Fluctuations, correlations and some other recent results from lattice QCD

Swagato Mukherjee
Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA
E-mail: swagato@bnl.gov

Abstract. I summarize recent results from lattice QCD on a few selected topics which are of interest to the heavy-ion physics community. Special emphasis is placed upon observables related to fluctuations of conserved charges and their connection to event-by-event fluctuations in heavy-ion collision experiments.

1. Transition temperature of QCD

At high temperatures and/or densities ordinary hadronic matter is expected to undergo a transition to a new form of matter, viz. the Quark Gluon Plasma (QGP). The spontaneously broken chiral symmetry of Quantum Chromodynamics (QCD) is also expected to become restored at this point. The temperature at which such a transition takes place is generally referred to as the QCD transition temperature ($T_c$). The value of $T_c$ is one of the most basic input from lattice QCD to the heavy-ion phenomenology. At present almost all the precision state-of-the-art finite temperature/density lattice QCD computations are being performed using computationally cheaper staggered fermion discretization scheme. At any non-zero lattice spacing ($a$) staggered fermions give rise to a distorted hadron spectrum, which apart from containing a single Goldstone pion also contains 15 unphysical pions. Masses of these unphysical pions are larger than the Goldstone pion and the physical hadron spectrum is obtained only in the continuum limit $a \to 0$. Since the chiral property of the staggered fermions are sensitive to the masses of these unphysical pions it is essential to reduce their masses (relative to the mass of the Goldstone pion) while studying the QCD transition.

One of the major progress made during the last couple of years in reducing this lattice artifact is the use of Highly Improved Staggered Quark (HISQ) action. The HISQ action largely reduces the masses of these unwanted pions even for relatively coarser lattices and consequently facilitates the continuum $a \to 0$ extrapolation using moderate values lattice spacings. In this conference the HotQCD collaboration presented [1] their latest results on $T_c$ obtained from observables related to the chiral symmetry restoration using two different types of fermion discretization (viz. HISQ and Asqtad actions) giving consistent results in the continuum $a \to 0$ limit. HotQCD collaboration
has also performed interpolations/extrapolations of their results to the physical values of quark masses using \(O(N)\) scaling analysis. At the physical quark masses the continuum extrapolated value for the transition temperature is \([1, 2]\) — \(T_c = 157 \pm 4 \pm 3 \pm 1\) (HotQCD preliminary). These latest results from the HotQCD collaboration is in excellent agreement with the previously published results \(T_c = 147 - 157\) MeV, obtained using observables which are sensitive to the light quarks) of the Wuppertal-Budapest collaboration \([3, 4]\).

2. Universal properties of the chiral transition

The nature of the QCD transition depends crucially on the values of the quark masses. As for example, Fig. 1(a) shows a sketch of the nature of the transition as functions of the quark masses for a theory with two degenerate light (up and down) quarks with masses \(m_l = m_u = m_d\) and a heavier strange quark with mass \(m_s\) at zero baryon chemical potential. In the limit \(m_l \to 0\) and \(m_s \to \infty\), the relevant symmetry is isomorphic to the 3-d \(O(4)\) spin model and the transition is second order belonging to the 3-d \(O(4)\) universality class. For \(m_l = m_s \to 0\) the transition is first order. In the intermediate quark mass region a (rapid) crossover takes place from the hadronic to the QGP phase. The first order region is separated from the crossover region by a line of second order phase transitions belonging to the 3-d Ising \(Z(2)\) universality class. The first order region, the second order \(Z(2)\) and the second order \(O(4)\) lines meet at a tri-critical point characterized by a certain value \(m_s^{tc}\) of the strange quark mass. While it is well established that for the physical values of the quark masses \(m_l = m_l^{phys}, m_s = m_s^{phys}\) the transition is a crossover \([5]\) the location of the physical point in the context of Fig. 1(a) remains an open issue. More specifically, if \(m_s^{phys} > m_s^{tc}\) then in the limit \(m_l \to 0\) one should see a second order transition belonging to the 3-d \(O(4)\) universality class. On the other hand, if \(m_s^{phys} < m_s^{tc}\) then in \(m_l \to 0\) limit the transition should be first order.

