Broken and Unbroken Symmetries in Low-Dimensional Quantum Magnets

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We present a theoretical analysis of the properties of low-dimensional quantum magnets in applied magnetic fields. Through the nonlinear σ model, we use a spin stiffness analysis, a 1/N expansion, and a renormalization group approach to describe the broken-symmetry regimes of finite magnetization, and especially the low-field regime where symmetry is restored via quantum fluctuations. Broken symmetry states are discussed in terms of deconfined, gapless spin excitations, while in the symmetric state the gapped excitations are confined. The analysis is relevant to a variety of laboratory systems, particularly those exhibiting Haldane physics.

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I. INTRODUCTION

The importance of low-dimensional spin systems in revealing fundamental quantum mechanical properties has been recognized since Haldane's conjecture[1] concerning the effects of quantum fluctuations in integral- and half-integral-spin antiferromagnetic (AF) chains. The key quantity is the topological term arising from the quantum spin phase, and similar considerations have since been extended to anisotropic and higher-order interactions, higher dimensions (planes), and coupled chains (spin ladders) — largely driven by materials and experiment. Magnetic flux within a sample can alter the effective spin magnitude. Features visible in an applied field include spin gaps and magnetization plateaus. Magnetic materials with field-accessible exchange interactions are primarily metalloorganics. Examples on which experimental interest has focused are the Haldane ($S = 1$) chain NENP[2], the planar system CFTD[3], and the two-chain spin ladder CuHpCl[4,5]. We shall focus on the ladder geometry of CuHpCl, the best-characterized sample in recent literature.

We will study the quantum AF system in an external magnetic field using the nonlinear σ model (NLsM). While this widely-applied treatment is in fact semiclassical, being truly valid only in the limit of large on-site spin S, it has in the past formed the basis for many fundamental deductions concerning the quantum limit of antiferromagnetic spin systems. We will demonstrate here its validity in the case of all effectively integral-spin quantum systems in appreciable magnetic fields, and provide justification for this result in terms of suppression of quantum fluctuations by the field.

The present contribution provides an illustrative example related to symmetry breaking in condensed matter systems. Indeed, we shall see that the O(3) symmetry of the spin Hamiltonian and its low-energy description in terms of the nonlinear σ model is broken on a purely classical level. However, this symmetry becomes completely restored by strong quantum fluctuations. This is a well-known property of the NLsM and has served in the past as an instructive model for illustrating the effect of asymptotic freedom (or "confinement of excitations")[6]. We shall see, however, that in the presence of a magnetic field the quantum fluctuations can be suppressed for fields that are sufficiently strong but that are still experimentally accessible, with the consequence that the full O(3) symmetry can not be restored and the spin system is left with the lower XY or O(2) symmetry. The XY symmetry (in the plane perpendicular to the applied field direction) is still high enough such that there is no true long range order, and, instead, there will be only quasi-long range order characterized by spin-spin correlation functions of XY type that decay in space only with a power law. There is a large number of examples known in condensed matter systems, in particular in magnetic systems, where the quantum fluctuations restore the symmetry which is broken on a classical level. Examples for this are tunneling processes in superparamagnets, where a large magnetic moment can fluctuate in its direction between two degenerate positions and thereby restore the symmetry that would be broken otherwise. For further reading and related references we refer the interested reader to Ref.[7].

The Hamiltonian for the ladder system in a magnetic field $\mathbf{b} = \tilde{g}\mu_B \mathbf{B}$ may be written as

$$H = \sum_{i,m=1,2} \left(J\mathbf{S}_{m,i} \cdot \mathbf{S}_{m,i+1} + J'\mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} + \mathbf{b} \cdot \mathbf{S}_{m,i} \right), \tag{1.1}$$

where J is the superexchange interaction between spins in each chain and J' the interchain, or ladder "rung", interaction. We choose N_x-site chains with periodic boundary conditions in both directions, and the geometry shown in Fig. 1, such that $J_x = J$, $J_y = J'/2$, $\mathbf{B} = (0, 0, B)$, and $\mathbf{S}_{m,N+i} = \mathbf{S}_{m,i}$. Following the standard procedure in the derivation of the NLsM, the spin is written as $\mathbf{S}_{m,i} \simeq S[(-1)^{i+m}\mathbf{n}_{m,i} + a\mathbf{l}_{m,i}]$, where $\mathbf{n}_{m,i}$ is the staggered spin of unit magnitude, and $\mathbf{l}_{m,i}$ describes the spin fluctuations perpendicular to $\mathbf{n}_{m,i}$. On proceeding to the continuum limit, the Hamiltonian is expressed as

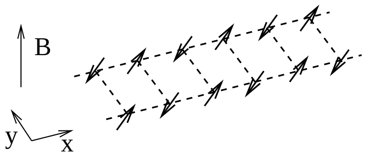

FIG. 1. Representation of two-chain ladder system and coordinate axes.

$$H = \int d\mathbf{r} \left(\frac{1}{2} S^2 \sum_{j=x,y} J_j \left[(\partial_j \mathbf{n})^2 + 4\mathbf{l}^2 \right] - \frac{S}{a} \mathbf{l} \cdot \mathbf{b} \right). \tag{1.2}$$

