

Two-Dimensional CP^2 Model with θ -Term and Topological Charge Distributions

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Topological charge distributions in the two-dimensional CP^2 model with the θ -term are calculated. In strong coupling regions, the topological charge distribution is approximately given by a Gaussian form as a function of the topological charge, and this behavior leads to a first order phase transition at $\theta = \pi$. In weak coupling regions, this distribution exhibits non-Gaussian form, and the first order phase transition disappears. The free energy as a function of θ displays “flattening” behavior at $\theta = \theta_f < \pi$ when we calculate the free energy directly from the topological charge distribution. A possible origin of this flattening phenomenon is proposed.

§1. Introduction

Quantum chromodynamics (QCD) admits a topological term, i.e., θ -term. This term leads to “strong CP violation”. Experimentally, the magnitude of the θ parameter, which controls the magnitude of strong CP violation, is severely limited to a tiny value ($|\theta| \lesssim 10^{-9}$). Lattice gauge theory (LGT), formulated by Wilson¹⁾ and developed by Creutz,²⁾ has allowed for a realistic progress in understanding the nature of QCD. In LGT, in which Euclidean space-time is adopted, the usual gauge coupling is a purely real quantity. On the other hand, the θ -term appears as a purely imaginary quantity. Combining both of these leads to a complex coupling. The action given by this complex coupling constant gives a complex-valued Boltzmann weight. Except for a few cases, all works in LGT have been done for real couplings. It is, however, very important to understand complex coupling cases, i.e., system with a θ -term. Monte Carlo simulations confront a difficulty caused by the complex Boltzmann weight. Monte Carlo simulation in this case was made possible to some extent by Bhanot et al.,^{3),4)} Wiese⁵⁾ and Karliner et al.^{6),7)}

The method is summarized as follows.

- 1) First we obtain the topological charge⁸⁾ distribution $P(Q)$ with the use of the Boltzmann weight defined by the real coupling constant. The Fourier series

$$Z(\theta) = \sum_Q P(Q) e^{i\theta Q}$$

gives the partition function $Z(\theta)$ for a system with a θ -term.

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- 2) There are some technical problems in obtaining the topological charge distribution. Since the topological charge distribution is a rapidly decreasing function, we use a “set method”, in which the whole range of Q is divided into a number of sets. In each set, an MC simulation is performed. Even after dividing into sets, the distribution is still rapidly decreasing, so we use a “trial distribution method,” in which the Boltzmann weight is normalized by some appropriate trial function so as to realize the slowly changing topological charge distribution. This method was applied to a two-dimensional $U(1)$ system with a θ -term. Wiese showed that a first order phase transition is observed at $\theta = \pi$ for all real couplings.⁵⁾

A two-dimensional CP^{N-1} system has many qualitative similarities with four-dimensional QCD, such as asymptotic freedom, confinement, deconfinement phase (Higgs phase) and topological excitations (instanton).

Schierholz studied a two-dimensional CP^3 system with a θ -term.⁹⁾ He observed that, 1) with strong coupling, a first order phase transition occurs at a critical value $\theta_c = \pi$, and that 2) with weak coupling, there is deviation of the position of the first order transition from $\theta_c = \pi$ to smaller values. He conjectured that $\theta_c \rightarrow 0$ as $\beta \rightarrow \infty$ (weak coupling limit) and that the continuum limit value of θ is zero.

If this conjecture is valid, it gives a quite important physical result, but almost no confirmation has been made by other groups. One of the aims of the present paper is to investigate this issue.^{10),*)}

We briefly summarize approaches other than MC. We analyzed a two-dimensional $U(1)$ system with a θ -term¹¹⁾ using the group character expansion method.¹²⁾ The topological charge distribution $P(Q)$ is found to be given by a Gaussian function $\exp(-\kappa_V Q^2)$ for all β . This leads to the result that the partition function is given by the third elliptic theta function $\vartheta_3(\nu, \tau)$. This implies the interesting fact that the partition function has an infinite number of zeros as a function of $z = e^{i\theta}$, where θ is extended to complex values. In the infinite volume limit, these infinite numbers of partition function zeros accumulate at $z = -1$ according to $\kappa_V \propto 1/V$. Thus, a first order phase transition is expected at $\theta = \pi$ in the limit $V \rightarrow \infty$, where $V = L^2$ denotes the volume of system.

A four-dimensional Z_N gauge system with a θ -term has been discussed by Cardy and Rabinovici.¹³⁾ They pointed out that the θ -term leads to symmetries under dual transformation of the Hamiltonian and that this symmetry leads to very rich phase structures, namely, the confinement phase, Higgs phase (deconfinement phase), and condensation of electric and magnetic charges (oblique confinement).¹⁴⁾ Their argument is based on free energy and is rather qualitative. It is of great interest to investigate this system by MC simulation or another method (e.g., renormalization group method).

In a previous paper,¹⁵⁾ we performed an MC simulation on a CP^1 system with

*) After completion of the main part of this paper, we were informed that a similar investigation was made by J. C. Plefka and S. Samuel (Phys. Rev. **D56** (1997), 44). We would like to thank Burkhalter for informing us of this paper.

a θ -term in the strong and weak coupling regions. In strong coupling regions, a first order phase transition is observed at $\theta = \pi$.^{16),17)} In the weak coupling regions,¹⁸⁾ we observed that the topological charge distribution apparently deviates from a Gaussian form. The free energy in the weak coupling regions is approximately given by a $\cos \theta$ form. This indicates that only a few small values of Q control the topological charge distribution. In intermediate coupling regions, the obtained results were not so clear. In order to avoid the effect of statistical error as much as possible, we used a fitted analytic form for $P(Q)$ to obtain $Z(\theta)$, $F(\theta)$, etc. Then, even in the weak coupling region, we observed no flattening behavior, but a change of behavior of $Z(\theta)$ and $F(\theta)$. The power series fit to $P(Q)$ has the following properties:

- 1) For β small (strong coupling regions), it is simply given by a Gaussian form ($\exp(-\kappa_V Q^2)$).
- 2) For β large (weak coupling regions), we need a Q^4 term in the polynomial fit of the exponent of $P(Q)$.
- 3) For β intermediate, a power series fit suffers from a quite large χ^2 value.

In this paper, a CP^2 model with a θ -term will be studied using the MC method.¹⁹⁾ The emphasis is put on intermediate coupling regions ($\beta = 3 \sim 4$). From $P(Q)$ we obtain $Z(\theta)$, and we obtain the free energy per unit volume as $F(\theta) = -(1/V) \ln Z(\theta)$. $F(\theta)$ grows smoothly for smaller θ and exhibits “flattening” at some value θ_f , beyond which it becomes almost flat. For example, at $\beta = 3.5$ and $L = 20$ (100000 = 100 k iterations), flattening is observed at $\theta = \theta_f \sim 0.57\pi$. Does it correspond to the “first order phase transition” found by Schierholz in CP^3 system?

