Phase Transitions in Spin Systems at Zero Temperature

V. M. Kontorovich and V. M. Tsukernik

Institute of Radio Physics and Electronics, Academy of Sciences, Ukrainian SSR

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Singularities of thermodynamic quantities in finite quantum spin chains are considered; they occur at points of reorganization of the ground state at $T \to 0$. Transition points with respect to the field correspond to limiting values of the zeros of the partition function on the real axis in the complex H-plane. The variation of the character of a singularity as $N \to \infty$ is investigated.

As is well known, at a temperature other than zero, thermodynamic quantities can have a singularity only in the limit $N \to \infty$ (where N is the number of particles in the system). Yang and Lee[1] related the occurrence of a singularity at $N \to \infty$ to the behavior of the zeros of the partition function as functions of the activity y, considered as a complex variable; this makes the occurrence of a singularity extremely graphic. (In the spin systems considered below, the number of particles N plays the role of the volume, the partition function plays the role of the grand partition function, and the number of excitations plays the role of the number of particles.) For arbitrary finite N, the partition function is proportional to a polynomial in y and has no zeros on the positive real semiaxis in the y-plane. According to Yang and Lee,[1-4] the occurrence of a nonanalytic partition function at $y > 0$ and $N \to \infty$ is due to the approach of at least one of the zeros indefinitely close to the semiaxis $y > 0$.

Singularities can arise also at finite N, if the temperature approaches zero. This possibility follows from the fact that $T = 0$ is a singular point of the function $\exp(-E/T)$. On the other hand, the occurrence of a singularity at zero temperature means simply a nonanalyticity of the energy of the ground state as a function of the external parameters. In this case it is convenient to speak of a phase transition at zero temperature. Such phase transitions are possible also in one-dimensional systems, where they can be followed in detail.

The present paper considers the thermodynamic properties of one-dimensional spin systems with a finite number of particles—the Ising model and the quantum xy-model, in which there is a singularity with respect to the external magnetic field at $T \to 0$. Here it is convenient to follow the behavior of the zeros in the complex H-plane. The character of the singularity in the limiting case $N \to \infty$ can differ significantly from the case of a finite number of spins.[1)]

1. ISING CHAIN WITH ANTIFERROMAGNETIC INTERACTION

Before considering a quantum system, we shall discuss the Ising model. In contrast to the ferromagnetic Ising model, where the zeros of the partition function in the complex plane of the activity $y = \exp(-2H/T)$ are located on the unit circle,[1] for the antiferromagnetic Ising chain the zeros lie on the negative real semiaxis $y < 0$. In fact, the zeros of the partition function

$$Z = \sum_{\{\sigma\}} e^{-\beta\mathcal{H}}, \quad \mathcal{H} = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - H\sum_i \sigma_i \tag{1}$$

can be calculated in closed form[1,2] and can be expressed in the form

$$\begin{gathered} y_m^{\pm} = -1 - 2x_m^2(\lambda-1) \pm [[2x_m^2(\lambda-1)+1]^2-1]^{1/2}, \\ \lambda = e^{-4\beta J}, \quad x_m = \cos\frac{\pi}{2}\frac{2m+1}{N}, \quad m = 0, 1, \ldots \left[\frac{N-1}{2}\right]. \end{gathered} \tag{2}$$

In the antiferromagnetic case ($J < 0$), $\lambda > 1$ and, as is clear from (2), all the zeros are real and negative. For odd N there is a value m_0 for which $x_{m_0} = 0$; this corresponds to $y_{m_0} = -1$ independently of temperature. The other zeros for $T = \infty$ ($\lambda = 1$) are located at the point $y = -1$ and for low temperature ($\lambda \gg 1$) are asymptotically equal to

$$y_m^- \approx -4x_m^2\lambda, \quad y_m^+ \approx -(4x_m^2\lambda)^{-1}. \tag{3}$$

For $T \to 0$, as is clear from (3), the zeros approach indefinitely close to the positive real semiaxis; this implies the possibility of occurrence of a singularity at zero temperature for certain values of the magnetic field. These values coincide with those points on the real axis of the complex H-plane to which the zeros of the partition function tend for $T \to 0$. From the expression (3) we get (see Fig. 1)

$$\begin{gathered} H_m^{\pm} \approx \left(\frac{\pi i}{2} \pm \ln 2|x_m|\right)T \pm 2|J| \quad (x_m \neq 0), \\ H_{m_0} = i\frac{\pi}{2}T \text{ (for odd N)}. \end{gathered} \tag{4}$$

Here a single branch of the logarithm is chosen. Thus for $T \to 0$ the zeros $H_m^{\pm}$ tend to the points $\pm 2|J|$, whereas the root H_{m_0} (for odd N) tends to zero.[2)] These singular points are independent of N. Therefore the character of the singularity (a transition of the first kind with respect to the field) is retained even for $N \to \infty$.

