Developments in Finite Temperature QCD on the Lattice with Dynamical Quarks

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I report on some recent developments in nonperturbative studies of finite temperature QCD with dynamical quarks on the lattice. I discuss new studies of improved lattice actions and their application to finite temperature QCD. I also summarize the status of lattice investigations about the order of the finite temperature QCD transition for the case of two flavors of degenerate light quarks, using both staggered and Wilson lattice fermions.

§1. Introduction

The finite temperature transition in QCD is characterized by recovery of the spontaneously broken chiral symmetry and also by breakdown of the confinement at temperatures higher than a critical value $T_c$. Because both of these characteristic properties of QCD are essentially non-perturbative in nature, the most systematic way of studying the transition is to investigate it on the lattice.

A large number of numerical simulations have been performed to clarify the nature of the QCD transition from the first principles of QCD. In order to make a precise prediction for the real world from the results obtained on finite lattices, we perform an extrapolation to the limit of vanishing lattice spacing, the continuum limit. For a reliable extrapolation, we have to simulate on sufficiently fine lattices. On the other hand, in a study of finite temperature QCD, the spatial lattice size should be sufficiently large in order to approximately realize the thermodynamic limit. With the limitation of the currently available computer power, this means that we have to suppress the lattice size in the time direction $N_t$; currently $N_t \approx 4-6$ is used for major simulations of QCD with dynamical quarks (full QCD). Because the temperature on the lattice is given by $T = 1/N_t a$ with $a$ the lattice spacing, the corresponding lattices become rather coarse; for $T \sim T_c \approx 100-200\text{MeV}$, $a \sim 0.2-0.4\text{fm}$. Subsequent lattice artifacts sometimes make the analysis and interpretation of lattice results not straightforward.

Here, recent developments in improved lattice actions opened us a possibility
to reduce the lattice artifacts already on coarse lattices and, therefore, to extract accurate results for finite temperature QCD transition with the present computer power. In section §2, I report these developments in improved lattice actions and their application to finite temperature QCD.

In a phenomenological study of quark-gluon plasma in heavy ion collisions and in the early Universe, the most fundamental information required is the order of the QCD phase transition. Recently, there have been several developments in lattice QCD on this issue, especially for the case of two flavors of degenerate light quarks. In sect. 3, I report about the status of these recent studies using both staggered and Wilson lattice fermions. This also includes one of the first fruitful applications of improved actions to the study of QCD at finite temperatures.

For other developments in lattice QCD, I refer reviews in recent Lattice conferences.

§2. Improvement of the lattice action

An action on the lattice is chosen such that the continuum action is recovered when we let the lattice spacing $a \rightarrow 0$ in the action. For the gluon part of the action, the minimal choice is the standard one-plaquette action by Wilson, which is the most local and geometrically the simplest lattice gauge action. On the lattice, however, we have freedom to introduce less local terms to the action without affecting the continuum limit. Here, the speed of approach to the continuum limit does depend on the choice of the action. Therefore, a judicious choice of the action can suppress lattice artifacts in physical observables even at moderate values of the lattice spacing. Such actions are called “improved actions”. Importance of improvement is much stressed recently (for reviews see Refs. 3, 4).

The basic idea behind improvement may be obtained by considering the lattice derivative; the naive derivative $\Delta_x f(x) = \frac{1}{2a} [f(x+a) - f(x-a)]$ converges to the continuum derivative with an error of $O(a^2)$. We can reduce this error down to $O(a^4)$ by replacing $\Delta_x \rightarrow \Delta_x - \frac{a^2}{6} \Delta_x^3$ which operates on fields at up to next nearest neighbor points. Similar substitution is effective also to obtain a lattice action that approaches to the continuum action much smoothly. The life is, however, not so easy, because what we want to obtain is not a smoother lattice action, but an action which leads to smaller discretization errors in the physical observables $\langle P \rangle = Z^{-1} \int \mathcal{D}\phi P[\phi] e^{-S[\phi]}$ which can be obtained only after a non-perturbative calculation, in general. Many different strategies have been proposed to obtain such $S$. Two major approaches are the renormalization group methods proposed first by Wilson, and the perturbative improvements by Symanzik. In any case, improved lattice actions contain additional terms (interactions that usually have a wider spatial size) compared with the standard action. Because such additional terms makes the simulation quickly difficult and time-consuming, the efficiency of improvement should be tested for each of the new terms introduced.