Does the flattening mentioned above really indicate a phase transition? We should be careful about the statistical error induced by the simulation. For example, after N sweeps (= iterations), we would have a statistical error of order

$$\delta P = |\text{error}| \sim 1/\sqrt{N}.$$

Note that δP is defined as positive.

“Set method” and “trial function (distribution) method” (see §2.2 Algorithm) will give us a $P(Q)$ exhibiting a decrease with a great number of orders of magnitude (e.g. 1 to 10^{-100} in some cases) between $Q = 0$ and a large value of Q . If the observed $P(Q)$ is fit with a smooth function $P_S(Q)$, it can be expressed as

$$P(Q) = P_S(Q) + \Delta P(Q),$$

where $\Delta P(Q)$ is the difference between the observed $P(Q)$ and the function $P_S(Q)$ used for the fitting. Quantity $|\Delta P(Q)|$ will be approximately given by $\delta P \times P(Q)$. The quantity $\Delta P(Q)$ can be either positive or negative (or zero), since it represents a fluctuation. The value of $|\Delta P(Q)|$ is approximately an order of $(1/\sqrt{N})P(Q)$, and $\Delta P(Q)$ itself is expected to be small at large Q . The partition function $Z(\theta)$, however, is given by a Fourier series, and the error in evaluation of $Z(\theta)$ is controlled by the largest one, i.e., $|\Delta P(0)| \sim \delta P \sim 1/\sqrt{N}$. The topological charge distribution $P(Q)$ is a rapidly decreasing function. When we estimate $Z(\theta)$ from

$$Z(\theta) = \sum_Q P(Q)e^{i\theta Q},$$

the value of $Z(\theta)$ will also be a rapidly decreasing function of θ , and the quantity $\Delta P(0)$ will play an important role at large θ . Since the partition function obtained from $P_S(Q)$ is a rapidly decreasing function, the true $Z_S(\theta)$ will be masked by the error $\Delta P(0)$ at large θ , which is much larger than $P_S(Q)$ itself at large Q . This effect leads to a shape of $Z(\theta)$ with flattening at some θ_f , like the illustration in Fig. 1 ($\theta_f \sim 0.55\pi$ in this figure).

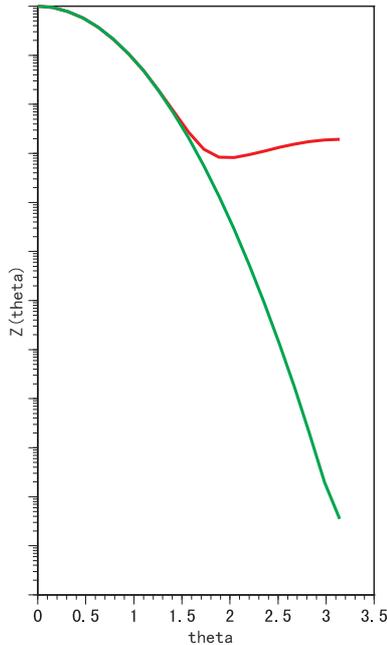


Fig. 1. An illustration of the partition function as a function of θ . Plotted here are the direct Fourier series (curve with flattening behavior) and that (Gaussian curve) calculated from smooth fit to $P(Q)$.

The value of $Z(\theta)$ almost coincides with $Z_S(\theta)$ for $\theta < \theta_f$, but it deviates greatly from $Z_S(\theta)$ for $\theta \gtrsim \theta_f$. $Z_S(\theta)$ will become quite small as $\theta \rightarrow \pi$, but the obtained $Z(\theta)$ does not exhibit such suppression.

In this way, the combined method of “set” and “trial function” leads to satisfactory results for $P(Q)$, but we still encounter difficulty in obtaining the correct $Z(\theta)$ for large values of θ .

In order to confirm the physical flattening (if it exists), we need sufficient accuracy in $Z(\theta)$ over a huge range of magnitudes. For example, to confirm the behavior of the partition function down to 10^{-8} , we need $N \sim 10^{16}$ iterations.

To obtain information about flattening with available computer facilities, we should analyze at larger β or with smaller volume V , since $P(Q)$ decreases faster when β is large or when V is small, and the partition function $Z(\theta)$, which is the Fourier transform of $P(Q)$, decreases slowly when β is large or when V is small. In these regions $Z(\theta)$ will be

reliably estimated over the entire region of θ ($0 \leq \theta \leq \pi$).

§2. CP^2 model in two dimensions

2.1. CP^2 model in two dimensions

We define the CP^2 model with a θ -term in the two-dimensional Euclidean lattice space. The CP^2 model consists of three component complex scalar fields,

$$z_\alpha(n) = \begin{pmatrix} z_1(n) \\ z_2(n) \\ z_3(n) \end{pmatrix}, \quad (2.1)$$

at each site n with the constraint,

$$\sum_{\alpha=1}^3 z_{\alpha}^*(n)z_{\alpha}(n) = 1. \tag{2.2}$$

The action, which is $U(1)$ gauge invariant, is given by

$$S_{\theta}[z] = S[z] - i\theta Q[z], \tag{2.3}$$

$$S = \beta \sum_{n=1}^{L^2} \sum_{\mu=1,2} \left\{ 1 - \sum_{\alpha=1}^3 |z_{\alpha}^*(n)z_{\alpha}(n + \mu)|^2 \right\}, \tag{2.4}$$

where Q is the topological charge, and $z_{\alpha}(n)$ is coupled with $z_{\alpha}(n + \mu)$ at the nearest neighbor site $n + \mu$ ($\mu = 1, 2$).

The topological charge Q is counted by A_{\square} as

$$Q = \frac{1}{2\pi} \sum_{\square} A_{\square} \tag{2.5}$$

in the updating process, where the plaquette contribution A_{\square} is given by

$$A_{\square} = (1/2) \sum_{\mu\nu} \{A_{\mu}(n) + A_{\nu}(n + \mu) - A_{\mu}(n + \nu) - A_{\nu}(n)\} \epsilon_{\mu\nu} \quad \text{mod} \quad 2\pi,$$

where $\exp(iA_{\mu}(n)) \equiv z^{\dagger}(n)z(n + \mu)/|z^{\dagger}(n)z(n + \mu)|$, i.e., $A_{\mu}(n) \equiv \arg(z^{\dagger}(n)z(n + \mu))$. The link variables $A_{\mu}(n) \equiv \arg(z^{\dagger}(n)z(n + \mu))$ are defined in

$$A_{\mu}(n) \in [-\pi, \pi].$$

The topological charge Q is given by the winding number, i.e., the quantity that represents the number of times the field $A_{\mu}(n)$ covers $U(1)$ space when we move around the boundary of the whole space-time once.