Since the parameter $\beta(H + 2J)$ can be arbitrary, the axymptotic form Z_0 of the partition function near the singular point $T = 0$, $H = 2|J|$ differs from the exact expression[2] only by replacement of hyperbolic functions of H/T by exponential. The relatively compli-

[1)]The research was reported at the Tenth Ural Winter School of Theoretical Physics[5].

[2)]The singularity at $H=0$ for odd N means that the "excess" spin orients itself along an arbitrarily weak field. In the case of the ferromagnetic Ising model, all the zeros in the H-plane tend to zero for $T \to 0$.

cated form of the asymptotic form near a singular point corresponds to the fact that at $T \to 0$, $[N/2]$ of the zeros of the partition function approach indefinitely close to this point.[3)]

2. PHASE TRANSITION IN ONE-DIMENSIONAL QUANTUM SYSTEMS

We consider the simplest exactly solvable spin-model[7-9] (the xy-model) with the Hamiltonian

$$\mathscr{H} = -J\sum_{n}(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) - H\sum_{n=1}^{N} s_n^z \tag{5}$$

where s_n is the spin operator at the n-th site ($s = 1/2$); the sum over n in the first term is carried out over the range 1 to $N-1$ in the case of an open chain and from 1 to N in the case of a closed chain, for which $S_{N+1} = s_1$. The properties of the open and closed chains are significantly different for finite N.

a) The Hamiltonian (5) for an open chain reduces to a quadratic form in the Fermi creation and annihilation operators:

$$\mathscr{H} = -\frac{NH}{2} - \frac{J}{2}\sum_{n=1}^{N-1}(a_n^+ a_{n+1} + a_{n+1}^+ a_n) + H\sum_{n=1}^{N} a_n^+ a_n. \tag{6}$$

The connection of the Fermi with the spin operators is given by the equations[10]

$$a_n = \prod_{m<n} \sigma_m s_n^+, \quad \sigma_m = 1 - 2s_n^- s_n^+,$$

which are invertible.

Diagonalization of the Hamiltonian (6) is accomplished by means of a Fourier sine transformation. As a result, the system reduces to an ideal gas of fermions:

$$\mathscr{H} = \sum_{q=1}^{N} \varepsilon_q a_q^+ a_q - \frac{NH}{2}, \quad \varepsilon_q = H - J\cos k_q, \quad k_q = \frac{\pi q}{N+1}, \tag{7}$$

for which the partition function factors:

$$Z = e^{\beta NH/2}\prod_{q=1}^{N}\{1 + \exp[\beta(J\cos k_q - H)]\}. \tag{8}$$

As is clear from (8), $Ze\exp(-\beta NH/2)$ is a polynomial of the N-th degree in the variable $\exp(-\beta H)$. This property is due, first, to the Fermi character of the spectrum of the system, when the number of states for finite N is finite, and, second, to the fact that the Zeeman energy commutes with the Hamiltonian. The zeros

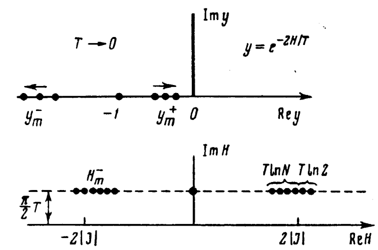

FIG. 1. Location of the zeros of the partition function of an antiferromagnetic Ising chain in the complex plane of the activity y and in the complex plane of the field H, at finite N and at $T \to 0$.

of the partition function in the H-plane have, according to (8), the form (see Fig. 2)

$$H_q = J\cos k_q + i\pi T, \quad q = 1, 2, \ldots, N. \tag{9}$$

For $T \to 0$, the zeros (9) fall on the real axis, at the points $H_q^0 = J\cos k_q$. In contrast to the antiferromagnetic Ising model considered above, where there was a single limiting value for all the roots when $H > 0$, here all the limiting values are different and independent of the sign of J.

On the other hand, at the points H_q^0 there occurs a reorganization of the ground state of the system. In fact, since the energy levels of the system are according to (7) determined by the equation

$$E_{\{n\}} = \sum_q \varepsilon_q n_q - \frac{NH}{2}, \quad n_q = 0, 1,$$

the energy of the ground state is equal to

$$E_0 = \sum_{H<J\cos k_q}(H - J\cos k_q) - NH/2. \tag{10}$$

Hence it is clear that with increase of the field, a reorganization of the ground state occurs at points where ϵ_q vanishes. The corresponding term in the sum (10) disappears, and the magnetization increases discontinuously by unity.