2.1. Comparison of improved actions
Fig. 1. Static quark potential obtained by a full QCD simulation performed on $12^3 \times 32$ lattices using various lattice actions. The coupling parameters $\beta = 6/g^2$ and $K$ are adjusted such that we obtain the lattice spacing $a \approx 0.2\text{fm}$ and the ratio of the pseudo-scalar and vector meson masses $m_{PS}/m_V \approx 0.8$.

Improved lattice actions have been studied mainly in quenched QCD (QCD without dynamical quark loops). In finite temperature QCD, however, dynamical quarks are essential. Quite recently, the CP-PACS Collaboration have performed a systematic investigation of how various terms added to the gauge and quark actions, taken separately, affect light hadron observables in full QCD. A new dedicated parallel computer CP-PACS is used for the simulation. The effect of improvement is studied comparing, for the gauge part of the action, the standard one plaquette action ($P$) and an improved action ($R$) that contain $1 \times 2$ rectangular loops with the coefficients obtained by a renormalization group study, and for the quark action, the standard Wilson quark action ($W$) and an improved Wilson quark action containing the so called clover term ($C$). Simulations are carried out in two-flavor QCD. Because the extent of improvement to be clearer at a coarser lattice spacing, we adjust the gauge coupling parameter $6/g^2$ such that the lattice spacing becomes $a \sim 0.2\text{fm}$.

Figure 1 summarizes the results for the static quark potential using the four different combinations for the action ($PW$, $PC$, $RW$, and $RC$). Different symbols correspond to potential data measured in different spatial directions on the hypercubic lattice, along the vector indicated in the figure. The jagged result for the standard
action (PW) means that the rotational symmetry is sizably violated on this coarse lattice. A drastic improvement of the rotational symmetry is seen when we replace the gauge action with the R action, as observed previously also in the quenched case. In this regard, the quark action has much less effect. Fig. 2 shows the results for light hadron masses. The solid curve represents the result of a phenomenological mass formula by Ono, which is approximately reproduced also on the lattice when \(a < \sim 0.1\)fm for the PW action. We see that improvement of the quark action makes the spectrum quite close to the phenomenological curve already at \(a \approx 0.2\)fm.

These results are very encouraging: They show that, even with the presently available computing power, it may be possible to obtain accurate results near the continuum limit also in full QCD, when we use an improved action.

2.2. Improved actions for full QCD at finite temperatures

One of the first systematic applications of improved action to the study of finite temperature QCD has been done by the Tsukuba group. Their motivation to adopt an improved action is to remove severe lattice artifacts encountered in a finite temperature simulation of QCD with the standard Wilson quark action. Using the RW action discussed in the previous subsection, these lattice artifacts are shown to be well removed. Further physical outputs from this study will be discussed in Sec. 3.2.

Through this study, it became clear that improvement of the lattice action is essential in order to study several important topics in finite temperature QCD. Other major research groups have also began to study the finite temperature QCD with improved actions.

The MILC Collaboration combined a Symanzik type improved gauge action and
the clover quark action $C$, and found good improvement similar to that observed in the case of the $RW$ action. Comparing these results together with an unpublished PC data, we conclude that the big reduction of the lattice artifacts noted in the simulation of finite temperature QCD is mainly due to improvement of the gauge action. The MILC Collaboration studied also an improved staggered quark action, aiming at a better flavor symmetry on a coarse lattice.

