THE THERMODYNAMICS OF LINEAR SPIN CHAINS IN A TRANSVERSE MAGNETIC FIELD

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A one-dimensional system of spins ($s = 1/2$) with a strongly anisotropic nearest neighbor interaction and situated in a homogeneous magnetic field directed along a chosen axis is considered. Exact formulas are obtained for the thermodynamic characteristics of such a system. It is shown that at $T = 0$ and for a certain value of the magnetic field strength H_0 the magnetic susceptibility has a singularity of a logarithmic or a fractional power nature. The nature of the singularity as well as the value of the field strength H_0 depends on the ratio between the interaction constants.

1. IN this paper we consider the thermodynamic properties of a spin chain with a strongly anisotropic nearest neighbor interaction. It is assumed that there exists a particular direction along which an effective magnetic field acts on the system. This field can either be external, or it can be a field associated with the anisotropy of the system. The part of the interaction associated with the transverse spin components has the nature of an effective spin-spin interaction. The corresponding Hamiltonian has the form

$$\mathcal{H} = -\sum_l J_{jk} s_l^j s_{l+1}^k - \mu H \sum_l s_l^z, \qquad (1)$$

where s_l is the spin operator at the l-th lattice point (the spin is equal to $1/2$): J_{jk} is the symmetric tensor of the interaction constants associated with the transverse components ($j, k = x, y$); H is the magnetic field; μ is the Bohr magneton.

The Hamiltonian (1) can be diagonalized, and this enables us to obtain exact formulas for the thermodynamic characteristics of the system. The cyclic spin components ($s_l^{\pm} = s_l^x \pm i s_l^y$, $s^z = 1/2 - s_l^- s_l^+$) can be transformed into the Fermi creation and annihilation operators a_l^+, a_l with the aid of the Wigner factor (cf., for example, [1-3]):

$$s_l^- = a_l^+ \prod_{m<l} (1 - 2a_m^+ a_m), \qquad s_l^+ = \prod_{m<l} (1 - 2a_m^+ a_m) a_l. \qquad (2)$$

On substitution of formulas (2) into (1) the Hamiltonian assumes the form

$$\mathcal{H} = -\frac{J_{xx}+J_{yy}}{4} \sum_l (a_l^+ a_{l+1} + a_{l+1}^+ a_l) - \mu H \sum_l \left(\frac{1}{2} - a_l^+ a_l\right) - \left(\frac{J_{xx}-J_{yy}}{4} + \frac{i}{2} J_{xy}\right) \sum_l a_l^+ a_{l+1}^+ - \left(\frac{J_{xx}-J_{yy}}{4} - \frac{i}{2} J_{xy}\right) \sum_l a_{l+1} a_l.$$

Going over to the Fourier transforms of the operators a_l^+ and a_l:

$$a_l = \frac{1}{\sqrt{N}} \sum_\lambda e^{i\lambda l} a_\lambda, \qquad a_l^+ = \frac{1}{\sqrt{N}} \sum_\lambda e^{-i\lambda l} a_\lambda^+,$$

we obtain

$$\mathcal{H} = -\frac{N\mu H}{2} + \sum_\lambda \left(\mu H - \frac{J_{xx}+J_{yy}}{2} \cos\lambda\right) a_\lambda^+ a_\lambda - \frac{i}{4}(J_{xx} - J_{yy} + 2iJ_{xy}) \sum_\lambda a_\lambda^+ a_{-\lambda}^+ \sin\lambda - \frac{i}{4}(J_{xx} - J_{yy} - 2iJ_{xy}) \sum_\lambda a_\lambda a_{-\lambda} \sin\lambda. \qquad (3)$$

Diagonalization of the Hamiltonian (3) is accomplished with the aid of the canonical u,v-transformation:

$$a_\lambda = u_\lambda c_\lambda + v_\lambda^* c_{-\lambda}^+, \qquad a_{-\lambda} = -u_\lambda c_{-\lambda} + v_\lambda^* c_\lambda^+,$$
$$|u_\lambda|^2 + |v_\lambda|^2 = 1. \qquad (4)$$

