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Sign problem and the chiral spiral on the finite density lattice

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We investigate the sign problem of the fermion determinant at finite baryon density in $(1+1)$ dimensions, in which the ground state in the chiral limit should be free from the sign problem by forming a chiral spiral. To confirm it, we evaluate the fermion determinant in the continuum theory at the one-loop level and find that the determinant becomes real as expected. The conventional lattice formulation to implement a chemical potential is, however, not compatible with the spiral transformation. We discuss an alternative of the finite-density formulation and numerically verify the chiral spiral on the finite density lattice.

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I. INTRODUCTION

QCD has profound contents to be explored with external parameters such as the temperature T, the baryon chemical potential μ_B (that is equal to the quark chemical potential μ_q multiplied by the number of colors N_c), the magnetic field B, and so on [1]. The direct calculation based on QCD is, however, feasible only in some limited ranges of these parameters. In particular along the direction of increasing μ_q, perturbative QCD is not really useful unless the density is high enough to accommodate color superconductivity [2,3]. Moreover, the numerical simulation based on lattice QCD breaks down with finite μ_q. The most serious obstacle lies in the fact that the Monte Carlo importance sampling is invalid for the finite-density case due to the complex fermion determinant, which is commonly referred to as the sign problem [4].

The sign problem is also relevant in analytical computations [5,6]. At finite T, the temporal component of the gauge field A_4 plays a special role, and its expectation value is given a gauge-invariant interpretation, namely, (the phase of) the Polyakov loop, $L \equiv \mathcal{P}\exp[ig\int_0^\beta dx_4 A_4]$. Because the traced Polyakov loop is an order parameter for quark deconfinement, many efforts have been devoted to the computation of the effective potential for L [7–9]. With the contribution from the fermion determinant [10], the effective potential at nonzero μ_q has turned out to take a complex value, and thus the physical meaning as a grand potential or thermal weight is obscure. This is how we observe the sign problem using the perturbative calculation.

Since the resolution of the sign problem is still far from our hands, it is instructive to study density-like effects that cause no sign problem. Theoretical attempts along this line include the imaginary chemical potential [11], the isospin chemical potential [12], the chiral chemical potential [13], dense QCD with two colors or with adjoint matter [4,14], the magnetic field [15], and so on. Among them the magnetic field leads to a quite suggestive change in the state of quark matter. The most drastic consequences result from the Landau quantization and the dominance of the lowest Landau levels for spin-$1/2$ fermions. In the strong-B limit, quarks are reduced to a $(1+1)$-dimensional system.

The nature of chiral symmetry breaking is affected accordingly by the strong-B effects [16]; the spontaneous breaking of chiral symmetry inevitably occurs in the $(1+1)$-dimensional system (or in the lowest-Landau-level approximation [17]), which is called magnetic catalysis. This phenomenon is analogous to superconductivity, which is also triggered by the low-dimensional nature of the Fermi surface. In chiral model studies [18], the chiral phase transition is delayed toward a higher temperature due to magnetic catalysis, while in the finite-T lattice QCD simulation it has been recognized that the chiral crossover temperature gets smaller with increasing B, which is called inverse magnetic catalysis or magnetic inhibition [19]. Another interesting example from the $(1+1)$-dimensional nature is the topological phenomenon such as the chiral magnetic effect [20] that might be detectable with the noncentral collision of positively charged heavy ions through charge separation or photon emission [21].

Such a $(1+1)$-dimensional quark matter provides us with further useful information; the ground state of the $(1+1)$-dimensional chiral system at finite density (with a large number of internal degrees of freedom) is known to form a chiral spiral [22,23]. In the strong-B limit, therefore, the "chiral magnetic spiral" would be the ground-state candidate of finite-density and magnetized quark matter [24]. The essential idea of Ref. [24] was that the explicit μ_q dependence is rotated away in $(1+1)$ dimensions, and this procedure transforms the homogeneous chiral condensate to form a spiral in the chiral basis. This at the same time implies that the sign problem should no longer be harmful once the dimensional reduction occurs.

One might have thought that the strong-B limit is such a special environment having loose relevance to our realistic world. It has been argued, however, that quark matter at high density even without B already exhibits characteristics of a pseudo-$(1+1)$-dimensional system locally on the Fermi surface [25], and the whole Fermi surface should be covered by low-dimensional patches [26]. Besides, the p-wave pion condensation in nuclear matter having the same spiral structure is still a vital possibility beyond the normal nuclear density [27]. In this way, it is definitely worth considering the sign problem and the ground-state structure in $(1+1)$-dimensional systems both for academic interest and for practical purposes.