The Bielefeld group also extended their study of improved pure gauge theories to include improved staggered and Wilson quark actions. One of their motivations is to achieve a faster convergence of thermodynamic quantities to the large $N_t$ limit: Thermodynamic quantities have errors of $O(1/N_t^2)$ on the lattice because the relevant fluctuations include those with spatial size $\sim 1/T = N_t a$, that feel discretization errors when $N_t$ is not large enough. These errors are automatically removed when we take the continuum limit $a \to 0$ keeping the temperature $T = 1/N_t a$ fixed, i.e., $N_t \to \infty$ simultaneously. [Practically, $N_t \geq 8$ is required to obtain thermodynamic quantities at $T \sim O(T_c)$ to an accuracy of several percent in quenched QCD using the standard one-plaquette action.] Because an improved action has improved short-distance properties, we expect these errors to be also smaller with improved actions.

In spin models and also in quenched QCD, good improvements are reported using a class of improved actions called fixed point actions ("perfect actions"), which are designed to be at the UV fixed point of a renormalization group transformation and therefore to remove all lattice artifacts when infinite number of coupling parameters are introduced. Trials to construct a fixed point action for full QCD are also made.

§3. Order of the chiral transition in two-flavor QCD

Let us now turn our attention to the topics of the order of the QCD transition from the high temperature quark-gluon-plasma phase to the low temperature hadron phase, which is supposed to occur at the early stage of the Universe and possibly at heavy ion collisions. It is, in particular, crucial to know whether the transition is a first order phase transition or a smooth transition (second order phase transition or crossover).

The nature of the QCD transition is considered to depend on the number of quark flavors $N_F$ sensitively. The physically interesting cases are the case of two and three flavors of degenerate light quarks ($N_F = 2$ and 3), and also a more realistic...
case of two light and one heavy quarks ($N_F = 2 + 1$). The case $N_F = 2$ corresponds to the case where the third quark is much heavier than the relevant energy scale for thermal processes near the critical temperature, $m_s \gg T_c$, while the case $N_F \geq 3$ corresponds to the case $m_s \ll T_c$.

Using universality hypothesis, the nature of the finite temperature QCD transition near the chiral limit can be studied by a Ginzburg-Landau effective theory respecting the chiral symmetry of QCD, the effective $\sigma$ model. For $N_F \geq 3$, a first order transition is predicted. For $N_F = 2$, on the other hand, the order of the transition is not quite definite in the effective $\sigma$ model; a first order transition is predicted when the anomalous axial $U_A(1)$ symmetry is effectively restored at the transition temperature, while a second order transition is expected otherwise. Because the $U_A(1)$ breaking operator is a relevant operator whose coefficient grows towards the IR limit under a renormalization group transformation, the transition is more likely to be second order. A non-perturbative study is required to determine the order of the transition conclusively.

Therefore, understanding the nature of the QCD transition for $N_F = 2$ is an important step toward the clarification of the transition in the real world.

When the chiral transition is second order, we expect that the transition turns into an analytic crossover at non-zero $m_q$, while when the chiral transition is first order, it will remain to be first order for small $m_q$. However, it is difficult to numerically distinguish between a very weak first order transition and a crossover, especially at small $m_q$. In order to confirm the expected crossover numerically, we have to study the lattice size dependence to see if the formation of singularity (e.g. the increase of the peak height of a susceptibility with increasing the lattice volume) stops on sufficiently large lattices. This becomes more and more difficult at small $m_q$.

Here, the universality provides us with useful scaling relations that can be confronted with numerical results of QCD, in order to test the nature of the transition: It is plausible from an effective $\sigma$ model that, when the chiral transition is of second order, QCD with two flavors belongs to the same universality class as the three dimensional O(4) Heisenberg model. The O(4) model is much simpler than the $\sigma$ model, and its scaling properties are well studied. For example, at small external field $h$ near the critical temperature $T_c$, for $h = 0$, the pseudo-critical temperature $T_{pc}(h)$ and the peak height of the magnetic and thermal susceptibilities follow $T_{pc} - T_c \sim h^{z_g}$, $\chi_m^{\text{max}} \sim h^{-z_m}$, and $\chi_t^{\text{max}} \sim h^{-z_t}$, where $z_g = 1/\beta \delta$, $z_m = 1 - 1/\delta$, and $z_t = (1 - \beta)/\beta \delta$ in terms of the O(4) critical exponents $\beta$ and $\delta$. Here the values of $\beta$ and $\delta$ for the O(4) model are well established. In QCD, we identify $T \sim 6/g^2$, $h \sim m_q$, and $M \sim \langle \bar{\Psi}\Psi \rangle$.