Going over to the Heisenberg representation for the operators a_λ:

$$a_\lambda(t) = \exp(i\mathcal{H}t/\hbar) a_\lambda \exp(-i\mathcal{H}t/\hbar),$$

we obtain the "equation of motion"

$$\dot{a}_\lambda = \frac{i}{\hbar}\left\{\left(-\mu H + \frac{J_{xx}+J_{yy}}{2}\cos\lambda\right) a_\lambda + \frac{i}{2}(J_{xx} - J_{yy} + 2iJ_{xy}) a_{-\lambda}^+ \sin\lambda\right\}. \qquad (5)$$

Since in terms of the operators c_λ and c_λ^+ the Hamiltonian must be diagonal we have

$$c_\lambda(t) = c_\lambda \exp(-i\varepsilon_\lambda t/\hbar), \quad c_\lambda^+(t) = c_\lambda^+ \exp(i\varepsilon_\lambda t/\hbar),$$

where ϵ_λ is the energy of the corresponding quasiparticle. Taking this into account and substituting (4) into (5) we obtain a system of equations to determine u_λ and v_λ:

$$[-\mu H + {}^1/_2(J_{xx}+J_{yy})\cos\lambda + \varepsilon_\lambda]u_\lambda + {}^1/_2 i(J_{xx}-J_{yy}+2iJ_{xy})v_\lambda \sin\lambda = 0,$$
$${}^1/_2 i(J_{xx}-J_{yy}-2iJ_{xy})u_\lambda\sin\lambda + [-\mu H + {}^1/_2(J_{xx}+J_{yy}) \times \cos\lambda - \varepsilon_\lambda]v_\lambda = 0.$$

From here we have

$$\varepsilon_\lambda = (A_\lambda^2 + |B_\lambda|^2)^{1/2};$$
$$A_\lambda = {}^1/_2(J_{xx}+J_{yy})\cos\lambda - \mu H,$$
$$B_\lambda = i[{}^1/_2(J_{xx}-J_{yy}) + iJ_{xy}]\sin\lambda. \quad (6)$$

Here u_λ and v_λ, apart from a phase factor, are respectively equal to

$$u_\lambda = \frac{|B_\lambda|}{[2\varepsilon_\lambda(A_\lambda+\varepsilon_\lambda)]^{1/2}}, \qquad v_\lambda = -\left[\frac{A_\lambda+\varepsilon_\lambda}{2\varepsilon_\lambda}\right]^{1/2}\frac{|B_\lambda|}{B_\lambda}.$$

We then have

$$\mathcal{H} = -\frac{N\mu H}{2} - \sum_\lambda \varepsilon_\lambda |v_\lambda|^2 + \sum_\lambda \varepsilon_\lambda c_\lambda^+ c_\lambda$$

or

$$\mathcal{H} = \sum_\lambda (c_\lambda^+ c_\lambda - {}^1/_2)\varepsilon_\lambda. \quad (7)$$

Thus, the chain of interacting spins under consideration is reduced to a Fermi gas of noninteracting quasiparticles. Because of this it is possible to evaluate all the thermodynamic quantities. The free energy of the system is, in accordance with (7), equal to

$$F = -T\sum_\lambda \ln\left\{2\operatorname{ch}\frac{\varepsilon_\lambda}{2T}\right\}. \quad (8)^*$$

From this we immediately obtain the expression for the magnetic moment of the system and for its energy

$$M = \frac{1}{2}\sum_\lambda \frac{\partial\varepsilon_\lambda}{\partial H}\operatorname{th}\frac{\varepsilon_\lambda}{2T}, \quad (9)^\dagger$$

$$E = -\frac{1}{2}\sum_\lambda \varepsilon_\lambda \operatorname{th}\frac{\varepsilon_\lambda}{2T}. \quad (10)$$

Since an investigation of the general formulas is too awkward we restrict ourselves to a consideration of three special cases:

a) $J_{xx} = 2J, \quad J_{yy} = J_{xy} = 0;$
b) $J_{xx} = J_{yy} = J, \quad J_{xy} = 0;$
c) $J_{xx} = J_{yy} = 0, \quad J_{xy} = J.$

2. Case a) corresponds to the one-dimensional Ising model with a transverse magnetic field. It should be noted that the problem of ordering in the system discussed by Vaks and Larkin[4] taking quantum effects into account leads to this model.