The present work reports that the conventional lattice formulation at finite density becomes problematic even for describing the expected ground state of such an idealized $(1+1)$-dimensional system. First we shall illuminate how the sign problem is irrelevant in $(1+1)$ dimensions by performing the perturbative calculation. Then, we will proceed to the lattice formulation to find that the conventional introduction of μ_{q} [28] cannot realize the transformation properties in the continuum theory. We choose an alternative that is optimal to yield a chiral spiral and conduct the numerical test to confirm a spiral formation on the lattice.

II. PERTURBATIVE CALCULATION

Let us first evaluate the fermion determinant at finite μ_{q} and a high enough T that justifies the perturbative treatment. At the one-loop level in the deconfined phase, we should keep the Polyakov-loop A_4 background and carry out the Gaussian integration with respect to quantum fluctuations of gluons. After taking the summation over the Matsubara frequency, we can write the determinant $\mathcal{M}[A_4]$ (for a single flavor throughout this work) down as

$$\begin{aligned}\mathcal{M}[A_4] &= \mathcal{N}\mathrm{e}^{-T^d V_d \Gamma[A_4]}\\ &= \mathcal{N}\exp\left\{\alpha_d \int \frac{V_d d^d p}{(2\pi)^d}\right.\\ &\left.\quad\times \operatorname{tr}\ln\left[(1+L\mathrm{e}^{-(\varepsilon-\mu_{\mathrm{q}})/T})(1+L^\dagger \mathrm{e}^{-(\varepsilon+\mu_{\mathrm{q}})/T})\right]\right\},\end{aligned} \tag{1}$$

where d and V_d represent the spatial dimension and the spatial volume, respectively, and the dispersion relation is $\varepsilon=\sqrt{p^2+m^2}$. We note that the spin degeneracy factor α_d depends on d: $\alpha_3=2$ and $\alpha_1=1$. For practical convenience, we rotate the color basis as $ULU^\dagger = \mathrm{diag}(\mathrm{e}^{\mathrm{i}\pi\phi_1}, \mathrm{e}^{\mathrm{i}\pi\phi_2}, \mathrm{e}^{\mathrm{i}\pi\phi_3})$, where $\phi_1+\phi_2+\phi_3=0$ should hold to satisfy $\det(ULU^\dagger)=1$.

For the massless case ($m=0$), we can perform the full analytical integration for arbitrary d. In particular, a choice of $d=3$ yields the well-known Weiss–Gross-Pisarski-Yaffe-type potential [8] that takes the following polynomial form [1,10,29]:

$$\Gamma[\phi] = -\frac{4\pi^2}{3}\sum_{i=1}^{N_{\mathrm{c}}} B_4\left[\left(\frac{1+\phi_i}{2}\right)_{\mathrm{mod}\ 1} - \frac{\mathrm{i}\tilde{\mu}_{\mathrm{q}}}{2}\right], \tag{2}$$

where the Bernoulli polynomial appears as $B_4(x) = x^2(1-x)^2 - 1/30$ [9]. We also introduced the dimensionless chemical potential as $\tilde{\mu}_{\mathrm{q}} \equiv \mu_{\mathrm{q}}/(\pi T)$ for notational simplicity. While we choose $N_{\mathrm{c}}=3$ in our QCD study, Eq. (2) is valid for any $\mathrm{SU}(N_{\mathrm{c}})$ groups.

The apparent presence of the imaginary part in Eq. (2) corresponds to the sign problem. Indeed, the phase of the fermion determinant is nothing but $-T^d V_d \mathrm{Im}\Gamma$ (mod 2π). To gain a more informative view, we make a plot for $\mathrm{Im}\Gamma[\phi]$ in the upper panel of Fig. 1 as a function of ϕ_1 and ϕ_2 (with $\phi_3=-\phi_1-\phi_2$). It is clear from the figure that the imaginary part has a nontrivial dependence on the gauge configuration ϕ_1 and ϕ_2.