The full Euclidean action $\mathcal{S}_E = \mathcal{S}_{WZ} + \int d\tau H$ in space $\mathbf{r} = (x, y)$ and inverse temperature τ contains a Berry-phase, or Wess-Zumino, term whose origin lies in the solid angle subtended by the fluctuating quantum spin phases:

$$\mathcal{S}_{WZ} = i \frac{S}{a^2} \int d\tau \, d\mathbf{r} \left[\dot{\phi} - a \mathbf{l} \cdot (\mathbf{n} \times \dot{\mathbf{n}}) \right] + 4\pi i S \left(P_1 + P_2 \right). \tag{1.3}$$

Here, ϕ is the azimuthal angle, and $P_1 = P_2 = (1/4\pi) \int d\tau \, dx \, (\mathbf{n} \times \dot{\mathbf{n}}) \cdot \partial_x \mathbf{n}$ are topological terms which give the Pontryagin index on each chain when $\partial_y \mathbf{n} = 0$, as is the case in a ladder of only two chains. The last term in Eq. (1.3) is therefore $i(4\pi P_1)2S$, demonstrating that the system will have integral-spin characteristics for any value of S, and the topological term may thus be ignored[8,9].

Integrating out the fluctuations $\mathbf{l}$ about the staggered spin configuration of $\mathbf{n}$, subject to the orthogonality constraint $\mathbf{n} \cdot \mathbf{l} = 0$, yields the classical solution

$$\mathbf{l}_{\rm cl} = \frac{1}{4aS\bar{J}} \left\{ i \left(\mathbf{n} \times \dot{\mathbf{n}} \right) + \left[\mathbf{b} - \mathbf{n} \left(\mathbf{b} \cdot \mathbf{n} \right) \right] \right\}, \tag{1.4}$$

where $\bar{J} = J_x + J_y$. Finally, the corresponding action for the quasi-one-dimensional (1D) ladder system, in 1+1 Euclidean dimensions denoted by μ, is

$$\mathcal{S}_E = \frac{1}{2g} \int d\tau \, dx \, \Big\{ (\partial_\mu \mathbf{n})^2 - \left[\mathbf{b}^2 - (\mathbf{n} \cdot \mathbf{b})^2 \right] + 2i \mathbf{b} \cdot (\mathbf{n} \times \dot{\mathbf{n}}) \Big\}, \tag{1.5}$$

where $g = (2/N_y S)\sqrt{\bar{J}/J_x}$ is the bare coupling constant, and the integral over τ is from zero to $L_T = c\beta$, with $c = 2Sa\sqrt{J_x \bar{J}}$ the effective spin-wave velocity. (We use $\hbar = 1$ throughout.) We have left explicit the number of chains N_y in the ladder. For the compound under consideration, $J_y > J_x$ and $N_y = 2$, giving an effectively rigid rung coupling.

The form of the NLsM in an external field given by Eq. (1.5) has been derived previously[10], and its implications considered in the low-field limit[11]. Below we examine its effects at all field strengths. The field induces a hard-axis anisotropy through the term $(\mathbf{n} \cdot \mathbf{b})^2$, i.e., the spins will tend to align with $\mathbf{n}$ in the plane normal to $\mathbf{b}$. Writing $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ in spherical coordinates, and expanding to quadratic order in $\vartheta = \theta - \pi/2$ (the field is along the z axis), the Lagrangean density

$$\mathcal{L}_E = \frac{1}{2g} \left\{ \left[\left(\dot{\phi} + ib \right)^2 + (\partial_x \phi)^2 \right] - \vartheta \left[\partial_\mu^2 + \left(\dot{\phi} + ib \right)^2 \right] \vartheta \right\} \tag{1.6}$$

separates into contributions from in-plane and out-of-plane fluctuations if $|b| > \dot{\phi} \equiv \omega$. We shall return to this condition below.

II. SPIN STIFFNESS ANALYSIS

To gain initial insight into the effect of the magnetic field, we consider the spin stiffness of the ladder system using the method of Ref.[12]. We take (Fig. 2) the staggered spin configuration to be subject to a twist ψ in the plane, $\mathbf{n}(\tau, 0) = (1, 0, 0)$ and $\mathbf{n}(\tau, L) = (\cos\psi, \sin\psi, 0)$. This is conveniently represented by $\mathbf{n} = \mathcal{R}(x)\sigma$, where $\mathcal{R}$ is a matrix for rotation by $\psi x/L$ about the z axis, and $\boldsymbol{\sigma}$ a 3-component vector with value $(1,0,0)$ at the spatial endpoints. The cross-term in $(\partial_\mu \mathbf{n})^2$ and the third term in Eq. (1.5) are total derivatives in x and τ respectively, and may be discarded. This is equivalent to considering only paths with no winding in the Euclidean space, and gives the action the form

$$\mathcal{S}_E = \frac{1}{2g} \int d\mathbf{x} \, (\partial_\mu \boldsymbol{\sigma})^2 + \left(\frac{\psi^2}{L^2} - \frac{b^2}{c^2} \right) \left(1 - \sigma_3^2 \right). \tag{2.1}$$

To 1-loop order in g, the spin stiffness is given by

$$\begin{aligned} \rho_s &= \frac{1}{2} cL \left. \frac{\partial^2 F}{\partial \psi^2} \right|_{\psi=0} \\ &= \frac{cL}{2L_T} \left. \frac{\partial^2}{\partial \psi^2} \right|_{\psi=0} \left\{ \frac{LL_T}{2g} \left[\frac{\psi^2}{L^2} - \frac{b^2}{c^2} \right] + \frac{1}{2} \mathrm{Tr} \ln \left[\mathbf{k}^2 - \frac{\psi^2}{L^2} + \frac{b^2}{c^2} \right] \right\} \\ &= \rho_s^0 \left[1 - \frac{g}{LL_T} \sum_{\mathbf{k}} \frac{1}{\mathbf{k}^2 + (b/c)^2} \right], \end{aligned} \tag{2.2}$$

where $\rho_s^0 = c/2g$ is the classical value and the sum includes both quantum and thermal (through the finite "length" L_T) corrections to first order.