The partition function as a function of the coupling constant β and θ is

$$Z(\theta) = \frac{\int Dz^* Dz \exp(-S[z] + i\theta Q[z])}{\int Dz^* Dz \exp(-S[z])}, \tag{2.6}$$

where Dz denotes integration over all fields, and the free energy $F(\theta)$ is given by

$$F(\theta) = -\frac{1}{V} \ln Z(\theta), \tag{2.7}$$

where V is the volume of the lattice space.

We would like to compute θ vacua effects, but the complex Boltzmann factor $e^{i\theta Q}$ prevents us from performing an ordinary Monte Carlo simulation. In order to overcome this difficulty, we follow Wiese's idea. The updating is restricted to fields in the topological sector. Thus the phase factor $e^{i\theta Q[z]}$ is replaced by a constant and can be factored out from the functional integral. We can perform ordinary Monte

Carlo simulation using the real action $S[z]$. The partition function is given by the summation of the topological charge distribution $P(Q)$ weighted by $e^{i\theta Q}$ in each Q sector. In practice, we get the topological charge distribution $P(Q)$ using the action at $\theta = 0$ through the Monte Carlo simulation. We obtain the partition function $Z(\theta)$ by taking the Fourier transform of $P(Q)$:

$$Z(\theta) = \sum_Q e^{i\theta Q} P(Q), \quad (2.8)$$

where $P(Q)$ is

$$P(Q) \equiv \frac{\int Dz^{*(Q)} Dz^{(Q)} \exp(-S[z])}{\int Dz^* Dz \exp(-S[z])}. \quad (2.9)$$

The integration measure $Dz^{(Q)}$ is restricted to fields in the topological sector labeled by the topological charge Q . Note that $\sum_Q P(Q) = 1$.

The expectation value of an observable O is given in terms of $P(Q)$ as

$$\langle O \rangle_\theta = \frac{\sum_Q P(Q) \langle O \rangle_Q e^{-i\theta Q}}{\sum_Q P(Q) e^{-i\theta Q}}, \quad (2.10)$$

where $\langle O \rangle_Q$ is the expectation value of O at $\theta = 0$ for a given Q sector

$$\langle O \rangle_Q = \frac{\int Dz^{*(Q)} Dz^{(Q)} O e^{-S[z]}}{\int Dz^{*(Q)} Dz^{(Q)} e^{-S[z]}}. \quad (2.11)$$

2.2. Algorithm

We measure the topological charge distribution $P(Q)$ using a Monte Carlo simulation with the Boltzmann weight $\exp(-S)$, where S is defined by Eq. (2.4). The standard Metropolis method is used to update configurations. To calculate $P(Q)$, we count the number of times the configuration of Q is visited by the histogram method. The distribution $P(Q)$ damps very rapidly as $|Q|$ becomes large. We need to calculate $P(Q)$ at largest possible number of $|Q|$, which would contribute to $F(\theta)$, $\langle Q \rangle_\theta$ and $\langle Q^2 \rangle_\theta$, because they are obtained by Fourier transformation of $P(Q)$ and the derivatives of the partition function by θ . In order to obtain $P(Q)$ at larger Q , we apply a) the set method and b) the trial distribution method.

The set method

The entire range of Q is divided into a number of sets S_i ($i = 1, 2, \dots$). Monte Carlo updatings are done in each set S_i ($S_i = \{Q \mid 3(n-1) \leq Q \leq 3n\}$). In the process, we start from a configuration within the set S_i , and we produce a tentative configuration C_t . When Q of this tentative configuration C_t remains within one of

the bins in S_i , the configuration C_t is accepted, and the count of the corresponding Q value is increased by one. On the other hand, when C_t leaves the set S_i , C_t is rejected, and the count of the Q value of the old configuration is increased by one. This is done for all sets S_i ($i = 1, 2, \dots$).

The trial distribution method

The topological charge distribution $P(Q)$ is still a rather rapidly decreasing function of Q even in each set. The number of counts in each set is sharply peaked at the smallest Q , and there are almost no counts at larger values of Q , so the statistical weight is modified by introducing trial distributions $P_t(Q)$ for each set. Namely the Boltzmann weight is replaced by $\exp[-S]/P_t(Q)$. This is to remedy $P(Q)$, which decreases too rapidly, even within a set in some cases. We make the counts at $Q = 3(i - 1)$, $3(i - 1) + 1$, $3(i - 1) + 2$ and $3i$ in each set S_i become almost the same. As the trial distributions $P_t(Q)$, we apply the form

$$P_t(Q) = A_i \exp \left[-\frac{C_i(\beta)}{V} Q^2 \right], \tag{2.12}$$

where the values of $C_i(\beta)$ and A_i depend on the set S_i . That is, the action during the updating is modified to an effective one such as $S_{\text{eff}} = S + \ln P_t(Q)$.

To reproduce the normalized distribution $P(Q)$ in the whole range of Q from the counts in each set, we perform a matching as follows:

- i) In each set S_i ($i = 1, 2, \dots$), the number of counts is multiplied by $P_t(Q)$ at each Q . We denote the multiplied value by $N_i(Q)$, which is hopefully proportional to the desired topological charge distribution $P(Q)$.
- ii) In order to match the values in two neighboring sets S_i and S_{i+1} , we rescale $N_{i+1}(Q)$ so that $N_{i+1}(Q) \rightarrow N_{i+1}(Q) \times r$, where $r = N_i(Q = 3i)/N_{i+1}(Q = 3i)$ is the ratio of the number of counts at the right edge of S_i to that at the left edge of S_{i+1} . These manipulations are performed over all the sets.
- iii) The rescaled S_i are normalized to obtain $P(Q)$ such that

$$P(Q) = \frac{N_i(Q)}{\sum_i \sum_Q N_i(Q)}. \tag{2.13}$$

§3. Numerical results. I

We use a square lattice with periodic boundary conditions. We measure $P(Q)$ with various lattice sizes ($V = L^2$) and coupling constants (β). The error analysis is discussed in a previous paper.¹⁵⁾ To check the algorithm, we calculated the internal energy. It agrees with the analytical results of the strong and weak coupling expansions. Using the calculated $P(Q)$, we estimate the free energy $F(\theta)$ and its derivative $\langle Q \rangle_\theta$. To obtain $Z(\theta)$, we use two methods.