A more interesting case is for $d=1$ corresponding to quark matter under the dimensional reduction. In this case we have

$$\Gamma[\phi] = 2\pi\sum_{i=1}^{N_{\mathrm{c}}} B_2\left[\left(\frac{1+\phi_i}{2}\right)_{\mathrm{mod}\ 1} - \frac{\mathrm{i}\tilde{\mu}_{\mathrm{q}}}{2}\right]. \tag{3}$$

Here, we again used the Bernoulli polynomial as defined by $B_2(x) = x^2 - x + 1/6$. It is quite reasonable that $B_4(x)$ in Eq. (2) for $d+1=4$ is replaced with $B_2(x)$ in Eq. (3) for $d+1=2$. The imaginary part for $d=1$ is given as

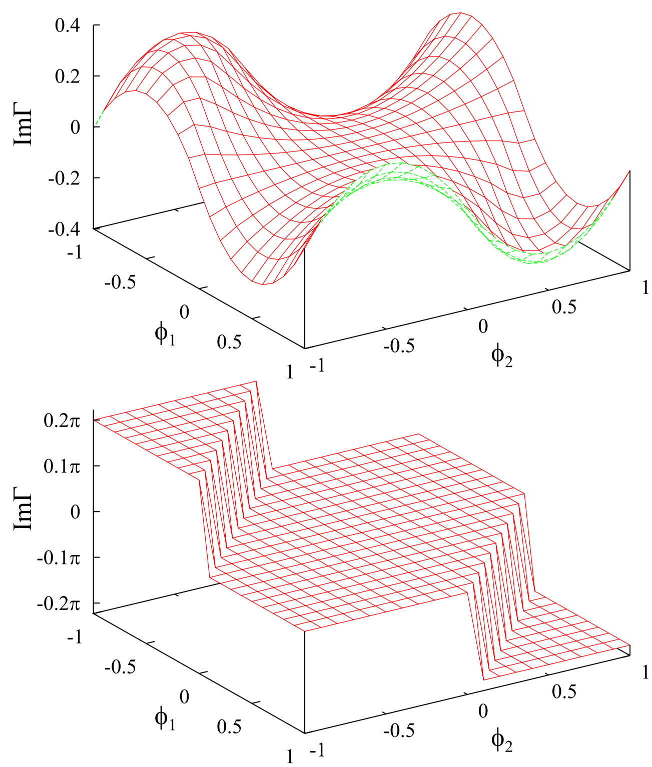

FIG. 1 (color online). (Upper) Imaginary part of $\Gamma[\phi]$ for $d=3$ at $\tilde{\mu}_{\mathrm{q}}=0.1$ shown as a function of ϕ_1 and ϕ_2. (Lower) Imaginary part of $\Gamma[\phi]$ for $d=1$ at $\tilde{\mu}_{\mathrm{q}}=0.1$.

$$\mathrm{Im}\Gamma[\phi] = \begin{cases} 0 & (-1 < \phi_1 + \phi_2 < 1), \\ -2\pi\tilde{\mu}_q & (\phi_1 + \phi_2 \geq 1), \\ +2\pi\tilde{\mu}_q & (\phi_1 + \phi_2 \leq -1). \end{cases} \tag{4}$$

This behavior is visually shown in the lower panel of Fig. 1. The step emerges when $(1+\phi_3)/2 = (1-\phi_1-\phi_2)/2$ exceeds the boundary of modular one. As is clear from the above expression, $\mathrm{Im}\Gamma$ takes a constant $\pm 2\pi\tilde{\mu}_q$, which is $\pm 0.2\pi$ in our numerical setup ($\tilde{\mu}_q = 0.1$) for Fig. 1.

With a more careful deliberation on the phase-space volume, we see that an imaginary part in the region $|\phi_1 + \phi_2| \geq 1$ has no contribution since this finite value is quantized as $TV_1 \mathrm{Im}\Gamma = 2\pi n$ with an integer n. To see this, let us consider the branch-cut contribution from the logarithm in the integrand of Eq. (1), which appears when the real part in the logarithm turns negative, i.e., $\mathrm{Re}[e^{i\pi\phi_i - (|p|-\mu_q)/T}] < -1$. The momentum integration under this condition picks up the phase-space volume satisfying $|p| < \mu_q$, that is, $\pm\sum_{\text{Phase Space}} 2\pi\theta(\mu_q - |p|) = \pm 2\cdot 2\pi\lfloor V_1\mu_q/2\pi\rfloor$, where $\lfloor \cdots \rfloor$ represents the floor function. It reproduces Eq. (4) multiplied with TV_1 in a quantized form. As conjectured, no sign problem arises in perturbative analyses in the $(1+1)$-dimensional continuum theory.