We restrict our analysis to the low-temperature, or "quantum" case $L_T > L$. Evaluating the summation between the spatial limits π/L and π/a, and introducing the "magnetic length" $L_m = \pi c/b$, we obtain the expression

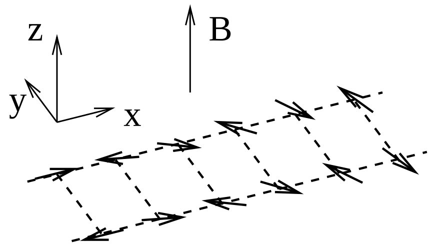

FIG. 2. Ladder system with twisted staggered moment.

$$\rho_s = \rho_s^0 \left[1 + \frac{g}{2\pi} \ln \left(\frac{a/L + \sqrt{(a/L)^2 + (a/L_m)^2}}{(1 + \sqrt{1 + (a/L_m)^2})} \right) \right]. \tag{2.3}$$

The system length L in Eq. (2.3) can be substituted by a correlation length ξ, beyond which segments of the ladder behave independently, and ξ computed from the condition $\rho_s = 0$. We emphasize that ρ_s is otherwise a local stiffness, meaningful only on length scales $L \le \xi$. In the weak-field limit ($L_m \to \infty$) one recovers the result[12] $\xi_0 = ae^{2\pi/g} = ae^{\alpha\pi S}$, where $\alpha = \sqrt{J_x/\bar{J}}$. The general solution can be expressed as

$$\begin{aligned} \xi(B) &= 2L_m^*/[1 - (L_m^*/L_m)^2] \\ &\equiv \xi_0/[1 - (B/B^*)^2], \end{aligned} \tag{2.4}$$

from which we see that the correlation length diverges at the critical field B^*, where $L_m^* = a\sinh(2\pi/g)$. For fields $B < B^*$ the system has only short-range correlations, and the finite correlation length may be written as $\xi(B) = ae^{\alpha\pi\tilde{S}}$, where $\tilde{S} = S\left[1 - (g/2\pi)\ln\left(1 - (L_m^*/L_m)^2\right)\right]$ is a growing value of the effective spin. There is no spontaneous breaking of the $O(3)$ spin symmetry. For $B > B^*$, the field enforces a long-ranged correlation throughout the system[13], and it is most convenient to write the spin stiffness as $\rho_s = \rho_s^0\,[1 - (g/2\pi)\ln(1 + L_m/a)]$, a quantity which recovers the bare value as $B \to \infty$. Finally, at the transition B^*, it is clear from Eq.(2.4) that the diverging correlation length corresponds to the closing of a gap Δ to spin excitations according to $\Delta \propto 1 - (B/B^*)^2$. This situation is summarized in Fig. 3. We stress that Δ is the gap to in-plane (ϕ) fluctuations (Eq. 1.6), whereas out-of-plane (θ) modes remain gapped with mass b. This result indicates a lowering of the spin symmetry from $O(3)$ to $O(2)$.

However, the magnetization $M = \partial F/\partial B|_{\psi=0}$ calculated in the spin stiffness framework is not zero in the low-field regime, as would be required of a system with no broken symmetry. This is a consequence of the approximation implicit in deriving the free energy $F(b,\psi)$, Eq. (2.2), that the field b be large on the scale of $|\dot{\phi}|$. Thus, the spin stiffness analysis, while qualitatively revealing, is not reliable at low fields.

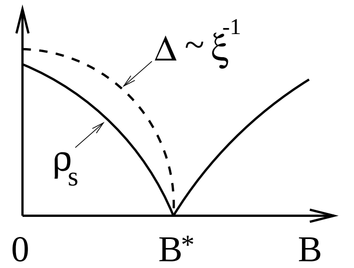

FIG. 3. Schematic behavior of spin stiffness and correlation length, or spin gap, with applied field.

III. 1/N APPROXIMATION

The situation in the weak-field regime may be addressed by a $1/N$ expansion[6], which is expected to be appropriate in describing phases with only short-range correlations. The staggered spin $\mathbf{n}$ is taken to exist in an N-dimensional spin space, in which only the component n_z is selected by the field, and a controlled expansion may be performed in the small parameter $1/N$. The relevant parts of the $O(N)$ action are

$$\mathcal{S}_E = \frac{1}{2g}\int d\mathbf{x}\,\left[(\partial_\mu \mathbf{n})^2 - \bar{b}^2\left(1 - n_z^2\right) - i\lambda\left(\mathbf{n}^2 - 1\right)\right], \tag{3.1}$$

where $\bar{b} = b/c$, and the constraint $\mathbf{n}^2 = 1$ is made explicit with the Lagrange multiplier λ. The saddle-point value of λ is given by

$$\frac{1}{g} = (N-1)\sum_{\mathbf{k}} \frac{1}{\mathbf{k}^2 + i\lambda} + \sum_{\mathbf{k}} \frac{1}{\mathbf{k}^2 + i\lambda + \bar{b}^2}, \tag{3.2}$$