Thus for finite N, we are dealing with a system of "phase transitions" of the first kind with respect to the field at $T = 0$. Near each of the transition points, it is possible to separate out a singular part of the thermodynamic quantities, for which only one of the zeros (9) makes a significant contribution. Thus for the singular part of the susceptibility near $H = H_q^0$ at $\beta \to \infty$ we have

$$\chi_{\text{sing}} = -\frac{\partial^2 F_{\text{sing}}}{\partial H^2} = \beta\frac{\exp[-\beta(H_q^0 - H)]}{\{1 + \exp[-\beta(H_q^0 - H)]\}^2}. \tag{11}$$

Hence[4)] $\chi_{\text{sing}} \to 0$ for $\beta \to \infty$, if $H \neq H_q^0$, and $\chi_{\text{sing}} \sim \beta$ for H_q^0; finally, $\chi_{\text{sing}} = \delta(H - H_q^0)$ in the limit $T = 0$.

For zero temperature and finite N, the susceptibility $\chi(H) = \sum_{q=1}^{N}\delta(H - H_q^0)$. If we compare H to energy and H_q^0 to the energy levels of the system, then $\chi(H)$ corresponds to the density of states. For $N \to \infty$, the relative size of the jump of magnetization at each transition point approaches zero, and the singularity at this point

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3)This is due to a peculiar degeneracy, which is easy to perceive directly in (1). In fact, if we write (1) in the form

$$Z = \sum_{n=-N}^{N} e^{\beta(H+2J)n}\sum_{\Sigma\sigma_i=n}\exp\left[\beta J\left(\sum_i \sigma_i\sigma_{i+1} - 2n\right)\right],$$

then in the inside sum at $T \to 0$ it is sufficient to retain only those terms that correspond to the "ground" state of the Hamiltonian, in the argument of the exponential. For these states (in which all the spins oriented opposite to the field are separated by oppositely directed spins), all terms with $n \geq 0$ must be taken into account simultaneously, since $(\Sigma\sigma_i\sigma_{i+1} - 2n)$ is equal to $(-N)$ for $n \geq 0$ or $-N - 4n$ for $n < 0$. On omitting the small terms with $n < 0$ (a majority of the spins oriented opposite to the field) and on taking into account that the statistical weight of a "ground" state with given n can be directly calculated from combinatorial considerations[6] and is equal to $N(N-k)^{-1}C_{N-k}^{k}$ ($n \equiv N - 2k$, where k is the number of spins directed opposite to the field), we arrive at the asymptotic form Z_0 of the partition function.

4)We note that the points $H = H_q^0$, where χ has singularities, are points of degeneracy of the ground state. This fact is of very general character and is not related to the model.

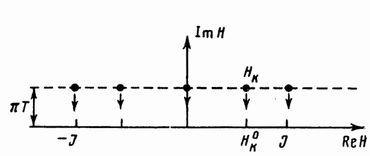

FIG. 2. Zeros of the partition function of a quantum xy-chain in the complex H-plane at $T \to 0$.

disappears. At the band edges for $H = \pm J$ there occurs a square-root singularity in the density of states[9,11] (transition of the second kind with respect to the field):

$$\chi = \pi^{-1}(J^2 - H^2)^{-1/2}, \quad |H| < J, \quad T = 0,$$

The singularity of the susceptibility χ with respect to temperature is retained at $N \to \infty$ only if $H = \pm J$; in this case it changes from linear ($\chi \sim \beta$) to square-root ($\chi \sim \beta^{1/2}$). This result is obtained as a consequence of the fact that inside a band, the fundamental contribution to χ gives a part of the spectrum that is linear with respect to $q - q_0$ in the expansion of $H_q^0 - H$, whereas at the edge it is quadratic.

b) For the closed chain, we shall restrict ourselves to the case of odd N. We transform (5) by introducing the Fermi operators a_n and a_n^+, related to the spin operators as follows:[12]

$$s_n^+ = \sigma_{n+1}\sigma_{n+3} \ldots \sigma_{n-2} a_n, \quad \sigma_k = 1 - 2a_k^+ a_k. \tag{12}$$

