REMARKS ON THE REWEIGHTING METHOD IN THE CHEMICAL POTENTIAL DIRECTION

SHINJI EJIRI

Department of Physics, University of Wales Swansea,
Singleton Park, Swansea, SA2 8PP, U.K.

We comment on the reweighting method in the chemical potential ($\mu_q$) direction. We study the fluctuation of the reweighting factor during Monte-Carlo steps. We find that it is the absolute value of the reweighting factor that mainly contributes to the shift of the phase transition line ($\beta_c$) by the presence of $\mu_q$. The phase fluctuation is a cause of the sign problem, but the effect on $\beta_c$ seems to be small. We also discuss $\beta_c$ for Iso-vector chemical potential and $\beta_c$ determined from simulations with imaginary chemical potential.

1. Introduction

The study of QCD at finite temperature and finite density is currently one of the most attractive topics in particle physics. The heavy-ion collision experiments aiming to produce the quark-gluon plasma are running at BNL and CERN, for which the interesting regime is rather low density. Moreover a new color superconductor phase is expected in the region of low temperature and high density. Numerical study by Monte-Carlo simulations of Lattice QCD is a powerful means of investigating aspects of the phase transition but the Monte-Carlo method is not applicable directly at finite density because the fermion determinant is complex for non-zero quark chemical potential $\mu_q$. Most of the studies at $\mu_q \neq 0$ are done by the reweighting method performing simulations at Re($\mu_q$) = 0\textsuperscript{1,2,3}.

In this paper, we make a comment on the reweighting method for the chemical potential direction. The interesting point is that there are two simulation parameters, $\beta = 6/g^2$ and $\mu = \mu_q a$. We perform a simulation at a suitable point ($\beta_0, \mu_0$) and, in order to calculate an observable at another point ($\beta, \mu$), we modify the Boltzmann weight. Then, if the

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modification factors (reweighting factors) for $\beta$ and $\mu$ are correlated during Monte-Carlo steps, there could exist a parameter subspace in which the effect of the modification is cancelled and changes of all physical quantities are small. Therefore it is interesting to investigate the correlation between the reweighting factors and to confirm if such a direction exists. It is also interesting to discuss the relation between that direction and the phase transition line, since we naively expect the physics is similar along the phase transition line. Moreover, increase of the error due to the reweighting could be reduced by the cancellation, which may explain why Fodor and Katz could calculate $\beta_c$ for rather large $\mu$.

2. Fluctuation of the reweighting factor

The reweighting method is based on the following identity:

$$
\langle O \rangle_{(\beta, \mu)} = \frac{1}{Z_{(\beta, \mu)}} \int DUO(e^{-S_\beta})^N e^{-S_\mu} = \frac{\langle O e^\Delta F e^{\Delta G} \rangle_{(\beta_0, \mu_0)}}{\langle e^\Delta F e^{\Delta G} \rangle_{(\beta_0, \mu_0)}}.
$$

Here $M$ is the quark matrix, $S_\beta$ is the gauge action, $N_f$ is the number of flavors, $F = N_0(\ln \det M(\mu) - \ln \det M(\mu_0))$, $G = (\beta - \beta_0)P$, $P = -\partial S_\beta / \partial \beta$, and $\Delta f = f - \langle f \rangle$. The expectation value $\langle O \rangle_{(\beta, \mu)}$ can in principle be computed by simulation at $(\beta_0, \mu_0)$ by this identity. In this study, we put $\mu_0 = 0$. If $O$ and $e^\Delta F e^{\Delta G} = e^F G / (e^F e^{G(f)})$ fluctuate with a correlation during Monte-Carlo steps, $\langle O \rangle_{(\beta, \mu)}$ has $\mu$ and $\beta$ dependence. Otherwise, the $\mu$ and $\beta$ dependence cannot be obtained, e.g. if $e^F G$ does not fluctuate, $e^\Delta F e^{\Delta G} = 1$ and $\langle O \rangle_{(\beta, \mu)}$ does not change. Roughly speaking, the difference of $\langle O \rangle_{(\beta, \mu)}$ from $\langle O \rangle_{(\beta_0, 0)}$ increases as the magnitude of fluctuations of $F$ and $G$ increases.