This question can be addressed by studying the the universal scaling behavior of the
chiral transition as a function of decreasing light quark mass while keeping the strange quark mass fixed at its physical value. In the vicinity of a second order phase transition the behavior of the free energy of a system is largely governed by the universal scaling properties—

\[ f(m_l, m_s, T, \mu_B) = h^{1+1/\delta} f_s(z) + f_{\text{reg}}(m_l, m_s, T, \mu_B), \]

where \( h = m_l / (h_0 m_s) \) and \( t = (T - T_0) / (t_0 T_0) \) are, respectively, the explicit (chiral) symmetry breaking field and the reduced temperature variable. \( T_0 \) denotes the critical temperature in the chiral limit \((h \to 0)\) and \( z = t h^{-1/\delta} \) is the so-called scaling variable. The scaling properties of the order parameter \((\sim \partial f / \partial h)\) is given by

\[ M = m_s \langle \bar{\Psi} \Psi \rangle / T^4 = h^{1/\delta} f_G(z), \]

where \( \langle \bar{\Psi} \Psi \rangle \) is the chiral condensate. The critical exponents \((\beta, \delta)\) and the scaling functions \((f_s(z), f_G(z))\) uniquely characterize the universality class of the transition. The parameters \( t_0, h_0 \) and \( T_0 \) are non-universal, i.e. they depend on the action, lattice spacing, value of the bare strange quark mass etc. The function \( f_{\text{reg}}(m_l, m_s, T, \mu_B) \) is not related to universal scaling properties and depicts the usual non-critical regular part of the free energy.

Recently such scaling studies were performed in Ref. [6] by the BNL-Bielefeld collaboration using p4fat3 staggered quark action. These studies show that in the limit \( m_l \to 0 \), keeping \( m_s = m_s^{\text{phys}} \), the chiral transition belongs to 3-d \( O(N) \) universality class. As for example, Fig. 1(b) shows that the properly scaled order parameter, \( h^{-1/\delta} M \), agrees with the relevant \( O(N) \) scaling function \( f_G(z) \) for \( m_l \lesssim m_s / 20 \) which corresponds to a Goldstone pion mass of \( m_\pi \simeq 150 \) MeV. These studies indicate that the \( m_s^{\text{phys}} \) is probably larger than \( m_s^{\text{tc}} \). Furthermore, they also indicate that the physical QCD \((m_l \simeq m_s / 27)\) may also lie within the scaling regime of the actual chiral transition. However, these studies where performed using p4fat3 staggered action which is known to have large discretization errors. Hence, in order to confirm these results similar studies have to be performed using the HISQ action. Such studies are currently underway.

3. Curvature of the phase transition line for small \( \mu_B \)

Based on the indications from the scaling studies mentioned in the previous section the conjectured phase diagram of QCD in the limit of massless light quarks is depicted in Fig. 2(a). At zero chemical potential \((\mu_B)\) the chiral transition is second order, belonging to the 3-d \( O(4) \) universality class. This \( O(4) \) chiral phase transition line extends in the \( T - \mu_B \) plane and meets the 1st order phase transition line emanating from the \( T = 0 \) axis at the so-called QCD (tri-)critical point which belongs to 3-d \( Z(2) \) universality class. The universal scaling properties of the chiral transition has been extended [7] to compute the curvature of the \( O(4) \) chiral critical line for small values of baryon chemical potential \( \mu_B / T \ll 1 \). Since the baryon chemical potential does not explicitly break the chiral symmetry, from the perspective of the universal scaling properties of the chiral transition, \( \mu_B \) is equivalent to the thermal variable. Further,

\[ \dagger \] As mentioned before in Section II for staggered fermions at non-zero lattice spacings there is only one Goldstone pion in the chiral limit as opposed to three in the continuum. Hence, for staggered fermions the relevant symmetry group is 3-d \( O(2) \) instead of the 3-d \( O(4) \) of the continuum.
due to \(CP\)-symmetry of the free energy, the reduced temperature variable must be even in \(\mu_B\) —  

\[ t = \left[ (T - T_0)/T_0 + \kappa_B (\mu_B/T)^2 \right] / t_0. \]

