Conundrums at Finite Density

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Introduction

- QCD Partition Function : $Z_{QCD} = \mathrm{Tr}\ \exp[-(H_{QCD} - \mu_B N_B)/T]$ $= \sum_{n_B} z^{n_B} Z^C(n_B, T)$, where fugacity $z = \mu_B/T$.

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- Price to pay : Massive Computations, since integrations have to be done over quark and gluon fields.

- Remember : Euclidean Path Integral properly defined by discretizing the space-time on which the fields are defined. Only Gaussian integrals defined otherwise.

The $\mu \neq 0$ problems : I. Divergences

♠ Well-known that no new divergences arise in field theories with nonzero temperature and/or density.

♢ So what are these divergences ? Are they lattice artifacts ? Are there any striking conceptual issues worth discussing ?

The $\mu \neq 0$ problems : I. Divergences

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♢ So what are these divergences ? Are they lattice artifacts ? Are there any striking conceptual issues worth discussing ?

♡ Recall that the naıvely discretized fermionic action is

$$S^F = \sum_{x,x'} \bar{\psi}(x) \left[\sum_{\mu=1}^{4} D^\mu(x,x') + ma\delta_{x,x'} \right] \psi(x'),$$

where

$$D^\mu(x,x') = \frac{1}{2}\gamma^\mu \left[U_x^\mu \delta_{x,x'-\hat{\mu}} - U_{x'}^{\mu\dagger} \delta_{x,x'+\hat{\mu}} \right].$$

♣ Easy to follow the canonical method to write a current conservation equation: $\sum_\mu \Delta_\mu J_\mu^{lat} = 0$, and obtain the conserved charge.

$\diamondsuit$ Conserved charge is the natural point-split for $N = \sum_x \bar{\psi}(x)\gamma^4[U_x^{4\dagger}\psi(x+\hat{4}) + U_x^4\psi(x-\hat{4})]/2$. Adding the chemical potential to the action above therefore amounts to weights $f(a\mu) = 1 + a\mu$ & $g(a\mu) = 1 - a\mu$ to forward and backward time links respectively.

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♣ This leads to μ-dependent a^{-2} divergences in energy density and quark number density even in the free theory!

$$\begin{aligned} \epsilon &= c_0 a^{-4} + c_1\mu^2 a^{-2} + c_3\mu^4 + c_4\mu^2 T^2 + c_5 T^4 \\ n &= d_0 a^{-3} + d_1\mu a^{-2} + d_3\mu^3 + d_4\mu T^2 + d_5 T^3 . \end{aligned} \tag{1}$$

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♠ Subtracting off vacuum contribution at $T = 0 = \mu$, eliminates the leading divergence in each case but the μ-dependent divergence persists.

♡ Hasenfratz-Karsch (PLB 1983) & Kogut et al. (PRD 1983) proposed to modify the weights to $\exp(\pm a\mu)$ to obtain finite results while simultaneously Bilić-Gavai (EPJC 1984) showed $(1 \pm a\mu)/\sqrt{(1 - a^2\mu^2)}$ also lead to finite results.

$\diamondsuit$ Indeed, in general *any* set of functions f, g, satisfying $f(a\mu) \cdot g(a\mu) = 1$ with $f(0) = f'(0) = 1$ suffice (Gavai, PRD 1985).

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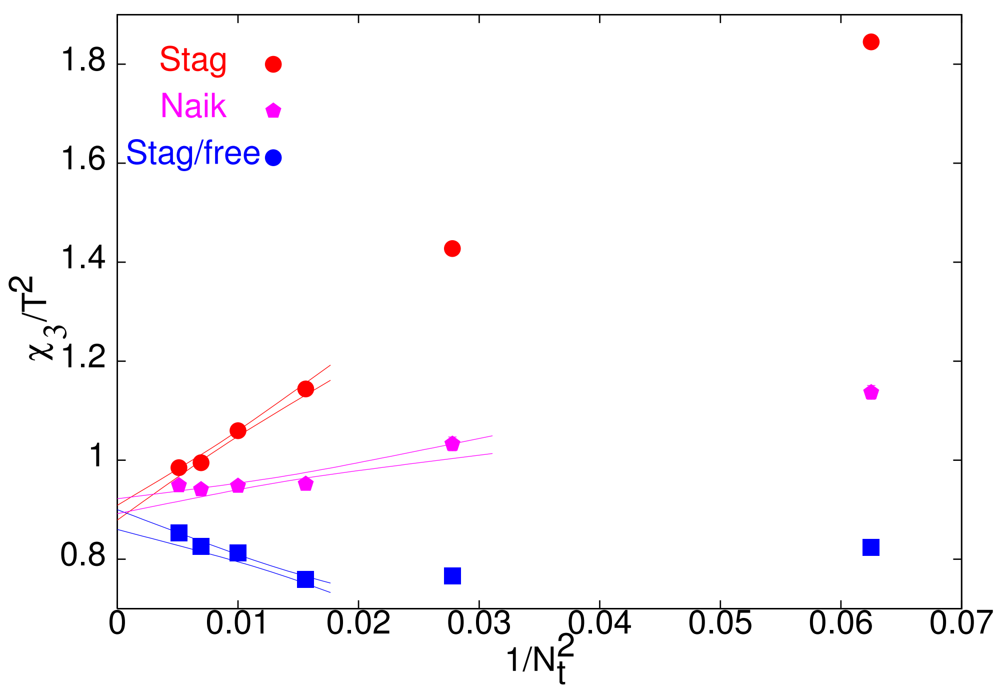
♡ Note that the analytical proof was *only* for free quarks & thus pert. theory. Numerical computations had to be performed to show that it worked for the non-perturbative interacting case as well (Gavai-Gupta PRD 67, 034501 (2003)) :



$\diamondsuit$ Question : Why, and how, does lattice introduce this divergence? or Does it really ?

