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Critical behavior of the one-dimensional $S=1$ XY model with single-ion anisotropy

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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.\(^2\)\(^3\) One of the systems presently of great interest\(^4\)\(^5\)\(^6\) is the spin-1 anisotropic Heisenberg chain in the presence of a uniaxial symmetry-breaking field, namely,

$$\mathcal{H} = -\frac{1}{2} \sum_{i=1}^{N} J_{i} (S_{i}^{x} S_{i+1}^{y} + S_{i}^{y} S_{i+1}^{x} + \Delta S_{i}^{z} S_{i+1}^{z}) + D \sum_{i} (S_{i}^{z})^{2} .$$

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 double rotor [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 $D=0.4$ was given by finite-ring calculations.\(^3\)\(^4\)\(^7\) Moreover, it has been suggested that in the $(D, \Delta)$ 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,\(^8\)\(^9\)\(^10\) 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,

$$\mathcal{H} = \mathcal{H}_0 + V$$

with

$$\mathcal{H}_0 = D \sum_{i} (S_{i}^{z})^{2}$$

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

$$V = -\frac{1}{2} \sum_{i} J_{i} (S_{i}^{z} S_{i+1}^{z} + S_{i}^{+} S_{i}^{-}) .$$

Now, one can write the partition function as

$$Z = \text{Tr} \left[ e^{-\beta \mathcal{H}_0} T \exp \left( -\int_{0}^{\beta} d\tau \, V(\tau) \right) \right] ,$$

where $T$ is the “inverse-temperature” ordering which reorders a product of operators from left to right in order of decreasing $\beta$. The $\tau$ dependence of the perturbation $V$ is given by

$$V(\tau) = e^{\frac{\beta}{M}} V_{0} e^{-\frac{\beta}{M}} .$$

To write the partition function in a convenient form, we make use of the following identity:\(^10\)

$$\exp \left[ \frac{1}{2} \sum_{i} J_{i} S_{i}^{z} S_{i+1}^{z} \right] = \text{const} \times \int_{-\frac{M}{2}}^{\frac{M}{2}} \prod_{i=1}^{N} d\phi_{i} \exp \left[ -\frac{1}{2} \sum_{i} \phi_{i} (J^{-1})_{i,j} \phi_{j} + \sum_{i} \phi_{i} S_{i}^{z} \right] ,$$

preceded by a discretization of the values of $\tau$ in the exponential of (5), that is,

$$\int_{0}^{\beta} d\tau \, V(\tau) = \lim_{M \to \infty} \sum_{M=1}^{M} V(\beta m/M) ,$$

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

$$Z = Z_0 \int \mathcal{D}X \mathcal{D}Y \exp \left[ -\frac{1}{2} \int_{0}^{\beta} d\tau \sum_{i} X_i (J^{-1})_{i,j} X_j + Y_i (J^{-1})_{i,j} Y_j \right] T \exp \left[ \int_{0}^{\beta} d\tau \sum_{i} [S_{i}^{z} X_i(\tau) + S_{i}^{+} Y_i(\tau)] \right] ,$$

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

$$\int \mathcal{D}X = \lim_{M \to \infty} \int_{-\frac{M}{2}}^{\frac{M}{2}} \prod_{i=1}^{N} \prod_{m=1}^{M} dX_i(\beta m/M) .$$
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 $\tau$-independent random field which exactly mimics the interactions of the original system.\(^\text{11}\)

The expectation value of (9) may be rewritten in terms of the cumulant averages, again taken with respect to the noninteracting ensemble of $K_0$; thus

$$Z = Z_0 \int dX dY \exp[-H_{\text{eff}}(X(\tau), Y(\tau))]$$

with the effective Hamiltonian $H_{\text{eff}}$ given by

$$H_{\text{eff}} = -\frac{1}{2} \int_0^\beta d\tau \sum_i \left[ \langle X_i(\tau) (J^{-1})_i X_i(\tau) + Y_i(\tau) (J^{-1})_i Y_i(\tau) \rangle \right]$$

$$- \left\langle T \exp \int_0^\beta d\tau \sum_i \langle S_i^x(\tau) X_i(\tau) + S_i^y(\tau) Y_i(\tau) \rangle \right\rangle_c,$$

(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.\(^\text{12}\) In this new form, however, the order parameter is $\tau$ 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,

$$H_{\text{eff}} = H_0 + H_2 + H_4 + \cdots,$$

(13)

where $H_0$ is the first term of (12), $H_2$ and $H_4$ the first two terms obtained by expanding the exponential factor,

$$H_2 = -\frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T | F(\tau_1) F(\tau_2) \rangle_{c},$$

