

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 resonating-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 Haldane³ 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 vectors.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

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

where $\hat{S}_i^\beta(i)$ 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 $\alpha, \beta = 1, \dots, N$ are summed over. We will use a Schwinger boson representation of the spin states, in which $\hat{S}_i^\beta(i) = b_\alpha^\dagger(i) b^\beta(i)$, $i \in A$ sublattice, and $\hat{S}_i^\beta(j) = -\bar{b}^{\beta\dagger}(j) \bar{b}_\alpha(j)$, $j \in B$ 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 Auerbach⁶ 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 integral⁸ 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-Stratonovich 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 $N \rightarrow \infty$ limit.⁸ This is equivalent to solving the mean-field Hamiltonian

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

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 Q can be taken real, positive by a gauge transformation. The Hamiltonian

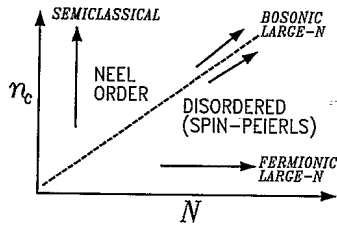


FIG. 1. Phase diagram of the square-lattice $SU(N)$ antiferromagnet as a function of the spin n_c [$=2S$ for $SU(2)$]. The phase boundary between Néel order and its absence behaves as $n_c/N \rightarrow 0.19$ as $N \rightarrow \infty$ (Ref. 6). Earlier work examined the semiclassical (Refs. 3 and 4) 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).

an H_{MF} can be diagonalized by Bogoliubov'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 $d=1$, $\Delta \rightarrow 0$ as $n_c/N \rightarrow \infty$; in $d=2$, $\Delta \rightarrow 0$ as temperature $T \rightarrow 0$ 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 $T < T_{N\acute{e}el}(n_c/N)$, 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_{MF} has the form for $\Delta > 0$

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

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 Sutherland¹⁰ 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_{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 in-

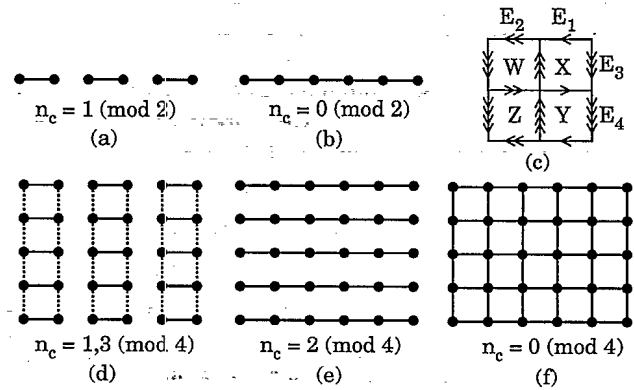


FIG. 2. Symmetry of the ground states: Solid lines denote larger values of $\langle \hat{S}(i) \cdot \hat{S}(i+1) \rangle$ for a link; no line, smaller values; and dashed line, intermediate values. (a), (b) $d=1$ chain. (c) Definition of the four plaquette sublattices W, X, Y, Z and the electric fields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

dependent) transformations; since our system has two sites per unit cell, there are two such invariances: (i) uniform, $b \rightarrow e^{i\phi} b$, $\bar{b} \rightarrow e^{i\phi} \bar{b}$; and (ii) staggered, $b \rightarrow e^{i\phi} b$, $\bar{b} \rightarrow e^{-i\phi} \bar{b}$. 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 $i \in A$)

$$Q_{i, i+\hat{\eta}} = [\bar{Q} + q_{\hat{\eta}}(i + \frac{1}{2}\hat{\eta})] \exp[i\theta_{\hat{\eta}}(i + \frac{1}{2}\hat{\eta})],$$

$$i\lambda(i) = \bar{\lambda} + i\lambda_1(i), \quad i\lambda(i+\hat{x}) = \bar{\lambda} + i\lambda_2(i+\hat{x}),$$

and in momentum space,

$$A_{\hat{\eta}}(\mathbf{k}) = \frac{1}{2} [\theta_{\hat{\eta}}(\mathbf{k}) - \theta_{-\hat{\eta}}(\mathbf{k})] = -A_{-\hat{\eta}}(\mathbf{k}),$$

$$M_{\hat{\eta}}(\mathbf{k}) = \frac{1}{2} [\theta_{\hat{\eta}}(\mathbf{k}) + \theta_{-\hat{\eta}}(\mathbf{k})] = M_{-\hat{\eta}}(\mathbf{k}),$$

$$A_\tau(\mathbf{k}) = \frac{1}{2} [\lambda_1(\mathbf{k}) - \lambda_2(\mathbf{k})],$$

$$M_\tau(\mathbf{k}) = \frac{1}{2} [\lambda_1(\mathbf{k}) + \lambda_2(\mathbf{k})].$$

