Anisotropic Ferromagnetic Quantum Domains

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We study a model for anisotropic ferromagnetic quantum domain walls. The large degeneracy of the ground state in the extreme anisotropic (Ising) limit, associated with the translational invariance of the "kink center," is lifted in the quantum system in a peculiar way. The critical point, at which the Hamiltonian is invariant under the quantum group U_q [SU(2)], is exactly determined by a cluster method. We also find the ground state wave function at the critical point. Some generalizations of these results for arbitrary spin and dimension are obtained.

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A simple model of a spin-S quantum Heisenberg ferromagnet with a domain wall is given by the spin Hamiltonian

$$\mathcal{H} = -J\sum_{r,\delta}(S_r^x S_{r+\delta}^x + S_r^y S_{r+\delta}^y) - \Delta\sum_{r,\delta} S_r^z S_{r+\delta}^z - h\left(\sum_{r\in F_-} S_r^z - \sum_{r\in F_+} S_r^z\right), \quad (1)$$

where $J > 0$ and $\Delta \geq J$ are exchange parameters, and r is a lattice vector, with a neighbor $r + \delta$, on a d-dimensional cubic lattice of side L. The effective field $h > 0$ represents the interactions of the spins with the boundary surfaces F_+ (F_-) with positive (negative) normal vectors. In one dimension, a fully isotropic ($J = \Delta$) spin-$\frac{1}{2}$ quantum Heisenberg model for a ferromagnetic domain wall has been analyzed in a beautiful paper by Schilling [1]. In a later work by Alcaraz *et al.* [2], the solution of the eigenvalue problem in the presence of the antiparallel boundary fields required a nontrivial generalization of the *Bethe Ansatz*. Real materials, however, usually display some kind of anisotropy, It is therefore of special interest to study the more general case, with $J \neq \Delta$.

In this Letter, we are mainly concerned with the one-dimensional version of (1) with a Hamiltonian given by

$$\mathcal{H}_L = -J\sum_{i=1}^{L-1}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \Delta\sum_{i=1}^{L-1} S_i^z S_{i+1}^z - h(S_1^z - S_L^z). \quad (2)$$

It is instructive to analyze the classical version of (2). The classical candidates to the ground state are the ferromagnetic configuration $\uparrow\uparrow\ldots\uparrow\uparrow$ with energy $E_f = -S^2(L-1)\Delta$, the highly degenerated kink configuration $\uparrow\ldots\uparrow\downarrow\ldots\downarrow$ with energy $E_{\rm kink} = E_f + 2S^2\Delta - 2hS$, and the helical configuration of the form

$$\vec{S}_i = S(0, \sin[(i-1)\theta_n], \quad \cos[(i-1)\theta_n]); \quad i = 1,2,\ldots,L, \quad (3)$$

with step $\theta_n = \pi(2n+1)/(L-1)$, for $n = 0,1,2,\ldots$, and energy

$$E_H = E_f\frac{J+\Delta}{2\Delta}\cos\theta_n - 2hS. \quad (4)$$

At $\Delta = J$, for arbitrary values of h, the ground state is given by the degenerated helical configurations, with $\theta_n \ll 1$. However, for $\Delta > J$, the ground state is the nondegenerate ferromagnetic configuration, if $h < \Delta S$, or the $L - 1$ degenerate kink configuration, if $h > \Delta S$.

