

Study of $CP(N - 1)$ θ -Vacua by Cluster Simulation of $SU(N)$ Quantum Spin Ladders

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D-theory provides an alternative lattice regularization of the 2D $CP(N - 1)$ quantum field theory in which continuous classical fields emerge from the *dimensional* reduction of *discrete* $SU(N)$ quantum spins. Spin ladders consisting of n transversely coupled spin chains lead to a $CP(N - 1)$ model with a vacuum angle $\theta = n\pi$. In *D*-theory no sign problem arises and an efficient cluster algorithm is used to investigate θ -vacuum effects. At $\theta = \pi$ there is a first order phase transition with spontaneous breaking of charge conjugation symmetry for $CP(N - 1)$ models with $N > 2$.

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Field theories are usually quantized by path integration over classical field configurations. Performing the path integration for nonperturbative field theories such as QCD or $CP(N - 1)$ models [1] is a highly nontrivial task. *D*-theory is an alternative formulation of field theory in which classical fields emerge dynamically as collective excitations of discrete quantum variables (such as quantum spins) that undergo dimensional reduction [2]. Similar forms of dimensional reduction occur in string theory. The idea that a quantum field theory can emerge from the dynamics of quantum spins is familiar in condensed matter physics. In particular, Haldane has conjectured that the antiferromagnetic spin 1/2 chain is described by the 2D $CP(1) = O(3)$ model at $\theta = \pi$ [3–5]. In general, chains of half-integer spins are gapless and lead to $\theta = \pi$, while chains of integer spins have a gap and correspond to $\theta = 0$. Similarly, spin ladders consisting of n transversely coupled spin 1/2 chains correspond to $\theta = n\pi$ [6]. Also, the 2D $CP(1) = O(3)$ model at $\theta = 0$ results from the $(2 + 1)$ D quantum Heisenberg antiferromagnet by dimensional reduction [7,8]. In this Letter, studying θ -vacua effects in $CP(N - 1)$ models, we show that *D*-theory may significantly simplify the evaluation of highly nontrivial nonperturbative path integrals. $CP(N - 1)$ models are interesting 2D quantum field theories which share a number of important features with 4D QCD. These include asymptotic freedom, the dynamical generation of a mass gap, and an instanton topological charge leading to nontrivial θ -vacuum effects. It has been conjectured that $CP(N - 1)$ models with $N > 2$ have a first order phase transition at $\theta = \pi$ [9]. This is consistent with large N analytic results [10]. For finite N , however, the investigation of these nonperturbative problems is highly nontrivial. In particular, in contrast to $O(N)$ models and other 2D quantum field theories, $CP(N - 1)$ models with $N > 2$ cannot be solved with the Bethe ansatz.

The numerical investigation of lattice $CP(N - 1)$ models is also far from being straightforward, even at $\theta = 0$. Again, in contrast to $O(N)$ models which can be studied with the efficient Wolff cluster algorithm [11], no efficient

cluster algorithm is available for $CP(N - 1)$ models [12,13]. Still, at $\theta = 0$, a rather efficient multigrid algorithm was developed in [14]. However, at $\theta = \pi$ the situation is much worse due to a very severe sign problem: the contributions from odd topological charge sectors almost completely cancel those from even charge sectors. This makes it exponentially hard to access large lattices, which is necessary for reaching reliable conclusions about the phase structure. For this reason, previous numerical studies of θ -vacua were limited to moderate volumes [15,16] or relied on additional assumptions [17]. In the $CP(1) = O(3)$ case, a Wolff-type meron-cluster algorithm allows efficient simulations at $\theta = \pi$ [18]. Unfortunately, due to a no-go theorem [13] this algorithm cannot be extended to higher $CP(N - 1)$ models.

In this Letter, using *D*-theory, we develop a method which allows us for the first time to perform accurate unbiased numerical simulations of any $CP(N - 1)$ model at $\theta = \pi$. In the case of $CP(N - 1)$ models, the discrete *D*-theory variables are generalized quantum spins $T_x^a = \frac{1}{2}\lambda_x^a$ which generate an $SU(N)$ symmetry $[T_x^a, T_y^b] = i\delta_{xy}f_{abc}T_x^c$. Here, f_{abc} are the structure constants of $SU(N)$. The spins are located at the sites x of a square lattice with spacing a of size $L \times L'$, with $L \gg L'$ and with periodic boundary conditions. Hence, as shown in Fig. 1, we have a quantum spin ladder consisting of $n = L'/a$ transversely coupled spin chains of length L . The x direction of size L corresponds to the spatial dimension of the target $CP(N - 1)$ model, while the extra y dimension of finite extent L' will ultimately disappear via dimensional

