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O. F. de Alcantara Bonfim
University of Portland, bonfim@up.edu

T. Schneider

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O. F. de Alcantara Bonfim* and T. Schneider
IBM Zurich Research Laboratory, 8803 Rüschlikon, Switzerland
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We study the quantum critical behavior of the one-dimensional, $S=1$ XY model in the presence of a single-ion anisotropy. Using a path-integral approach, we obtain, at $T=0$ and for a positive anisotropy constant, a classical free-energy functional that allows discussion of the critical properties. The rescaling of frequencies is governed by the critical exponent $z=1$. Renormalization-group arguments reveal that at criticality the system belongs to the same universality class as the isotropic $2-d$ XY model.

The ground-state properties of spin chains have been widely studied in the past years; however, the emphasis has been on spin-$\frac{1}{2}$ chains, where in some cases exact solutions are available.[1] Only recently was it realized that properties for integer-spin systems may differ considerably from those with half-integer spins.[1,2] One of the systems presently of great interest[3,4] is the spin-1 anisotropic Heisenberg chain in the presence of a uniaxial symmetry-breaking field, namely,

$$\mathscr{H}=-\frac{1}{2}\sum_{\langle ij\rangle}J_{ij}(S_i^xS_j^x+S_i^yS_j^y+\Delta S_i^zS_j^z)+D\sum_i(S_i^z)^2 \ . \quad (1)$$

Here, the exchange J and single-ion anisotropy D have been chosen to be positive. Examples of current concern are $CsNiF_3$ (Ref. 5) ($\Delta=1$) and compounds like $RbNiCl_3$ and $CsNiCl_3$ (Ref. 6) for $\Delta\neq 1$. The above model with $\Delta=0$ can also be viewed as a truncated version of a quantum coupled rotator [the quantum O(2) model] where only the three lowest states are retained.[7] The two limiting cases for zero and infinite anisotropy have degenerate and nondegenerate ground states, respectively; hence, a phase transition is expected at $T=0$ at a particular value of D. Evidence for such a transition at $D\simeq 0.4$ was given by finite-ring calculations.[3,4,7] Moreover, it has been suggested that in the (D,Δ) plane, including $\Delta=0$, a critical line exists, exhibiting Kosterlitz-Thouless behavior.[3,4] However, these numerical calculations have not been able to identify the nature of this transition unambiguously. In this Rapid Communication, we shall investigate, by using a path-integral approach,[8-10] the quantum critical behavior of the above Hamiltonian for $\Delta=0$, driven to criticality by changes in the single-ion anisotropy parameter D. We show that the universal properties of this transition are equivalent to those of the $2-d$ classical XY model exhibiting a Kosterlitz-Thouless type of phase transition.

We shall separate (1) into two parts, namely,

$$\mathscr{H}=\mathscr{H}_0+V \quad (2)$$

with

$$\mathscr{H}_0=D\sum_i(S_i^z)^2 \quad (3)$$

as the unperturbed Hamiltonian with $D>0$, and for the perturbative part ($\Delta=0$)

$$V=-\frac{1}{2}\sum_{\langle ij\rangle}J_{ij}(S_i^xS_j^x+S_i^yS_j^y) \ . \quad (4)$$

Now, one can write the partition function as

$$Z=\mathrm{Tr}\left[e^{-\beta\mathscr{H}_0}T\exp\left(-\int_0^\beta d\tau\, V(\tau)\right)\right] \ , \quad (5)$$

where T is the "inverse-temperature" ordering which reorders a product of operators from left to right in order of decreasing β. The τ dependence of the perturbation V is given by

$$V(\tau)=e^{\tau\mathscr{H}_0}Ve^{-\tau\mathscr{H}_0} \ . \quad (6)$$

To write the partition function in a convenient form, we make use of the following identity:[10]

$$\exp\left(\frac{1}{2}\sum_{ij}J_{ij}S_iS_j\right)=\mathrm{const}\times\int_{-\infty}^{\infty}\prod_{i=1}^{N}d\phi_i\exp\left(-\frac{1}{2}\sum_{ij}\phi_i(J^{-1})_{ij}\phi_j+\sum_i\phi_iS_i\right) \ , \quad (7)$$

preceded by a discretization of the values of τ in the exponential of (5), that is,

$$\int_0^\beta d\tau\, V(\tau)=\lim_{M\to\infty}\frac{\beta}{M}\sum_{m=1}^{M}V(\beta m/M) \ , \quad (8)$$

which allows the partition function to be written as a functional integral

$$Z=Z_0\int\mathscr{D}X\mathscr{D}Y\exp\left(-\frac{1}{2}\int_0^\beta d\tau\sum_{ij}X_i(J^{-1})_{ij}X_j+Y_i(J^{-1})_{ij}Y_j\right)\left[T\exp\left(\int_0^\beta d\tau\sum_i[S_i^x(\tau)X_i(\tau)+S_i^y(\tau)Y_i(\tau)]\right)\right]_0 \ , \quad (9)$$