- (i) We use the measured $P(Q)$ directly to obtain $Z(\theta)$ (“direct method”).
- (ii) To avoid the error problems discussed in the Introduction, we first fit the measured $P(Q)$ with the appropriate function $P_S(Q)$, and then obtain $Z(\theta)$ by Fourier transforming from $P_S(Q)$ (“fitting method”).

3.1. Topological charge distribution $P(Q)$

In this subsection we discuss the topological charge distribution $P(Q)$. In Fig. 2, we show the measured $P(Q)$ for various values of β for a fixed volume ($L = 20$). These functions $P(Q)$ have different behavior in the strong coupling regions and the weak coupling regions. In strong coupling regions, $P(Q)$ exhibits Gaussian behavior. In weak coupling regions, $P(Q)$ deviates gradually from the Gaussian form. In order to investigate the strong coupling regions in detail, we use a chi-square-fitting for $\ln P(Q)$. Tables I and II display the results of the fittings, i.e., the coefficients a_n

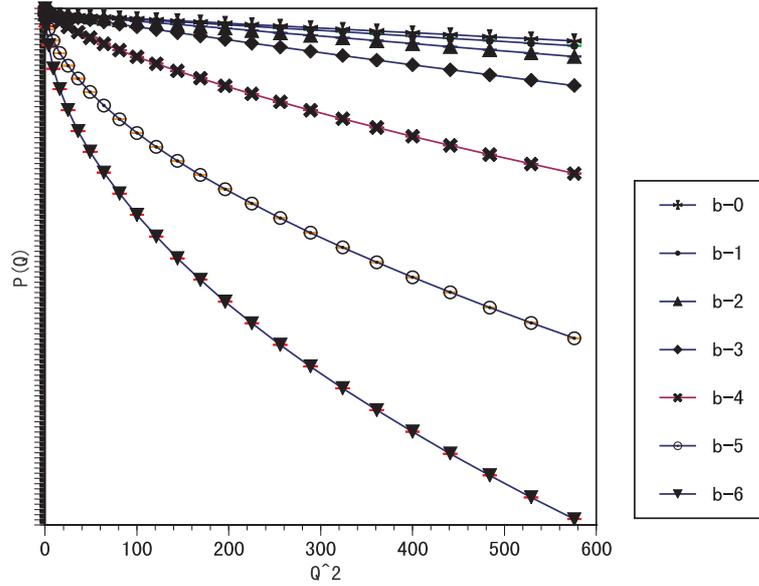


Fig. 2. Topological charge distribution $P(Q)$ vs Q^2 . The lattice size is $L = 20$. β ranges from 0 to 6. The results include errors and are plotted for $0 \leq Q \leq 24$. The total number of counts N in each set is 10^5 . $P(Q)$ ranges from 1 to 10^{-98} for the $\beta = 6$ case.

Table I. The results of chi-square-fitting for $\ln P(Q)$ in terms of the polynomial $a_0 + a_2 Q^2$ for various β , where “dof” represents the number of degrees of freedom.

| β | χ^2 | χ^2/dof | a_0 | a_2 |
|---------|----------|---------------------|--------|--------|
| 0 | 20.058 | 0.872 | -2.509 | -0.021 |
| 1 | 83.936 | 3.649 | -2.416 | -0.025 |
| 1.5 | 136.066 | 5.916 | -2.368 | -0.028 |
| 2 | 769.635 | 34.625 | -2.296 | -0.033 |

Table II. The result of chi-square-fitting for $\ln P(Q)$ in terms of the polynomial $\sum_n a_n Q^n$ for various β .

| β | χ^2 | χ^2/dof | a_0 | a_1 | a_2 | a_3 | a_4 |
|---------|----------|---------------------|-------------------------|--------|--------|------------------------|-------------------------|
| 2 | 27.835 | 1.392 | -2.273 | 0.006 | -0.035 | 5.123×10^{-5} | 1.359×10^{-7} |
| 3 | 30.561 | 1.528 | -1.950 | 0.01 | -0.069 | 5.765×10^{-4} | -2.904×10^{-6} |
| 4 | 3496.599 | 174.830 | -0.791 | -0.684 | -0.188 | 5.842×10^{-3} | -8.643×10^{-5} |
| 5 | 4027.247 | 201.362 | 4.147×10^{-3} | -4.468 | -0.159 | 6.161×10^{-3} | -1.015×10^{-4} |
| 6 | 5175.739 | 258.787 | -3.341×10^{-3} | -8.806 | -0.054 | 1.423×10^{-3} | -1.393×10^{-5} |

of the polynomial $\sum_n a_n Q^n$ for various β with the resulting χ^2/dof , where “dof” represents the number of degrees of freedom. (i) For $\beta \leq 1.5$, the functions $P(Q)$ are fit well by the Gaussian form. (ii) For $2 \leq \beta \leq 3$, terms up to quartic order are needed for a sufficiently good fit. (iii) For $4 \leq \beta$, the fit using the quartic polynomial turns out to be quite poor. Here we discuss the volume dependence. In strong coupling regions, $P(Q)$ is fit very well by the Gaussian form for all values of V :

$$P(Q) \propto \exp(-\kappa_V(\beta)Q^2), \tag{3.1}$$

where the coefficient $\kappa_V(\beta)$ ($= a_2$) depends on β and V . Figure 3 plots $\kappa_V(\beta)$ vs V for fixed β ($= 1.0$). We see that $\kappa_V(\beta)$ is clearly proportional to $1/V$:

$$\kappa = \frac{\alpha}{V}. \tag{3.2}$$

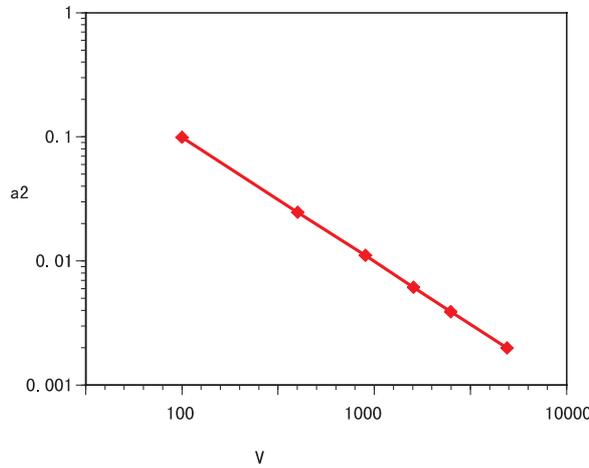


Fig. 3. a_2 vs V for $\beta = 1.0$ and $N = 10^5$.