Here we assume \(\mu_B/T << 1\) and consider only the leading order term in \(\mu_B/T\). The \(O(4)\) chiral transition line in \(T - \mu_B\) plane is defined by the condition \(t = 0\) and hence at the leading order in \(\mu_B\) the chiral transition temperature is given by  

\[ T_0(\mu_B)/T_0(0) = 1 - \kappa_B[\mu_B/T_0(0)]^2. \]

Thus \(\kappa_B\) is the curvature of the chiral transition line around \(\mu_B = 0\). The value of the this curvature parameter \(\kappa_B\) can be determined by studying the universal scaling properties of the so-called “thermal” susceptibility of the order parameter —  

\[ \chi_{m,B} = \partial^2 M/\partial(\mu_B/T)^2 = 2\kappa_B h^{(\beta-1)/\beta} f'_G(z)/t_0, \]

where \(f'_G(z)\) is a scaling function uniquely associated with the specific universality class. Once the non-universal scaling parameters \(t_0, h_0\) and \(T_0(0)\) is determined from the scaling analysis at \(\mu_B = 0\), as have been done in Ref. [6], scaling analysis of \(\chi_{m,B}\) can be preformed in order to determine the only unknown parameter \(\kappa_B\).

Such a scaling analysis of the “thermal” susceptibility of the order parameter was performed by the BNL-Bielefeld-GSI collaboration in Ref. [7], using p4fat3 staggered fermions with two different lattice spacings, and the curvature of the chiral transition line was determined to be \(\kappa_B = 0.0066(9)\). In Fig. 2(b) we show the scaling analysis of the “thermal” susceptibility of the order parameter from Ref. [7]. Once the the curvature of the chiral transition line is known it is possible to compare the phase boundary in \(T - \mu_B\) plane, given by \(T_0(\mu_B)/T_0(0) = 1 - \kappa_B[\mu_B/T_0(0)]^2\), with the (chemical) freeze-out curve [8]. This gives an idea about how far the chiral critical line is from the freeze-out of the heavy-ion collision experiments. Such comparison is shown in Fig. 2(c). In the limit \(m_l \to \infty\), i.e. for a pure gluonic theory, the transition temperature is independent of \(\mu_B\) and in the limit \(m_l \to 0\) the phase boundary is the one obtained by the BNL-Bielefeld-GSI collaboration in Ref. [7]. The transition line for the physical quark mass

\[ \kappa_B = \kappa_q/9. \]
Figure 3. (a) Second order susceptibility for the baryon number, (b) fourth order susceptibility for up quark number and (c) sixth order susceptibility for the electric charge. The new calculations for the HISQ action have been performed by the BNL-Bielefeld collaboration and that for the stout action are from the Wuppertal-Budapest collaboration [11]. The older data for the p4fat3 action is taken from Ref. [12]. The dotted lines indicate the values of these quantities for the hadron resonance gas (HRG) model and for the free fermionic gas (SB).

should lie in between these two limits. In fact, the phase boundary for the physical quark masses has also been computed recently from lattice QCD by the Wuppertal-Budapest collaboration [3, 9]. As can be seen from Fig. 2(c), the phase boundary for the physical quark mass almost coincides with that in the chiral limit and they agrees with the freeze-out curve [5] till $\mu_B \sim 150$ MeV and then slowly starts to deviate. However, one has to remember that the lattice computations for the phase boundary are at present performed only up to the leading order in $\mu_B$.