$\clubsuit$ It was argued [Hasenfratz-Karsch (PLB 1983)] that the divergence arises on the lattice due to the lack of a "formal" gauge symmetry: In continuum theory, μ term appears as a 4^{th} component of a constant (imaginary) gauge field. All the forms above restore this formal symmetry on lattice.

$$f(a\mu) \cdot g(a\mu) = 1 \Leftrightarrow F(a\mu) = \exp(\ln f(a\mu)). \tag{2}$$

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$\spadesuit$ Amusing to note though that **only irrelevant** terms distinguish the naıve $f, g = 1 \pm \mu a$ from those above : only $\mathcal{O}(\mu a)^2$ or higher.

$\heartsuit$ *Paradox :* These terms vanish from action as $a \to 0$ but do eliminate divergences. Apparent violation of universality ? !! Terms not there in the continuum theory, so divergences ?

♣ Problem : With *any* of these functions above, one has **no** conserved charge on lattice anymore ! Alternatively $Z \neq \exp(-\beta[H - \mu N])$ on the lattice for them. Possible only in the continuum limit of $a \to 0$.

♣ One cannot define an *exact* canonical partition function on lattice from the Z defined this way. $Z \neq z^n Z_n^C$ on lattice.

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♢ Finally, only quark loops winding around the T direction contribute to μ_B dependence since other loops have equal number of factors of f and g always.

♠ On the other hand, all quark loops contribute for f,$g = 1 \pm \mu a$, as indeed in the continuum case.

Divergences exist in Continuum too

- It turns out that contrary to common belief, divergences are **NOT** a lattice artifact. The "formal gauge" symmetry has nothing to do with them.

- Indeed lattice regulator simply makes it easy to spot them. Using a momentum cut-off Λ in the continuum theory, one can show the presence of $\mu\Lambda^2$ terms in number density easily (Gavai-Sharma, 1406.0474).

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- The quark number density, or equivalently (1/3) the baryon number density, is defined as,

$$n = \frac{T}{V}\frac{\partial \ln \mathcal{Z}}{\partial \mu}\Big|_{T=\mathrm{fixed}} \tag{3}$$

with $\mathcal{Z}$ for free fermions given by

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \mathrm{e}^{\int_0^{1/\mathrm{T}} \mathrm{d}\tau \int \mathrm{d}^3\mathrm{x}\left[-\bar{\psi}(\gamma_\mu\partial_\mu + \mathrm{m} - \mu\gamma_4)\psi\right]}, \tag{4}$$

- Evaluating n in the momentum space, the expression for the number density is

$$n = \frac{2iT}{V} \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{(\omega_n - i\mu)}{p^2 + (\omega_n - i\mu)^2} \equiv \frac{2iT}{V} \int \frac{d^3p}{(2\pi)^3} \sum_{\omega_n} F(\omega_n, \mu, \vec{p}), \quad (5)$$

where $p^2 = p_1^2 + p_2^2 + p_3^2$ and $\omega_n = (2n+1)\pi T$. The gamma matrices are all Hermitian.

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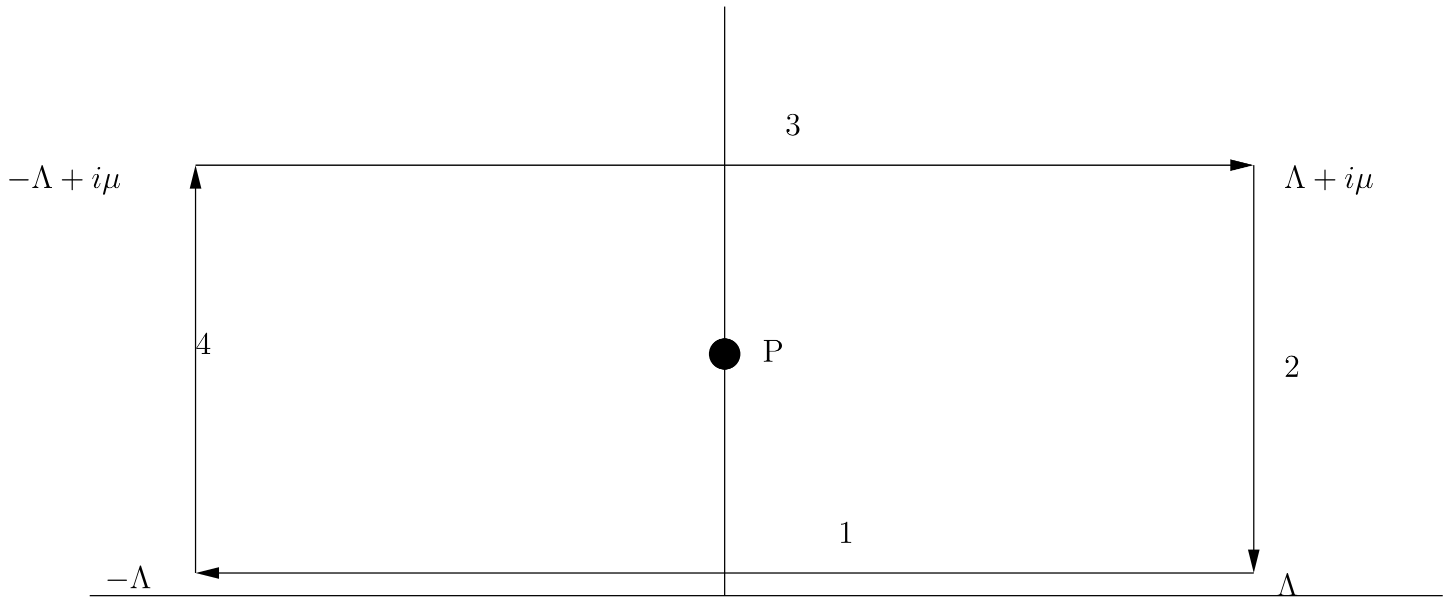
- In the usual contour method, the sum over n gets replaced as sum of integrals in the complex ω-plane:

$$n = \frac{2i}{\pi} \left[\oint_{Im\omega<0} \frac{F(\omega,\mu)d\omega}{\mathrm{e}^{\mathrm{i}\omega/\mathrm{T}} + 1} - \oint_{Im\omega>0} \frac{F(\omega,\mu)d\omega}{\mathrm{e}^{-\mathrm{i}\omega/\mathrm{T}} + 1} + \int_{-\infty}^{\infty} F(\omega,\mu)d\omega \right] . \quad (6)$$