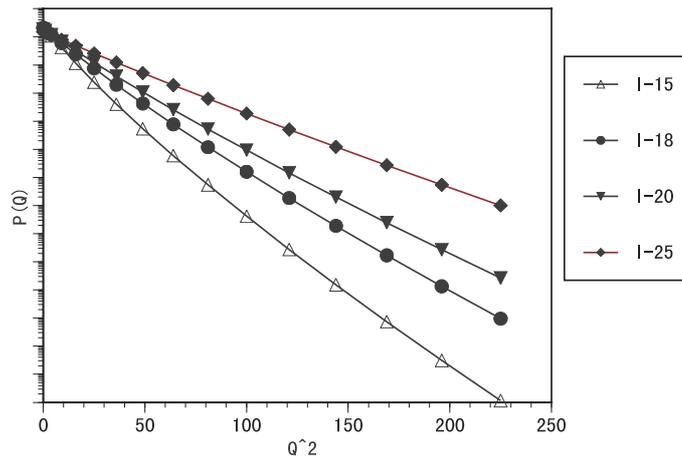


Fig. 4. $P(Q)$ vs Q^2 for $\beta = 3.45$ and $N = 5 * 10^5$.

This $1/V$ -dependence of the Gaussian behavior determines the phase structure of the strong coupling regions. This result agrees with the CP^1 result. Figure 4 displays the volume dependence of $P(Q)$ for $L = 15, 18, 20$ and 25 at $\beta = 3.45$. The parameters a_1^γ with $\gamma = 2.0$ at $\beta = 3.45$ (see Table V) give the V dependence. We find a slight deviation from the exact $1/V$ law, but a clear volume dependence is observed, which gives $\sim 1/V^{1.15}$, not so far from the $1/V$ law.

3.2. Free energy and expectation value of topological charge

The partition function $Z(\theta)$ is given as a function of θ by (2.8) from $P(Q)$. The free energy is

$$F(\theta) = -\frac{1}{V} \ln Z(\theta). \quad (3.3)$$

The expectation value of topological charge is

$$\langle Q \rangle_\theta = -(-i) \frac{dF(\theta)}{d\theta}. \quad (3.4)$$

In strong coupling regions, we have Gaussian behavior of $P(Q)$, and the $1/V$ -law appears to hold up to $L = 70$. It is natural to expect that this behavior persists at $V \rightarrow \infty$. Let us look at how the $1/V$ -law affects $F(\theta)$ and $\langle Q \rangle_\theta$. By setting $C(\beta) = 9.9$ in $P(Q) = \exp[-\frac{C(\beta)}{V}Q^2]$ for $\beta = 1.0$, we calculate $F(\theta)$ and $\langle Q \rangle_\theta$ from (2.8), (3.3) and (3.4). Figures 5 and 6 show their volume dependence. As V is increased, $F(\theta)$ very rapidly approaches a quadratic form from below. Its first moment $\langle Q \rangle_\theta$ develops a peak near $\theta = \pi$, and the position of the peak quickly approaches π as V increases. The jump in $\langle Q \rangle_\theta$ would arise at $\theta = \pi$ as $V \rightarrow \infty$. This indicates the existence of a first order phase transition at $\theta = \pi$.

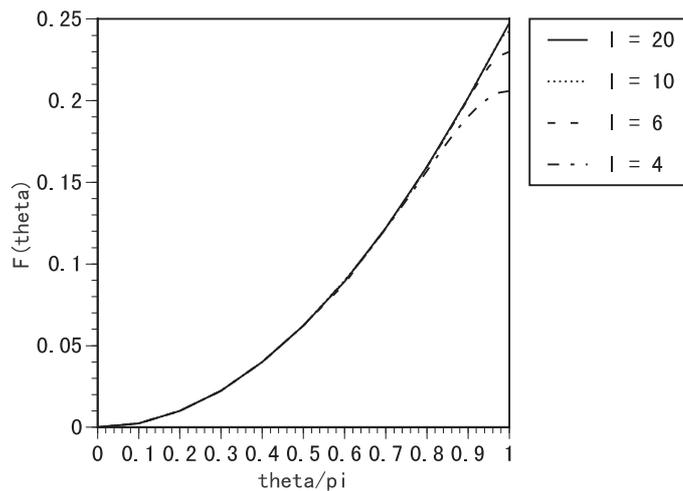


Fig. 5. Free energy vs θ in strong coupling regions. $L = 4, 6, 10, 20$.

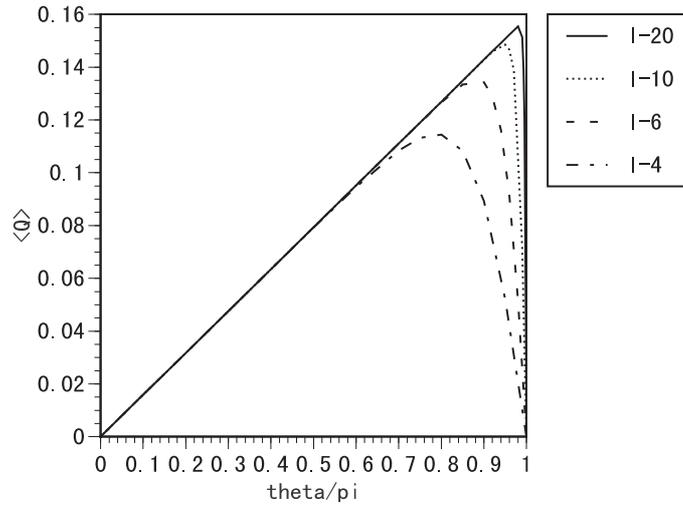


Fig. 6. $\langle Q \rangle$ vs θ in strong coupling regions. $L = 4, 6, 10, 20$.

§4. Numerical results. II

4.1. Flattening of free energy

Figure 7 displays $F(\theta)$ obtained by the “direct method” at $\beta = 3.45$. $F(\theta)$ exhibits “flattening” at some value θ_f above $L = 18$. For $\theta \leq \theta_f$, $F(\theta)$ is volume independent. For $\theta_f \leq \theta$, $F(\theta)$ is flat. θ_f decreases as V becomes large. (With $L = 25$, we cannot calculate $F(\theta)$ for $\theta \geq 0.7\pi$, because $Z(\theta)$ becomes negative.) This flattening phenomenon may correspond to similar behavior found by Schierholz, according to whom such flattening corresponds to the position of the first order phase transition (because $dF/d\theta$ is “discontinuous” at the sharp flattening of the free energy

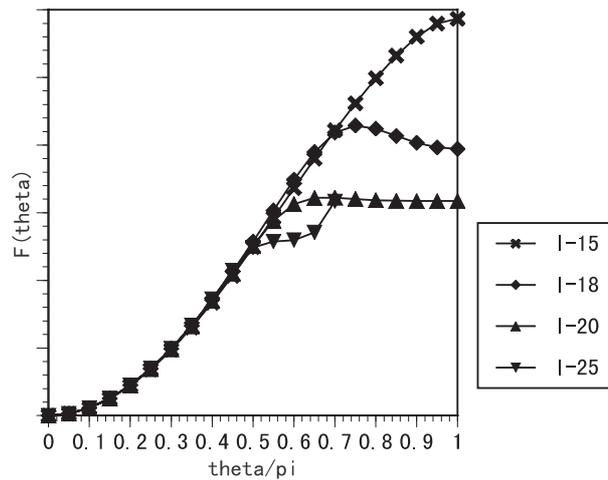


Fig. 7. Free energy vs θ at $\beta = 3.45$ and $L = 15, 18, 20, 25$. Flattening is clearly seen in $L = 18, 20, 25$.

