Study of QCD Thermodynamics at Finite Density by Taylor Expansion

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We discuss the phase structure and the equation of state for QCD at non-zero temperature and density. Derivatives of $\ln Z$ with respect to quark chemical potential μ_q up to fourth order are calculated for 2-flavor QCD, enabling estimates of the pressure, quark number density and associated susceptibilities as functions of μ_q via a Taylor series expansion. Also, the phase transition line for 2 and 3-flavor QCD and the critical endpoint in the (T, μ_q) plane are investigated in the low density regime.

§1. Introduction

We would like to report our recent study of QCD thermodynamics with a small but non-zero quark chemical potential μ_q by numerical simulations. The interesting regime for heavy-ion collision experiments is rather low density regime, e.g. $\mu_q/T_c \sim$ 0.1 for RHIC and $\mu_q/T_c \sim 0.5$ for SPS. The phase transition for 2-flavor QCD is known to be crossover at $\mu_q = 0$ and expected to become a first order phase transition at a critical endpoint. To find the endpoint is also an interesting topic in the low density regime, and it might be possible to detect the endpoint experimentally via event-by-event fluctuations in heavy-ion collisions.

We discuss the equation of state at non-zero baryon number density in §2. [1] The study of the equation of state gives the most basic information for the experiments. Quantitative calculations of thermodynamic quantities such as pressure and energy density are indispensable. In particular, since the number density fluctuation should be large around the critical endpoint, the susceptibility of the quark number density, given by the second derivative of pressure with respect to μ_q, is an important quantity. Several studies of the quark number susceptibility have been performed at $\mu_q = 0$. [2] Moreover, measurements of pressure and energy density at $\mu_q \neq 0$ were done using the reweighting method, [3] which allow the investigation of thermodynamic properties at non-zero baryon density. This approach, however, does not work for large μ_q and large lattice size due to the sign problem.

Our strategy is the following. We compute the derivatives of physical quantities with respect to μ_q at $\mu_q = 0$, and determine the Taylor expansion coefficients in terms of μ_q, [4,5] in which the sign problem does not arise. Because the pressure is an even

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function of μ_q, the μ_q^2-term is leading and μ_q^4-term is the next to leading, and in fact only these two terms are non-zero in the high temperature (Stefan-Boltzmann) limit. We compute the Taylor expansion coefficients up to fourth order. The fourth order term enables us to evaluate the μ_q-dependence of the quark number susceptibility near $\mu_q = 0$. By estimating the change of the susceptibility, we discuss the possibility of the existence of the critical endpoint in the phase diagram of T and μ_q [1].

In §3, we compute the Taylor expansion coefficients for the transition temperature T_c. [5] Some investigations of the phase structure on the (T, μ) plane have been done by the reweighting method [6] and simulations with imaginary chemical potential. [7], [8] Because the procedure to identify the phase transition point is complex, it is difficult to apply the method which we use in §2. Our method for T_c is the following. We use the reweighting method, but we perform a Taylor expansion for the quark determinant and the fermionic operators and neglect unnecessary higher order terms of μ_q for the calculation of the derivatives which we want. Then, in the region where the sign problem is not serious, we calculate the Taylor expansion coefficients. This method reduces computer time drastically in comparison with the original reweighting method and enables us to use rather large lattice size.

Finally, we discuss the critical endpoint again. Since a Taylor expansion must break down at the singular point, it seems to be difficult to find the position of the critical endpoint by the Taylor expansion. We focus on a property of 3-flavor QCD at very small quark mass. [9] The crossover phase transition becomes a first order phase transition at a critical quark mass also for $\mu_q = 0$. [10] Hence, by tracing out the position of the critical endpoint from that at $\mu_q = 0$ to finite μ_q in the vicinity of $\mu_q = 0$, we may be able to estimate the position of the critical endpoint for the real physical quark masses. We try it in §4. Section 5 presents our conclusions.