For spin $\frac{1}{2}$, in the extreme anisotropic limit $\Delta/J \to \infty$ (Ising limit), Eq. (2) is reduced to the Ising Hamiltonian

$$\mathcal{H}_{I,L} = -\frac{\Delta}{4}\sum_{i=1}^{L-1}\sigma_i\sigma_{i+1} - \frac{h}{2}(\sigma_1 - \sigma_L), \quad (5)$$

where $\sigma_i = \pm 1$, and we reproduce the classical picture with a phase transition, at $h = \Delta/2$, from the ferromagnetic ground state to the $(L-1)$ degenerated kink ground state. In this Ising limit it is easy to use the transfer matrix technique to write the canonical partition function

$$Z_N = \left[2\cosh\left(\frac{\beta\Delta}{4}\right)\right]^L\left\{\frac{\cosh\left(\frac{\beta\Delta}{2}\right) + \cosh(\beta h)}{4\left(\cosh\frac{\beta\Delta}{4}\right)^3}[1 + (\tanh\beta\Delta)^{L-3}] + \frac{1 + \cosh\left(\frac{\beta\Delta}{2}\right)\cosh(\beta h)}{4\left(\cosh\frac{\beta\Delta}{4}\right)^3}[1 - (\tanh\beta\Delta)^{L-3}]\right\}, \quad (6)$$

where β is the inverse of the temperature. For fixed L, in the $\beta \to \infty$ limit, we obtain the energy and the entropy of the ground state. If $h > \Delta/2$, the second term of Eq. (6) gives a nontrivial contribution, and we have the kink energy $E_k = -\Delta(L-1)/4 + \Delta/2 - h$ and entropy $\ln(L-1)$. If $h < \Delta/2$, this second

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term does not contribute, and we have the ground state ferromagnetic energy $E_f = -\Delta(L-1)/4$, in agreement with previous considerations.

How does this picture change in the quantum case? To consider a situation with finite values of Δ, let us make $J = 1$ and concentrate in the $S = \frac{1}{2}$ case. Following Bader and Schilling [3], we write $\mathcal{H}_L$ as a sum over "cell Hamiltonians" including two sites,

$$\mathcal{H}_L^{(1/2)} = \sum_{i=1}^{L-1} \mathcal{H}_i^C, \tag{7}$$

where

$$\mathcal{H}_i^C = -(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) - h(S_i^z - S_{i+1}^z). \tag{8}$$

If E_0^C is the lowest eigenvalue of $\mathcal{H}_i^C$ and E_0 is the ground state energy, we have

$$E_0 \geq (L-1)E_0^C. \tag{9}$$

By the variational principle, as the expectation value of $\mathcal{H}_L$ in the ferromagnetic ground state is given by $-(L-1)\Delta/4$, we have $E_0 \leq -(L-1)\Delta/4$. Also, we have $E_0^C = \min[(\Delta - 2\sqrt{4h^2+1})/4, -\Delta/4]$, from which we see that the ground state is ferromagnetic for

$$h < \tfrac{1}{2}\sqrt{\Delta^2 - 1}, \tag{10}$$

and a lattice of arbitrary size. However, if $h > (\Delta^2 - 1)^{1/2}/2$, a "kink-type" solution is expected. We remark that for $\Delta \longrightarrow \infty$ this agrees with the Ising bound $h > \Delta/2$, while for $\Delta = 1$ agrees with Schilling's result [1] (that is, for $h > 0$, the ground state is of "helical" type, as shown by a generalized *Bethe Ansatz*). This suggests that $h = h_c = (\Delta^2 - 1)^{1/2}/2$ is an exact result for the critical point, as we have indeed been able to check numerically and analytically. It is interesting to remark that in a recent work by Carneiro, de Oliveira, and Wreszinski [4] for a one-dimensional quantum model with competing interactions between first and second neighbors, the Bader-Schilling cluster method [3] yielded the exact location of the phase transition in the ground state with a cell of three sites. In the present case, just two sites were enough. This is rather surprising as we might have anticipated a monotone behavior with cluster size.