With $\hat{\eta}$ in a positive axis direction, the $A_{\hat{\eta}}, A_\tau$ are the components (A_τ) 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_{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 :

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

plus additional terms involving M and $q_{\hat{n}}$. Here $\bar{\tau} = c\tau$, $A_{\bar{\tau}} = A/c$, and $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$, where μ, ν run over $x, y, \dots, \bar{\tau}$, 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 $(i\Theta/2\pi) \int dx d\bar{\tau} F_{x\bar{\tau}}$, as suggested by semiclassical calculations¹² 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 , $\theta_{\hat{n}}(i + \frac{1}{2}\hat{n}, \tau) = \text{sgn}(\hat{n})\phi(\tau)$, 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 $\int dx d\bar{\tau} F_{x\bar{\tau}} = 2\pi l$. At $\tau=0$ we have the wave function $|\Omega\rangle$ in Eq. (2) with f_k real and the sum is over $k = 2\pi n/aN_s$, $n=1, \dots, N_s/2$. For $\tau > 0$ we find $\langle \Omega | d/d\tau | \Omega \rangle = 0$; as a result

$$|\Omega(\tau=\beta)\rangle \propto \exp\left[\sum_k f_k - 2\pi l/aN_s b_k^{\dagger} \bar{b}_k^{\dagger}\right] |0\rangle. \quad (3)$$

The gauge-invariant Berry phase is now just the change in the phase of the wave function, which for large N is

$$Z = \sum_{K, \{m_s\}} \frac{1}{K!} \prod_{s=1}^K \left[\sum_{\mathbf{R}_s} \int_0^{c\beta} \frac{d\bar{\tau}_s}{\rho a} \right] \exp[-S_m(\{m_s\})], \quad (4)$$

$$S_m(\{m_s\}) = \frac{N\pi}{2e^2} \sum_{s \neq t} \frac{m_s m_t}{[(\mathbf{R}_s - \mathbf{R}_t)^2 + (\bar{\tau}_s - \bar{\tau}_t)^2]^{1/2}} + \sum_s \left[NE_c m_s^2 + i \frac{n_c \pi}{2} \zeta_s m_s \right].$$

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 model¹⁶ can now be used to show

$P_{n_c} |\Omega(\tau=\beta)\rangle = (-1)^{n_c l} P_{n_c} |\Omega(\tau=0)\rangle$, 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 field¹³ $iF_{x\bar{\tau}} = e^2 p/N$, energy per site $\sim ce^2 p^2 a/N$, and a spin-Peierls order parameter

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

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 $p = \pm 1$, 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 Affleck¹⁴ 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} model¹³ 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 Haldane³ and its extension to SU(N).⁴

The subsequent analysis follows closely Polyakov’s solution¹⁶ 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

that the long-distance properties of Z are equivalent to those of $Z = \int D\chi \exp(-S_{sG})$ with

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

Here χ is the sine-Gordon field which was coupled to the instanton charge with the term $\exp(i\chi_s m_s)$, $g = e^2/4N\pi^2$, and $M^2 = (2/gpa) \exp(-NE_c)$ 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 $n_c = 0 \pmod{4}$, S_{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 $n_c \neq 0 \pmod{4}$ the uniform state $\chi_s = \text{const}$ is *unstable*. The rotation symmetry between the four sublattices W, X, Y, Z is therefore *spontaneously broken*. For $n_c = 1 \pmod{4}$ one stable minimum of S_{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_{eff} now implies an exponentially small (in N) but *nonzero spin-Peierls order* of the type shown in Fig. 2(d) with $\langle q_{\hat{x}} - q_{-\hat{x}} \rangle \sim (\gamma \lambda a) \pi g c M^2 / \sqrt{2}$. A very similar analysis can be performed for $n_c = 3 \pmod{4}$. For $n_c = 2 \pmod{4}$ the minima of S_{sG} lead to the static electric fields $iE_2 = iE_3 = -iE_4 = g M^2 / 4a$ 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 $1, 3 \pmod{4}$, 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 $n_c \pmod{3}$, which is consistent with Ref. 18. Our results also generalize to models where sublattice A has m rows in its Young tableau, requiring 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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¹⁹In this case the electric field oscillates in sign and we must include both fields A, M with $E_{\hat{\eta}}(i \pm \frac{1}{2} \hat{\eta}) = \pm \partial_{\tau} \theta_{\pm \hat{\eta}}(i \pm \frac{1}{2} \hat{\eta})$ for $i \in A$ and $\hat{\eta} > 0$ in the gauge $\lambda = \text{const}$. The coupling $i(q_{\hat{x}} + q_{-\hat{x}})[\gamma_1(2M_{\hat{\tau}} - \partial_{\tau} M_x) + \gamma_2(2M_{\hat{\tau}} - \partial_{\tau} M_y)] + (x \leftrightarrow y)$ in S_{eff} then leads to the spin-Peierls order shown in Fig. 2(e).