- Introduce a cut-off Λ for all 4-momenta at $T = 0$ for a careful evaluation of the last term. Together with the subtracted (μ=0) contribution, one can rewrite in the complex ω-plane:



- The $\mu\Lambda^2$ terms arise from the arms 2 & 4 in figure above. (Gavai-Sharma, arXiv 1406.0474) :

$$\begin{aligned}
\text{Sum of } 2+4 &= \int \frac{d^3p}{(2\pi)^3} \left(\int_2 + \int_4 \right) \frac{d\omega}{\pi} \frac{\omega}{p^2+\omega^2} \\
&= -\frac{1}{2\pi} \int \frac{d^3p}{2\pi^3} \ln \left[\frac{p^2+(\Lambda+i\mu)^2}{p^2+(\Lambda-i\mu)^2} \right] .
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\end{aligned}
$$

- One usually *assumes* this sum to cancel for $\mu \neq 0$ by setting Λ infinite. However, since $\Lambda \gg \mu$, expanding in μ/Λ, one finds the leading Λ^3 terms indeed cancel but there is a nonzero coefficient for the $\mu\Lambda^2$ term.

- Ignoring the contribution from the arms 2 & 4 amounts to a subtraction of the 'free theory divergence' in continuum !

- Note also that the arms 2 & 4 make a finite contributions to the μ^3 term as well.

- Why did this remain unnoticed, even in text books ?

- Often one uses T as the cut-off in analytic computations and does frequency sums on $\omega_n = (2\pi n + 1)T$ *first* [Kapusta-Gale Book].

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- Since these divergences exist in the continuum, and are simply subtracted for the free theory, one may follow the prescription of subtracting the free theory divergence by hand on Lattice as well.

Testing the idea

- In order to test whether the divergence is truly absent in simulations as well, one needs to take the continuum limit $a \to 0$ or equivalently $N_t \to \infty$ at fixed $T^{-1} = aN_t$.

- This was tested for quenched QCD. (Gavai-Sharma, 1406.0474). For $m/T_c = 0.1$, $N_t = 4$, 6, 8, 10 and 12 lattices were employed. On 50-100 independent configurations different susceptibilities were computed at $T/T_c = 1.25$, & 2.

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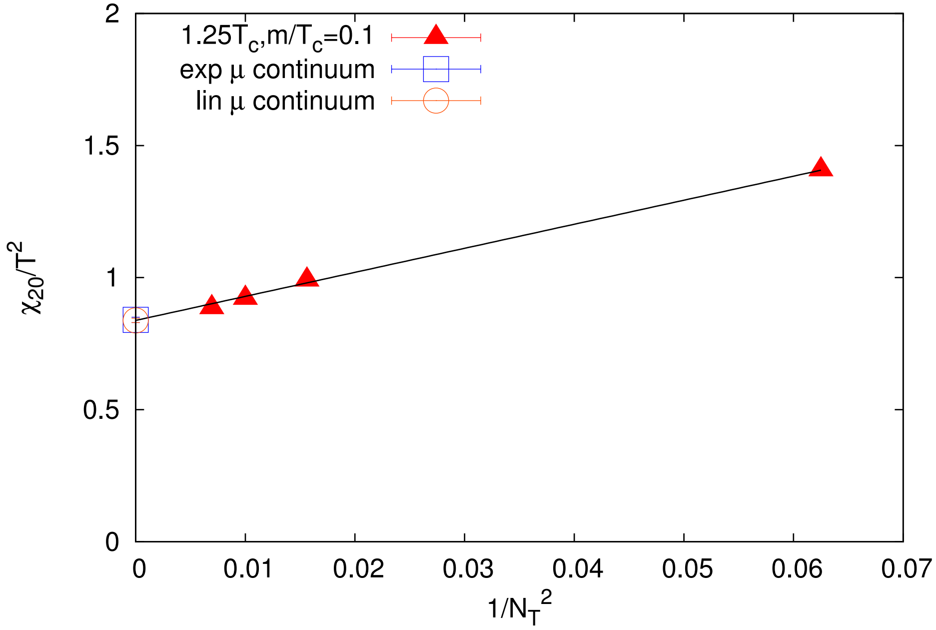
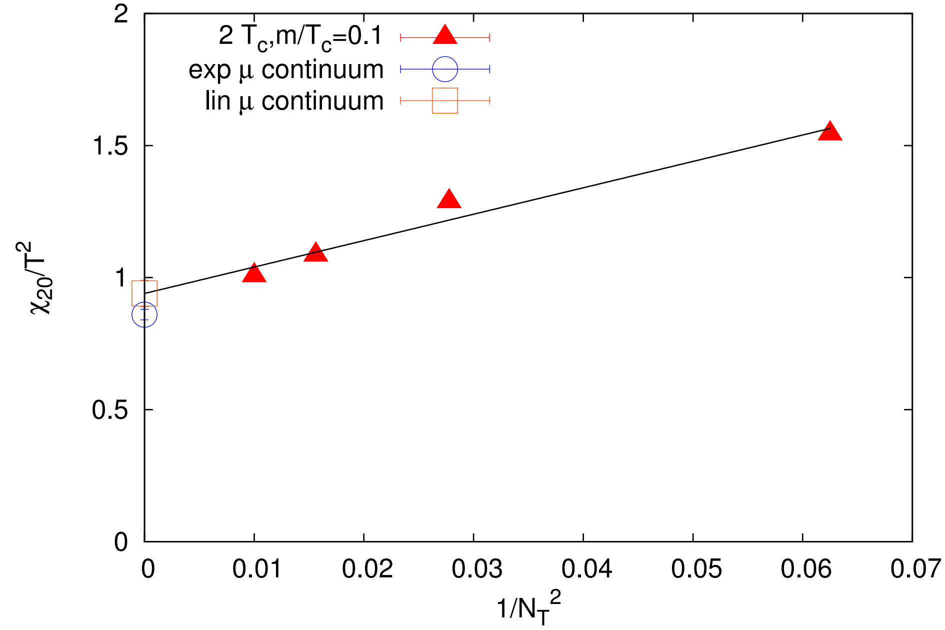
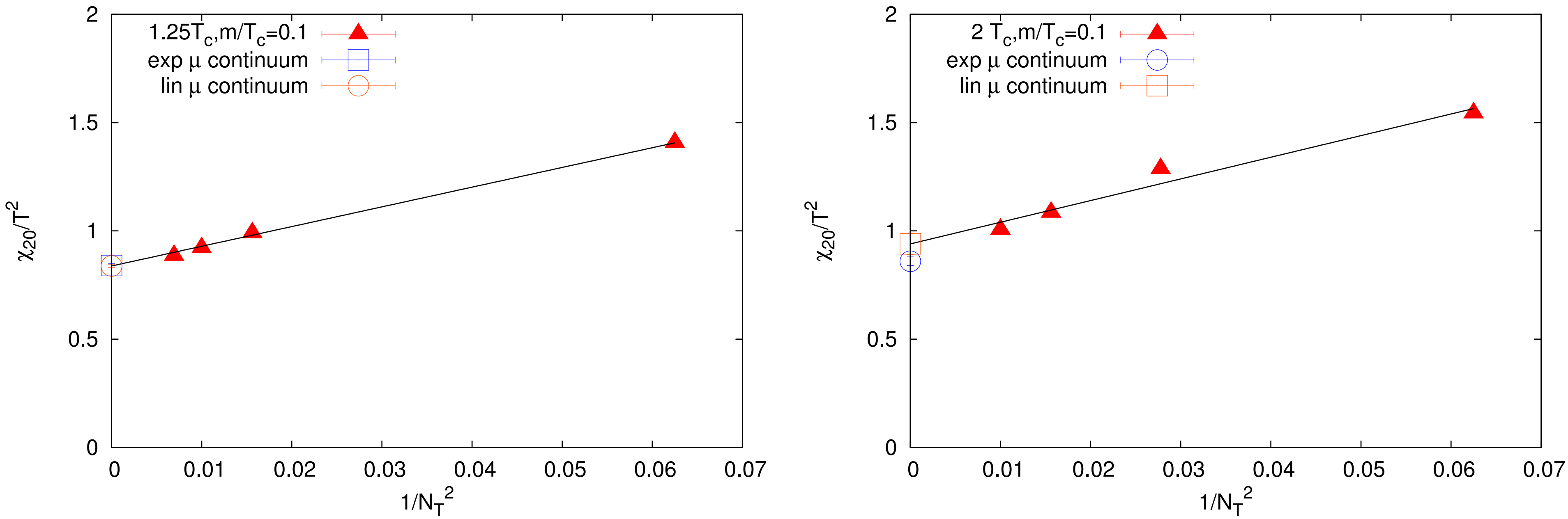
- $1/a^2$-term for free fermions on the corresponding $N^3 \times \infty$ lattice was subtracted from the computed values of the susceptibility.