It is also surprising that at $h = h_c$ the Hamiltonian is invariant under the quantum group U_q [SU(2)]. This can be seen upon setting

$$h_c = \tfrac{1}{4}(q - q^{-1}) \quad \text{and} \quad \Delta = \tfrac{1}{2}(q + q^{-1}), \tag{11}$$

as suggested in a paper by Pasquier and Saleur [5]. Since q is real ($\Delta > 1$) and hence cannot be a root of unity, the theory of representations of U_q [SU(2)] is essentially equivalent to the theory of U [SU(2)]. In the isotropic case, for $q = 1$, with $h = h_c = 0$, the state $\Omega^f = |\downarrow \ldots \downarrow\rangle$ is a ground state and corresponds to the highest eigenvalue $S(S+1)$, with $S = (L-1)/2$, of the total spin (Casimir operator). Therefore, there exist degenerate states $(S_L^+)^p \Omega^f$, $p = 1, \ldots, (L-1)$, at higher values of $S_L^z = -(L-1)/2 + 1, \ldots, (L-1)$, respectively. Of course, this breaks down for the antiferromagnet, where the ground state, characterized by $S^z = S = 0$, is therefore unique by the Lieb-Mattis theorem [6]. Similarly, for $h = h_c$, and using the Bader-Schilling argument given above, we show that Ω^f is a ground state, with energy

$$E_L = -\left(\frac{q + q^{-1}}{4}\right)\left(\frac{L-1}{2}\right). \tag{12}$$

As in the case $q = 1$, Ω^f lies on the eigenspace corresponding to the highest eigenvalue of the Casimir operator of U_q [SU(2)],

$$C_2(q) = \left[S^z \pm \tfrac{1}{2}\right]^2 + X_\mp X_\pm, \tag{13}$$

where $[2H] = (q^{2H} - q^{-2H})/(q - q^{-1})$, and S^z and $X_\pm$ are the generators of the Lie algebra of U_q [SU(2)] with

$$[S^z, X_\pm] = \pm X_\pm, \tag{14}$$

and

$$[X_+, X_-] = [2S^z]. \tag{15}$$

On each copy of the Hilbert space $\mathbf{C}^{2S+1}$, for a spin quantum number S, the step operator X_+ acts as

$$X_+ = \left\{\frac{[S - S^z][S + S^z + 1]}{(S - S^z)(S + S^z + 1)}\right\}^{1/2} S_+. \tag{16}$$

Using all these facts, it is possible to show that the ground state wave function in each sector $m = \sum_i S_i^z$ is degenerate and given by

$$\Psi_{0,L}^{(m)} = \sum_{\{s\}} q^{\sum_{j=1}^L j s_j} |s_1, s_2, \ldots, s_L\rangle, \tag{17}$$

where $s_i = \pm 1/2$ and $|s_1, s_2, \ldots, s_L\rangle$ is the basis where S^z is diagonal.

In the classical and Ising cases, for $h \geq h_c$, we have an enormous degeneracy due to the position of the kink center. How is this degeneracy lifted in the quantum case? A generalization of an ingenious argument by Schilling [1], which follows an idea of Griffiths [7], may be adapted to the present case. The *Bethe Ansatz* solution [2] for the Hamiltonian (2) gives the eigenenergies in the sectors with $\nu = 0, 1, 2, \ldots,$ down spins,

$$E(\{k_j\}) = -(L-1)\Delta/4 + \sum_{j=1}^{\nu} (\Delta - \cos k_j), \tag{18}$$

where $\{k_j\}$ is the set of roots of the equations

$$e^{i2(L+1)k_j} = \frac{[1 - (\Delta - 2h)e^{ik_j}][1 - (\Delta + 2h)e^{ik_j}]}{[1 - (\Delta - 2h)e^{-ik_j}][1 - (\Delta + 2h)e^{-ik_j}]} \prod_{j \neq l = 1}^{\nu} \frac{B(-k_j, k_l)}{B(k_j, k_l)}, \tag{19}$$

where

$$B(k,k') = (1 - 2\Delta e^{ik'} + e^{i(k+k')})(1 - 2\Delta e^{-ik} + e^{i(k+k')}). \quad (20)$$