4. Fluctuation, correlations: lattice QCD meets experiments

Although lattice QCD has proven to be a successful technique for performing ab-initio, quantitative studies of QCD a direct computation at non-zero baryon chemical potential is, unfortunately, plagued by the infamous sign problem. However, important information at non-zero chemical potentials may be obtained using the well established numerical technique of Taylor expansion of the QCD partition function with respect to the baryon chemical potential [10]. In this method one Taylor expands the partition function $(Z)/$free energy $(f)/$pressure $(P)$ in power series of the $\mu_B$ around $\mu_B = 0$—

$$P(\mu_B, T)/T^4 = \sum_{n=0}^{\infty} (1/n!)(\chi_B^R(T)(\mu_B/T)^n$$,

where $VT^3\chi_B^R(T) = [\partial^n Z(\mu_B, T)/\partial(\mu_B/T)^n]_{\mu_B=0}$ and $V$ is the volume of the system. $\chi_B^R$ are the generalized baryon number susceptibilities and since they are defined at $\mu_B = 0$ usual lattice QCD simulations at zero chemical potential can be used to compute these susceptibilities. Similar susceptibilities $\chi_Q^R$, $\chi_S^R$ etc. can be defined from the Taylor expansions of the pressure with respect to the electric charge chemical potential $\mu_Q$, the strangeness chemical potential $\mu_S$ etc.

Since the generalized susceptibilities are derivatives of the free energy with respect to the chemical potentials universal scaling properties of these susceptibilities can also be readily predicted. From discussions in Sections 2 and 3 it can be inferred...
that two derivatives of the free energy with respect to $\mu_B$ is equivalent to a single
derivative with respect $T$ and consequently the scaling behavior of the susceptibilities
are— $\chi_n^B \sim \hbar^{(1-\alpha-n/2)} f_s^{(n/2)}(z) + C_{n,\text{reg}}$. Here $f_s^{(n/2)}(z)$ are unique scaling functions
and $C_{n,\text{reg}}$ are contributions from the non-critical regular part of the free-energy. In
order to understand the universal scaling behavior of the generalized susceptibilities
it is also important to note that for 3-d $O(4)$ universality class the critical exponent
$-1 < \alpha < 0$. In Fig. 3(a) we show the second order baryon number susceptibility. Close
to $T_c$, $\chi_2 \sim C_{2,\text{reg}} \mp A_\pm |(T - T_c)/T_c|^{(1-\alpha)}$ is non-divergent and behaves like the energy
density. While for $T < T_c$ the new lattice data is in good agreement with the hadron
resonance gas model, for $T > T_c$ approach towards the ideal gas value is much smoother
and slower compared to the older data from the p4fat3 action [12]. Also note the good
agreement between the new data coming from the HISQ (BNL-Bielefeld collaboration)
and the stout [11] actions. Close to $T_c$ the behaviors of the higher order susceptibilities
are also consistent with there expected scaling behaviors. The fourth order susceptibility
(see Fig. 3(b)) $\chi_4 \sim C_{4,\text{reg}} \mp A_\pm |(T - T_c)/T_c|^{-\alpha}$ remains non-divergent and behaves like
the specific heat by always staying positive and showing a cusp like structure in the
vicinity of $T_c$. The sixth order susceptibility $\chi_6 \sim \mp A_\pm |(T - T_c)/T_c|^{-(1+\alpha)}$ changes
sign across $T_c$ (see Fig. 3(c)) and diverges at $T_c$ in the chiral limit. Based on the later
observation that even for $\mu_B \approx 0 \chi_6 < 0$ in the vicinity of $T_c$, it has been recently argued
[13] that if the measured values of the sixth order moments of the conserved charges
come out to be negative for the on-going heavy-ion collision experiments at the Large
Hadron Collider (LHC) then it may indicate that the transition from the hadronic to
the QGP phase happens very close to the freeze-out curve.