The energy spectrum in this case, as follows from (6), has the form

$$\varepsilon_\lambda = [(J-\mu H)^2 + 4\mu HJ\sin^2\lambda/2]^{1/2}.$$

As can be seen the energy spectrum has a gap defined by the difference $J - \mu H$. This gap vanishes for $J = \mu H$, and this should lead to singularities in the thermodynamics. It turns out that the magnetic susceptibility has a logarithmic singularity with respect to the parameter $|J - \mu H|/J$ at $T = 0$, viz.:

$$\chi|_{T=0} \approx -\frac{\mu^2 N}{2\pi J}\ln\frac{|J-\mu H|}{J} \quad (|J-\mu H| \ll J).$$

It is curious that the specific heat in the two-dimensional Ising model has the same singularity with respect to the temperature at the transition point in zero magnetic field. In an analogous manner one can obtain

$$\chi|_{\mu H = J} \approx \frac{\mu^2 N}{2\pi J}\ln\frac{J}{T} \quad (T \ll J).$$

Thus, the model under consideration leads to a logarithmic singularity in the magnetic susceptibility at an isolated point ($\mu H = J$, $T = 0$) of the (T, H) plane. But the specific heat has no singularities, and at the same time for $T \ll J$ near the point $\mu H = J$ the quantity $C \approx \pi NT/6J$, while far from this point $C \sim \exp(-|\mu H - J|/T)$.

3. In case b) the energy of the quasiparticle is equal to

$$\varepsilon_\lambda = |J\cos\lambda - \mu H|.$$

Such a dispersion law corresponds to the fact that for $\cos\lambda < \mu H/J$ "particles" are excited with energies $\epsilon_\lambda = \mu H - J\cos\lambda$, while for $\cos\lambda > \mu H/J$ "holes" are excited with energies $\epsilon_\lambda = J\cos\lambda - \mu H$. In the absence of a magnetic field the contributions of the "particles" and of the "holes" to the magnetic moment of the system are equal in absolute value, so that the spontaneous magnetization is equal to zero. For a magnetic field H different from zero ordering of the spins parallel to the field occurs. If at the same time the temperature is equal to zero, then, as follows from formula (9), the magnetic moment is equal to

$$M_0 = \frac{\mu N}{2} - \frac{\mu N}{\pi}\arccos\frac{\mu H}{J}. \quad (11)$$

From this it can be seen that for $\mu H = J$ the quan-

*ch = cosh.
†th = tanh.

tity $M_0 = \mu N/2$, i.e., the magnetization, attains a nominal value, and this is analogous to the classical result for a uniaxial ferromagnet with a negative anisotropy constant.[5] But in our case, in contrast to the classical one, the dependence of $M_0(H)$ is nonlinear.

From expression (11) we obtain

$$\chi_0 = (\mu^2 N / \pi J) [1 - (\mu H)^2 / J^2]^{-1/2},$$

i.e., the magnetic susceptibility at $T = 0$ has a fractional power singularity with respect to the field H at the point $\mu H = J$. We note that the corresponding classical result does not yield a singularity in χ, but only a discontinuity.

For $\mu H = J$ and $T \ll J$, as can be easily shown, the magnetic susceptibility has a fractional power singularity with respect to the temperature:

$$\chi|_{\mu H = J} \approx \mu^2 N / \pi (2JT)^{1/2}.$$

The specific heat, as in case a), has no singularities, and for $T \ll J$ the magnitude of $C|_{H=0} \sim T$, while $C|_{\mu H = J} \sim \sqrt{T}$.

4. Case c) with the dispersion law

$$\varepsilon_\lambda = [(\mu H)^2 + J^2 \sin^2 \lambda]^{1/2}$$

is analogous to case a) with the only difference that the gap disappears at $H = 0$. Therefore the magnetic susceptibility has a logarithmic singularity at the point $H = 0$, $T = 0$.

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