in which the magnetic-field term appears only at $O(1/N)$. The Lagrange field λ functions as a mass, or, equivalently, as a correlation length. Writing the saddle-point solution as $i\lambda = c^2\pi^2/\xi(B)^2$ and carrying out the summation at low temperatures, we obtain an expression analogous to $\rho_s = 0$ emerging from Eq.(2.3),

$$\begin{aligned} 1 = -\frac{g}{2\pi}\ln &\left[\left(\frac{a/\xi}{1 + \sqrt{1 + (a/\xi)^2}}\right)^{N-1}\right. \\ &\times \left.\left(\frac{\sqrt{(a/\xi)^2 + (a/L_m)^2}}{1 + \sqrt{1 + (a/\xi)^2 + (a/L_m)^2}}\right)\right]. \end{aligned} \tag{3.3}$$

In the weak-field regime, $\xi \ll L_m$ and one finds $\xi \simeq (1/2)ae^{2\pi/Ng}[1 + (a^2/8NL_m^2)e^{4\pi/g}]$. This is an $O(1/N)$ correction to the previous result, but there is also a difference of a power of $1/N$ in the exponent. Taking the field derivative, the result $\partial_b(c\pi/\xi)^2 = -2b/N$ ensures that the magnetization contribution from the $\mathbf{k}$ summation terms in F are identically zero to $O(1/N)$. At the same order, the derivative of the constant term $b^2 + c^2\pi^2/\xi^2$ is $2b(1 - 1/N)$. The behavior required of a gapped system is obtained in the weak-field regime on making the well-recognized identification, deduced by comparison with exact renormalization-group results[6], $N \to N-2$. For the $O(3)$ magnet, the magnetization is zero at all fields $B < B^*$. The saddle-point solution for $\xi(B)$, Eq. (3.3), becomes precisely that deduced from Eq. (2.3), and the critical field B^* is the same. Thus, for the $O(3)$ case, we have deduced the expected gapped state, with no breaking of spin rotational symmetry.

For completeness, we note the strong-field results of the $1/N$ treatment. When the magnetic length is small ($L_m \ll \xi$), the correlation length $\xi \simeq (1/2)ae^{2\pi/g(N-1)}(a/L_m)^{1/(N-1)}$ has a direct field dependence. The magnetization is given to leading order by $M \simeq -C + 2bL_m^2/[(N-1)\xi^2]$. The quantity appearing in these expressions is not N but $N-1$, indicating again the lowering of symmetry in the field direction above a finite critical field B^*. However, these expressions are not applicable in the $O(3)$ case. In summary, the spin stiffness and $1/N$ techniques taken together yield a consistent picture at both weak and strong magnetic fields.

IV. RENORMALIZATION-GROUP STUDY

To quantify the regimes of validity of the foregoing analyses, we consider a renormalization-group (RG) approach to the NLsM in an applied field. The action in the form

$$\mathcal{S}_E = \frac{1}{2g}\int d\mathbf{x}[(\partial_\mu \mathbf{n})^2 - \bar{b}^2(1-n_z^2) + 4i\bar{b}n_x\dot{n}_y] \quad (4.1)$$

may be reexpressed in terms of variables ϕ, representing in-plane fluctuations of $\mathbf{n}$, and $\sqrt{g}\sigma_z = n_z$, representing out-of-plane fluctuations. The latter is chosen to facilitate a perturbative expansion in g, which yields

$$\mathcal{L}_E = \frac{1}{2g}\left(A - \bar{b}^2\right) - \frac{1}{2}\sigma_z(-\partial_\mu^2 + \bar{b}^2 - A)\sigma_z + O(g), \quad (4.2)$$

where $A = (\partial_\mu\phi)^2 + 2i\bar{b}\dot{\phi}$ denotes the in-plane terms, which, because $\phi(\tau,x)$ is assumed to vary slowly, can be taken to be a small constant (no fast Fourier modes) in the momentum shell $\gamma\pi/a < |\mathbf{k}| < \pi/a$ ($\gamma \to 1$). By expanding in A, the form of Eq. (4.2) is recovered, but with new coefficients $g(a')$ and $\bar{b}(a')^2$ given by

$$\frac{1}{g(a')} = \frac{1}{g_0} - \mathrm{Tr}'\frac{1}{-\partial_\mu^2 + \bar{b}^2},$$
$$\bar{b}(a')^2 = \bar{b}_0^2 - g_0\mathrm{Tr}'\ln\left(-\partial_\mu^2 + \bar{b}_0^2\right). \quad (4.3)$$

The integrals represented by the partial traces are performed over an isotropic momentum shell $\Lambda_T = \Lambda$ by appeal to the conformally invariant properties in $1+1$ dimensions. Alterations arising from considering instead a rectangular momentum shell should affect only non-universal prefactors. Differentiation with respect to the flow parameter $l = \ln(a'/a)$ leads to the coupled RG equations

$$\frac{dg}{dl} = \frac{g^2}{2\pi}\frac{1}{1+\bar{\beta}^2}, \quad (4.4)$$
$$\frac{d\bar{\beta}^2}{dl} = 2\bar{\beta}^2 - \frac{g^2}{2\pi}\ln\left(1+\bar{\beta}^2\right). \quad (4.5)$$

