{40}(T=0)$
4			-0.062487	-0.142923
8	1.25		-0.062499	-0.142661
10		0.1	-0.062501	-0.142620
12			-0.062502	-0.142607
4			-0.062541	-0.142999
6	2		-0.062500	-0.142611
8		0.1	-0.062508	-0.142677
10			-0.062512	-0.142718

Table 1: The $T=0$ ideal gas subtraction terms at different volumes and temperatures for the second and fourth order QNS used in this work.

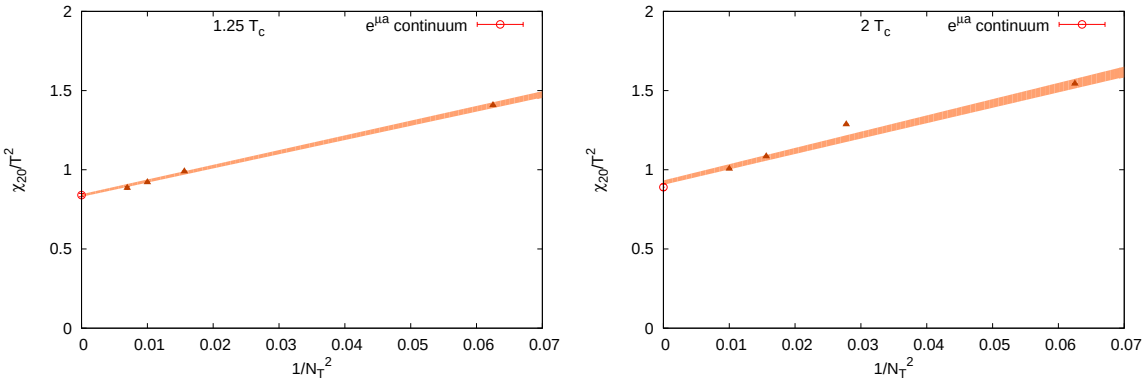

Figure 2: The continuum extrapolated results for the second order quark number susceptibilities in quenched QCD for a quark mass $m/T_c = 0.1$ at $1.25T_c$ (left) and $2T_c$ (right) compared to the corresponding results using the e$^{\mu a}$ method.

order QNS with a quark mass $m/T_c = 0.1$ is shown in Figure 2. We do not observe any divergent term as evident from the positive slope of the data. Moreover, our extrapolated continuum result coincides with the earlier result obtained with the $\exp(\pm a\mu)$ action [5, 22], marked with red open circles on the vertical axis of each figure. In other to check that there are no mass dependent divergent terms we calculated the second order QNS with a still lower quark mass $m/T_c = 0.01$, the continuum extrapolated results shown in the left panel of Figure 3. We indeed confirm absence of any new divergences from the slope of the fitted curve. Furthermore, removing the free theory $T=0$ artifacts from the fourth order QNS also gives the correct continuum limit as evident from the right panel of Figure 3. For the QNS χ_n , $n \geq 6$, the additional artifacts in the linear μ method are $\mathcal{O}(a^{n-4})$, hence do not affect the continuum extrapolation of the lattice results. Moreover these terms reduce the cut-off effects compared to the e$^{\mu}$a-method and facilitate a smoother approach to the continuum [19].

4. Summary

We did a comprehensive study of the possible origin of the μ^2/a^2 divergences in the quark