- Expect χ_{20}/T^2 to behave as $\chi_{20}/T^2 = c_1(T) + c_2(T)N_T^2 + c_3(T)N_T^{-2} + \mathcal{O}(N_T^{-4})$.





- Absence of any quadratically divergent term is evident in the positive slope of the data. Logarithmic divergence cannot be ruled out with our limited N_t data.



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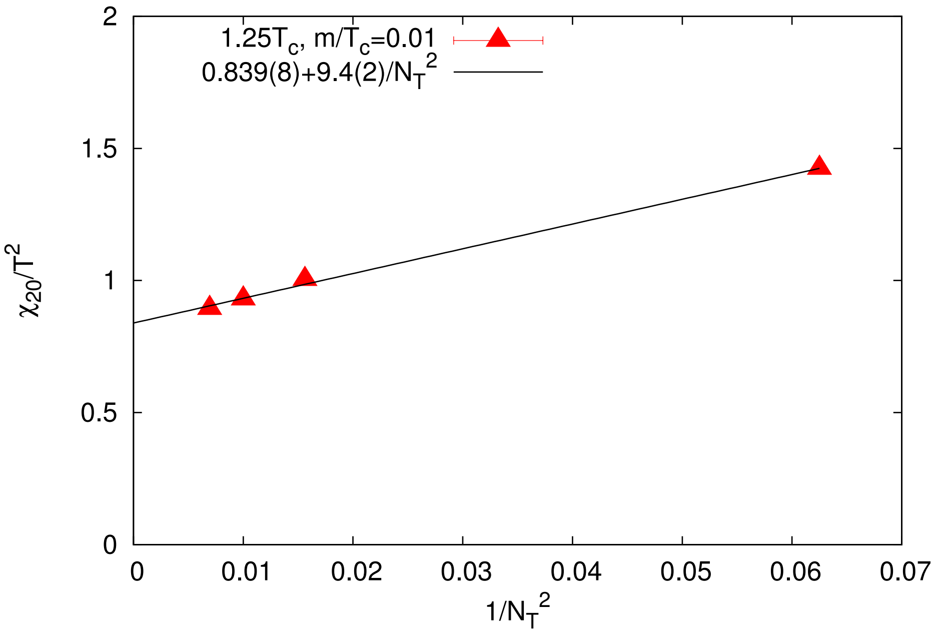
- Furthermore, the extrapolated continuum result coincides with the earlier result obtained with the $\exp(\pm a\mu)$ action (Swagato Mukherjee PRD 2006).

- Lowering the mass by a factor of 10 to $m/T_c = 0.01$ the exercise was repeated at a lower temperature on $T/T_c = 1.25$.



- Again no divergent term is evidently present in the slope of the data.

- Higher order susceptibility show similar finite result in continuum limit.

The $\mu \neq 0$ problem : II. Quark Type

- Mostly staggered quarks used in these simulations. Broken flavour and spin symmetry on lattice. Moreover, NO flavour singlet $U_A(1)$ symmetry or anomaly. Critical point needs $N_f = 2$ and anomaly to persist by T_c.