$F(\theta)$). Our interpretation about the flattening found in our numerical calculations is different. The shift of θ_f (flattening position) with the size of the volume in our calculations is closely related to the statistical error existing in the estimate of $Z(\theta)$ in the Fourier series. The magnitude of the statistical error δP in the simulation of N measurements is essentially given by

$$\delta P \sim \frac{1}{\sqrt{N}}. \quad (4.1)$$

The statistical error $\Delta P(Q)$ at Q in the topological charge distribution $P(Q)$ decreases rapidly as Q becomes large in the set method,

$$\Delta P(Q) \sim \delta P \times P(Q), \quad (4.2)$$

where $\delta P = \text{constant}$, and then $\Delta P(Q)$ is a rapidly decreasing function of Q . The largest contribution of $\Delta P(Q)$ comes from that at $Q = 0$,

$$\Delta P(0) \sim \delta P \times P(0). \quad (4.3)$$

Then $Z(\theta)$ contains the error of $P(0)$ with a magnitude $\Delta P(0) \sim \delta P$. The partition function $Z(\theta)$ is also a rapidly decreasing function of θ , and thus $Z(\theta)$ becomes of the order of $\Delta P(0) \sim \delta P$ at $\theta \sim \theta_f$. In such a case, the rapidly decreasing function $Z(\theta)$ for $\theta > \theta_f$ cannot be estimated accurately.

We now present the results of our simulation. In Table III we list the flattening position θ_f for various lattice sizes L and coupling constants β , $\beta = 3.45$ and $\beta = 3.5$.

Table III. The flattening position θ_f for various lattice sizes L . We also list the values of $\theta_f \times L$.

| β | L | θ_f | $\theta_f \times L$ |
|---------|-----|------------|---------------------|
| 3.45 | 15 | 0.83π | 12.4π |
| | 18 | 0.7π | 12.6π |
| | 20 | 0.6π | 12.1π |
| | 25 | 0.51π | 12.8π |
| 3.5 | 20 | 0.57π | 11.4π |
| | 30 | 0.38π | 11.4π |

energy $F(\theta) = -\frac{1}{V} \ln Z(\theta)$ is given by the quadratic function θ^2 . For $L = 15$ to $L = 25$, the calculated $F(\theta)$ is almost V -independent. Since $Z(\theta) = \sum_Q P(Q)e^{i\theta Q}$ suffers from the statistical error δP , flattening is expected at the value of θ where the free energy becomes of order

$$VF(\theta_f) \sim -\ln(\delta P) \quad (4.5)$$

and we obtain the relation

$$\theta_f \sim V^{-1/2}. \quad (4.6)$$

Of course, δP may lead to a negative value of $Z(\theta)$ for $\theta \gtrsim \theta_f$. With $\beta = 3.45$, however, $L = 15, 18$ and 20 simulations with $N = 5 \times 10^5$ iterations all give positive

From these results, we observe that the flattening position scales as $\theta_f \propto L^{-1} = V^{-1/2}$ for each β , where $V = L^2$. What is the reason for this $V^{-1/2}$ -law? At these values of β , $P(Q)$ is approximately given by the Gaussian form

$$P(Q) \propto \exp(-\kappa_V(\beta)Q^2), \quad (4.4)$$

and the Fourier transform $Z(\theta)$ of this Gaussian form is also a Gaussian form, $Z(\theta) = \exp(-\alpha_V\theta^2)$. Then the free energy

Table IV. The free energy and partition function for $\beta = 3.45$ and $L = 20$.

| θ | $F(\theta)$ | $Z(\theta)$ | $\delta Z(\theta)$ |
|----------|------------------|------------------|--------------------|
| 0 | 0 | 1.00 | $1.37 * 10^{-3}$ |
| 0.1π | $5.65 * 10^{-4}$ | $7.98 * 10^{-1}$ | $1.23 * 10^{-3}$ |
| 0.2π | $2.23 * 10^{-3}$ | $4.10 * 10^{-1}$ | $9.97 * 10^{-4}$ |
| 0.3π | $4.92 * 10^{-3}$ | $1.40 * 10^{-1}$ | $9.06 * 10^{-4}$ |
| 0.4π | $8.48 * 10^{-3}$ | $3.37 * 10^{-2}$ | $8.94 * 10^{-4}$ |
| 0.5π | $1.26 * 10^{-2}$ | $6.59 * 10^{-3}$ | $8.94 * 10^{-4}$ |
| 0.6π | $1.56 * 10^{-2}$ | $1.92 * 10^{-3}$ | $8.94 * 10^{-4}$ |
| 0.7π | $1.61 * 10^{-2}$ | $1.59 * 10^{-3}$ | $9.06 * 10^{-4}$ |
| 0.8π | $1.59 * 10^{-2}$ | $1.71 * 10^{-3}$ | $9.97 * 10^{-4}$ |
| 0.9π | $1.59 * 10^{-2}$ | $1.76 * 10^{-3}$ | $1.23 * 10^{-3}$ |
| π | $1.59 * 10^{-2}$ | $1.76 * 10^{-3}$ | $1.37 * 10^{-3}$ |

$Z(\theta)$ for all θ ($0 \leq \theta \leq \pi$). Only the $L = 25$ case leads to negative $Z(\theta)$ for $\theta \gtrsim 0.7\pi$. We would expect both positive excess fluctuation and negative excess fluctuation. Thus the reason that positive excess results were more often observed in $\beta = 3.45$ simulations remains unknown. Numerical results for $Z(\theta)$ and $F(\theta)$ are given in Table IV for $\beta = 3.45$ and $L = 20$ case. The value of $Z(\theta)$ in the flat region is the same order as $\delta P \sim 1/\sqrt{N} \sim 1.4 \times 10^{-3}$ ($N = 5 \times 10^5$).