These represent an extension of the usual RG equations to include a magnetic field B, contained in $\bar{\beta} = a'\bar{b}(a')$. Eq. (4.4) is the conventional "β-equation", the terminology given to the renormalization of the coupling constant, with an additional field term in the denominator. Clearly, a strong field restricts flow to the strong-coupling (disordered) limit, and thus acts to suppresses quantum fluctuation effects, pointing to the "deconfinement of excitations" at suitably high field. Eq. (4.5) expresses the renormalization of the magnetic field according (in the first term) to the dynamical exponent $z = 1$, but with a suppression of this flow at strong coupling. A caveat regarding above RG equations, however, has to be made at this point. The NLsM in the presence of a magnetic field can be expressed as a gauge theory where the field plays the role of a gauge potential[14]. From this it is concluded[14] that the field itself cannot be renormalized, otherwise the gauge invariance would be violated. This conclusion stands in contrast to what we find from our Wilson momentum shell RG treatment in Eq.(4.5), where the second term, $\frac{g^2}{2\pi}\ln(1+\bar{\beta}^2)$, indeed gives a renormalization of the field. This issue deserves further investigation, and it is not clear at the time of writing if such a term would not occur if we used a more systematic field-theoretic renormalization procedure instead. Also, if we take into account the saturation in the NLsM (as discussed further in Sec.V) additional magnetic field terms appear for which the argument[14] based on gauge invariance can not be used. However, since this field renormalization is rather weak anyway, we will ignore this apparent inconsistency in the following discussion. Finally, the RG equations possess a variety of interesting limiting cases, whose detailed study we also defer to a future publication[15]. We concentrate here on the fixed points, in order to obtain a qualitative picture of the RG flow diagram.

Seeking first a fixed point by a weak-field expansion around $\bar{\beta}_* = 0$, we find

$$\frac{dg}{dl} \simeq \frac{g^2}{2\pi}, \qquad \frac{d\ln\bar{\beta}^2}{dl} = 2 - \frac{d\ln g}{dl}, \quad (4.6)$$

which may be solved to yield

$$\frac{g_0}{g} = 1 - \frac{g_0}{2\pi}l, \qquad \bar{\beta} = \bar{\beta}_0 e^l\left(1 - \frac{g_0}{2\pi}l\right)^{1/2}. \quad (4.7)$$

The fixed point $(g_*, \bar{\beta}_*) = (\infty, 0)$ is evidently stable if the flow is stopped at $l_* = 2\pi/g_0$. The system will flow

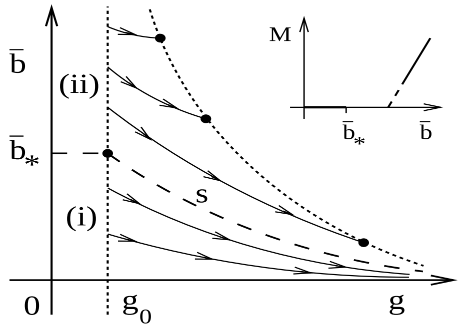

FIG. 4. RG flow diagram for g and $\bar{b}$. Strong- and weak-coupling regimes are separated by separatrix s.

to this strong-coupling regime if the starting value $\bar{\beta}_0$ is sufficiently small. The length scale $\mathcal{L}_* = ae^{l_*}$ at which the flow stops may be compared with the spatial and thermal dimensions (L, L_T) of the system to calculate directly the effects of finite size and temperature[15].

At strong fields ($\bar{\beta} \to \infty$), $dg/dl = 0$, or $g = g_0$, and similarly $d \ln \bar{\beta}^2 = 2dl$, from which it follows that $\bar{b}(l) = \bar{b}_0$, *i.e.* in this regime neither the coupling nor the field is renormalized.

Numerical solution of Eqs.(4.4,4.5) leads to the flow diagram in Fig. 4, which has the following interpretation. The regime (i) of weak initial B-field is the strong-coupling condition, with confinement of (gapped) excitations. Here, the assumption of small g becomes inconsistent, but one may still deduce the critical length scale $\mathcal{L}_*$, and that the magnetization $M = 0$. In this region $O(3)$-symmetry is restored by quantum fluctuations. In contrast, the regime (ii) of strong initial B-field corresponds to weak coupling, where g and $\bar{b}$ are only weakly renormalized. Here, the excitations are deconfined on a length scale $\bar{\xi}(B)$ whose flow is governed by B. In this region, quantum fluctuations are suppressed by the magnetic field, and the broken $O(3)$ symmetry cannot be restored.

The properties of the broken- and unbroken-symmetry phases may be further contrasted by considering the correlation length ξ in each regime. This is a physical quantity and so does not change under the RG flow, whence $d\xi/da' = 0$ and

$$\frac{\partial g}{\partial l}\frac{\partial \xi}{\partial g} + \frac{\partial \bar{\beta}^2}{\partial l}\frac{\partial \xi}{\partial \bar{\beta}^2} + \xi = 0. \tag{4.8}$$

At low fields, we find that $-\partial\xi/\xi \simeq 2\pi \partial g/g$, which has the solution $\xi_0 = \xi e^{2\pi(1/g_0 - 1/g)}$. If one assumes that $\xi \to a$ (the bare lattice constant), as the system flows to the strong-coupling limit ($1/g_0 \to 0$), then $\xi_0 = ae^{2\pi/g_0}$ returns the same, finite physical correlation length as in the previous analyses. For high values of the initial field we have $-2\partial\xi/\xi \simeq \partial\bar{\beta}^2/\bar{\beta}^2$, which leads to the relation $\xi_0 = \xi\mathcal{L}/a$ ($\bar{b}_0$ is invariant) under the RG flow. Thus, for any finite ξ during the flow, the bare correlation length ξ_0 is the system size L or L_T, corresponding to the quasi-long-range order expected of an XY system in one spatial dimension.

