Valence-Bond and Spin-Peierls Ground States of Low-Dimensional Quantum Antiferromagnets

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The large-N limit of a nearest-neighbor SU(N) antiferromagnet on a bipartite lattice exhibits in dimensions $d \geq 2$ a zero-temperature phase transition between a Néel-ordered state and a resonanting-valence-bond state. Here it is shown in $d=1,2$ that topological effects produce spin-Peierls or valence-bond-solid order in the non-Néel phase with a ground-state degeneracy which varies periodically with "spin" for fixed N, with periodicity given by the coordination number of the lattice. Thus a non-Néel phase of the spin-$\frac{1}{2}$ Heisenberg model on a square lattice would be a spin-Peierls state with a fourfold degeneracy due to broken lattice rotational symmetry.

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Following the discovery of high-temperature superconductivity,[1] it has been proposed that the phenomenon is linked to a $T=0$ disordered (i.e., non-Néel) phase of the Heisenberg antiferromagnet on a square lattice.[2] We examine here nearest-neighbor generalizations of the standard Heisenberg model on bipartite lattices in dimensions $d=1,2$ all of which have a two-sublattice Néel state as their classical ground state. We find that *topological effects radically influence the nature of the disordered phase, producing in general a spin-Peierls or valence-bond-solid state.* The degeneracy of this state varies periodically with the magnitude of the "spin" at each lattice site in accordance with the recent prediction of Haldane[3] and its generalization to SU(N).[4] In $d=2$, the elementary spin excitations are confined (i.e., permanently bound) pairs of "spinons" and there is a spinless collective mode with an energy gap at all wave vectos.[5] Our results for the phase diagram and ground states are summarized in Figs. 1 and 2.

We study a family of models with Hamiltonian

$$H=\frac{J}{N}\sum_{\langle i,j\rangle}\hat{S}_\alpha^\beta(i)\hat{S}_\beta^\alpha(j)\,, \qquad (1)$$

where $\hat{S}_\alpha^\beta(i)$ are the generators of SU(N), $\langle i,j\rangle$ denotes pairs of nearest neighbors ("links") on a d-dimensional hypercubic lattice, and repeated indices $\alpha,\beta=1,\ldots,N$ are summed over. We will use a Schwinger boson representation of the spin states, in which $\hat{S}_\alpha^\beta(i)=b_\alpha^\dagger(i)b^\beta(i)$, $i\in A$ sublattice, and $\hat{S}_\alpha^\beta(j)=-\bar{b}^{\beta\dagger}(j)\bar{b}_\alpha(j)$, $j\in B$ sublattice; the $\bar{b}$ bosons are implied by the placement of indices to transform as the conjugate representation to b, which are in the fundamental representation of SU(N). If we impose the constraint $b_\alpha^\dagger b^\alpha=n_c$ or $\bar{b}^{\alpha\dagger}\bar{b}_\alpha=n_c$ at each site, then the states are in an irreducible representation of SU(N) which has a Young tableau with one row of n_c boxes (the totally symmetric representation) on sublattice A, and the conjugate of this on sublattice B ($N-1$ rows, n_c columns). In the familiar case of $N=2$ [SU(2) or O(3) Heisenberg model], these are the usual Schwinger bosons, and all sites have spin $S=n_c/2$. This representation has been used previously by Arovas and Auerbach[6] to obtain a $1/N$ expansion with $n_c\propto N$ in order to study mainly the Néel-ordered phase.

We may represent the partition function of our models by an imaginary-time functional integral[8] of

$$\mathcal{L}=\sum_{i\in A}\left[b_\alpha^\dagger(i)\left(\frac{d}{d\tau}+i\lambda(i)\right)b^\alpha(i)-i\lambda(i)n_c\right]+\sum_{j\in B}\left[\bar{b}^{\alpha\dagger}(j)\left(\frac{d}{d\tau}+i\lambda(j)\right)\bar{b}_\alpha(j)-i\lambda(j)n_c\right]$$
$$+\sum_{i\in A,\hat{\eta}}\left[\frac{N}{J}|Q_{i,i+\hat{\eta}}|^2-Q_{i,i+\hat{\eta}}^*b^\alpha(i)\bar{b}_\alpha(i+\hat{\eta})+\text{H.c.}\right]$$