Once we found the flattening phenomena in regions of rather large β , we investigated the strong coupling region again to see whether it is a phenomenon peculiar to weaker coupling regions. Surprisingly, a similar phenomenon was found also in strong coupling regions. In Fig. 1 (§1), we showed the case of $\beta = 1.0$, which is sufficiently strong; the chi-square fitting with the Gaussian form is quite good (Table I). Figure 1 was the result obtained for $\beta = 1.0$ and $L = 10$ for 500 k iterations. Again, the position of flattening is consistent with the value estimated from δP . As is seen above, the calculation of the partition function with (2.8) using the observed value of $P(Q)$ directly will be called the “direct method”. In this method $Z(\theta)$ incurs statistical error of the order δP , and flattening occurs at θ_f . On the other hand, in the set method, the topological charge distribution itself is obtained over quite a wide range of Q . We first fit this distribution with an appropriate analytical function and using the fitted function $P_S(Q)$ (“smooth”), we can evaluate $Z(\theta)$. This latter method will be called the “fitting method”. In strong coupling regions, the indirect method leads to a Gaussian function for $P(Q)$, and the Fourier series again gives a Gaussian function of θ for $Z(\theta)$. It gives a smooth θ^2 -type free energy distribution up to $\theta = \pi$. There, no flattening phenomena appear.

Actually, in $U(1)$ LGT, it is known that $P(Q)$ is Gaussian for all β , and there is a θ^2 -type free energy distribution up to $\theta = \pi$. But if we use the observed $P(Q)$ directly to obtain the partition function, it causes flattening phenomena.

4.2. Strong and weak coupling region

As is seen in Table I, $\ln P(Q)$ can be fit by a Gaussian form accurately up to $\beta = 1.5$, but beyond this value the fit becomes worse, and higher power terms are necessary. Up to $\beta = 3.5$ a quartic function fits rather well, but still the most dominant power is 2 in this region (see Table II). For $\beta \geq 4.0$ the power series up to

Table V. The result of chi-square-fitting for $\ln P(Q)$ in term of the series starting from $a_0^\gamma + \sum_{n=1} a_n^\gamma |Q|^{\gamma+n-1}$ for various β .

| β | χ^2 | χ^2/dof | γ | a_0^γ | a_1^γ | a_2^γ | $a_3^\gamma * 10^6$ | $a_4^\gamma * 10^8$ |
|---------|----------|---------------------|----------|--------------|--------------|--------------|---------------------|---------------------|
| 0 | 24.14 | 1.207 | 2.08 | -2.512 | -0.0194 | 0.000293 | -9.32 | 11.8 |
| 1 | 22.45 | 1.123 | 1.96 | -2.418 | -0.0260 | -0.000155 | 3.73 | -3.59 |
| 2 | 29.70 | 1.485 | 2.06 | -2.267 | -0.0324 | 0.000383 | -11.2 | 15.2 |
| 3.45 | 23.19 | 1.160 | 2.0 | -1.661 | -0.122 | 0.00261 | -39.1 | 1.84 |
| 4 | 38.98 | 1.949 | 1.59 | -0.927 | -0.607 | 0.0104 | -251 | 287.5 |
| 5 | 319 | 15.950 | 1.12 | -0.0274 | -4.317 | -0.0157 | -588 | 684 |
| 6 | 2813 | 140.65 | 1.09 | -0.00156 | -7.534 | -0.0209 | 268 | -1210 |

order 4 is not sufficient, as is seen from Table II. The value of chi-square becomes quite bad for $\beta \geq 4.0$. In the weaker coupling region ($\beta \gtrsim 4.0$), we tried another type of function, which is a series starting from some power γ :

$$\ln P(Q) = a_0^\gamma + \sum_{n=1} a_n^\gamma |Q|^{\gamma+n-1}. \tag{4.7}$$

This drastically improves the chi-square fit in the range $4.0 \gtrsim \beta \gtrsim 5.0$ (see Table V and compare with Table II). The chi-square value for $\beta = 4$ was 3497 in Table II, it becomes 38.98 in Table V. From Table V, we understand that the leading power γ is 2 for $\beta \lesssim 3.5$, and the leading power becomes 1 for $\beta \gtrsim 5$. Thus we will call this region the “weak coupling region”. $\beta = 4.0$ is an “intermediate” value, since the leading power γ is about 1.59, which is just between the values of $\gamma = 2$ (Gaussian in strong coupling regions) and $\gamma = 1$ (weak coupling regions).

In weak coupling regions, excitation of the topological charge is suppressed more strongly as β becomes larger. For example,

$$\frac{P(2)}{P(1)} = \frac{1}{1.12}, \quad \frac{1}{3.3}, \quad \frac{1}{126} \tag{4.8}$$

for $\beta = 2.0, 4.0, 5.0$, respectively.

In contrast with the weak coupling case, a large topological charge configuration is relatively important, and a Gaussian distribution is obtained in the strong coupling region. This leads to the partition function $\vartheta_3(\nu, \tau)$, a third elliptic theta function. Here $\nu = \theta/(2\pi)$ and $\tau = i\kappa_V(\beta)/\pi$. Note that θ is extended to complex values. This function clearly exhibits a distribution of partition function zeros leading to a first order phase transition at $\theta = \pi$.

In weak coupling regions the large topological charge contribution is suppressed. In this region $-\ln P(Q)$ is given approximately by $a_1^\gamma |Q|$ (with $\gamma \sim 1.0$). This form of $P(Q)$ leads to a partition function given by the generating function of Chebyshev Polynomials:

$$\begin{aligned} Z(\theta) &= \sum_{Q=-\infty}^{\infty} c^{|Q|} e^{i\theta Q} \\ &= \frac{1 - c^2}{1 - 2c \cos \theta + c^2}. \end{aligned} \tag{4.9}$$

In weak coupling regions, the value of c is quite small, and c^2 in this equation can be discarded. This leads to an expectation value of the topological charge given almost by the $\sin \theta$ form:

$$i\langle Q \rangle = \frac{1}{V} \frac{dZ}{d\theta} / Z \sim \frac{2c}{V} \sin \theta, \tag{4.10}$$

when $|c| \ll 1$. At $\beta = 6.0$, $L = 20$, we have $c = 1.34 \times 10^{-4}$, $2c/V \sim 6.68 \times 10^{-7}$. Actually, the calculated $i\langle Q \rangle$ exhibits sine function-type behavior over the whole range of θ in weak coupling regions. No discrete phase transition is expected at $\theta = \pi$ in weak coupling regions. To determine whether there is a continuous phase transition (second order one) requires further precise investigation such as study of the correlation length.