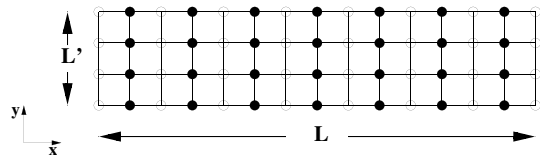


FIG. 1. Spin ladder geometry: the open circles belong to sublattice *A*, while the filled circles form sublattice *B*.

reduction. We consider nearest-neighbor couplings which are antiferromagnetic along the chains and ferromagnetic between different chains. Hence, the lattice naturally decomposes into two sublattices A and B with even and odd sites along the x direction, respectively. Note that neighboring sites along the transverse y direction belong to the same sublattice. The spins T_x^a on sublattice A transform in the fundamental representation $\{N\}$ of $SU(N)$, while the ones on sublattice B are in the antifundamental representation $\{\bar{N}\}$ and are thus described by the conjugate generators $-T_x^{a*}$. The quantum spin ladder Hamiltonian is given by

$$H = -J \sum_{x \in A} [T_x^a T_{x+\hat{1}}^{a*} + T_x^a T_{x+\hat{2}}^a] - J \sum_{x \in B} [T_x^{a*} T_{x+\hat{1}}^a + T_x^{a*} T_{x+\hat{2}}^{a*}], \quad (1)$$

where $J > 0$, and $\hat{1}$ and $\hat{2}$ are unit vectors in the spatial x and y directions, respectively. Note that, in the $SU(2)$ case, the $\{2\}$ and $\{\bar{2}\}$ representations are unitarily equivalent. In particular, by a unitary transformation, one can turn $-T_x^{a*}$ into T_x^a . This is not possible for $N > 2$. By construction, the system has a global $SU(N)$ symmetry, i.e., $[H, T^a] = 0$, with the total spin given by

$$T^a = \sum_{x \in A} T_x^a - \sum_{x \in B} T_x^{a*}, \quad (2)$$

which satisfies the $SU(N)$ algebra $[T^a, T^b] = if_{abc} T^c$.

A priori it is not obvious that the $(2+1)$ D quantum spin ladder provides a viable regularization of the 2D continuum $CP(N-1)$ field theory. As a necessary prerequisite, the quantum spin ladder does indeed have the global $SU(N)$ symmetry of $CP(N-1)$ models. Using the coherent state technique of [19], one finds that, at zero temperature, the infinite system (with both $L, L' \rightarrow \infty$) undergoes spontaneous symmetry breaking from $SU(N)$ to $U(N-1)$. It should be noted that the choice of the $SU(N)$ spin representations (in this case, $\{N\}$ and $\{\bar{N}\}$) has an influence on the breaking pattern. Because of spontaneous symmetry breaking, there are massless Goldstone bosons—in this case, spin waves—described by fields in the coset space $SU(N)/U(N-1) = CP(N-1)$. The $CP(N-1)$ fields $P(x, y, t)$ are Hermitean $N \times N$ projector matrices, i.e., $P^2 = P$, with $\text{Tr} P = 1$. Using chiral perturbation theory, the lowest-order terms in the Euclidean effective action for the spin waves are given by

$$S[P] = \int_0^\beta dt \int_0^L dx \int_0^{L'} dy \text{Tr} \left\{ \rho'_s \partial_y P \partial_y P + \rho_s \left[\partial_x P \partial_x P + \frac{1}{c^2} \partial_t P \partial_t P \right] - \frac{1}{a} P \partial_x P \partial_t P \right\}. \quad (3)$$

Here $\beta = 1/T$ is the inverse temperature, ρ_s and ρ'_s are spin stiffness parameters for the x and y direction, respectively, and c is the spin wave velocity. The action is invariant under global transformations $P' = \Omega P \Omega^\dagger$ with

$\Omega \in SU(N)$. The last term in the integrand of Eq. (3) is purely imaginary and is related to the topological charge

$$Q[P] = \frac{1}{\pi i} \int_0^\beta dt \int_0^L dx \text{Tr} [P \partial_x P \partial_t P], \quad (4)$$

which is an integer in the second homotopy group $\Pi_2[CP(N-1)] = \mathbf{Z}$, and thus y independent. Hence, the y integration in the last term of Eq. (3) can be performed trivially. This yields $i\theta Q[P]$ where the vacuum angle is given by $\theta = L'\pi/a = n\pi$. Here a is the lattice spacing of the quantum spin ladder and $L'/a = n$ is the number of transversely coupled spin chains. Hence, for even n the vacuum angle is trivial, while for odd n it is equivalent to $\theta = \pi$. The same topological term is also generated when one uses a single antiferromagnetic spin chain with larger representations of $SU(N)$. When one chooses a completely symmetric representation with a Young tableau containing n boxes in a single row on sublattice A and its antirepresentation on sublattice B , the resulting vacuum angle is again given by $\theta = n\pi$.