§2. Taylor expansion of pressure in terms of μ_q

Pressure is given in terms of the grand partition function $Z(T, V, \mu_q)$ by $p/T^4 = (1/VT^3) \ln Z$. However, the direct calculation of $\ln Z$ is difficult, hence most of the work done at $\mu_q = 0$ for the calculation of pressure is done by using the integral method, [11], [12] where the first derivative of pressure is computed by simulations, and the pressure is obtained by integration along a suitable integral path. For $\mu_q \neq 0$, direct Monte Carlo simulation is not applicable; in this case we proceed by computing higher order derivatives of pressure with respect to μ_q/T at $\mu_q = 0$, and then estimate $p(\mu_q)$ using a Taylor expansion,

$$\left.\frac{p}{T^4}\right|_{T,\mu_q} = \left.\frac{p}{T^4}\right|_{T,0} + \sum_{n=1}^{\infty} c_n(T) \left(\frac{\mu_q}{T}\right)^n, \tag{2.1}$$

where $c_n = (1/n!)\partial^n(p/T^4)/\partial(\mu_q/T)^n|_{\mu_q=0}$. Explicitly writing

$$c_2 = \frac{N_\tau}{2!N_\sigma^3}\mathcal{A}_2, \qquad c_4 = \frac{1}{4!N_\sigma^3 N_\tau}(\mathcal{A}_4 - 3\mathcal{A}_2^2), \tag{2.2}$$
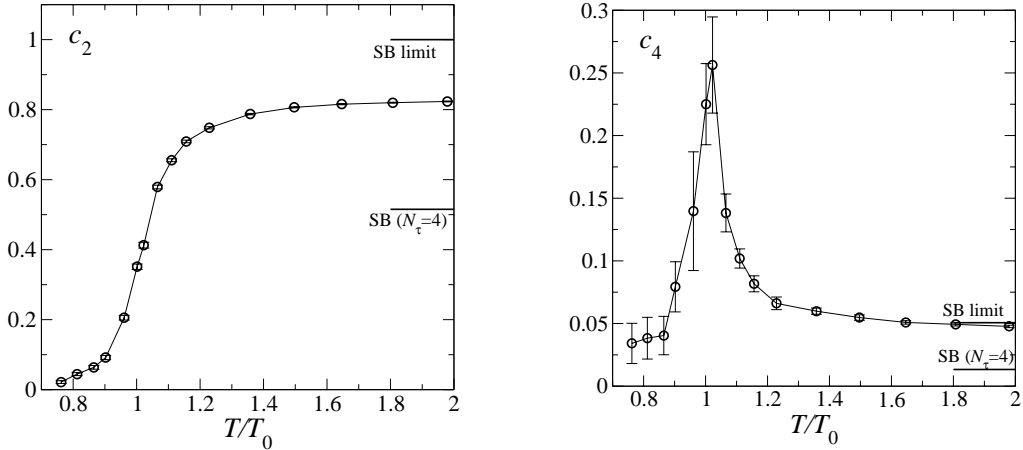
Fig. 1.   Coefficients of Taylor expansion, c_2 (left) and c_4 (right). T_0 is T_c at $\mu_q = 0$.

$$\mathcal{A}_2 = \left\langle \frac{N_f}{4} \frac{\partial^2 (\ln \det M)}{\partial \mu^2} \right\rangle + \left\langle \left(\frac{N_f}{4} \frac{\partial (\ln \det M)}{\partial \mu} \right)^2 \right\rangle,$$

$$\mathcal{A}_4 = \left\langle \frac{N_f}{4} \frac{\partial^4 (\ln \det M)}{\partial \mu^4} \right\rangle + 4 \left\langle \left(\frac{N_f}{4} \right)^2 \frac{\partial^3 (\ln \det M)}{\partial \mu^3} \frac{\partial (\ln \det M)}{\partial \mu} \right\rangle + 3 \left\langle \left(\frac{N_f}{4} \right)^2 \left(\frac{\partial^2 (\ln \det M)}{\partial \mu^2} \right)^2 \right\rangle$$

$$+ 6 \left\langle \left(\frac{N_f}{4} \right)^3 \frac{\partial^2 (\ln \det M)}{\partial \mu^2} \left(\frac{\partial (\ln \det M)}{\partial \mu} \right)^2 \right\rangle + \left\langle \left(\frac{N_f}{4} \frac{\partial (\ln \det M)}{\partial \mu} \right)^4 \right\rangle,$$