The off-diagonal susceptibilities $\chi_{BS}^{11}$, $\chi_{QS}^{11}$ etc., are measures of correlations among
different conserved charges. As a result these quantities are good probes for the degrees
of freedom inside QGP. As for example, inside QGP where strange quarks ($B = 1/3$, $S = -1$) are the relevant degrees of freedom strangeness can only exists in direct
conjunction with the baryon number. On the other hand, at very low temperatures in the
hadronic phase where the relevant strangeness carrying excitation are the kaons ($B = 0$)
there is no apparent correlation among the baryon number and strangeness. Based on
these observations the observable baryon strangeness correlation $C_{BS} = -3\chi_{11}^{BS}/\chi_2^S$ was proposed in Ref. [14]. In Fig. 4(a) we show the this quantity computed using the
HISQ (by BNL-Bielefeld collaboration) as well as using the stout [11] action. Below $T_c$
this quantity is in very good agreement with the results predicted by the HRG model
indicating that at these temperatures the strangeness is truly carried by the hadrons.
On the other hand, for $T \gtrsim 250$ MeV the baryon strangeness correlation is quite close to
its ideal gas value indicating that above these temperatures the strangeness and baryon
number are carried by the strange quarks. Also note that the lattice data from both
the actions are in excellent agreement with each other.

So far we discussed the physics of the generalized susceptibilities at zero chemical
potentials. However, susceptibilities for non-zero values of chemical potentials have more
direct relevance for the heavy-ion collision experiments. These can be obtained from
the Taylor series expansions of the susceptibilities themselves, e.g. the baryon number susceptibilities at $\mu_B > 0$ are given by— $\chi_n^B(\mu_B, T) = \sum_{k=0}^{\infty} (1/k!)\chi_{n+k}(0, T)(\mu_B/T)^k$. These generalized susceptibilities are measures of the moments of the conserved charge distributions. As for example— $VT^3\chi_1^B(\mu_B, T) = \langle N_B \rangle$, $VT^3\chi_2^B(\mu_B, T) = \langle (\delta N_B)^2 \rangle$, $VT^3\chi_3^B(\mu_B, T) = \langle (\delta N_B)^3 \rangle$, $VT^3\chi_4^B(\mu_B, T) = \langle (\delta N_B)^4 \rangle - 3\langle (\delta N_B)^2 \rangle^2$ etc. measure different moments of the distribution of the net baryon number $N_B(\mu_B, T)$, where $\delta N_B(\mu_B, T) = N_B(\mu_B, T) - \langle N_B(\mu_B, T) \rangle$. On the other hand, such moments of conserved charges have also been measured by the STAR experiment [15] using event-by-event fluctuations in the Relativistic Heavy Ion Collider (RHIC) at various energies ($\sqrt{s_{NN}}$ ). As for example, in heavy-ion collision experiments one measures the moments— mean $M_B(\sqrt{s_{NN}}) = \langle N_B \rangle$, variance $\sigma^2_B(\sqrt{s_{NN}}) = \langle (\delta N_B)^2 \rangle$, skewness $S_B(\sqrt{s_{NN}}) = \langle (\delta N_B)^3 \rangle / \sigma^3_B$, kurtosis $K_B(\sqrt{s_{NN}}) = \langle (\delta N_B)^4 \rangle / \sigma^4_B - 3$ etc. Assuming— (i) experiments measure conserved charge distributions of a thermalized system, (ii) measured moments characterize the chemical freeze-out condition and (iii) $T(\sqrt{s_{NN}})$ and $\mu_B(\sqrt{s_{NN}})$ at the chemical freeze-out can be modeled by the hadron resonance gas model [8], the experimentally measured volume independent combinations of the moments can be related to the ratios of susceptibilities computed from lattice QCD— $\sigma^2_B(\sqrt{s_{NN}})/M_B(\sqrt{s_{NN}}) = \chi_2^B(\mu_B, T)/\chi_1^B(\mu_B, T)$, $\sigma^2_B(\sqrt{s_{NN}})S_B(\sqrt{s_{NN}}) = \chi_3^B(\mu_B, T)/\chi_2^B(\mu_B, T)$, $\sigma^2_B(\sqrt{s_{NN}})K_B(\sqrt{s_{NN}}) = \chi_4^B(\mu_B, T)/\chi_2^B(\mu_B, T)$ etc. .