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- Introduction of μ a la "Formal" gauge symmetry by Bloch & Wettig (PRL 2006 & PRD2007).

- Unfortunately BW-prescription breaks the lattice chiral symmetry ! (Banerjee, Gavai & Sharma PRD 2008; PoS (Lattice 2008); PRD 2009) Furthermore, anomaly for it depends on μ unlike in continuum QCD (Gavai & Sharma PRD 2010).

- Good News : Action with Continuum-like (flavour & spin) symmetries for quarks at nonzero μ and T proposed already. (Gavai & Sharma , arXiv : 1111.5944).

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- It was shown why this is physically the right thing to do. Using Domain Wall formalism, one discovers that such an action counts only the physical (wall) modes.

- Bad News (or is it?): Chirally invariant Overlap action with nonzero μ only in the linear form, i.e., with the divergence. Interestingly, even the exponential form leads to divergences in this case [Narayanan-Sharma JHEP 1110(2011)151].

The $\mu \neq 0$ problem : III. Complex Measure

Physical(thermal expectation) value of an observable $\mathcal{O}$ is

$$\langle \mathcal{O} \rangle = \int DU \left[\frac{\exp(-S_G)\ \mathrm{Det}^{N_f}\ M(m,\mu)}{\mathcal{Z}} \right] \mathcal{O},$$

where the QCD partition function $\mathcal{Z}$ is

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Typically 8-9 million dimensional integral and M is million $\times$ million. Probabilistic methods are therefore used to evaluate $\langle \mathcal{O} \rangle$.

$\Longrightarrow$ Simulations can be done IF Det^{N_f} $M > 0$ for any set of $\{U\}$. However, Det M is a complex number for all $\mu \neq 0$: The Phase/sign problem

Lattice Approaches

Several Approaches proposed in the past two decades : None as satisfactory as the usual $T \neq 0$ simulations. Still scope for a good/great idea !

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- A partial list :
  - Suitable variables for measure (Chandrasekharan EPJA 90(2013); Gattringer Pos LATTICE 2013).
  - Two parameter Re-weighting (Z. Fodor & S. Katz, JHEP 0203 (2002) 014).
  - Density of States (Langfeld & Lucini PRD 90 (2014)).
  - Imaginary Chemical Potential (Ph. de Forcrand & O. Philipsen, NP B642 (2002) 290; M.-P. Lombardo & M. D'Elia PR D67 (2003) 014505).
  - Taylor Expansion (R.V. Gavai and S. Gupta, PR D68 (2003) 034506 ; C. Allton et al., PR D68 (2003) 014507).
  - Canonical Ensemble (K. -F. Liu, IJMP B16 (2002) 2017, S. Kratochvila and P. de Forcrand, Pos LAT2005 (2006) 167.)
  - Complex Langevin (G. Aarts and I. O. Stamatescu, arXiv:0809.5227 and its references for earlier work).
- Why Taylor series expansion? — i) Ease of taking continuum and thermodynamic limit & ii) Better control of systematic errors.

The $\mu \neq 0$ problem : IV. Topology

♣ The Overlap Dirac operator spectra has been used to understand the nature of the high temperature phase.

♢ Number of low eigen modes do get depleted as $T \uparrow$. (Edwards-Heller-Kiskis-Narayanan, PRL '99, NPB (PS) '00, PRD '01; Gavai-Gupta-Lacaze, PRD '02)

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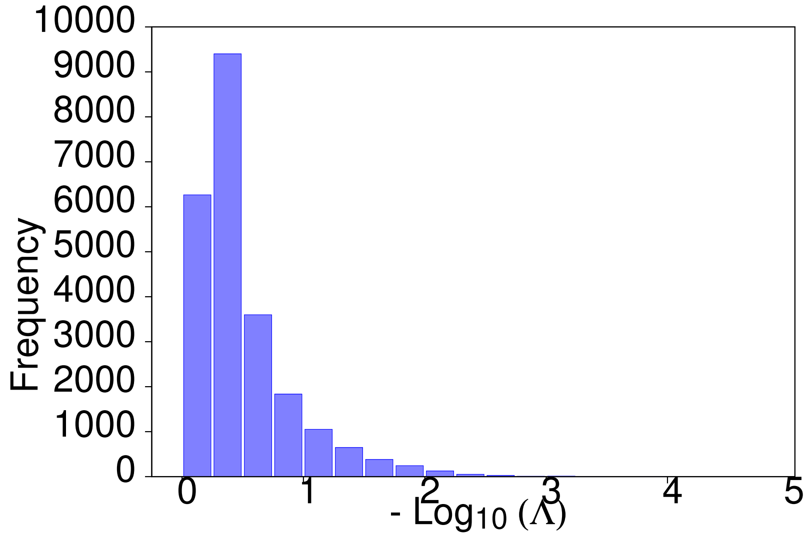
♠ What about finite μ ? This question has been addressed at nonzero isospin density in QCD as well as two colour QCD, both of which do not have a sign problem.

♡ A lot of work on both cases, studying the phase structure. In particular, both are known to show an increase in number density and the Polyakov loop at the same place.

♣ However very little/no change is seen the number of zero modes or topological susceptibility. (Bali-Endrődi-Gavai-Mathur, 1610.00233, Lat2017; Iida-Itou-Lee 1920.07872)

♡ Zooming in on the eigenvalue distribution on the log scale to see if the near-zero modes have any difference in the two phases.