for staggered type quarks on an $N_\sigma^3 \times N_\tau$ lattice, and the coefficients for odd terms are zero. M is the quark matrix. μ is a chemical potential in lattice units, $\mu \equiv \mu_q a$. Here, we used a property that the odd derivatives of $\ln \det M$ are purely imaginary and the even derivatives are real. [5] These derivatives are computed by the random noise method, which saves computer time. Furthermore, we do not need simulations at $(T, \mu_q) = (0, 0)$ for the subtraction to normalize the value of p, since the derivatives of $p|_{T=0, \mu_q=0}$ with respect to μ_q are, of course, zero. This also reduces computer time.

We compute the pressure up to $O(\mu_q^4)$ using 2-flavors of p4-improved staggered fermion [13] at a bare quark mass $ma = 0.1$ on a $16^3 \times 4$ lattice. Then the quark number density n_q and quark number susceptibility χ_q are calculated up to $O(\mu_q^3)$ and $O(\mu_q^2)$, respectively. These are obtained by the derivatives of pressure; $n_q/T^3 = \partial(p/T^4)/\partial(\mu_q/T)$, $\chi_q/T^2 = \partial^2(p/T^4)/\partial(\mu_q/T)^2$, The details are given in Ref. 1). In Fig. 1, we plot the data for c_2 (left) and c_4 (right). Both of them are very small at low temperature and approach the Stefan-Boltzmann (SB) limit in the high temperature limit, as expected. The remarkable point is a strong peak of c_4 around T_c.

We can understand this peak via two arguments. One is a prediction from the hadron resonance gas model, [14] which is an effective model of the free hadron gas in the low temperature phase. The model study predicts $c_4/c_2 = 0.75$ and our results are consistent with this prediction for $T < T_c$; in fact, as T increases c_4/c_2 remains constant until $T \approx T_c$, whereupon it approaches the SB limit.

The other point is from a discussion of the convergence radius of the Taylor expansion. We expect that the crossover at $\mu_q = 0$ changes to a first order transition at a point $\mu_q/T_c \sim O(1)$. [6,9] Then, the analysis by Taylor expansion must break
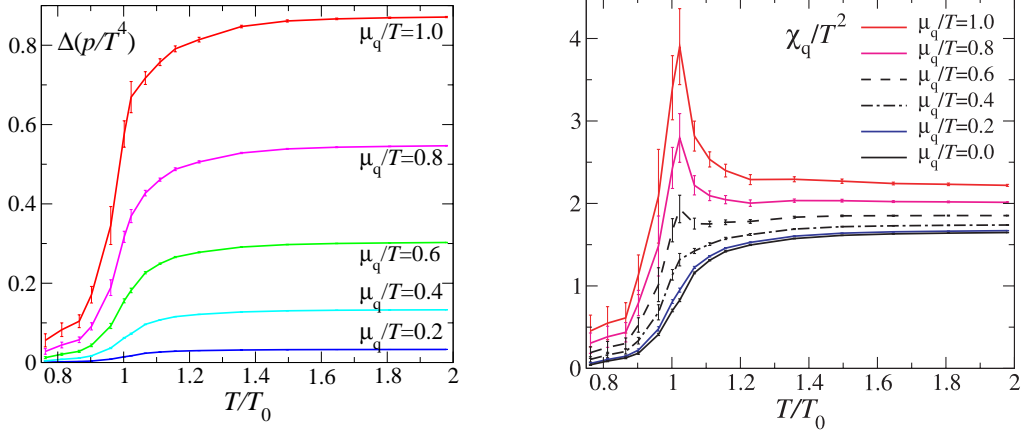
Fig. 2. Difference of pressure from $\mu_q = 0$ (left) and Quark number susceptibility (right) as a function of T for each fixed μ_q/T. T_0 is T_c at $\mu_q = 0$.

down in that regime, i.e. the convergence radius should be smaller than the value of μ_q/T at the critical endpoint. We define estimates for the convergence radius by $\rho_n \equiv \sqrt{|c_n/c_{n+2}|}$. We compute ρ_0 and ρ_2 from $c_0 \equiv p/T^4(0)$, c_2 and c_4. It is found that both ρ_0 and ρ_2 are quite large at high temperature as expected from the SB limit, $\rho_2^{SB} \simeq 2.01, \rho_4^{SB} \simeq 4.44$. On the other hand, around T_c, these are $O(1)$, since c_2 and c_4 are of the same order, so that our results around T_c suggest a singular point in the neighborhood of $\mu_q/T_c = 1$.