over the fields b, $\bar{b}$, Q, and λ. Here the $\lambda(i)$ fix the boson number at each site, τ dependence of all fields is implicit, Q was introduced by a Hubbard-Stratonvich decoupling of H, and $\hat{\eta}$ runs over nearest-neighbor vectors and has length a. The Lagrangian $\mathcal{L}$ possesses a U(1) gauge invariance under arbitrary τ-dependent changes of phase of b, $\bar{b}$, provided corresponding changes in Q,λ are made; the functional integral over $\mathcal{L}$ faithfully represents the partition function as long as we fix a gauge, e.g., by the condition $d\lambda/d\tau=0$ at all sites.

The $1/N$ expansion of the free energy can be obtained by integrating out of $\mathcal{L}$ the N-component $b,\bar{b}$ fields to leave an effective action for Q,λ having coefficient N (since $n_c\propto N$); minimizing with respect to the "mean-field" values of Q,λ gives the $N\to\infty$ limit.[8] This is equivalent to solving the mean-field Hamiltonian

$$H_{\text{MF}}=\sum_{i\in A,\hat{\eta}}[N|\bar{Q}|^2/J-\bar{Q}b^\alpha(i)\bar{b}_\alpha(i+\hat{\eta})+\text{H.c.}]+\bar{\lambda}\sum_{i\in A}[b_\alpha^\dagger(i)b^\alpha(i)-n_c]+\bar{\lambda}\sum_{j\in B}[\bar{b}^{\alpha\dagger}(i)\bar{b}_\alpha(i)-n_c]\,.$$

In writing H_{MF} we used the fact that $i\lambda(i)=\bar{\lambda}$ and $Q_{i,i+\hat{\eta}}$ are found to be uniform and independent of $\hat{\eta}$ at the saddle point. The constant $\bar{\lambda}$ is found to be real and $\bar{Q}$ can be taken real, positive by a gauge transformation. The Hamiltoni-

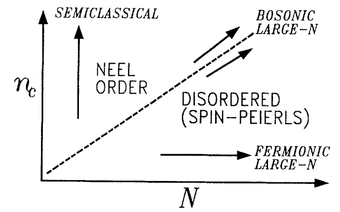

FIG. 1. Phase diagram of the square-lattice SU(N) antiferromagnet as a function of the spin n_c [$=2S$ for SU(2)]. The phase boundary between Néel order and its absence behaves as $n_c/N \to 0.19$ as $N \to \infty$ (Ref. 6). Earlier work examined the semiclassical (Refs. 3 and 4) and the fermionic large-N limits (Refs. 4, 6, and 7); the latter has spin-Peierls order with the symmetry of Fig. 2(d) for *all* n_c. This paper examines the bosonic large-N region in the disordered phase close to the transition line. In $d=1$, the Néel region is absent, while for $d>2$, a similar phase boundary is found (Ref. 4).

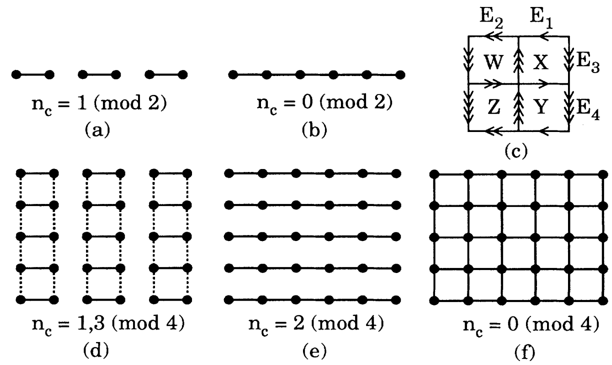

FIG. 2. Symmetry of the ground states: Solid lines denote larger values of $\langle \hat{S}(i)\cdot\hat{S}(i+1)\rangle$ for a link; no line, smaller values; and dashed line, intermediate values. (a),(b) $d=1$ chain. (c) Definition of the four plaquette sublattices W,X,Y,Z and the electric fields on the links. (d)–(f) Symmetry of ground states for square lattice near phase boundary in Fig. 1, of degeneracy 4,2,1, respectively.