While the infinite $(2+1)$ D system has massless Goldstone bosons, the Coleman-Hohenberg-Mermin-Wagner theorem forbids the existence of massless excitations once the y direction is compactified to a finite extent L' . As a consequence, the Goldstone bosons then pick up a nonperturbatively generated mass gap $m = 1/\xi$ and thus have a finite correlation length ξ . Interestingly, for sufficiently many transversely coupled chains, the correlation length becomes exponentially large

$$\xi \propto \exp(4\pi L' \rho_s / cN) \gg L', \quad (5)$$

and the system undergoes dimensional reduction to the 2D $CP(N-1)$ field theory with the action

$$S[P] = \int_0^\beta dt \int_0^L dx \text{Tr} \left\{ \frac{c}{g^2} \left[\partial_x P \partial_x P + \frac{1}{c^2} \partial_t P \partial_t P \right] - n P \partial_x P \partial_t P \right\}. \quad (6)$$

The coupling constant of the dimensionally reduced theory is given by $1/g^2 = L' \rho_s / c$. The mechanism of dimensional reduction is well known from quantum antiferromagnets [7,8] and occurs in all D -theory models. It has also been discussed for $SU(2)$ quantum spin ladders [6]. The dimensional reduction of ladder systems has already been used in the D -theory construction of the 2D $O(3)$ model at nonzero chemical potential. The corresponding sign problem has been solved with an efficient meron-cluster algorithm [20]. In this Letter, we extend the D -theory construction to $CP(N-1)$ models, which allows us to simulate them reliably at $\theta = 0$ and π .

One advantage of D -theory is that it allows us to construct quantum field theories using simple discrete degrees of freedom instead of the usual continuum classical fields. In particular, the partition function $Z = \text{Tr} \exp(-\beta H)$ of the $SU(N)$ quantum spin ladder can be written as a path integral using a basis of discrete $SU(N)$

spin states $q \in \{u, d, s, \dots\}$ on sublattice A and $\bar{q} \in \{\bar{u}, \bar{d}, \bar{s}, \dots\}$ on sublattice B . For $SU(2)$ this corresponds to the usual \uparrow and \downarrow spins. These can be simulated with the very efficient loop-cluster algorithm [21,22] which can even operate directly in continuous Euclidean time [23]. As mentioned in [24], this algorithm extends to $SU(N)$ in a straightforward manner.

We have used this cluster algorithm to investigate if $CP(N-1)$ models with $N > 2$ have a first order phase transition at $\theta = \pi$ where the charge conjugation symmetry C is spontaneously broken. A natural quantity that suggests itself as an order parameter for such a phase transition would be the topological charge $Q[P]$, which indeed is C odd, i.e., $Q[CP] = Q[P^*] = -Q[P]$. Note that C is explicitly broken for $\theta \neq 0, \pi$. At $\theta = \pi$ it is not broken explicitly because then the Boltzmann weight $\exp(i\theta Q[P]) = (-1)^{Q[P]}$ is C invariant. The topological charge itself is defined only in the framework of the target continuum theory. In the discrete spin system another order parameter, which is also C odd, is more easily accessible. In the basis of quantum spin states q, \bar{q} we define an order parameter $Q[q, \bar{q}]$ by counting the number of spin flips in a configuration. $Q[q, \bar{q}]$ receives a contribution 1 if a pair of nearest-neighbor spins along the x direction, $q_x \bar{q}_{x+\hat{i}}$, flips to another state, $q'_x \bar{q}'_{x+\hat{i}}$, at some moment in time. A spin flip from $\bar{q}_x q_{x+\hat{i}}$ to $\bar{q}'_x q'_{x+\hat{i}}$, on the other hand, contributes -1 to $Q[q, \bar{q}]$. In the quantum spin ladder, charge conjugation corresponds to replacing each spin state q_x by $q_{x+\hat{i}}$ (which is the conjugate of $\bar{q}_{x+\hat{i}}$). Indeed, $Q[q, \bar{q}]$ changes sign under this operation while the action remains invariant.