§5. Conclusions and discussion

In this paper we have numerically investigated a two-dimensional CP^2 model with a θ -term. The topological charge distribution was determined using a Monte Carlo method based on “set method” (see §2.2) and “trial function method”. Then this distribution was used to obtain the partition function $Z(\theta)$ as a function of the theta parameter.

The topological charge distribution $P(Q)$ is Gaussian in strong coupling regions ($\beta \lesssim 1.5$). In the $\beta = 2 \sim 3.5$ region, the exponent of $P(Q)$ cannot be simply given by Q^2 , but additional higher powers are necessary (Tables I and II). Still, the leading contribution comes from the Q^2 term (Table V).

In weak coupling regions, i.e., $\beta \gtrsim 4.5$, the leading power of the exponent of $P(Q)$ is $|Q|$. A sharp decrease in $P(Q)$ at larger $|Q|$ is observed.

At $\beta = 4$, which is between the strong and weak coupling regions, the leading power of the exponent of $P(Q)$ is characterized by $|Q|^{1.59}$. The behavior $|Q|^{1.59}$ is between that in the strong coupling region, Q^2 , and that in the weak coupling region, $|Q|^1$.

The free energy as a function of θ was investigated. We observed a “flattening” of the θ -distribution of the free energy at θ_f . In our analysis, the main reason for this flattening is attributed to the statistical fluctuation δP of $P(Q)$ at $Q = 0$ and $\delta P \sim O(1/\sqrt{N})$, where N is the number of measurements. The volume dependence at each β is explained by this interpretation.

The topological charge distribution $P(Q)$ was measured over a wide range of Q . However, a direct method to obtain $Z(\theta)$ through Fourier series with direct use of the measured topological charge distribution $P(Q)$ leads to flattening caused by δP . We attempted to obtain an approximate form of $P(Q)$ by the fitting method. The smooth function $P_S(Q)$ obtained by fitting and used to evaluate $Z_S(\theta)$ has the following properties. In the strong coupling region, the Gaussian topological charge distribution leads to $Z_S(\theta)$ with the third elliptic theta function ϑ_3 , and it leads to an infinite number of zeros of the partition function, leading to a first order phase transition at $\theta = \pi$ in the infinite volume limit. In the weak coupling region, $Z_S(\theta)$

is approximated by the functional form

$$Z_S(\theta) = \frac{1 - c^2}{1 - 2 \cos \theta + c^2}, \quad (c \ll 1) \quad (5.1)$$

which is the generating function of Chebyshev polynomials. Due to this form, the expectation value of topological charge is

$$i\langle Q \rangle \propto \sin \theta. \quad (5.2)$$

No first order phase transition at $\theta = \pi$ is expected.

Let us summarize the situation concerning the flattening phenomena.

- 1) Flattening is observed when we calculate $Z(\theta)$ and $F(\theta)$ with the “direct method”. No flattening is obtained with the “indirect (fitting) method”. The situation regarding flattening is essentially the same for CP^1 , CP^2 and CP^3 cases. (We have checked the CP^1 system and CP^3 system. Results will be reported in the forthcoming papers.)
- 2) In a previous paper on CP^1 , we used only the “indirect method” in order to avoid a misinterpretation of the effect coming from statistical fluctuations as the physical effect. This is the reason that we did not observe flattening phenomena in the previous paper. Note that the occurrence of flattening is not peculiar to CP^2 or CP^3 . Such a phenomenon is observed also in CP^1 if we use the “direct method”. In this paper we tried both “direct” and “indirect” methods and observed flattening in the former case but not in the latter case.
- 3) Our present understanding based on our simulation is that a flattening phenomenon is due to statistical fluctuations.

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Appendix A

— Integration Measure —

In this appendix, we briefly discuss the measure of integration. The measure is defined as

$$dz_1 dz_2 dz_3 \delta(|z_1|^2 + |z_2|^2 + |z_3|^2 - 1). \quad (A.1)$$

The complex numbers z_i ($i = 1, 2, 3$) are given by two real numbers, x_i and y_i as $z_i = x_i + iy_i$. The measure becomes

$$dx_1 dy_1 dx_2 dy_2 dz_3 \delta(x_1^2 + y_1^2 + x_2^2 + y_2^2 + x_3^2 + y_3^2 - 1). \quad (A.2)$$

When the parameters x_i and y_i ($i = 1, 2, 3$) are changed to polar coordinates (k_i, a_i ($i = 1, 2, 3$)), we have

$$x_i = k_i \cos a_i, \tag{A.3}$$

$$y_i = k_i \sin a_i, \tag{A.4}$$

where $k_i \geq 0$ and $0 \leq a_i \leq 2\pi$. The measure becomes

$$k_1 k_2 k_3 dk_1 dk_2 dk_3 \delta(k_1^2 + k_2^2 + k_3^2 - 1) da_1 da_2 da_3. \tag{A.5}$$

We translate the parameters from k_1, k_2, k_3 to 3-dimensional polar coordinates (l, t_1, t_2) as

$$k_1 = l \sin t_1 \cos t_2, \tag{A.6}$$

$$k_2 = l \sin t_1 \sin t_2, \tag{A.7}$$

$$k_3 = l \cos t_2, \tag{A.8}$$

$$l^5 \delta(l^2 - 1) dl \sin^3 t_1 \cos t_1 dt_1 \sin t_2 \cos t_2 dt_2 da_1 da_2 da_3, \tag{A.9}$$

where $l \geq 0$ and $0 \leq t_1, t_2 \leq \frac{\pi}{2}$. Here the measure we use in the Monte Carlo simulation finally becomes

$$dm dn da_1 da_2 da_3, \tag{A.10}$$

after integration over l is performed. The variables m and n are given by

$$m = \frac{1}{8} \left(\cos 2t_1 - \frac{1}{4} \cos 4t_1 \right), \tag{A.11}$$

$$n = \frac{1}{4} \cos 2t_2. \tag{A.12}$$

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Note added in proof: It is an interesting problem to study numerically to what extent the first order phase transition at $\theta = \pi$ persists beyond the strong coupling region. In connection to the existence of the phase transition in the continuum theory, Asorey and Falceto show that the first order phase transition does not occur at $\theta = \pi$ (M. Asorey and F. Falceto, Phys. Rev. Lett. **80** (1998), 234). A possibility of the higher order transition is certainly not excluded.

The flattening behavior of the free energy is observed in a matrix model (R. A. Janik, M. A. Nowak, G. Papp and I. Zahed, hep-ph/9901390). It is shown that the results are sensitive to the numerical precision, which is similar to the lattice simulations. They also claim that such behavior also depends on the density of the winding modes.

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