where the average is taken with respect to the noninteracting ensemble defined by $\mathscr{H}_0$ (with respective partition function Z_0). The measure of the functional integral is defined as

$$\int\mathscr{D}X=\lim_{M\to\infty}\int_{-\infty}^{\infty}\prod_{i=1}^{N}\prod_{m=1}^{M}dX_i(m\beta/M) \ , \quad (10)$$

and similarly for the Y component. Here, N stands for the total number of spins in the chain. In the present form, we have effectively replaced the original interacting system of quantum spins by a noninteracting one subjected to a τ-independent random field which exactly mimics the interactions of the original system.[11]

The expectation value of (9) may be rewritten in terms of the cumulant averages, again taken with respect to the noninteracting ensemble of $\mathscr{H}_0$; thus

$$Z = Z_0 \int \mathscr{D}X\,\mathscr{D}Y \exp\{-\mathscr{H}_{\text{eff}}[X(\tau),Y(\tau)]\} \tag{11}$$

with the effective Hamiltonian H_{eff} given by

$$\mathscr{H}_{\text{eff}} = \frac{1}{2}\int_0^\beta d\tau \sum_{ij}[X_i(\tau)(J^{-1})_{ij}X_j(\tau) + Y_i(\tau)(J_{ij}^{-1})Y_j(\tau)] - \left\langle T\exp\int_0^\beta d\tau \sum_i [S_i^x(\tau)X_i(\tau)+S_i^y(\tau)Y_i(\tau)]\right\rangle_c , \tag{12}$$

where c stands for cumulant average. The effective Hamiltonian obtained here is the quantum generalization of the classical Landau-Ginzburg-Wilson free-energy functional which is the starting point of the renormalization group devised by Wilson.[12] In this new form, however, the order parameter is τ dependent. The origin of this extra variable can be traced back to the noncommutativity of the quantum-mechanical operators in the original Hamiltonian.

Since we are interested in the critical behavior of the system, we shall keep only the relevant terms of (12), namely,

$$\mathscr{H}_{\text{eff}} = \mathscr{H}_0 + \mathscr{H}_2 + \mathscr{H}_4 + \cdots , \tag{13}$$

where H_0 is the first term of (12), $\mathscr{H}_2$ and $\mathscr{H}_4$ the first two terms obtained by expanding the exponential factor,

$$\mathscr{H}_2 = -\frac{1}{2!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T\{F(\tau_1)F(\tau_2)\}\rangle_c , \tag{14}$$

$$\mathscr{H}_4 = -\frac{1}{4!}\int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_4 \langle T\{F(\tau_1)\ldots F(\tau_4)\}\rangle_c , \tag{15}$$

with

$$F(\tau) = \sum_i [X_i(\tau)S_i^x(\tau) + Y_i(\tau)S_i^y(\tau)] .$$

The cumulant average in (15) is given by

$$\langle T\{F(\tau_1)\ldots F(\tau_4)\}\rangle_c = \langle T\{F(\tau_1)\ldots F(\tau_4)\}\rangle_0 - 3\langle T\{F(\tau_1)F(\tau_2)\}\rangle_0 \times \langle T\{F(\tau_3)F(\tau_4)\}\rangle_0 . \tag{16}$$

A further simplification of (13) is achieved by taking the Fourier transform over the spatial and temperature variables, defined by

$$X_i(\tau) = \frac{1}{\beta}\sum_{\omega_n}\int_k \exp[i(kr_i+\omega_n\tau)]\psi_i^x(k,\omega_n) , \tag{17}$$

where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies. Thus, in the Fourier-Matsubara space one obtains

$$\mathscr{H}_{\text{eff}} = \frac{\beta}{2}\int_q \{[J^{-1}(k) - \beta m_2^{xx}(\omega)][|\psi^x(q)|^2 + |\psi^y(q)|^2] + \mathscr{H}_4 + \cdots\} . \tag{18}$$

Here, $J(k)$ is the Fourier transform of J_{ij}, and the second-order cumulant average $m_2^{\alpha\alpha}$ $(\alpha = x,y)$ is given by

$$m_2^{\alpha\alpha}(\omega_1,\omega_2)\delta_{\omega_1+\omega_2,0} \equiv \frac{1}{\beta^2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 l^{i(\tau_1\omega_1+\tau_2\omega_2)}\langle TS^\alpha(\tau_1)S^\alpha(\tau_2)\rangle_c . \tag{19}$$

This gives

$$m_2^{\alpha\alpha}(\omega) = \frac{2d}{\beta(D^2+\omega^2)}\frac{1-e^{-\beta D}}{1+2e^{-\beta D}}, \quad \alpha = x,y . \tag{20}$$