an $H_{\rm MF}$ can be diagonalized by Bogoluibov's method and we find two modes for each wave vector in the (reduced) Brillouin zone, of energy $\omega_{\mathbf{k}}=(\bar\lambda^2-4d^2\bar{Q}^2\gamma_{\mathbf{k}}^2)^{1/2}$, where $\gamma_{\mathbf{k}}=(1/2d)\sum_{\hat\eta}e^{i\mathbf{k}\cdot\hat\eta}$ and $\bar\lambda\sim\bar{Q}\sim J$. At $\mathbf{k}=0$, $\omega_{\mathbf{k}}=\Delta=(\bar\lambda^2-4d^2\bar{Q}^2)^{1/2}\geq 0$ is the energy gap. In $d=1$, $\Delta\to 0$ as $n_c/N\to\infty$; in $d=2$, $\Delta\to 0$ as temperature $T\to 0$ for all $n_c/N\geq 0.19$, and for $n_c/N<0.19$, the gap Δ remains nonzero at $T=0$. For $d>2$, Δ vanishes above some critical value of n_c/N for all $T<T_{\rm N\acute{e}el}(n_c/N)$, the Néel-ordering temperature. Cases where $\Delta=0$ require $\langle b\rangle,\langle\bar b\rangle$ to be nonzero due to condensation into the zero-energy states, which is identified physically as long-range Néel order.[9] In this paper, we shall be interested in the *disordered* state at $T=0$ and $d=1,2$ ($n_c/N<0.19$ for $d=2$) where SU(N) symmetry is *unbroken.*

When $\Delta\ll J$, the long-wavelength $b,\bar b$ excitations have a relativistic spectrum with speed of "light" (spin-wave velocity) $c\sim\bar\lambda a/d^{1/2}$ and mass Δ/c^2. The ground state of $H_{\rm MF}$ has the form for $\Delta>0$

$$|\Omega\rangle\propto\exp\left(\sum_{\mathbf{k}}f_{\mathbf{k}}b_{\mathbf{k}\alpha}^{\dagger}\bar b_{-\mathbf{k}}^{\alpha\dagger}\right)|0\rangle\,, \qquad (2)$$

which represents a condensate of singlet pairs of bosons ("valence bonds"); the bonds have ends on opposite sublattices and their characteristic size is c/Δ. When projected onto n_c bosons per site, $|\Omega\rangle$ is an SU(N) generalization of the short-range resonating-valence-bond states of Sutherland[10] and Liang, Doucot, and Anderson,[10] which are thus *exact* in the present large-N limit provided the distribution of bond lengths is chosen correctly. The eigenmodes of $H_{\rm MF}$ are clearly *bosons* in agreement with recent calculations.[11]

We now consider the fate of the U(1) gauge invariance of $\mathcal{L}$ in the mean-field theory of the disordered state. It is useful to examine first *global* (site and τ independent) transformations; since our system has two sites per unit cell, there are two such invariances: (i) uniform, $b\to e^{i\phi}b$, $\bar b\to e^{i\phi}\bar b$; and (ii) staggered, $b\to e^{i\phi}b$, $\bar b\to e^{-i\phi}\bar b$. Clearly the "uniform" symmetry is broken by the nonzero value of $\bar Q\sim\langle b^\alpha\bar b_\alpha\rangle$ while the "staggered" symmetry is not. Considering the full group of *local* gauge transformations we see that it splits into two parts: the uniform part which is broken, and the staggered part which is not. Fluctuations of Q and λ can be written in the form (for each unit cell labeled by $i\in A$)

$$Q_{i,i+\hat\eta}=[\bar Q+q_{\hat\eta}(i+\tfrac12\hat\eta)]\exp[i\theta_{\hat\eta}(i+\tfrac12\hat\eta)]\,,$$
$$i\lambda(i)=\bar\lambda+i\lambda_1(i),\quad i\lambda(i+\hat x)=\bar\lambda+i\lambda_2(i+\hat x)\,,$$

and in momentum space,

$$aA_{\hat\eta}(\mathbf{k})=\tfrac12[\theta_{\hat\eta}(\mathbf{k})-\theta_{-\hat\eta}(\mathbf{k})]=-aA_{-\hat\eta}(\mathbf{k})\,,$$
$$M_{\hat\eta}(\mathbf{k})=\tfrac12[\theta_{\hat\eta}(\mathbf{k})+\theta_{-\hat\eta}(\mathbf{k})]=M_{-\hat\eta}(\mathbf{k})\,,$$
$$A_\tau(\mathbf{k})=\tfrac12[\lambda_1(\mathbf{k})-\lambda_2(\mathbf{k})]\,,$$
$$M_\tau(\mathbf{k})=\tfrac12[\lambda_1(\mathbf{k})+\lambda_2(\mathbf{k})]\,.$$