In lattice QCD, an additional complication should be noted because no known lattice fermions have the full chiral symmetry on finite lattices. Two conventional lattice fermions are the staggered and Wilson fermions. In the formulation of staggered fermions, the flavor-chiral symmetry $SU(N_F)_L \times SU(N_F)_R \times U(1)$ of massless $N_F$-flavor QCD is explicitly broken down to $U(N_F/4)_L \times U(N_F/4)_R$ at $a > 0$. Moreover, this action is local only when $N_F$ is a multiple of 4. For the physically interesting cases $N_F = 2$ and 3, a usual trick is to modify by hand the
power of the fermionic determinant in the numerical path-integration. This necessarily makes the action non-local, that poses conceptually and technically difficult problems. With the Wilson fermion action, on the other hand, the flavor symmetry is manifest also on the lattice, and the action is local for any \( N_F \). This feature is quite attractive in a study of the \( N_F \) dependence of the QCD transition. However, the chiral symmetry is explicitly broken at \( a > 0 \), that requires additional tedious analyses of chiral properties.

These broken symmetries of lattice fermions are expected to restore in the continuum limit. On a coarse lattice used in a finite temperature simulation, however, we may encounter sizable deviations from the scaling behavior expected in the continuum limit. Therefore, the appearance of the O(4) scaling is also a useful touchstone to test the recovery of the chiral symmetry on the lattice when the chiral transition is of second order.

### 3.1. Results with staggered quarks

The O(4) scaling was first tested on the lattice for staggered quarks by the Bielefeld group. Based on simulations on an \( 8^3 \times 4 \) lattice at \( m_q a = 0.02, 0.0375, \) and 0.075 using the standard action, they obtained \( z = 0.77(14) \), \( z_m = 0.79(4) \), and \( z_t = 0.65(7) \), where the corresponding O(4) values are 0.537(7), 0.794(1), and 0.331(7). The result for \( z_m \) is consistent with the O(4) value while other exponents are in disagreement with the O(4) values.

Possible causes of the discrepancy are (i) \( m_q \) is not small enough to see the critical behavior in the chiral limit, and (ii) the spatial lattice volume is not large enough to obtain the observables in the thermodynamic limit. Two additional caveats are in order for \( N_F = 2 \) staggered quarks: (iii) The symmetry in the chiral limit at \( a > 0 \) is O(2) instead of O(4). Practically, however, the values of the O(2) exponents are almost indistinguishable from the O(4) values with the present numerical accuracy. (iv) The action is not local. Therefore, an assumption behind the universality argument can be violated so that some non-universal behavior may appear. The correct continuum chiral limit with the O(4) symmetry will be obtained only when
we first take the continuum limit $a \rightarrow 0$ and then take the chiral limit. In addition to these points, we also have to check technical details in the numerical simulation; the accuracy of the methods to simulate the system, such as the the finite step-size error and the dependence on the convergence criterion for fermion matrix inversion.

A systematic study of the quark mass dependence as well as the lattice volume dependence is in order. We performed a series of simulations on $8^3 \times 4$, $12^3 \times 4$, and $16^3 \times 4$ lattices at $m_q a = 0.01$, 0.02, 0.0375, and 0.075. The Bielefeld group also extended their study to larger spatial lattices. The results obtained are consistent with each other. It turned out that determination of critical exponents on $8^3 \times 4$ lattices suffers from a sizable finite lattice-size effect for $m_q a < 0.0375$.