Before concluding our RG analysis, we also consider its qualitative predictions for the system magnetization, a measurable quantity. This may be calculated as

$$M = \frac{\tilde{g}\mu_B a}{c}\frac{\partial F}{\partial \bar{\beta}_0} = \frac{\tilde{g}\mu_B a}{c}\left(\frac{\partial \bar{\beta}}{\partial \bar{\beta}_0}\frac{\partial F}{\partial \bar{\beta}} + \frac{\partial g}{\partial \bar{\beta}_0}\frac{\partial F}{\partial g}\right). \tag{4.9}$$

Once again, for weak fields we find that $\partial g/\partial\bar{\beta}_0 = 0$ and $\partial\bar{\beta}/\partial\bar{\beta}_0 = e^l\sqrt{1 - g_0 l/2\pi}$, where the latter expression will introduce the characteristic length scale $\mathcal{L}$ of the short-range correlated phase. Now for any $F(\bar{b})$ analytic in $\bar{b}$,

$$M(B_0) \sim \sqrt{1 - \frac{g_0}{2\pi}\ln\frac{\mathcal{L}}{a}}, \tag{4.10}$$

so the invariant quantity $M(B_0)$ flows to zero as $\mathcal{L} \to \mathcal{L}^*$. The RG framework returns the vanishing of the magnetization in the regime where quantum fluctuations ensure no spontaneous symmetry breaking. At high fields the magnetization is finite, but its saturation in the physical system limits the useful information which can be deduced from the RG approach.

V. COMPARISON WITH EXPERIMENT

We close with a comparison between the preceeding physical ideas and experiments performed on the two-chain, $S = 1/2$ spin ladder material CuHpCl. The magnetization[4] illustrates the transition from the gapped regime of unbroken symmetry, and the nature of the broken-symmetry phase, while nuclear magnetic resonance (NMR) measurements of spin relaxation rates[17] reveal some characteristics of the spin correlation functions in both types of ground state.

The magnetization is represented schematically by

$$M = -\tilde{g}\mu_B N_x N_y (b/4\bar{J}) + M_d + M_f + O(1/S). \tag{5.1}$$

The first term contains contributions linear in B from the quadratic part in Eq. (1.5). M_d represents the effect of the dynamical term in the trace (*cf.* Eq. (2.2)) due to out-of plane (θ) fluctuations of $\mathbf{n}$. M_f arises from in-plane fluctuations ($\dot{\phi}$), and gives rise to a sawtooth form leading to magnetization steps[15], a finite-size effect which will not be considered further here. While the linear term is always present, we have shown that below a threshold field B^*, where the system has a spin gap, it is canceled by the corresponding correlation-length term. Above an upper threshold B_{c2}, the magnetization will saturate at the value $M_s = \tilde{g}\mu_B S N_s$ ($N_s = N_x N_y$). This effect is not contained in the NLsM as presently applied.

In what follows we shall apply M_s as a simple cutoff, but let us first describe parenthetically how saturation may be systematically included in the model by applying a constraint on the total spin[15]. In addition to the

$\mathbf{n}\cdot\mathbf{l}=0$ and the $\mathbf{n}^2=1$ constraints, there is a constraint enforcing conservation of spin. For a field along the z axis, the conserved quantity is $S^z \equiv \langle\{\mathbf{\Omega}\}|\widehat{S}^z|\{\mathbf{\Omega}\}\rangle \to S\int dx\, l^z$, where the continuum limit was taken in the final step. Whereas the first two constraints are purely local, in that they must be enforced at each spacetime point, this final constraint is local in time, but global in space. All constraints are handled in similar fashion — inserting (functional) delta functions into the measure of the propagator:

$$\langle\{\mathbf{\Omega}\}_b|\, e^{-\beta H}\, |\{\mathbf{\Omega}\}_a\rangle \\ = \int \mathcal{D}\mathbf{n}(x,\tau)\int \mathcal{D}\mathbf{l}(x,\tau)\ [\text{constraints}]\, e^{-\mathcal{S}_E[\mathbf{n},\mathbf{l}]}. \quad (5.2)$$

After integrating out the (now constrained) fluctuation field $\mathbf{l}$, as well as all the Lagrange multipliers, one is left with the Euclidean action

$$\mathcal{S}[\mathbf{n}] = \mathcal{S}_{WZ} + \frac{1}{2g}\int d\tau\, dx\, \left[(\partial_x\mathbf{n})^2 + (\partial_\tau\mathbf{n})^2\right] \\ - \frac{1}{2g}\int d\tau\, \frac{(D[\mathbf{n}]+2iN_s\sigma)^2}{A[\mathbf{n}]} - SN_s\beta b\sigma, \quad (5.3)$$