We discuss the correlation between $e^F$ and $e^G$. Since $e^F$ is complex, we separate it into a phase factor and an amplitude. As is shown in Ref.\(^3\), the phase factor and the amplitude can be written by the odd terms and the even terms of the Taylor expansion of $\ln \det M$, respectively, since the odd terms are purely imaginary and the even terms are real at $\mu = 0$. Denoting $e^F = e^{i\theta} |e^F|$ and $F = \sum_{n=1}^{\infty} R_n \mu^n$, $|e^F| = \exp\{\sum_{n=1}^{\infty} \text{Re} R_{2n-1} \mu^{2n-1}\}$, and $e^{i\theta} = \exp\{i \sum_{n=1}^{\infty} \text{Im} R_{2n-1} \mu^{2n-1}\}$. We study these correlations in the vicinity of the simulation point $(\beta_0, 0)$. Up to $O(\beta - \beta_0, \mu^2)$, the reweighting factor is $e^{i\theta} |e^F| e^G \approx 1 + R_1 \mu + R_1^2 \mu^2 / 2 + R_2 \mu^2 + P(\beta - \beta_0)$. We compute the correlations, $(\Delta(R_1^2 / 2) \Delta P)$, $(\Delta R_2 \Delta P)$, and $(\Delta(R_1^2 / 2) \Delta R_2)$, which correspond to the correlations of $(e^{\theta}, e^G)$, $(|e^F|, e^G)$ and $(e^{i\theta}, |e^F|)$, respectively. Here, $(\Delta R_1 \Delta P)$ is zero at $\mu = 0$ because $R_1$ is purely imaginary.
We use the configurations in Ref. 3, which are generated by the $N_f = 2$ p4-improved staggered action on a $16^3 \times 4$ lattice. The results are summarized in Table 1. We find that the correlation between $|e^F|$ and $e^G$ is very strong in comparison with the other correlations, which means that the contribution to an observable can be separated into two independent parts: from $e^{i\theta}$, and from a combination of $|e^F| \times e^G$.

Table 1. Correlations among $R_1^2$, $R_2$, and $P$. $N_{\text{site}} = 16^3 \times 4$.

| $m$ | $\beta$ | $\langle (\Delta(R_1^2/2)\Delta P)N_{\text{site}}^{-1}\rangle$ | $\langle \Delta R_2 \Delta P \rangle N_{\text{site}}^{-1}$ | $\langle (\Delta(R_1^2/2)\Delta R_2)N_{\text{site}}^{-1}\rangle$ |
|-----|--------|--------------------------------|----------------|--------------------------------|
| 0.1 | 3.64   | 0.006(29)                     | 0.312(33)      | 0.034(10)                     |
|     | 3.65   | 0.059(21)                     | 0.434(29)      | 0.056(10)                     |
|     | 3.66   | 0.055(15)                     | 0.410(26)      | 0.022(5)                      |
|     | 3.67   | 0.032(15)                     | 0.397(28)      | 0.031(5)                      |
| 0.2 | 3.75   | 0.037(18)                     | 0.287(26)      | 0.029(7)                      |
|     | 3.76   | 0.019(10)                     | 0.353(23)      | 0.018(3)                      |
|     | 3.77   | 0.037(10)                     | 0.359(24)      | 0.017(3)                      |

To make the meaning of this result clearer, we consider the following partition function, introducing two different $\mu$, $\mu_o$ and $\mu_e$,

$$Z = \int DU e^{R_1 \mu_o + R_3 \mu_e + \cdots + R_2 \mu_e^2 + R_4 \mu_e^4 + \cdots} (\det M)_{\mu=0}^{N_f} e^{-S_g}$$

Then, $\langle \Delta R_1^2 \Delta P \rangle = \langle (\Delta R_1)^2 \Delta P \rangle = \frac{\partial^3 \ln Z}{\partial \mu_o^2 \partial \mu_e} N_{\text{site}}$, $2 \langle \Delta R_2 \Delta P \rangle = \frac{\partial^3 \ln Z}{\partial \mu_e^2 \partial \mu_o} N_{\text{site}}$, at $\mu = 0$, where $\chi_S$ and $\chi_{NS}$ are the singlet and non-singlet quark number susceptibilities. The result in Table 1 means that $\frac{\partial^3 \ln Z}{\partial \mu_e^2 \partial \mu_o} < < \frac{\partial^3 \ln Z}{\partial \mu_o^2 \partial \mu_o}$, i.e. $\mu_o$ in the phase factor ($\mu_o$) does not contribute to the $\beta$-dependence of $Z$ and $\mu$ in the amplitude ($\mu_e$) is more important for the determination of $\beta_c$. Moreover, these correlations have a relation with the slope of $\chi_S$ and $\chi_{NS}$ in terms of $\beta$. Since $\chi_S - \chi_{NS}$ is known to be small, this result may not change even for small quark mass.