From the lattice-size dependence of the magnetic susceptibility $\chi_m$ for fixed value of quark mass, shown in Fig. 3(a), we conclude that the transition is a crossover for $m_q a \geq 0.02$; the peak height $\chi_m^{\text{max}}$ for $m_q a = 0.02$ stabilizes on spatial lattices larger than $12^3$. For $m_q a = 0.01$, on the other hand, $\chi_m^{\text{max}}$ is increasing up to our largest spatial lattice of $16^3$. If this increase is maintained up to infinite volume, then we have a first order transition at this quark mass. However, examining the lattice volume dependence of Monte Carlo time histories and histograms, we could not find any clear indication of a first-order transition at $m_q a = 0.01$. Furthermore, when we rescale the lattice volume by zero-temperature pion correlation length, we find that the lattice volume $16^3$ for $m_q a = 0.01$ approximately corresponds to the volume $12^3$ for $m_q a = 0.02$, where the increase of $\chi_m^{\text{max}}$ terminates [Fig. 3(b)]. Therefore, it is possible that the increase of $\chi_m^{\text{max}}$ for $m_q a = 0.01$ seen in our data is a transient effect.

Assuming that the finite size effect is sufficiently small on the $16^3 \times 4$ lattice, we fit the data at the four values of $m_q a$. We find $z_g = 0.64(5)$, $z_m = 1.03(9)$, and $z_t = 0.82(12)$. (Removing the data for $m_q a = 0.01$ gives slightly smaller but consistent values with larger errors.) The results for $z_g$ and $z_m$ sizably deviate from the O(2) or O(4) values. We also studied other exponents related to energy expectation value, which also largely deviate from O(2) and O(4) values. On the other hand, the identity $z_g + z_m - z_t = 1$ expected for a second-order fixed point with two relevant operators is approximately satisfied. Thus, the exponents are consistent with a second-order transition at $m_q = 0$. Our study of the scaling function also shows a similar trend: With measured values of exponents, data for the susceptibility $\chi_m$ exhibits a reasonable scaling as a function of $\beta$ and $m_q a$, although results are much worse when we adopt the O(4) exponents.

In summary, we find the determination of the nature of the two-flavor chiral transition with staggered quarks using the standard action to involve subtle problems. While our data so far do not contradict a second-order transition at $m_q = 0$, the exponents take quite unexpected values, at least in the range $m_q a \geq 0.01$. Evidently further work, possibly on larger spatial sizes and smaller quark masses, is needed to clarify this important problem.

### 3.2. Results with Wilson quarks

We now study the issue using Wilson quarks. It turned out that Wilson quarks in the standard action lead to several unexpected phenomena on lattices with $N_t = 4$
and 6: On these lattices, the transition becomes once very sharp when we increase $m_q$ from the chiral limit, in contrary to the expectation in the continuum limit that the chiral transition becomes weaker when we increase $m_q$. Together with other strange behaviors of physical quantities near the transition point, this phenomenon is identified as an effect of lattice artifacts. Therefore, we apply an improved action.

With the RW action discussed in Sec. 2.1, we first find that the lattice artifacts observed with the standard action are well removed. We also find that the physical quantities are quite smooth around the transition point at $m_q > 0$, as shown in Fig. 4. The straight line envelop of $m_\pi^2$ at finite temperature ($N_t = 4$) shown in Fig. 4(b) agrees with $m_\pi^2$ obtained at low temperature ($N_t = 8$), and corresponds to the PCAC relation $m_\pi^2 \propto m_q$ expected in the low-temperature phase. The smoothness of the physical observables strongly suggests that the transition is a crossover at $m_q > 0$.

Concerning the nature of the transition in the chiral limit, we find that the transition becomes monotonically weaker when we increase $6/g^2$ (see Fig. 4). Because the transition point shifts to larger $6/g^2$ at larger $m_q$, increasing $6/g^2$ corresponds to increasing $m_q$ for the transition. We also note that $m_\pi^2$ in the chiral limit monotonically decreases to zero as we decrease temperature from above towards the chiral transition point. $m_\pi^2$ at the transition temperature for finite $m_q$ also shows a similar monotonic decrease when we decrease $m_q$. These results suggest that the chiral transition is continuous.