We have used the cluster algorithm to simulate $SU(N)$ quantum spin ladders for $N = 3, 4$, and 5 , with $n = L'/a \in \{2, 3, \dots, 7\}$. The spatial size L/a has been varied between 20 and 300, and the inverse temperature βJ was chosen between 15 and 200. Our simulations confirm the existence of a first order phase transition with sponta-

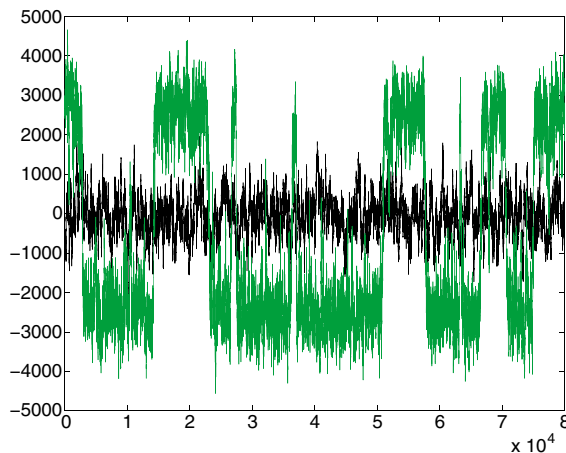


FIG. 2 (color online). Monte Carlo time histories of the order parameter $Q[q, \bar{q}]$ for the $CP(3)$ model at $\theta = 0$ ($n = 4$, $L = 180a$, $\beta J = 50$) and $\theta = \pi$ ($n = 3$, $L = 200a$, $\beta J = 80$).

neous C breaking at $\theta = \pi$ for all $N > 2$. As expected, there is no phase transition at $\theta = 0$. Figure 2 shows Monte Carlo time histories of $Q[q, \bar{q}]$ for $SU(4)$ spin ladders with $n = 3$ and 4 which correspond to $CP(3)$ models at $\theta = \pi$ and 0 , respectively. For $n = 3$ one observes two coexisting phases with spontaneous C breaking, while for $n = 4$ there is only one phase which is C symmetric. For $n = 5$ and thus $\theta = \pi$, one again finds a first order phase transition as in the $n = 3$ case. Figure 3 shows the probability distribution of $Q[q, \bar{q}]$ for an $SU(5)$ spin ladder with $n = L'/a = 7$, which corresponds to a $CP(4)$ model at $\theta = \pi$. The double peak structure again implies a first order phase transition. A first order phase transition is also observed in the $CP(2)$ case.

At this point, we have shown that D -theory indeed verifies the conjectured θ -vacuum structure of $CP(N-1)$ models. In order to demonstrate that we approach the continuum limit of an asymptotically free field theory, we have determined the correlation length $\xi(n)$ (defined using the second moment method [13]) in the $CP(2)$ case as a function of $n = L'/a$, which controls the coupling $1/g^2 = L'\rho_s/c$. One obtains $\xi(2) = 4.82(4)a$, $\xi(4) = 17.6(2)a$, and $\xi(6) = 61(2)a$, which indeed shows the exponential increase of the correlation length characteristic for an asymptotically free theory.

In D -theory, $CP(N-1)$ models at $\theta = 0$ can also be obtained by dimensional reduction of an $SU(N)$ quantum ferromagnet with the Hamiltonian

$$H = -J \sum_{x,\mu} T_x^a T_{x+\hat{\mu}}^a. \quad (7)$$

In this case, using a symmetric $SU(N)$ representation with a Young tableau containing n boxes, the symmetry again breaks spontaneously to $U(N-1)$ and the low-energy effective action for the spin waves takes the form

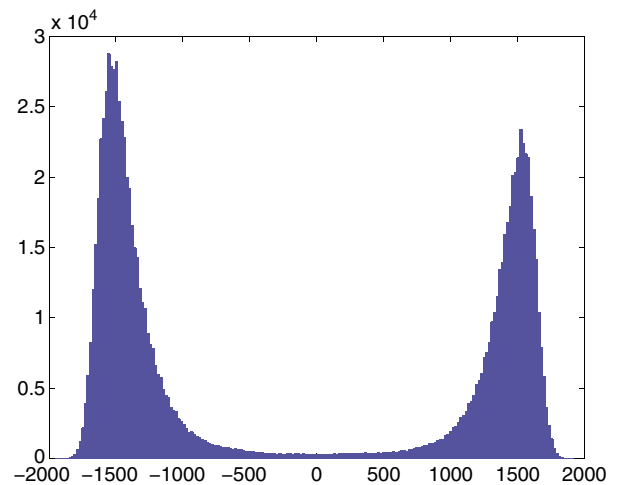


FIG. 3 (color online). Probability distribution of the order parameter $Q[q, \bar{q}]$ for the $CP(4)$ model at $\theta = \pi$ ($n = 7$, $L = 40a$, $\beta J = 6$). Because of limited statistics, the two peaks are sampled unevenly.