III. LATTICE FORMULATION

This analytical observation is, however, not easy to be validated on the lattice. To make the point clear, let us take a pseudo-$(1+1)$-dimensional system discarding two transverse (first and second) components. Then, in Euclidean space-time with the longitudinal (third) and the temporal (fourth) components, the Lagrangian density, $\mathcal{L}_{\text{eff}} = \bar{\psi}D(\mu_q)\psi$, with $D(\mu_q) = \gamma^3(\partial_3 - igA_3) + \gamma^4(\partial_4 + \mu_q - igA_4)$ defines the theory. Here, we consider the most interesting case of $m = 0$ only. Then, we can confirm that μ_q is superficially erased by the following rotation: $\psi \to \psi = U\psi'$, $\bar{\psi} \to \bar{\psi} = \bar{\psi}'U$ with $U = \exp(-\mu_q\gamma^3\gamma^4 x_3)$. The chemical potential can be factorized out by the unitary transformation, $D(\mu_q) = U^\dagger D(0) U^\dagger$, and thus the fermion determinant is independent of μ_q. Strictly speaking, this rotation also causes a shift in momenta carried by ψ' and $\bar{\psi}'$, and such a shift gives rise to a nontrivial μ_q dependence through the chiral anomaly [22]. For the moment, it suffices for our purpose of seeing the spiral if we focus on the tree-level elimination of the μ_q term, and we will not go into the anomalous μ_q dependence.

In the conventional lattice formulation [28], μ_q is introduced as

$$\begin{aligned} \bar{\psi}\gamma^4(\partial_4 + \mu_q)\psi &= (\bar{\psi}e^{-\mu_q x_4})\gamma^4\partial_4(e^{\mu_q x_4}\psi) \\ &\simeq \frac{1}{2}\bar{\psi}(x)\gamma^4 e^{\mu_q}\psi(x+\hat{4}) \\ &\quad - \frac{1}{2}\bar{\psi}(x)\gamma^4 e^{-\mu_q}\psi(x-\hat{4}). \end{aligned} \tag{5}$$

If we apply the unitary transformation U on the lattice, we find $UD(\mu_q)U$ as

$$\begin{aligned} &\frac{1}{2}\{\bar{\psi}'(x)[(\gamma^3\cos\mu_q - \gamma^4\sin\mu_q)\psi'(x+\hat{3}) + \gamma^4 e^{\mu_q}\psi'(x+\hat{4})] \\ &-\bar{\psi}'(x)[(\gamma^3\cos\mu_q + \gamma^4\sin\mu_q)\psi'(x-\hat{3}) \\ &+\gamma^4 e^{-\mu_q}\psi'(x-\hat{4})]\} \end{aligned} \tag{6}$$

apart from the link variables. In the continuum limit (i.e. the lattice spacing $a \to 0$), where $\mu_q a$ goes vanishingly small, the explicit μ_q dependence disappears as anticipated from the continuum theory. In this sense, such an incomplete cancellation in Eq. (5) is a lattice artifact, and yet, this is crucial for the sign problem and the formation of the chiral spiral.

One quick remedy for the noncancellation problem is to alter the way one formulates μ_q on the lattice. We propose to introduce the chemical potential as $D(\mu_q) = U^\dagger D(0) U^\dagger$, i.e. (see Ref. [30] for a similar proposal),

$$\begin{aligned} &\bar{\psi}(\gamma^3\partial_3 + \gamma^4\mu_q)\psi \\ &\quad = (\bar{\psi}U^\dagger)\gamma^3\partial_3(U^\dagger\psi) \\ &\quad \simeq \frac{1}{2}\bar{\psi}(x)(\gamma^3\cos\mu_q + \gamma^4\sin\mu_q)\psi(x+\hat{3}) \\ &\qquad - \frac{1}{2}\bar{\psi}(x)(\gamma^3\cos\mu_q - \gamma^4\sin\mu_q)\psi(x-\hat{3}) \end{aligned} \tag{7}$$

(with link variables omitted). In this form, it may look trivial at first glance that the unitary transformation can get rid of the μ_q dependence. However, the situation is not so trivial. One can actually prove that the eigenvalues of this fermion operator appear as a quartet: λ, $-\lambda$, λ^*, and $-\lambda^*$. In other words, the fermion determinant is always real regardless of the dimensionality! Needless to say, this cannot be a resolution of the sign problem. Because $\sin\mu_q$ is accompanied by $\cos q_3$ in the momentum space of Eq. (7), the sign of μ_q changes for the fermion doublers in the $\hat{3}$ direction. Therefore, if we interpret the doublers as different quark flavors, μ_q as it appears in Eq. (7) represents the isospin chemical potential rather than the quark chemical potential, so that the determinant is always real! This also means that the new formulation as in Eq. (7) cannot produce a chiral spiral.