For a more decisive test about the nature of the transition, a scaling study is required. From the universality argument we expect that magnetization $M$ near the second order transition point can be described by a single scaling function:

$$M/h^{1/\delta} = f(t/h^{1/\delta})$$

(3.1)

where $h$ is the external magnetic field and $t = [T - T_c]/T_c$ the reduced temperature.
When the QCD transition is of second order in the chiral limit, the chiral condensate should satisfy this scaling relation with O(4) exponents $1/\beta\delta = 0.537(7)$ and $1/\delta = 0.2061(9)$, and the O(4) scaling function $f(x)$. Our results for $M$ are shown in Fig. 5(a). We make a fit of $M$ to the scaling function obtained for an O(4) model, by adjusting $\beta_{ct}$ and the scales for $t$ and $h$, with the exponents fixed to the O(4) values. Figure 5(b) shows our result with $\chi^2/df = 0.61$. The scaling ansatz works remarkably well with the O(4) exponents. Our recent study shows that the situation holds also when we include data in the $t \leq 0$ region. On the other hand, a change of the exponents quickly makes the fit worse: For example, when we use the MF exponents suggested by Kocić and Kogut as a possibility for two-flavor QCD, the data no more falls on the MF scaling function.

The success of this scaling test with the O(4) exponents strongly suggests that the chiral transition is of second order in the continuum limit. It also indicates that the chiral violation due to the Wilson fermion action is sufficiently small with our improved action, for the values of $m_q$ and $6/g^2$ studied here.

§4. Summary

A simulation of finite temperature QCD sometimes suffers from sizable lattice artifacts caused by the coarseness of the lattice. Due to a requirement of large spatial lattice size for the thermodynamic limit, and also due to physical requirements to study a wide range of the parameter space, it is hard to remove these lattice artifacts when we use the standard lattice actions. Recent developments in improved lattice actions opened us a possibility to perform accurate simulations of finite temperature QCD with the present power of computers. A comparative study of improved full QCD actions shows that an efficient reduction of lattice artifacts can be achieved.
already on lattices with $a \sim 0.2$ fm, as used in major finite temperature simulations.

Among the topics of finite temperature QCD, intensive lattice studies have been made recently on the nature of the chiral transition in QCD with two degenerate light quarks. Understanding it is an important step toward the clarification of the transition in the real world including the non-degenerate s quark. Numerical simulations show that the transition for $N_F = 2$ is analytic crossover down to a very small value of the quark mass. In order to further determine the nature of the transition in the chiral limit, we have to study the scaling property and compare it with the $O(4)$ scaling expected theoretically for the case of a second order transition.

Using the standard action for the staggered quark, we find the determination of the nature of the two-flavor chiral transition to involve subtle problems. While our data do not contradict a second-order transition at $m_q = 0$, the critical exponents take quite unexpected values. It is not yet clear whether this strange behavior is caused by large sub-leading terms in the scaling relations, or by the non-universality caused by the non-locality of the two-flavor staggered quark action. If the latter is the case, application of an improved action may solve the problem.

A study of the issue using the Wilson quark has been difficult due to severe lattice artifacts encountered when we use the standard action. We find that these lattice artifacts are removed when we use an improved gauge action combined with the standard Wilson quark action. Furthermore, we find that the chiral condensate remarkably follows the scaling relation with $O(4)$ exponents and $O(4)$ scaling function. This strongly suggests that the chiral transition in two-flavor QCD is of second order.

This second order transition for the case $m_s = \infty$ should turn into a first order transition when we decrease $m_s$, as observed for the degenerate $N_F = 3$ case. Because $m_s \simeq 150 – 200$ MeV is just of the same order of magnitude as the expected values of $T_c$, we have to fine-tune the value of $m_s$ in order to study the nature of the transition in the real world. Unfortunately, the lattice simulations performed so far for the $N_F = 3$ and $N_F = 2 + 1$ cases do not have that accuracy yet because, using standard lattice actions, we have sizable systematic errors due to lattice artifacts. At the moment, both possibilities of a first order transition and an analytic crossover are remaining for the physical point.

Encouraged with the success of the scaling study for two-flavor QCD using an improved action, we began test simulations for $N_F = 3$ and $2 + 1$ applying the same improved action. Many lattice groups began to simulate finite temperature QCD using improved actions. It may, however, take several more years to re-accumulate the basic data in a wide range of the many-dimensional full QCD parameter space, that is required to clarify the nature of the QCD transition in the real world.

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