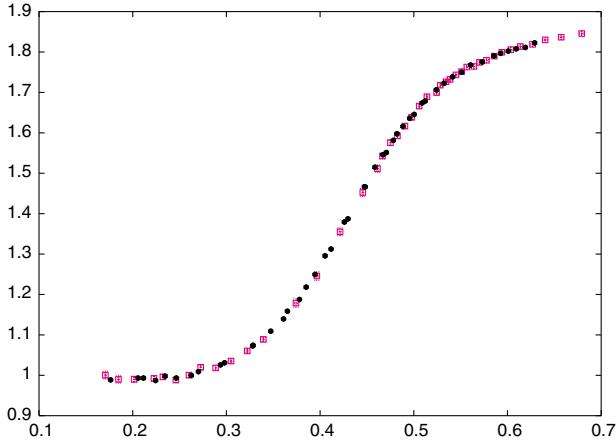


FIG. 4 (color online). Monte Carlo data for the universal finite-size scaling function $F(z)$ of the 2D CP(2) model at $\theta = 0$. The black points represent D -theory data from an SU(3) quantum ferromagnet at $\beta J = 5.5$ and 6, while the open squares correspond to data obtained with the standard Wilson lattice field theory at $1/g^2 = 2.25$ and 2.5.

$$S[P] = \int_0^\beta dt \int d^2x \text{Tr} \left[\rho_s \partial_\mu P \partial_\mu P - \frac{2n}{a^2} \int_0^1 d\tau P \partial_\tau P \partial_\tau P \right] \rightarrow \beta \rho_s \int d^2x \text{Tr} [\partial_\mu P \partial_\mu P], \quad (8)$$

where x now represents a 2D space-time coordinate. The Wess-Zumino term with the quantized prefactor n involves an interpolated field $P(x, t, \tau)$ ($\tau \in [0, 1]$) with $P(x, t, 1) = P(x, t)$ and $P(x, t, 0) = \text{diag}(1, 0, \dots, 0)$. The Wess-Zumino term vanishes after dimensional reduction and one obtains the action of the 2D CP($N-1$) model at $\theta = 0$ with $1/g^2 = \beta \rho_s$. In order to verify explicitly that this defines the CP($N-1$) model in the continuum limit, we now compare physical results obtained with the SU(N) quantum ferromagnet and the Wilson formulation using the standard lattice action

$$S[P] = -\frac{2}{g^2} \sum_{x, \mu} \text{Tr} [P_x P_{x+\hat{\mu}}]. \quad (9)$$

The continuum limit is reached as $g \rightarrow 0$. A convenient physical quantity characteristic for a given model is the universal finite-size scaling function $F(z) = \xi(2L)/\xi(L)$. Here $\xi(L)$ is the correlation length in a finite system of size L (again obtained from the second moment method), and $z = \xi(L)/L$ is a finite-size scaling variable that measures the size of the system in physical units. Figure 4 shows Monte Carlo data for $F(z)$ obtained both from D -theory and from the standard Wilson approach. Up to small scaling violations, the agreement of the two data sets confirms that the SU(N) quantum ferromagnet indeed provides a valid lattice regularization of 2D CP($N-1$) models. Thanks to the cluster algorithm, the D -theory framework allows calculations that are much more accurate than the ones using Wilson's approach.

To summarize, D -theory provides us with a powerful algorithmic tool, a cluster algorithm that even works efficiently at $\theta = \pi$. Despite great efforts, this remains impossible within Wilson's lattice field theory. D -theory also provides a natural definition of QCD in which 4D gluons arise by dimensional reduction of discrete quantum links and quarks arise as domain wall fermions located at the boundary of a $(4+1)$ D space-time [2]. The present study suggests that—using the D -theory regularization—ideas that originated from condensed matter physics may also significantly simplify the evaluation of the QCD path integral. In this way, even the QCD θ -vacuum may become accessible to numerical studies.

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