Thus, we must cope with the doubler problem to treat μ_q as a quark chemical potential. In this work we shall naively add the Wilson term, $r_W\bar{\psi}\partial^2\psi$ (where we choose $r_W = 1$) to make heavy doublers decouple from the dynamics. In order not to violate the transformation properties, $D(\mu_q) = U^\dagger D(0) U^\dagger$, we must implement the Wilson term according to Eq. (7) as $r_W\bar{\psi}\partial^2\psi \to r_W(\bar{\psi}U^\dagger)\partial^2(U^\dagger\psi)$. In this case the fermion determinant becomes real only for discrete values of μ_q, which is quantized as $\mu_q = (\pi/N)n$, where N is the number of lattice sites along the x_3 direction. Because the Wilson term has an explicit x_3 dependence, we

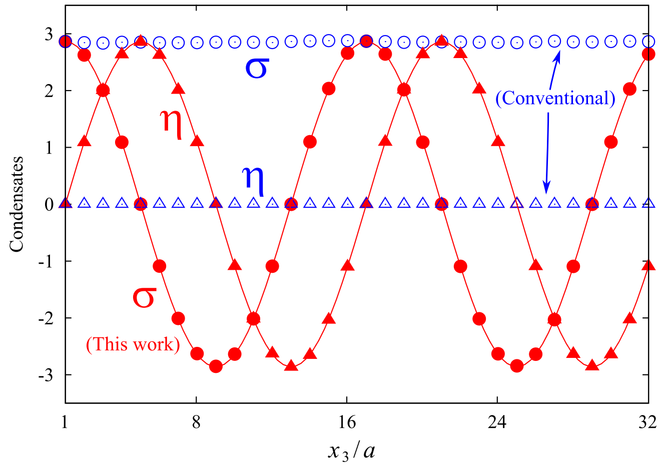

FIG. 2 (color online). Condensates σ and η at $\mu_q = 2\pi/N$ (with $N = 32$) as a function of x_3 in lattice units. The closed circles and triangles represent the results from our new formulation, while the open circles and triangles represent those from the conventional one. The solid curves are $2.86\cos[2\mu_q(x_3 - a)]$ and $2.86\sin[2\mu_q(x_3 - a)]$, which fit the oscillation behavior.

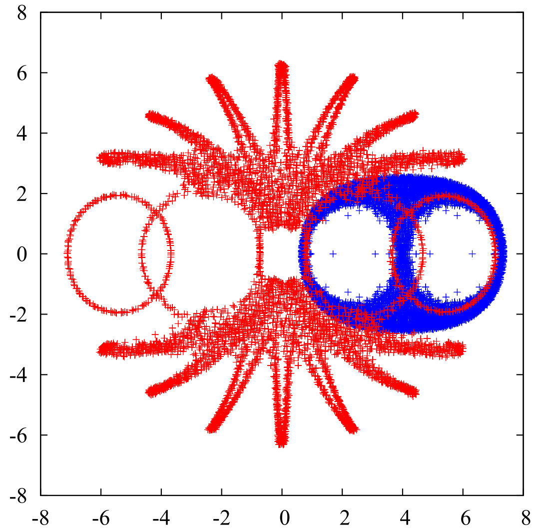

FIG. 3 (color online). Eigenvalue distribution of the finite-μ_q fermion operator on the 32×32 lattice ($N = 32$) for the gauge configuration corresponding to Fig. 2. Results with $\mu_q = 2\pi/N$ (red dots) are overlaid on those with $\mu_q = 0$ (blue dots).

must require $e^{2\mu_q\gamma^3\gamma^4 N} = 1$ to keep the action invariant under the shift $x_3 \to x_3 + N$.