For $\Delta \geq 1$ the roots $\{k_u\}$ that minimize the energy (18) are purely imaginary, corresponding to "bound states," because the surface term in Eq. (2) acts like an attractive potential for spin deviations. By making $\rho_\mu = e^{ik_\mu}$, with

$$0 < \rho_1 \leq \rho_2 \leq \cdots \leq \rho_\nu < 1, \quad (21)$$

and defining the variables $(x_1, x_2, \ldots, x_\nu)$ by

$$x_1 = [1 - (\Delta - 2h)\rho_1][1 - (\Delta + 2h)\rho_1],$$
$$x_\mu = \rho_{\mu-1}\rho_\mu + 1 - 2\Delta\rho_\mu, \; \mu = 2, \ldots, \nu \quad (22)$$

we can write Eq. (19) as a fixed-point equation [1]

$$x_\mu = \Omega_{mu}(x_1, \ldots, x_\nu) G_\mu(x_1, \ldots, x_\nu),$$
$$\Omega_\mu(x_1, \ldots, x_\nu) = \rho_\mu^{2L+1}, \quad (23)$$

for $\mu = 1, 2, \ldots, \nu$ and where $G_\mu(x_1, \ldots, x_\nu)$ is independent of L and finite for all $(x_1, x_2, \ldots, x_\nu)$ compatible with (21). The solution of (23) for $L \to \infty$ is $x_\mu = 0$, for $\mu = 1, 2, \ldots, \nu$, which gives

$$\rho_1 = \rho_1^{\pm} = \frac{1}{\Delta \pm 2h}, \; \rho_\mu = \frac{1}{2\Delta - \rho_{\mu-1}};$$
$$\mu = 2, \ldots, \nu, \quad (24)$$

and the energy

$$E_\nu^\infty - E_0^\infty = \sum_{\mu=1}^{\nu} [\Delta - \tfrac{1}{2}(\rho_\mu + \rho_\mu^{-1})]. \quad (25)$$

However, the solution ρ_1^- must be discarded since it contradicts (21) for $h > 0$, and the solution ρ_1^+ is valid for $h > h_c = \sqrt{\Delta^2 - 1}/2$. We can easily see that for $h > h_c$ all individual contributions $\Delta - (\rho_\mu + 1/\rho_\mu)/2$ to the energy (25) are negative for $h > h_c$ and are zero for $h = h_c$. Hence at $h = h_c$ the ground state is L degenerated, and for $h > h_c$ the energy is nondegenerate but decreases with the number of down spins. Hence in the framework of the *Bethe Ansatz,* the degeneracy is lifted and the ground state for $h > h_c$ is in the sector with $\nu = L/2$ down spins. In order to better analyze the lifting of degeneracies let us consider the gaps between the two lowest states in the sectors with ν and $\nu - 1$ down spins,

$$G_{\nu,\nu-1} = E_\nu^\infty - E_{\nu-1}^\infty = \Delta - \tfrac{1}{2}(\rho_\nu + \rho_\nu^{-1}). \quad (26)$$

In the case $\Delta = 1$ we can iterate [1] Eq. (24) and obtain $G \simeq 1/L^2$, for $\nu \simeq L/2$, which is expected since at $\Delta = 1$ the model in massless with a classical dispersion relation $E \sim k^2$. For $\Delta > 1$, from Eqs. (24) and (25), we obtain

$$G_\nu \sim \exp\Big[-2\nu \,\Big|\, \ln\Big(\Delta - \sqrt{\Delta^2 - 1}\Big) \,\Big|\Big], \quad (27)$$

for $\nu \sim o(L/2)$ which shows that the gap vanishes even more quickly than in the case $\Delta = 1$ case. The exponential vanishing is reasonable since now the model is massive. It should be remarked that this behavior resembles the classical degeneracies. However, the sectors with $\nu \sim o(1)$ do not vanish as $L \to \infty$, giving a true lifting of degeneracies in the thermodynamic limit.