Next, we calculate pressure and quark number susceptibility in a range of $0 \leq \mu_q/T \leq 1$ which is within the radius of convergence discussed above, Using the data of c_2 and c_4, p/T^4 and χ_q/T^2 is obtained by $\Delta(p/T^4) \equiv p(T, \mu_q)/T^4 - p(T, 0)/T^4 = c_2(\mu_q/T)^2 + c_4(\mu_q/T)^4 + O(\mu_q^6)$, and $\chi_q/T^2 = 2c_2 + 12c_4(\mu_q/T)^2 + O(\mu_q^4)$.

We draw $\Delta(p/T^4)$ for each fixed μ_q/T in Fig. 2 (left) and find that the difference from $p|_{\mu_q=0}$ is very small in the interesting regime for heavy-ion collisions, $\mu_q/T \approx 0.1$ (RHIC) and $\mu_q/T \approx 0.5$ (SPS), in comparison with the value at $\mu_q = 0$, e.g. the SB value for 2-flavor QCD at $\mu_q = 0$: $p^{SB}/T^4 \simeq 4.06$. The effect of non-zero quark density on pressure at $\mu_q/T = 0.1$ is only 1%. Also, the result is qualitatively consistent with that of Ref. 3) obtained by the reweighting method.

Figure 2 (right) is the result for χ_q/T^2 at fixed μ_q/T. We find a pronounced peak for $m_q/T > 0.5$, whereas χ_q does not have a peak for $\mu_q = 0$. This suggests the presence of a critical endpoint in the (T, μ_q) plane.

This discussion can be easily extended to the charge fluctuation χ_C. The spike of χ_C at T_c is weaker than that of χ_q, which means the increase of the charge fluctuation is smaller than that of the number fluctuation as μ_q increases. [1]

§3. Phase transition line in the (T, μ_q) plane

Next, we investigate the phase transition temperature as a function of μ_q by performing a Taylor expansion around $\mu_q = 0$. [5] In principle, the method via a Taylor expansion is applied for any physical observable. However, as the order of

the derivative becomes higher, the number of terms increases exponentially and there exist serious subtractions, so the method in the previous section does not suit a quantity which needs complex procedures for the measurement such as T_c.

We consider the following identity,

$$\langle \mathcal{O} \rangle_{(\beta,\mu)} = \langle \mathcal{O}W \rangle_{(\beta_0,0)} / \langle W \rangle_{(\beta_0,0)}, \qquad (3\cdot1)$$

where $W = e^{(N_f/4)(\ln \det M(\mu) - \ln \det M(0))} e^{-S_g(\beta) + S_g(\beta_0)}$ for staggered type quarks, S_g is the gauge action, and $\beta = 6/g^2$. An expectation value $\langle \mathcal{O} \rangle$ at (β,μ) is computed by a simulation at $(\beta_0,0)$. This is a basic formula of the reweighting method, but we expand $\ln \det M(\mu)$ and any operator of a fermionic observable using a Taylor series, e.g. $\ln \det M(\mu) - \ln \det M(0) = \sum_{n=1}^{\infty} [\partial(\ln \det M)/\partial \mu](\mu^n/n!)$. This formula is valid in a region that the $\ln \det M(\mu)$ does not have any singular point for each configuration. We moreover neglect the terms higher than $O(\mu^n)$, then the resulting expectation value contains the error of the higher order of μ but the error does not affect the calculation of the derivatives for the lower order than the neglected terms. In fact, if we expand into the form of the Taylor expansion from Eq. (3·1), we obtain the correct coefficients of the Taylor expansion for $\langle \mathcal{O} \rangle$ up to $O(\mu^n)$, and this expression is much simpler than the method discussed in the previous section. Here, we try to trace out the phase transition line for non-zero μ using this method.