For $\mu_q = (\pi/N)n$, the determinant returns to a real value. While the bulk properties are fixed by the whole quantity of the determinant, we emphasize here that the microscopic dynamics is far more nontrivial. If the vacuum at $\mu_q = 0$ has a nonzero and homogeneous chiral condensate $\sigma_0 \equiv \langle\bar\psi\psi\rangle \neq 0$, the rotated vacuum at $\mu_q \neq 0$ should yield $\sigma_0 = \langle\bar\psi'\psi'\rangle$ as well. In terms of the original basis, accordingly, we can expect $\sigma \equiv \langle\bar\psi\psi\rangle = \sigma_0\cos(2\mu_q x_3)$ and $\eta \equiv \langle\bar\psi\gamma^3\gamma^4\psi\rangle = \sigma_0\sin(2\mu_q x_3)$, which locally breaks chiral symmetry but does not break it globally, i.e., the average of the condensate vanishes: $\int d^2x\langle\bar\psi\psi\rangle = 0$.

In Fig. 2 we show the condensates as a function of x_3 defined by $\sigma(x_3) \equiv N_t^{-1}\sum_{x_4}\mathrm{tr}[D^{-1}(\mu_q)]$ and $\eta(x_3) \equiv N_t^{-1}\sum_{x_4}\mathrm{tr}[\gamma^3\gamma^4 D^{-1}(\mu_q)]$ (in lattice units). This is the result for one gauge configuration generated after 1000 quench updates using the Wilson gauge action with $\beta = 5.0$. If we use the conventional introduction of μ_q as in Eq. (5), only σ has a finite expectation value and the oscillatory pattern is hardly visible. With the new formulation as in Eq. (7), on the other hand, both σ and η take a finite value to develop a clear chiral spiral. [One should be careful when interpreting this result: the exact chiral limit with strict $(1+1)$ dimensions gives rise to no chiral condensate. This is why we set our problem in pseudo-$(1+1)$ dimensions and it is also why the Wilson term plays a role.]

Since the chiral condensate is related to the low-lying eigenvalues via the Banks-Casher relation, it is interesting to see how the eigenvalue distribution changes with the chiral spiral. The Wilson term breaks anti-Hermiticity, and the eigenvalues are complex even at $\mu_q = 0$, so that the original Banks-Casher relation needs a modification; the chiral condensate should be derived from the eigenvalues of $D^\dagger(0)D(0)$ rather than $D(0)$ [31]. In this work, we do not calculate the former, and yet, it is quite interesting to investigate the qualitative changes of the latter at finite μ_q. Figure 3 shows the eigenvalue distribution of $D(\mu_q)$ for $\mu_q = 0$ and $2\pi/N$ as introduced in Eq. (7). At $\mu_q = 0$ the eigenvalue distribution is the same as a conventional one. With increasing μ_q the distribution spreads to the negative real region, and when μ_q reaches a multiple of π/N, the determinant becomes identical to the $\mu_q = 0$ value, though the eigenvalue distribution looks totally different. Although the distribution appears to be symmetric for $\mu_q = (2\pi/N)n$ as seen in Fig. 3, there is no longer a quartet structure nor any pairwise symmetry. It is miraculous that the product of all these eigenvalues happens to be real.

IV. CONCLUSIONS

We have justified the idea that the sign problem is irrelevant in the $(1+1)$-dimensional system. This is caused by the chiral transformation that removes the chemical potential. We have first evaluated the determinant perturbatively in the continuum theory, and found that the imaginary part in the $(1+1)$-dimensional case vanishes unlike the $(3+1)$-dimensional situation that suffers from the sign problem.

For the discretized fermion on the $(1+1)$-dimensional lattice, the conventional way to impose a chemical potential causes the sign problem, which is a lattice artifact and should be absent in the continuum limit. In practice, however, this lattice artifact hinders the formation of the chiral spiral. To evade this problem, we have proposed a new method to introduce a chemical potential by twisting the Dirac operator along one of the spatial directions. In this case, the fermion determinant becomes real, but it turns out that such a chemical potential induces not a quark density but rather a doubler (or isospin) density if the doublers are not killed. We then find no chiral spiral. By diminishing spurious symmetry with doublers, we have successfully confirmed a clear chiral spiral. The eigenvalues of our fermion operator have a peculiar distribution, which suggests some relation between the distribution pattern and the formation of the chiral spiral. We leave this for future work.

Our formulation can be applied to more general dimensions. If the spiral structure is the genuine ground state at strong magnetic field or at high baryon density that brings about the dimensional reduction, the conventional formulation with μ_q is not an optimal choice. The present work has manifestly demonstrated the advantage of the new formulation to investigate the sign problem and the chiral spiral. It is also an intriguing future problem to study our method using the other fermions, particularly the overlap fermion that also exhibits a peculiar distribution of finite-density eigenvalues [32].

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