To conclude this paper let us present some results for higher spins ($S > \frac{1}{2}$) and higher lattice dimensions ($d > 1$). In both generalizations the model is not exactly integrable anymore, but our numerical results show that a phase transition of the same nature, as in the case $S = \frac{1}{2}$ and $d = 1$, takes place at $h = h_c = S\sqrt{\Delta^2 - 1}$. At $h = h_c$, all the lowest eigenenergies in the U(1) sectors with a given magnetization are degenerated with energy $E_0 = \Delta S^2 (L - 1)^d$, in a similar way as the $U_q(SU(2))$ chain. This result reproduces the classical situation when $\Delta \to \infty$. At $h = h_c$, defining $\Delta = (q + q^{-1})/2$, $h = h_c = S(q - q^{-1})/2$, and inspired by the wave function (17) obtained within the formalism of the quantum group (which does not even exist for $S \neq \frac{1}{2}$ or $d > 1$), we were surprisingly able to guess a form for the groundstate wave function, which turns out to be correct as we can prove using a finite induction method. In the one-dimensional case, for a given sector with $m = \sum_i S_i^z$, we obtain in the S^z basis

$$\Psi_0^{(m)} = \sum_{\{s\}} q^{\sum_{j=1}^{L} j s_j} \prod_{l=0}^{2S} \left[f_l^{\sum_{j=1}^{L} \delta_{s_j, S-l}} \right] |s_1, s_2, \ldots, s_L\rangle, \quad (28)$$

where

$$f_l = \begin{cases} 1 & \text{if } l = 0, \\ \sqrt{\dfrac{(2S)!}{l!(2S - l)!}} & \text{if } l = 1, 2, \ldots, S. \end{cases} \quad (29)$$

In the d-dimensional case the ground state wave functions are given by

$$\Psi_0^{(m)} = \sum_{\{s\}} \prod_r \left[q^{(i_1 + i_2 + \cdots + i_d)s_r} \prod_{l=0}^{2S} f_l^{\delta_{s_r, S-l}} \right] |s_{r_1} s_{r_2} \cdots\rangle, \quad (30)$$

where $r = (i_1, i_2, \ldots, i_d)$. In this last case we can even consider the introduction of different anisotropies Δ^δ and surface fields h^δ for each direction $\delta = 1, 2, \ldots, d$. At $h^\delta = h_c^\delta = S$, we have

$$[(\Delta^\delta)^2 - 1]^{1/2} = S(q_\delta - q_\delta^{-1})/2, \quad (31)$$

and the ground state wave function is given by

$$\Psi_0^{(m)} = \sum_{\{s\}} \prod_r \left[(q_1^{i_1} q_2^{i_2} \cdots q_d^{i_d})^{s_r} \prod_{l=0}^{2S} f_l^{\delta_{s_r, S-l}} \right] |s_{r_1} s_{r_2} \cdots\rangle, \quad (32)$$

The results for higher spins and lattice dimensions indicate that at $h = h_c$ these models have some special hidden symmetry. Following Ref. [8] we can show that for spin $\frac{1}{2}$ but for all dimensions these generalized Hamiltonians describe the asymmetric diffusion in nonequilibrium statistical mechanics [9]. The degeneracies of the ground state in this case are related to the conservation of the number of particles; the probability distribution of particles in the steady state of the lattice with free boundary conditions can be straightforwardly obtained from Eq. (28). A phase transition induced by the boundaries has been predicted in the case of a spin-$\frac{1}{2}$ chain with twisted boundary conditions [10], $S_{L+1}^{\pm} = \rho^{\pm L} S_1^{\pm}$; $S_L^z = S_1^z$, with $\rho \in \mathbf{R}$. However, for $\rho \neq 1$, the corresponding Hamiltonian is non-Hermitian (and hence unphysical), and the boundary conditions are lattice dependent. The present Letter gives the first application of quantum groups to a model with an independent origin in physics (that is, in the physics of magnetism). It also provides an illustration of a physical ground state phase transition induced by a surface term.

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