With $\hat\eta$ in a positive axis direction, the $A_{\hat\eta},A_\tau$ are the components $(\mathbf{A},A_\tau)$ of the gauge field for the unbroken, staggered U(1) symmetry, while the M's are related to the broken uniform symmetry. Note that the two modes of $H_{\rm MF}$ at each point $\mathbf{k}$ in the Brillouin zone have charges ±1 with respect to the staggered symmetry; i.e., they are particle and antiparticle.

We now give the form of the long-wavelength ($\gg a$) effective action of H in terms of the continuum fields $q_{\hat\eta}$, A, M, $z^\alpha=(b^\alpha+\bar b^{\alpha\dagger})/2$, $\pi^\alpha=(b^\alpha-\bar b^{\alpha\dagger})/2$, obtained after integrating out π:

$$S_{\rm eff}=\int d^dr\int_0^{c\beta}d\tilde\tau\left[\frac{a^{1-d}}{2\sqrt{d}}\left\{|(\partial_\mu-iA_\mu)z^\alpha|^2+\frac{\Delta^2}{c^2}|z^\alpha|^2\right\}+\frac{N}{4e^2}F_{\mu\nu}^2+iN\gamma\sum_{\hat\eta>0}(q_{\hat\eta}-q_{-\hat\eta})F_{\hat\eta\tilde\tau}\right]$$

plus additional terms involving M and $q_{\hat{\eta}}$. Here $\tilde{\tau}=c\tau$, $A_{\tilde{\tau}}=A_\tau/c$, and $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$, where μ,ν run over $x,y,\ldots,\tilde{\tau}$, is the electromagnetic field. The terms involving z come from $\mathcal{L}$ while the remaining terms come from integrating out $b,\bar{b}$ (or z) at one-loop order, giving the coefficient N. For $d<3$, $e^2\sim(\Delta/c)^{3-d}$ can be calculated in the continuum limit, but γ (needed for the spin-Peierls calculation below) has to be calculated using the underlying lattice regularization, giving $\gamma\sim a^{1-d}/\bar{\lambda}$. The z,A part of S_{eff} has just the form that would be expected by first passing to the continuum semiclassical limit of the Néel phase of H (Ref. 12) and then taking the large-N limit of the resulting CP^{N-1} model.[13]

So far S_{eff} contains only terms for small fluctuations, but no terms relating to topologically nontrivial gauge-field configurations. These terms, which are expected to be Berry phase factors in the functional integral, would be obtainable by integrating out $b,\bar{b}$ in the presence of a nontrivial background gauge field. This should be equivalent to our procedure below of calculating the phase due to adiabatic evolution of the ground state (2) in such a background. We discuss $d=1,2$ in turn:

(i) d=1.—The only relevant term which could be added to S_{eff} is $(i\Theta/2\pi)\int dx\,d\tilde{\tau}F_{x\tilde{\tau}}$, as suggested by semiclassical calculations[12] in the Néel-ordered phase which produce just this term, when written in CP^{N-1} language,[13] with $\Theta=\pi n_c$. This term survives destruction of Néel order and can be derived *directly* in the disordered phase as follows. Consider a spin chain with N_s sites (N_s even) and periodic boundary conditions. Choosing the configuration in the phase of Q, $\theta_{\hat{\eta}}(i+\frac{1}{2}\hat{\eta},\tau)=\text{sgn}(\hat{\eta})\phi(\tau)$, where $\phi(\tau)$ increases slowly from 0 at $\tau=0$ to the gauge equivalent value $2\pi l/N_s$ at $\tau=\beta$ (l integer), yields $\int dx\,d\tilde{\tau}F_{x\tilde{\tau}}=2\pi l$. At $\tau=0$ we have the wave function $|\Omega\rangle$ in Eq. (2) with f_k real and the sum is over $k=2\pi n/aN_s$, $n=1,\ldots,N_s/2$. For $\tau>0$ we find $\langle\Omega|d/d\tau|\Omega\rangle=0$; as a result

$$|\Omega(\tau=\beta)\rangle\propto\exp\left[\sum_k f_{k-2\pi l/aN_s}b^\dagger_{k\alpha}\bar{b}^{\alpha\dagger}_{-k}\right]|0\rangle\,. \tag{3}$$