(14)

$$H_4 = -\frac{1}{4!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_4 \langle T | F(\tau_1) \cdots F(\tau_4) \rangle_{c},$$

with

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

The cumulant average in (15) is given by

$$\langle T | F(\tau_1) \cdots F(\tau_4) \rangle_{c} = \langle T | F(\tau_1) \cdots F(\tau_4) \rangle_{0} - 3 \langle T | F(\tau_1) F(\tau_2) \rangle_{0} \times \langle T | F(\tau_1) F(\tau_4) \rangle_{0}.$$

(16)

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

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

(17)

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

$$H_{\text{eff}} = \frac{\beta}{2} \int_q \left[ (J^{-1}(k) - \beta m^{F^2}(\omega)) \langle |\psi^x(q)|^2 + |\psi^y(q)|^2 \rangle_{c} + H_4 + \cdots \right].$$

(18)

Here, $J(k)$ is the Fourier transform of $J_0$, and the second-order cumulant average $m^{F^2}(\omega)$ is given by

$$m^{F^2}(\omega_1, \omega_2) = \frac{1}{\beta^2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T | \psi^x(\tau_1) \psi^x(\tau_2) \rangle_{c}.$$  

(19)

This gives

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

(20)

We have also used the notation

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

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 $\omega_n$ by an integral over $\omega$ preceded by a rescaling of the fields$^3$

$$\psi^x(q) = e^{-\beta} \psi^x(q), \quad \sum_{\omega_n} = \beta \int_{-\infty}^{\infty} \frac{1}{2\pi} \int d\omega.$$

Therefore, (18) yields

$$H_{\text{eff}} = \frac{1}{4} \int_q \left[ J^{-1}(k) - \beta m^{F^2}(\omega) \right] \left[ \langle \phi^x(q) \rangle^2 + \langle \phi^y(q) \rangle^2 \right] - \frac{\beta^3}{4!} m^{F^4}(0) \int_q \cdots \int_q \sum_{\alpha=2} \phi^x(q_1) \phi^x(q_2) \phi^y(q_3) \phi^y(q_4) + \cdots.$$  

(21)

Here

$$J^{-1}(k) \equiv [J(0)]^{-1} + \frac{J}{J(0)} k^2, \quad q = -(q_1 + q_2 + q_3), \quad \beta m^{F^2}(\omega) = \frac{2}{D} \frac{2 - 2 D \omega^2}{D^3}, \quad \beta m^{F^4}(0) = -\frac{4!}{D^3}.$$  

The cumulant $m^{F^4}$ is the fourth-order term analog to (19). We have set the $\omega$ 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 \( \omega \) 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, 

\[
k = \left[ J(0)/J \right]^{1/2} q_x \quad \text{and} \quad \omega = \left[ D^3/2 J(0) \right]^{1/2} q_y, \]

thus 

\[
\mathcal{X}_{\text{eff}} = \frac{1}{2} \int \left[ 1 - \frac{4J}{D} + q^2 \right] \left[ |\phi^x(q)|^2 + |\phi^y(q)|^2 \right] + \frac{(2J)^2}{D^3} \times \int q_1 \ldots \int q_4 \delta(q_1 + q_2 + q_3 + q_4) \left[ \phi^x(q_1)\phi^x(q_2)\phi^x(q_3)\phi^x(q_4) + 2\phi^x(q_1)\phi^y(q_2)\phi^x(q_3)\phi^x(q_4) + \phi^x(q_1)\phi^x(q_2)\phi^y(q_3)\phi^x(q_4) \right],
\]

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 \( \Delta \), a critical line with the same critical properties as for \( \Delta = 0 \). The details of these calculations will be given elsewhere.\(^{15}\) For \( S = \frac{1}{2} \) 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 \( S_{\text{xy}}(q) \sim q^{-1+n(D)} \), dynamic scaling implies for small wave numbers \( q \)

\[
S_{\text{xy}}(q, \omega) \sim [\omega^2 - \omega^2(q)]^{-1+n/2}, \tag{23}
\]

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

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\(^2\)For a recent review, see T. Schneider and E. Stoll, IBM Zurich Research Laboratory Report (unpublished), and references therein.


\(^16\)O. F. de Alcantara Bonfim and T. Schneider (unpublished).