However, if we want to use Eq. (3·1), we must discuss a famous problem, called "sign problem". Because $\det M$ is complex at $\mu \neq 0$, if the complex phase fluctuates rapidly, the numerator and the denominator in RHS of Eq. (3·1) becomes vanishingly small, and then we cannot obtain the reliable answer for $\langle \mathcal{O} \rangle$. Of course, the phase fluctuation is zero at $\mu = 0$, but it becomes larger as μ increases. However, in the context of the Taylor expansion, the applicable range of the reweighting method is rather easy to estimate by evaluating the complex phase fluctuation. For small $\mu \equiv N_\tau^{-1}(\mu_q/T)$, the complex phase can be written by the odd terms of the Taylor expansion of $\ln \det M$. [5)] Denoting $\det M = |\det M|e^{i\theta}$,

$$\theta = \frac{N_f}{4} \sum_{n:\text{odd}} \text{Im}\left(\frac{\partial^n \ln \det M}{\partial \mu^n}\right) \mu^n. \qquad (3\cdot2)$$

The first term is $(N_f/4)\text{Im} \, \text{tr}[M^{-1}(\partial M/\partial \mu)]\mu$. From these equations, we find explicitly that the magnitude of θ is proportional to $\mu \equiv N_\tau^{-1}(\mu_q/T)$, $V \equiv N_\sigma^3$ and N_f. Moreover this can be computed by the noise method. Roughly speaking, the sign problem happens when the fluctuation of θ becomes larger than $O(\pi/2)$. Thus the sign problem is not serious for small μ and small volume, but that region becomes narrower and narrower as the volume increases.

We observed the complex phase fluctuation on a $16^3 \times 4$ lattice [5)] and found that the applicable range is not so small for this lattice size. The applicable range is narrower than the convergence radius discussed in §2, but it covers the interesting regime for the heavy-ion collisions at RHIC. We also found a tendency for the phase fluctuation to increase as quark mass decreases, and that the fluctuation is small in the high temperature phase.

In the region where the sign problem is not serious, we determine the phase transition line. Because the first derivative is expected to be zero from the symmetry
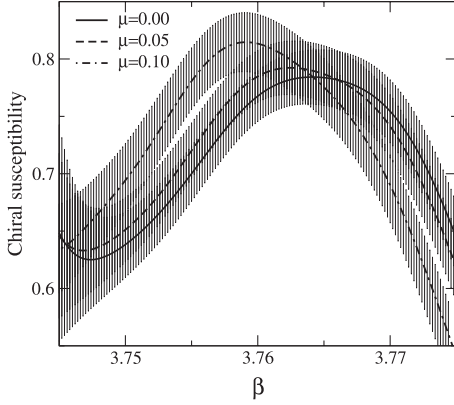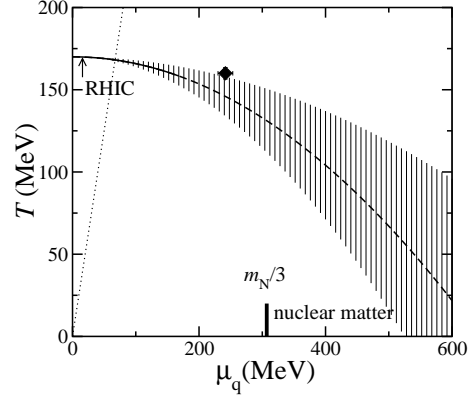
Fig. 3. Chiral susceptibility.