The gauge-invariant Berry phase is now just the change in the phase of the wave function, which for large N is $P_{n_c}|\Omega(\tau=\beta)\rangle=(-1)^{n_c l}P_{n_c}|\Omega(\tau=0)\rangle$, where P_{n_c} projects onto n_c bosons per site. This phase may be included in S_{eff} by using $\Theta=p\pi$, where $(-1)^p=(-1)^{n_c}$. Each choice of Θ corresponds to a different metastable state of the spin chain with a mean static electric field[13] $iF_{x\tilde{\tau}}=e^2p/N$, energy per site $\sim ce^2p^2a/N$, and a spin-Peierls order parameter

$$\langle\hat{S}(i)\cdot\hat{S}(i+1)-\hat{S}(i)\cdot\hat{S}(i-1)\rangle\sim N\bar{Q}\langle q_{\hat{x}}-q_{-\hat{x}}\rangle/J \sim\gamma e^2cp\,.$$

The ground state for n_c even is therefore obtained with the choice $p=0$ and is nondegenerate; the linear Coulomb force confines the spinons in pairs. For n_c odd the ground state corresponds to $p=\pm1$, and is *twofold degenerate with a nonzero spin-Peierls order parameter;* the spinons are domain walls interpolating between the two ground states. A schematic of the two ground states is shown in Figs. 2(a) and 2(b). The spin-Peierls order for n_c odd was anticipated by Affleck[14] though not shown directly for $n_c\sim N$. This picture is now expected to be correct for *all* $N>2$.[4,14]

(ii) d=2.—In the Néel-ordered state of the CP^{N-1} model, the Berry-phase term vanishes for any spin configuration which is smooth on the scale of the lattice spacing,[15] but is nonzero for space-time "hedgehog" singularities.[3] In the disordered phase, we use the correspondence between the electromagnetic field tensor $F_{\mu\nu}$ and the "topological charge" $i(\partial_\mu z^*_\alpha\partial_\nu z^\alpha-\partial_\nu z^*_\alpha\partial_\mu z^\alpha)$ of the CP^{N-1} model[13] to identify pointlike instanton configurations of the (2+1)-dimensional compact U(1) gauge theory[16,17] which have $\int F_{\mu\nu}dS_{\mu\nu}=2\pi m$ (the integral is over a sphere surrounding the singular point and m is an integer) as the remnants of the hedgehog of the Néel phase. The Berry phase of the instantons can be calculated in a manner very similar to that employed for $d=1$: We obtain a result (specified below) *identical* to the hedgehog Berry phase calculated by Haldane[3] and its extension to SU(N).[4]

The subsequent analysis follows closely Polyakov's solution[16] of (2+1)-dimensional compact QED. Neglecting all fields except A at distances $>c/\Delta$, the action is evaluated for each instanton configuration, to give the partition function

$$Z=\sum_{K,\{m_s\}}\frac{1}{K!}\prod_{s=1}^{K}\left[\sum_{\mathbf{R}_a}\int_0^{c\beta}\frac{d\tilde{\tau}_s}{\rho a}\right]\exp[-S_m(\{m_s\})]\,,$$
$$S_m(\{m_s\})=\frac{N\pi}{2e^2}\sum_{s\neq t}\frac{m_sm_t}{[(\mathbf{R}_s-\mathbf{R}_t)^2+(\tilde{\tau}_s-\tilde{\tau}_t)^2]^{1/2}}+\sum_s\left[NE_cm_s^2+i\frac{n_c\pi}{2}\zeta_sm_s\right]. \tag{4}$$