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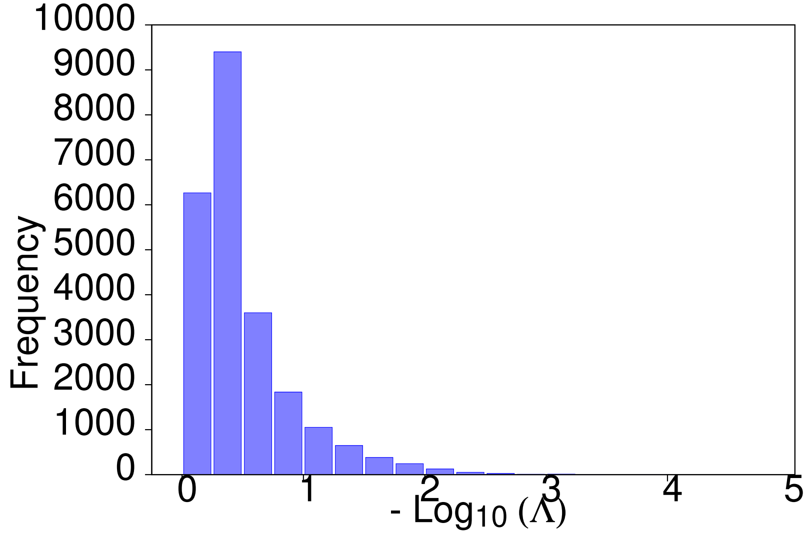

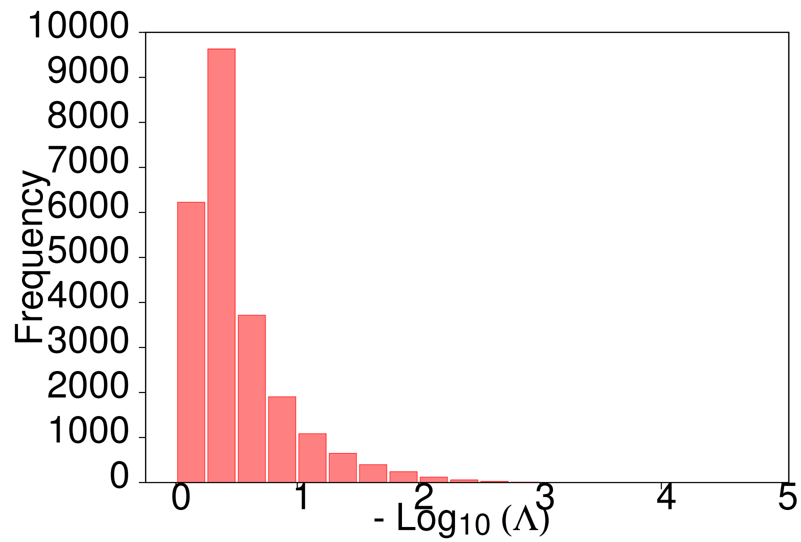

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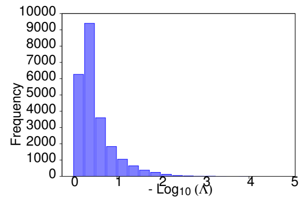
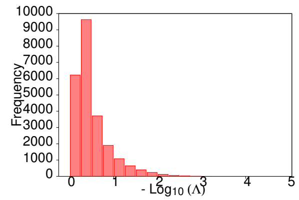
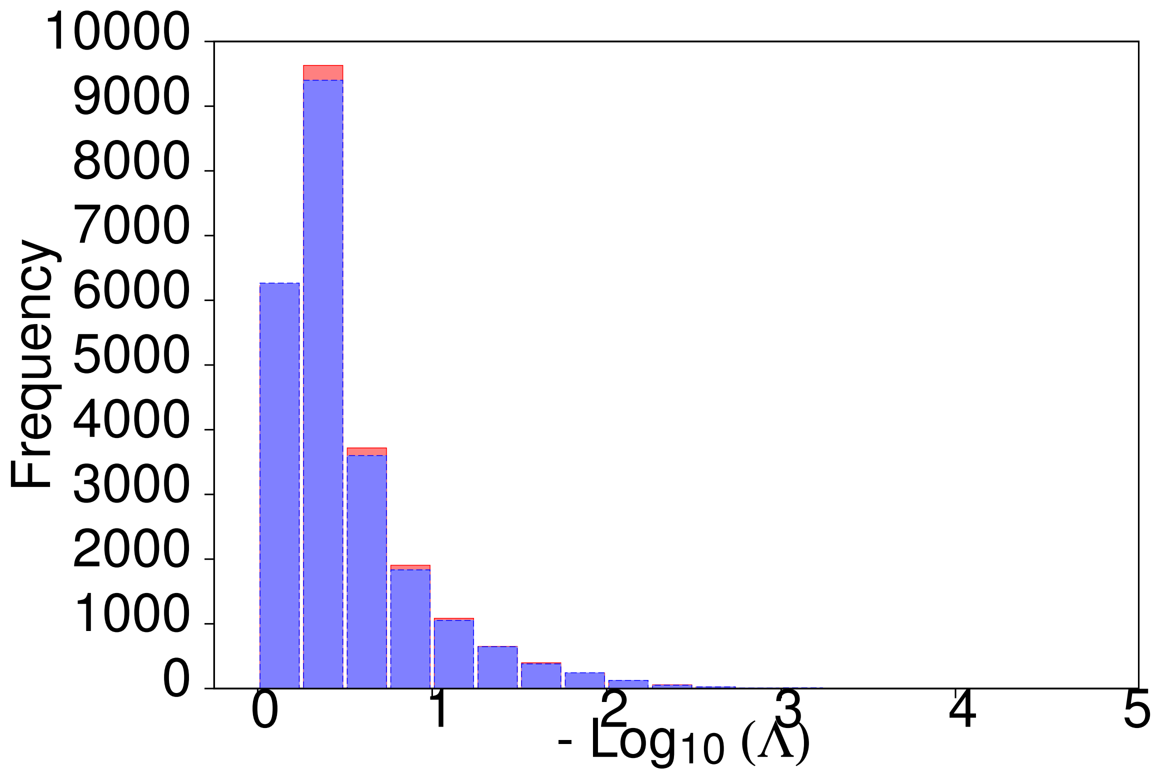
♡ $\mu_I/\mu_I^c = 1.5$: Similarity in the distribution as in the lower phase clearly indicated.







♡ No visible difference in the near-zero mode distributions.

What about Zero Modes?

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♢ Zero modes are *not* degenerate & come with specific chirality, +ve or -ve. Hence, these act as a direct measure of topology.