We have also used the notation

$$q \equiv (k,\omega_n), \quad \int_q \equiv \sum_{\omega_m}\frac{1}{2\pi}\int dk .$$

At $T=0$, the Matsubara frequencies will run over a continuum spectrum; hence, in the limit $\beta \to \infty$ we must replace the sums over ω_n by an integral over ω preceded by a rescaling of the fields[8]

$$\psi^\alpha(q) = \beta^{-1}\phi^\alpha(q), \quad \sum_{\omega_n} \to \beta\int_\omega \equiv \frac{\beta}{2\pi}\int d\omega .$$

Therefore, (18) yields

$$\mathscr{H}_{\text{eff}} = \frac{1}{2}\int_q [J^{-1}(k) - \beta m_2^{xx}(\omega)][|\phi^x(q)|^2 + |\phi^y(q)|^2] - \frac{\beta^3}{4!}m_4^{xxxx}(0)\int_{q_1}\cdots\int_{q_3}\sum_{a,b=x,y}\phi^a(q_1)\phi^a(q_2)\phi^b(q_3)\phi^b(q_4) + \cdots . \tag{21}$$

Here

$$J^{-1}(k) \simeq [J(0)]^{-1} + \frac{J}{J(0)^2}k^2, \quad q_4 = -(q_1+q_2+q_3) , \quad \beta m_2^{xx}(\omega) = \frac{2}{D} - \frac{2}{D^3}\omega^2, \quad \beta m_4^{xxxx}(0) = -\frac{4!}{D^3} .$$

The cumulant m_4^{xxxx} is the fourth-order term analog to (19). We have set the ω dependence on the fourth-order term equal to zero since this is the only relevant part as far as the critical region is concerned. The wave vector k and the Matsubara frequency ω appear in the propagator on the same footing (this gives a dynamical critical exponent $z=1$), allowing the definition of a two-dimensional wave vector $q=(q_x,q_y)$ by suitable rescaling of the frequency and wave vector, namely, $k=[J(0)/J]^{1/2}q_x$ and $\omega=[D^3/2J(0)]^{1/2}q_y$; thus

$$\mathscr{H}_{\text{eff}}=\frac{1}{2}\int_q\left[1-\frac{4J}{D}+q^2\right][|\phi^x(q)|^2+|\phi^y(q)|^2]+\frac{(2J)^2}{D^3}$$
$$\times\int_{q_1}\cdots\int_{q_1}\delta(q_1+q_2+q_3+q_4)[\phi^x(q_1)\phi^x(q_2)\phi^x(q_3)\phi^x(q_4)+2\phi^x(q_1)\phi^x(q_2)\phi^y(q_3)\phi^y(q_4)$$
$$+\phi^y(q_1)\phi^y(q_2)\phi^y(q_3)\phi^y(q_4)] \ , \qquad (22)$$

where the irrelevant multiplicative constants have been absorbed into the fields. The effective Hamiltonian (22) undergoes a continuous transition at the mean-field critical parameter $D/J=4$. It has an O(2) symmetry, and consequently belongs to the same universality class as the two-dimensional classical XY model which presents a Kosterlitz-Thouless type of phase transition.[13,14]

To summarize, using a functional integral approach we studied the critical properties at $T=0$ of a one-dimensional $S=1$ XY model with a single-ion anisotropy. At criticality, the system was mapped into the two-dimensional O(2) model, belonging to the Kosterlitz-Thouless universality class. For the general case, in the presence of the exchange anisotropy [Eq. (1)], we found for small Δ, a critical line with the same critical properties as for $\Delta=0$. The details of these calculations will be given elsewhere.[15] For $S=\frac{3}{2}$ our approach leads to a complex effective Hamiltonian indicating that there is no Kosterlitz-Thouless line.

Finally, we note that our results have important implications for the dynamics as well. In fact, because $z=1$ and at criticality $S_{xx}(q)\sim q^{-1+\eta(D)}$, dynamic scaling implies for small wave numbers q

$$S_{xx}(q,\omega)\sim[\omega^2-\omega^2(q)]^{-1+\eta/2} \ , \qquad (23)$$

where $\omega(q)\sim q^2$ and $\eta=\frac{1}{4}$. This result confirms the $1/s$-expansion expression[16] and extends it to the critical coupling. Moreover, it reveals that for small q values, $S_{xx}(q,\omega)$ probes transition from the ground state to the $\sum_i S_i^z=\pm 1$ continuum and exhibits a singularity along the bottom of this continuum.

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*Permanent address: Departamento de Fisica, Universidade Federal de Pernambuco, Cidade Universitaria, 50,000—Recife, Pernambuco, Brazil.

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