Note the following: (i) The instantons are represented by integer charges m_s located at $\mathbf{R}_s$, the centers of the plaquettes. (ii) ρ is a dimensionless constant of order unity. (iii) The $1/r$ interaction between instantons is valid at distances larger than the spin-correlation length c/Δ in contrast to the linear r interaction between hedgehogs on the ordered side. (iv) NE_c, the instanton core-action, is determined by the physics at length scales shorter than c/Δ; assuming that the instanton is better described as a hedgehog at these length scales, we expect $E_c\sim\bar{\lambda}/\Delta$. (v) The term proportional to ζ_s is the Berry phase of the instanton; we have $\zeta_s=0,1,2,3$ for $\mathbf{R}_s$ on sublattices W,X,Y,Z [Fig. 2(c)]. The well-known equivalence between the d-dimensional Coulomb gas and the sine-Gordon model[16] can now be used to show that the long-distance properties of Z are equivalent to those of $Z=\int D\chi \exp(-S_{\rm sG})$ with

$$S_{\rm sG}=\frac{g}{2}\int_0^{c\beta} d\tilde{\tau}\left\{\sum_{\langle s,t\rangle}(\chi_s-\chi_t)^2+\sum_s\{a^2(\partial_{\tilde{\tau}}\chi_s)^2-M^2\cos[\chi_s-(n_c\pi/2)\zeta_s]\}\right\}. \tag{5}$$

Here χ is the sine-Gordon field whch was coupled to the instanton charge with the term $\exp(i\chi_s m_s)$, $g=e^2/4N\pi^2$, and $M^2=(2/g\rho a)\exp(-NE_c)$ is the *exponentially* small instanton fugacity. In the transformation from Eq. (4) to Eq. (5) we have made the small-fugacity approximation of neglecting instantons with $|m_s|\geq 2$.

If $n_c=0(\mathrm{mod}4)$, $S_{\rm sG}$ is the usual sine-Gordon model. For small M, it is solved by expanding perturbatively around a minimum.[16] This gives a "screening length" in the instanton plasma $\sim aM^{-1}$ and confinement of z quanta (spinons) into pairs of size $\sim aM^{-1}$. The fluctuations in F give a collective mode of gap $\sim cM/a$. This closely resembles the properties of the valence-bond-solid states recently introduced for $n_c=2S=4$ in an SU(2) model,[18] and gives the full lattice symmetry [Fig. 2(f)].

For $n_c\neq 0(\mathrm{mod}4)$ the uniform state $\chi_s=\mathrm{const}$ is *unstable*. The rotation symmetry between the four sublattices W,X,Y,Z is therefore *spontaneously broken*. For $n_c=1(\mathrm{mod}4)$ one stable minimum of $S_{\rm sG}$ is given to order M^2 by $\chi_W=\chi_X=-\pi/4-M^2/4\sqrt{2}$, $\chi_Y=\chi_Z=-\pi/4+M^2/4\sqrt{2}$ (there are three other similar minima near $\pi/4$, $3\pi/4$, and $-3\pi/4$). This minimum has a static electric field [Fig. 2(c)]: $iE_3=iE_4=0$, $iE_1=iE_2=\pi g M^2/\sqrt{2}a$. The coupling between the electric field and the $q_{\hat{\eta}}$ field in $S_{\rm eff}$ now implies an exponentially small (in N) but *nonzero spin-Peierls order* of the type shown in Fig. 2(d) with $\langle q_{\hat{x}}-q_{-\hat{x}}\rangle\sim(\gamma\bar{\lambda}a)\pi g c M^2/\sqrt{2}$. A very similar analysis can be performed for $n_c=3(\mathrm{mod}4)$. For $n_c=2(\mathrm{mod}4)$ the minima of $S_{\rm sG}$ lead to the static electric fields $iE_2=iE_3=-iE_4=gM^2/4a$ and spin-Peierls order of the type shown in Fig. 2(e).[19] These states with broken lattice symmetry also give confinement of spinons and a massive spinless collective mode but with gap (inverse confinement scale) $\sim cM^2/a$ and cM^4/a for $n_c=2$ and 1,3(mod4), respectively. This completes our results.

A similar calculation can be carried out for other bipartite lattices, in particular the honeycomb lattice in $d=2$. This has coordination number 3 and the periodicity in ground-state properties is then in n_c(mod3), which is consistent with Ref. 18. Our results also generalize to models where sublattice A has m rows in its Young tableau, requireing that the bosons have U(m) gauge symmetry.[4] The only modification to our results is that in $d=1$ there are no soliton excitations connecting the ground states for n_c odd.

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