Iso-vector chemical potential Next, we discuss the model with Iso-vector chemical potential. If we impose a chemical potential with opposite sign for $u$ and $d$ quarks: $\mu_u = -\mu_d$, the Monte-Carlo method is applicable, since the measure is not complex. In Ref. 3, we discussed the difference of the curvature of the phase transition line in this case. Because we expect at $T = 0$ that pion condensation happens around $\mu_q \approx m_{\pi}/2$, if we consider that the phase transition line runs to that point directly, the curvature of the
transition line for Iso-vector $\mu$ should be much larger than that for usual $\mu$, since $m_\pi/2 << m_N/3$. However, as we discussed above, $\mu_o$ in Eq. 2 does not contribute the shift of $\beta_c$ and the difference from the usual $\mu$ is only in $\mu_o$, i.e. $\mu_o = 0$ for the Iso-vector case. Therefore the difference of the curvature might be small and the naive picture seems to be wrong. In practice, our result at small $\mu$ using the method in Ref. 3 supports that. Moreover Kogut and Sinclair 6 showed that $\beta_c$ from chiral condensate measurements is fairly insensitive to $\mu$ for small $\mu$ by direct simulations with Iso-vector $\mu$.

We estimate the fluctuation of the reweighting factor. The phase factor $e^{i\theta}$ gives a contribution independent from the other parts. As we discussed in Ref.3, these phase fluctuations cause the sign problem to become more severe as $\mu$ (or $\mu_o$) increases. The amplitude of the fermionic part and the gauge part are strongly correlated. Therefore the magnitude of the contribution to an observable is not simple. We compute the dispersion of $|e^F|e^G$ to estimate the fluctuation. Up to $O[\beta - \beta_0, \mu^2], \langle (\Delta |e^F|e^G|^2)^2 \rangle \approx \mu^4(\langle \Delta R^2 \rangle^2) + 2\mu^2(\beta - \beta_0)(\Delta R\Delta P) + (\beta - \beta_0)^2(\Delta P)^2$. Then, the line of constant dispersion is an ellipse. We write contour line in Fig. 1(left). Here the susceptibilities of $R_2$ and $P$ and the correlation of $R_2$ and $P$ are computed at the phase transition point, $\beta_c = 3.6497(16)$ for $m = 0.1$. We denote the lower and upper bounds of $\partial^2 \beta_c/\partial \mu^2 = -1.1(4)$ by bold lines. We find that there exists a direction along which the increase of the fluctuation is relatively small. That direction is roughly parallel to the phase transition line. Because we expect that physics is similar along
the transition line, if we consider that $|e^F|e^G$ is the important part for the calculation of $\beta_c$, this result suggests that the phase transition line is determined by the quite simple mechanism that the fluctuation of the reweighting factor itself is small along the transition line and physics is similar on that line.

**Imaginary chemical potential** In Fig. 1(left), we write also the region for $\mu^2 < 0$, i.e. imaginary $\mu$. de Forcrand and Philipsen$^7$ computed $\partial^2 \beta_c/\partial \mu^2$ performing simulations with imaginary $\mu$, assuming that $\beta_c$ is an even function in $\mu$ and analyticity in that region. Here, we confirm whether the results obtained by real and imaginary $\mu$ are consistent or not by the method in Ref.$^3$. We replace $\mu$ by $i\mu$ or $-i\mu$ and reanalyze for imaginary $\mu$. In Ref.$^3$, the reweighting factor has been obtained in the form of the Taylor expansion in $\mu$ up to $O(\mu^2)$, and the replacement is easy. We determined $\beta_c$ by the chiral susceptibility. The results of $|\beta_c(\mu) - \beta_c(0)|$ are written in Fig. 1(right). Errors are $O(\mu^4)$. The solid line is the result for real $\mu$. The results of $\mu \to i\mu$ and $\mu \to -i\mu$ are dashed and dot-dashed lines respectively. The slope at $\mu = 0$ is $(\partial^2 \beta_c/\partial \mu^2)/2$. We find that these results of the slope for real and imaginary $\mu$ are consistent.

3. Conclusions

We investigated the fluctuation of the reweighting factor. The contribution to the $(\beta, \mu)$ dependence of a physical quantity can be separated into the phase factor and the amplitude. Mainly the amplitude of the reweighting factor contributes to the determination of $\beta_c$. The fluctuation of the amplitude is small along the phase transition line, which is consistent with physics being similar along the transition line, while the fluctuation of the phase increases in proportion to $\mu$ and causes the sign problem. We also confirmed that the second derivative of the phase transition lines at $\mu = 0$ determined from imaginary $\mu$ is consistent with that from real $\mu$.

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