As net proton fluctuations can be treated as a proxy for the net baryon number fluctuations [16], in Fig. 4(b) we show a comparison of the experimentally measured moments of net proton distribution [15] to the lattice QCD calculations of the ratios of the baryon number susceptibilities using improved p4fat3 [17] and un-improved naive [18] staggered actions. As can been seen, the experimental data and the lattice QCD computations are in good agreement with each other and also with that from the hadron resonance gas calculations [19]. This, for the first time, shows a direct comparison.
between the heavy-ion collision experiments and lattice QCD computations. However, in order to make such comparisons it is essential to perform reliable computations of the higher order susceptibilities. As for example, in Fig. 4(c) we show the results for ratio $\chi_B^4/\chi_B^2$ computed in leading and next to leading orders of the Taylor expansion. As can be seen, around $\sqrt{s_{NN}} \sim 20$ GeV (i.e. $\mu_B \sim 200$ MeV) the contribution of the next to leading order term is much larger than the contribution of the leading order term. Moreover, at present these lattice results are not continuum extrapolated and were calculated using actions which are known to suffer from significant discretization effects and resulting in larger values for the transition temperature. Hence, in future, it is essential to carry out these lattice computations using HISQ like highly improved actions with accurate determination of the higher order susceptibilities. This is specially important for the observables like moments of net electric charge fluctuations as they are sensitive to light charged hadrons like the pions (see discussion in Section 1). Such calculations are currently in progress

Acknowledgments: The author is supported under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy.

References

[1] A. Bazavov and P. Petreczky, this proceeding.
[2] HotQCD collaboration, in preparation.
[3] Z. Fodor, this proceeding.
[4] S. Borsanyi et al., JHEP 1009, 073 (2010).
[5] Y. Aoki, G. Endrodi, Z. Fodor, S. D. Katz and K. K. Szabo, Nature 443, 675 (2006).
[6] S. Ejiri et al., Phys. Rev. D80, 094505 (2009).
[7] O. Kaczmarek et al., Phys. Rev. D83, 014504 (2011).
[8] J. Cleymans, H. Oeschler, K. Redlich and S. Wheaton, Phys. Rev. C73, 034905 (2006).
[9] G. Endrodi, Z. Fodor, S. D. Katz and K. K. Szabo, JHEP 1104, 001 (2011).
[10] C. R. Allton et al., Phys. Rev. D68, 014507 (2003); R. V. Gavai and S. Gupta, Phys. Rev. D68, 034506 (2003).
[11] C. Ratti, this proceeding.
[12] M. Cheng et al., Phys. Rev. D79, 074505 (2009).
[13] F. Karsch, this proceeding; V. Skokov, this proceeding; B. Friman et al., arXiv:1103.3511 [hep-ph].
[14] V. Koch, A. Majumber and J. Randrup, Phys. Rev. Lett. 95, 182301 (2005).
[15] T. Tarnowsky (STAR collaboration), this proceedings; M. M. Aggarwal et al (STAR collboration), Phys. Rev. Lett. 105, 022302 (2010).
[16] Y. Hatta and M. A. Stephanov, Phys. Rev. Lett. 91, 102003 (2003).
[17] C. Schmidt, Prog. Theor. Phys. Suppl. 186, 563 (2010).
[18] R. Gavai and S. Gupta, Phys. Lett. B696, 459 (2011).
[19] F. Karsch and K. Redlich, Phys. Lett. B695, 136 (2011).