where $D[\mathbf{n}] = \int dx\,(\mathbf{n}\times\dot{\mathbf{n}})_z$ and $A[\mathbf{n}] = \int dx\,(1-n_z^2)$. We also introduced the scaled spin $\sigma = S_z/(SN)$, $-1\le\sigma\le 1$. In this action, the field b appears only as linear coupling to the spin σ, just as in does in ferromagnets, but in marked contrast, for example, to Eqs. (1.5,1.6), where the field played the role of a hard-axis anisotropy. This linear coupling is directly due to the spin constraint. We can recover the previous action, Eq. (1.5), by allowing σ to fluctuate in time, relaxing the condition $|\sigma|\le 1$, and integrating over $\sigma(\tau)$. These steps undo the constraint. In evaluating the partition function, one must use the constrained action, Eq. (5.3), and sum over all degrees of freedom, including all allowed values of $|S_z|\le N_sS$. This procedure limits M to M_s at large fields, and provides a consistent description of the second phase transition which occurs at B_{c2}. For the present purposes, however, we shall not use the spin constraint just outlined, but instead treat saturation as a simple cutoff, particularly since this transition is from an XY phase with strongly suppressed quantum fluctuations to a fully polarized state, and is hence of less interest in the current context.

The contribution from fluctuations in the field direction is given consistently to lowest order in the small parameter c/b, and in limit of low T, by the constant $M_d = \frac{1}{2}N_x\tilde{g}\mu_B$. Next-order corrections from out-of-plane spin excitations have the form $M_d' \sim B\ln(B/\bar{J})$.

Specializing to the parameters of CuHpCl, the exchange constants deduced from magnetization and susceptibility measurements[4,5] are $J'=13.2$K and $J=2.4$K, whence $\bar{J}=13.3$T and $J_x=3.6$T. Taking the simplest case of constant M_d, and the lower critical field B_{c1} for onset where $M(B_{c1})=0$, we obtain $B_{c1}=\bar{J}/\tilde{g}\mu_B = 6.6$T. The saturation field B_{c2} is given from $M(B_{c2}) = M_s$ as $B_{c2} = (4S/\tilde{g}\mu_B)\bar{J} = 13.3$T. These values agree well with a linear extrapolation of the magnetization data at the lowest temperature in Ref. 4, which yields $B_{c1}=6.8$T and $B_{c2}=13.7$T. The computed magnetization is shown in Fig. 5, where the dashed line indicates the validity limit ($|b|\sim\omega_c\equiv c\pi/a$) of the calculation.

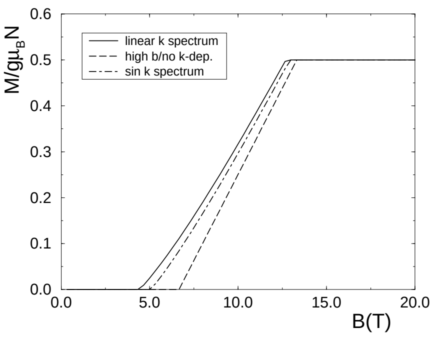

FIG. 5. Computed magnetization for the spin ladder system CuHpCl.

The NLsM prediction of linear magnetization appears closer to the data than a repulsive boson model[13] and other purely 1D approaches[16], which predict square-root cusps at B_{c1} and B_{c2} not evident in the data[4]. This may be indicative of a weak interladder coupling, which also causes the real material to display 3D order at intermediate B and low T. The gradient of the linear region can be written as

$$\chi^{\perp}_{\mathrm{NL}\sigma\mathrm{M}} = \frac{1}{N_s}\frac{N_xN_yS}{4\bar{J}S - 2\bar{J}/N_y} \\ = \chi^{\perp}_{\mathrm{AF}}\left(\frac{1}{1-1/(2N_yS)}\right), \quad (5.4)$$

where $\chi^{\perp}_{\mathrm{AF}} = (\tilde{g}\mu_B)^2/4\bar{J}a^2$ is the Néel susceptibility per unit volume, the result for a classical antiferromagnet. The last term expresses the variation from classical behavior as a function of spin magnitude and the number of coupled chains. That the magnetization adopts such a quasi-classical form in the broken-symmetry regime, at least in systems with no topological term, may be ascribed in part to suppression of quantum fluctuations by the field (effective beyond B_{c1}), and possibly also to the presence of higher-dimensional couplings.

Turning to NMR measurements, the experimental observable is the spin-lattice relaxation rate

$$\frac{1}{\mathrm{T}_1} = \lim_{\omega\to 0}\frac{2k_{\mathrm{B}}T}{\hbar\omega}\int\frac{dq}{2\pi}F_{ij}(\mathbf{q})\chi_{ij}(\mathbf{q},\omega,T), \quad (5.5)$$

which probes the dynamic susceptibility

$$\chi_{ij}(\mathbf{q},\omega,T) = \int d\tau\, dx\, e^{i\omega\tau + i\mathbf{q}\cdot\mathbf{x}} \\ \times\Theta(\tau)\,\langle[S_i(x,\tau),S_j(0,0)]\rangle_T. \quad (5.6)$$

The spin-spin correlation functions may be calculated in the NLsM framework using

$$\langle S_i(x,\tau)S_j(0,0)\rangle = (-1)^x\langle n_i(x,\tau)n_j(0,0)\rangle + (aS)^2\langle l_i(x,\tau)l_j(0,0)\rangle, \quad (5.7)$$

and used to compare the properties of the system at low and high fields.

In the low-field regime where full symmetry is retained, the gap Δ to all spin excitations results in exponentially decaying spin correlations, reflecting the short-range nature of the quantum disordered phase. By simple scaling, this translates to relaxation rates which are exponentially activated in temperature, for T below the characteristic energy scale Δ. This is observed in experiments for fields $B < B_{c1}$[17].