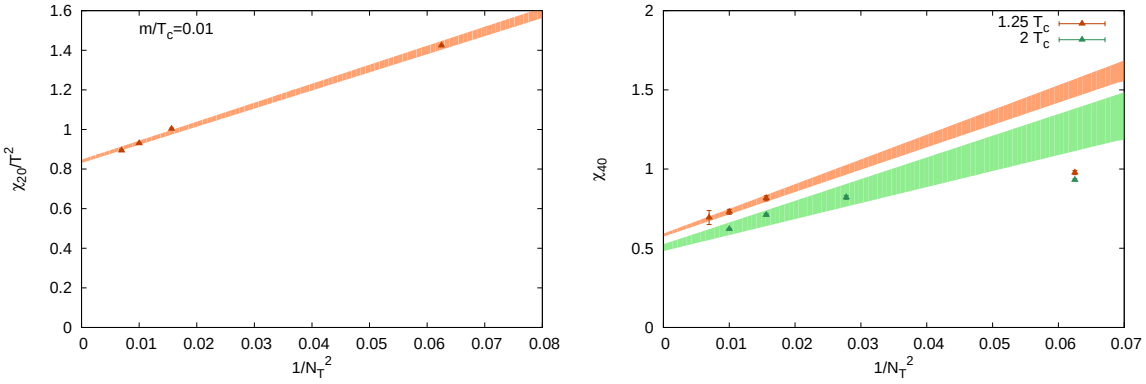

Figure 3: The continuum extrapolated results for the second order quark number susceptibilities for a lighter quark mass $m/T_c = 0.01$ at $1.25T_c$ (left) and the results for the fourth order susceptibility for the quark mass $m/T_c = 0.1$ (right).

number susceptibility on the lattice when we introduce chemical potential as a μN term in the fermion action, N being the conserved number density on the lattice. We found out that such a divergence explicitly exist for the QNS of free fermions with a cut-off regulator. The lattice regulator just faithfully reproduces this divergence for the free fermions as well. Conserved charges are not renormalized. Assuming therefore that the only divergence that would exist for QCD on the lattice is due to the μN term of the free theory, we did an explicit check in quenched QCD by taking the continuum limit of the second and the fourth order ideal gas subtracted QNS. We indeed find that there are no additional divergences that arise due to interactions. The divergence in the linear μ-method can be removed easily which gives us another path towards introducing μ on the lattice in addition to the most popular method [2] where one modifies the quark action at finite μ to remove these divergences explicitly. This method may be beneficial for calculating the higher order QNS with considerably less computational effort allowing us to calculate the Lattice EoS at finite baryon chemical potential and make progress towards measuring the critical end-point.

References

[1] G. Aarts, Proceeding of this conference .

[2] P. Hasenfratz and F. Karsch *Phys. Lett.* B125, 308 (1983); J. Kogut *et al., Nucl. Phys.* B 225, 93 (1983).

[3] N. Bilic and R. V. Gavai *Z. Phys.* C23, 77 (1984).

[4] R. V. Gavai, *Phys. Rev.* D32, 519 (1985).

[5] R. V. Gavai and S. Gupta, *Phys. Rev.* D67, 034501 (2003).

[6] R. V. Gavai and S. Gupta, *Phys. Lett.* B696, 459 (2011).

[7] R. V. Gavai and S. Sharma, *Phys. Rev.* D81, 034501 (2010).

[8] R. D. Pisarski and F. Wilczek, *Phys. Rev.* D29, 338 (1984).

[9] R. Narayanan and H. Neuberger, *Phys. Rev. Lett.* 71, 3251 (1993); H. Neuberger, *Phys. Lett.* B417, 141 (1998).

[10] D. Kaplan, *Phys. Lett.* B288, 342 (1992).

[11] P. Hasenfratz, V. Laliena and F. Neidermeyer, *Phys. Lett.* B427, 125 (1998).

[12] M. Luscher, *Phys. Lett.* B428, 342 (1998).

[13] T. Bhattacharya et. al., *Phys. Rev. Lett.* 113, 082001 (2014).

[14] J. Bloch and T. Wettig, *Phys. Rev. Lett.* 97, 012003 (2006);
J. Bloch and T. Wettig, *Phys. Rev.* D76, 114511 (2007).

[15] C. Gattringer and L. Liptak, *Phys. Rev.* D76, 054502 (2007).

[16] D. Banerjee, R. V. Gavai and S. Sharma, *Phys. Rev.* D78, 014506 (2008);
D. Banerjee, R. V. Gavai and S. Sharma, *PoS (LATTICE 2008)*, 177.

[17] R. V. Gavai and S. Sharma, *Phys. Lett.* B **716**, 446 (2012).

[18] R. Narayanan and S. Sharma, *JHEP* **1110**, 151 (2011);

[19] R. V. Gavai and S. Sharma, *Phys. Rev.* D85, 054508 (2012).

[20] R. V. Gavai and S. Sharma, `arXiv:1406.0474` [hep-lat].

[21] R. V. Gavai and S. Gupta, *Phys. Rev.* D78, 114503 (2008).

[22] S. Mukherjee, *Phys. Rev.* D74, 054508 (2006).