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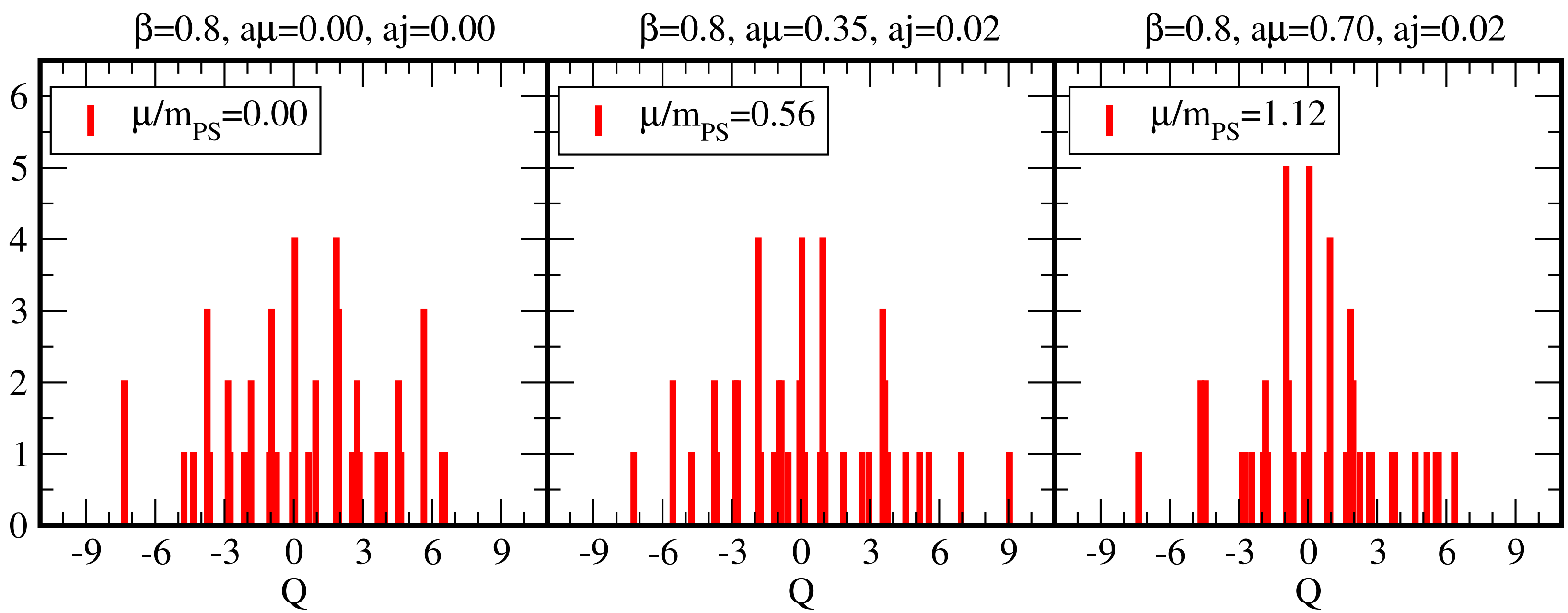
• For $\mu_I \neq 0$, we find for *same* number of configs (50) :

μ_I/μ_I^c	$N_{zero}^{0.11}$	$N_{zero}^{0.44}$
0.5	426	477
1.5	451	332
3.0	437	396
4.0	–	562

• No variation across μ_I^c for $\lambda/m_{ud} = 0.11$ & a mild dip for $\lambda/m_{ud} = 0.44$ (25% reduction at μ_I/μ_I^c=1.5)

Topology for Two-Color QCD

♡ Recently Iida-Itou-Lee arXiv:1910.07872 have reported similar results for topology for two-color QCD:



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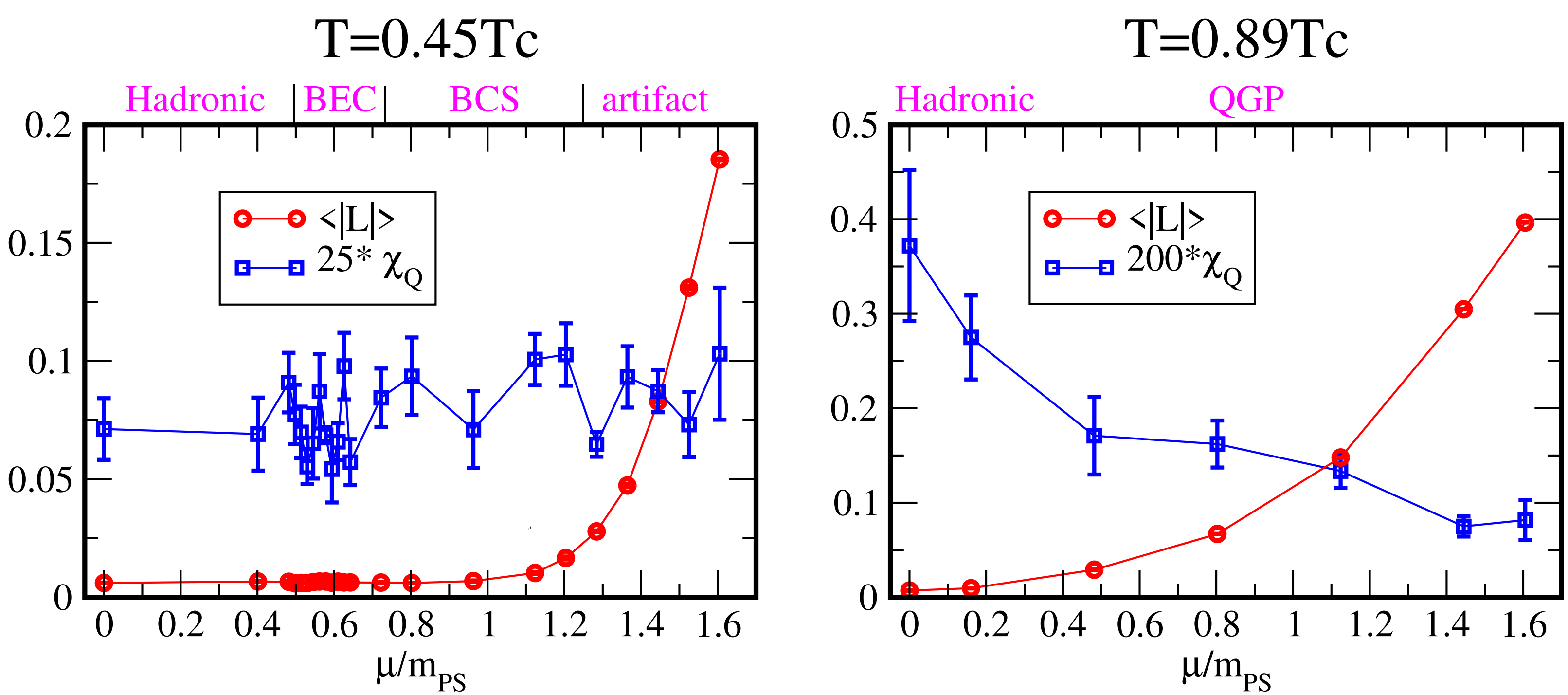
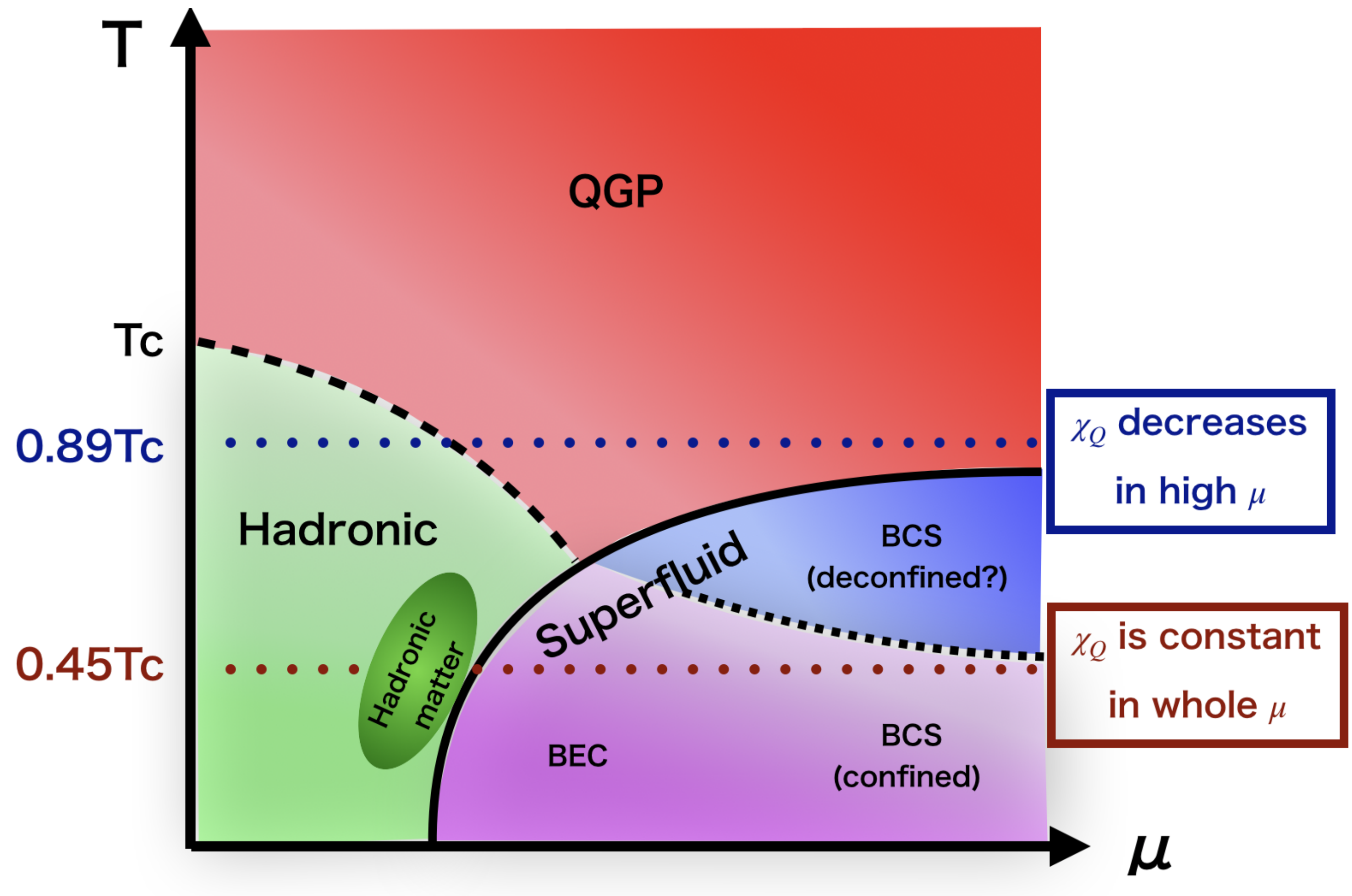


♠ Interestingly, they report both the decrease in χ_t in going to the high T phase, and no change in the low T phase as μ is changed.



Summary

- μ-dependent divergence is not unique to Lattice. Indeed, Lattice only reproduces faithfully what exists in the continuum field theory.

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Summary

- μ-dependent divergence is not unique to Lattice. Indeed, Lattice only reproduces faithfully what exists in the continuum field theory.

- Subtraction of free theory divergences suffices even nonperturbatively. Proof limited to numerical simulations only, but so it is for the exponential prescription where analytic proof exists only for free theory.

- Chiral invariance crucial for critical point investigations but insisting on it for overlap quarks at finite density seems to always lead to a μ-dependent divergence for free quarks.

- Simulations suggest that the distribution of Q or zero modes of Overlap Dirac operator across the phase transition in μ, where $\langle L \rangle$ takes-off, changes very little in the low T phase in contrast to the change to high T phase, which at $\mu = 0$ exhibits an exponential fall-off.