Above the critical field, as we have seen, the gap to XY (ϕ) excitations closes, and $\langle n_z(x,\tau)n_z(0,0)\rangle$ and $\langle l_+(x,\tau)l_-(0,0)\rangle$ depend directly on the gapped, out-of-plane fluctuations in θ, and remain short-ranged. However, $\langle l_z(x,\tau)l_z(0,0)\rangle \propto \partial_\tau^2\langle\phi(x,\tau)\phi(0,0)\rangle$, which leads to a power-law (or "long-ranged") decay of the correlation function parallel to the field direction,

$$\langle S_z(x,\tau)S_z(0,0)\rangle = \frac{A}{2\pi g}\left[\frac{a^2}{(x-i\tau)^2}+\frac{a^2}{(x+i\tau)^2}\right]. \quad (5.8)$$

Similarly, $\langle n_+(x,\tau)n_-(0,0)\rangle = \langle \exp(i\phi(x,\tau)-i\phi(0,0))\rangle$ yields

$$\langle S_+(x,\tau)S_-(0,0)\rangle = B\left(\frac{a^2}{x^2+\tau^2}\right)^{(g/4\pi)}, \quad (5.9)$$

a separate power-law form for the correlation function perpendicular to the field direction, which has a direct dependence on the bare coupling constant. The results for the long-ranged parts of both longitudinal and transverse correlation functions are very similar to those of a Luttinger-liquid description of the gapless, broken-symmetry phase[16]. In addition to the activated form in the gapped regimes at $B < B_{c1}$ and $B > B_{c2}$, the experimental measurements of $1/T_1$[17] show clear power-law divergence in the intermediate regime, fully consistent with expectations based on a model of symmetry breaking by the effect of the field on quantum fluctuations.

The foregoing analysis is not restricted to CuHpCl, but applies to any system with a trivial topological term, and thus exhibiting the physics of the Haldane gap. The primary example is the $S = 1$ AF chain, of which NENP is considered a prototypical case (but for the complication of a large single-ion anisotropy). The present study yields the same qualitative features of a gapped regime with zero magnetization, followed by approximately linear behavior towards saturation (not achieved), as in experiment[2]. Finally, there has been considerable recent interest in the possibility of field-induced magnetization plateaus in certain systems: in the NLsM approach these may be expected, for example in $S > 1$ chains, when the field strength is such that the projected in-plane spin $S\mathbf{n}_\perp$ is of integer amplitude, leading to a gapped phase.

VI. SUMMARY

In conclusion, the nonlinear σ model description of quantum antiferromagnets in an external field provides a versatile framework for illustrating the breaking and restoration of symmetries. The case of $O(3)$ spins has a variety of physical realizations, which illustrate clearly the transition from the gapped, short-range ordered phase where full spin symmetry is maintained by quantum fluctuations, to a gapless, quasi-long-range ordered regime where the $O(3)$ symmetry is reduced to $O(2)$ by the field.

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[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1993); Phys. Rev. Lett. **50**, 1153 (1983).

[2] Y. Ajiro, T. Goto, H. Kikuchi, T. Sakakibara, and T. Inami, Phys. Rev. Lett. **63**, 1424 (1989).

[3] A. Harrison, S. J. Clarke, T. E. Mason, G. J. McIntyre, and D. Visser, J. Magn. Magn. Mater. **104-107**, 557 (1992).

[4] G. Chaboussant, P. A. Crowell, L. P. Lévy, O. Piovesana, A. Madouri, and D. Mailly, Phys. Rev. B **55**, 3046 (1997).

[5] P. R. Hammar, D. H. Reich, C. Broholm, and F. Trouw, Phys. Rev. B **57**, 7846 (1998).

[6] A. M. Polyakov, *Gauge Fields and Strings*, (Harwood, London, 1986).

[7] D. Loss, in Dynamical Properties of Unconventional Magnetic Systems, A.T. Skjeltorp and D. Sherrington (eds.), NATO ASI Series E: Applied Sciences, Vol. 349, 1998 Kluwer Academic Publishers, p. 29-75.

[8] D. V. Kveshchenko, Phys. Rev. B **50**, 380 (1994).

[9] G. Sierra, J. Math. Phys. A **29**, 3289 (1996).

[10] H. J. Mikeska, J. Phys. C **13**, 2913 (1980); A. F. Andreev and V. I. Marchenko, Sov. Phys. Usp. **23**, 21 (1980).

[11] S. Allen and D. Loss, Physica A, **239**, 47 (1997).

[12] D. Loss and D. L. Maslov, Phys. Rev. Lett. **74**, 178 (1995).

[13] Before saturation there is no true long-range order, but the field imposes a quasi-long-range order of the XY-model type: I Affleck, Phys. Rev. B **43**, 3215 (1991).

[14] S. Sachdev, Z. Phys. B 94, 469 (1994).

[15] B. Normand, J. Kyriakidis, and D. Loss, in preparation.

[16] R. Chitra and T. Giamarchi, Phys. Rev. B **55**, 5819 (1997).

[17] G.Chaboussant, Y. Fagot-Revurat, M.-H. Julien, M. E. Hanson, C. Berthier, M. Horvatic, L. P. Lévy and O. Piovesana, Phys. Rev. Lett. **80**, 2713 (1998).