Fig. 4. Sketch of the phase diagram.

under exchange of μ to $-\mu$, we calculate the second derivative of T_c with respect to μ. Simulations are performed around the phase transition point β_c by using the p4-improved action at $ma = 0.1$ and 0.2, corresponding $m_\pi/m_\rho \approx 0.70$ and 0.85, on a $16^3 \times 4$ lattice. In Fig. 3, we plot chiral susceptibility as a function of β for $\mu = 0, 0.05$ and 0.1 at $ma = 0.2$. This calculation contains errors of $O(\mu^4)$. From this figure, we find that the peak position of the susceptibility moves left as μ increases, which means that β_c or T_c decreases as μ increases. Assuming the peak position is β_c, we determine the second derivative of β_c. The truncation error of $O(\mu^4)$ does not affect to this calculation. Combining with the results for the Polyakov loop susceptibility, we obtain $d^2\beta_c/d\mu^2 \approx -1.1$ and the quark mass dependence of $d^2\beta_c/d\mu^2$ for $ma = 0.1$ and 0.2 is not visible within the accuracy of our calculation. (However, we find large mass dependence for very small quark mass. See §4.)

The second derivative of T_c is given by

$$\frac{d^2 T_c}{d\mu_q^2} = -\frac{1}{N_\tau^2 T_c} \frac{d^2\beta_c}{d\mu^2} \bigg/ \left(a\frac{d\beta}{da}\right). \tag{3·3}$$

The beta function, $a(d\beta/da)$, is obtained from the string tension data in Ref. 11). We then find $(T_c/2)(d^2T_c/d\mu_q^2) = -0.07(3)$. We sketch the phase transition line from the curvature in Fig. 4. The diamond symbol is the critical point obtained by Ref. 6). The dotted line is the upper bound of the fit range to determine the curvature. At the relevant point for RHIC, this shift of T_c is very small from that at $\mu = 0$ and the result is roughly consistent with those obtained by the other groups. [6], [7]

Comparing the result of the equation of state, we also find that the lines of constant pressure and energy density are roughly consistent with the phase transition line for small μ_q, which suggest the change of pressure and energy density is small along the transition line. Moreover, by measuring the Polyakov loop, we can observe that the external quark current is screened by dynamical anti-quarks. [5]

§4.   Critical endpoint for 3-flavor QCD

Finally, we consider 3-flavor QCD. We perform simulations for $N_\mathrm{f} = 3$ at $ma = 0.1$ ($m_\pi/m_\rho \approx 0.68$) on $16^3 \times 4$ lattices, and at $ma = 0.005$ on $12^3 \times 4$ and $16^3 \times 4$ lattices, using the p4-improved action.[9] The result of the curvature at $ma = 0.1$ is $(T_c/2)(\mathrm{d}^2 T_c/\mathrm{d}\mu_q^2) = -0.045(10)$, where we keep μ for strange quark is zero, and $a(\mathrm{d}\beta/\mathrm{d}a)$ is obtained from the string tension data. The difference from $N_\mathrm{f} = 2$ is not large at $ma = 0.1$. However, a significant difference is observed between $ma = 0.005$ and 0.1 for $N_\mathrm{f} = 3$. Using a perturbative beta-function, we obtain $(T_c/2)(\mathrm{d}^2 T_c/\mathrm{d}\mu_q^2) = -0.025(6)$, and $-0.114(46)$ for $m = 0.1$ and 0.005, respectively. Although the perturbative beta-function gives almost a factor of 2 smaller result than the non-perturbative analysis, this suggests that the curvature of the transition line becomes stronger as the quark mass smaller.

The most interesting point for $N_\mathrm{f} = 3$ is the existence of the critical quark mass m_c on $\mu_q = 0$ axis between a first order phase transition at small m and crossover at large m. In order to identify m_c, we compute Binder cumulants constructed from the chiral condensate, $B_4 = \langle(\delta\bar\psi\psi)^4\rangle/\langle(\delta\bar\psi\psi)^2\rangle^2$. It has been verified that the critical point belongs to the Ising universality class, i.e. the value of B_4 at T_c for m_c is the same with that of 3-dimensional Ising model.[10] Moreover, we expect such a critical point at $\mu_q \neq 0$ even in the region of large m, hence it is very interesting to investigate how the critical point moves as a function of μ_q.

We apply the Taylor expanded reweighting method, explained in §3, with respect to quark mass, replacing μ to $\Delta m \equiv m - m_0$, where m_0 is a simulation point, and we investigate the quark mass dependence around the simulation point, $m_0 = 0.005$. The reweighting factor is computed up to $O[(\Delta m)^2]$. This analysis suggests a critical value of $m_c = 0.0007(4)$ for $\mu_q = 0$. At this point, the Binder cumulant is consistent with the value of the Ising model, and also the peak height of the chiral susceptibility $\chi_{\bar\psi\psi}$ shows scaling behavior indicating a first order phase transition, i.e. $\chi_{\bar\psi\psi} \sim V$, for the volume size $V = 12^3$ and 16^3 below about this point. The corresponding value of pseudoscalar meson mass at the critical point is $m_\pi^\mathrm{crit} = 67(18)$ MeV. Hereafter, we use the value of m_π at $T = 0$ for setting a physical scale of quark mass instead of the value of bare quark mass m.

Next, we investigate the critical point for finite μ using the Taylor expanded reweighting method with respect to μ, up to $O(\mu^2)$. Since the sign problem is serious for the analysis on the $16^3 \times 4$ lattice, we analyze only the data on the $12^3 \times 4$ lattice. The data of B_4 suggests $\mu^\mathrm{crit} = 0.074(13)$ or $\mu_q^\mathrm{crit}/T = 0.296(52)$. An estimate for the transition temperature at corresponding m_π is obtained from $T_c/\sqrt\sigma = 0.40(1) + 0.039(4)(m_\pi/\sqrt\sigma)$[15]. Then the critical value is $\mu_q^\mathrm{crit} = 52(10)$ MeV at the simulation point $ma = 0.005$. The corresponding m_π is about 170 MeV.

In the context of the Taylor expanded reweighting method for $(2+1)$-flavor QCD with up and down quark masses and strange quark mass, m_{ud} and m_s, the system is identical along the line of slope -2 near $m_{ud} = m_s$ line in the (m_{ud}, m_s) plane, since the first terms of reweighting factor in terms of Δm for m_{ud} and m_s are cancelled, i.e. if $(m_s - m^{(3f)})/(m_{ud} - m^{(3f)}) = -2$ is satisfied, the systems at (m_{ud}, m_s) and

$(m^{(3f)}, m^{(3f)})$ are the same for $m_{ud} \approx m_s$. We use this property for the extrapolation to the physical point. Using the lowest order chiral perturbation theory relation, $m_K^2/m_\pi^2 = (m_{ud} + m_s)/(2m_{ud})$, this line in the (m_{ud}, m_s) plane is translated to the line of slope $-1/2$ in the (m_π^2, m_K^2) plane. Hence, when $m_K^2 = -m_\pi^2/2 + 3m_\pi^{(3f)2}/2$, the physics at (m_π^2, m_K^2) is roughly corresponding to that of 3-flavor QCD with $m_\pi^{(3f)}$. For the physical value $m_\pi = 140$ MeV and $m_K \approx 500$ MeV, we obtain the corresponding pion mass for 3-flavor QCD, $m_\pi^{(3f)} = 416$ MeV. The extrapolation to this pion mass value is performed by a straight line in the (m_π^2, μ_q^2) plane using the two critical points which we found at $\mu_q = 0$ and $\mu_q \neq 0$ for 3-flavor QCD. We obtain the estimation of the critical point for the physical quark mass, $\mu_q^{\text{crit}} \approx 140$ MeV. This value is smaller than the value of about 240 MeV estimated by Ref. 6) for (2+1)-flavor QCD. Further study is required to improve this analysis.

§5. Conclusions

Taylor expansion coefficients were calculated up to $O(\mu^4)$ for pressure and up to $O(\mu^2)$ for phase transition temperature. We found that the differences of T_c and pressure from those at $\mu_q = 0$ are small for the interesting values of μ_q for the heavy-ion collisions at RHIC and SPS. The fluctuations in the quark number density increase in the vicinity of T_c and the susceptibilities start to develop a pronounced peak as μ_q is increased. This suggests the presence of a critical endpoint in the (T, μ_q) plane. Also, the critical endpoint for 3-flavor QCD near $\mu_q = 0$ was investigated. The extrapolation from the critical point at $\mu_q = 0$ suggests that the critical endpoint exists around $\mu_q/T_c \sim 1$ for the physical quark mass.

Acknowledgements

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