Since the Hamiltonian (5) contains products of spin operators s^+ and s^- at neighboring sites, we have with the aid of (12)

$$s_n^- s_{n+1}^+ = -\left(\prod_{k=1}^{N} \sigma_k\right) a_n^+ a_{n+1}.$$

As a result, we arrive at the Hamiltonian

$$\mathscr{H} = \frac{J}{2} \prod_k \sigma_k \sum_{n=1}^{N} (a_n^+ a_{n+1} + a_{n+1}^+ a_n) + H \sum_{n=1}^{N} a_n^+ a_n - \frac{NH}{2} \tag{13}$$

where, except for the common multiplier

$$\prod_k \sigma_k = \exp\left(i\pi \sum_{k=1}^{N} a_k^+ a_k\right)$$

the term with the interaction is quadratic in the Fermi operators.5) On going over to the Fourier form of the operators a_n,

$$a_\mu = \frac{1}{N^{1/2}} \sum_{n=1}^{N} a_n e^{-i\mu n}, \quad \mu \equiv \mu_m = \frac{2\pi m}{N}, \quad m = 0, \pm 1, \ldots, \pm \frac{N-1}{2}, \tag{14}$$

we reduce the Hamiltonian (13) to diagonal form:

$$\mathscr{H} = \sum_\mu [H + (-1)^{\mathfrak{N}} J \cos \mu] a_\mu^+ a_\mu - \frac{NH}{2} \tag{15}$$

Because of the presence of the sign-changing factor $(-1)^{\mathfrak{N}}$, where $\mathfrak{N} = \sum_\lambda a_\lambda^+ a_\lambda$ is the number-of-excitations operator, the spectrum of the closed chain, as is clear from (15), is of Fermi-liquid character. The energy of an elementary excitation depends on the parity of the number of excitations. The latter, obviously, is an integral of the motion of the system.

As follows from (15), the energy of the ground state coincides with the smaller of two energies, each of which is the smallest within the class of states with a given parity of the number of excitations $\mathfrak{N}$:

$$\begin{aligned} E_0 &= \sum_{H + J\cos\mu < 0} (H + J \cos \mu) - \frac{NH}{2}, \quad \mathfrak{N} - \text{even}, \\ E_0 &= \sum_{H - J\cos\mu < 0} (H - J \cos \mu) - \frac{NH}{2}, \quad \mathfrak{N} - \text{odd}. \end{aligned} \tag{16}$$

Each of these states is reorganized with change of field just as in the case considered above of the open chain; at points where the energy of the corresponding elementary excitation vanishes. But, as is clear from (16) and (15), in consequence of the symmetry of the spectrum with respect to replacement of μ by $-\mu$, in contrast to the open chain, in each such reorganization the number of excitations changes by two. But as can be seen from (16), the reorganization of the ground state occurs not at these points, but at points that alternate with them, where the energies with an even and an odd number of excitations become equal and, accordingly, the total spin changes by unity. The values of the field at which reorganization of the ground state occurs are determined by the equation

$$H_k^0 = \pm J \sin \frac{\pi k}{N} \Big/ \cos \frac{\pi}{2N}, \quad k = 1, \ldots, \frac{N-1}{2}. \tag{17}$$

We now consider the partition function of the closed chain. After removal of a multiplier $\exp(NH/2T)$, it becomes a polynomial of degree N in y:

$$Z^{(N)} = Z e^{-\beta NH/2} = \sum_{\mathfrak{N}=0}^{N} y^{\mathfrak{N}} Z_{\mathfrak{N}}, \quad Z_{\mathfrak{N}} = \sum_{\lambda \neq \ldots \neq \nu}^{N} \exp[\beta J (-1)^{\mathfrak{N}} (\cos \lambda + \ldots + \cos \nu)]. \tag{18}$$

By introduction of the quantity $x_\mu = \exp(\beta J \cos \mu)$, this polynomial can be reduced to the form

$$2Z^{(N)} = \prod_\mu (1 + y x_\mu^{-1}) + \prod_\mu (1 - y x_\mu^{-1}) + \prod_\mu (1 + y x_\mu) - \prod_\mu (1 - y x_\mu). \tag{19}$$

The quantities x_μ possess the properties

$$\prod_\mu x_\mu = \prod_\mu x_\mu^{-1} = 1.$$

Hence it is clear that $Z^{(N)}(y)$ is an inverted polynomial:

$$Z^{(N)}(y^{-1}) = y^{-N} Z^{(N)}(y). \tag{20}$$

One of its zeros is $y = -1$:

$$Z^{(N)}(-1) = -Z^{(N)}(-1) = 0$$

(compare the antiferromagnetic Ising chain for odd N). Because of (20), $Z^{(N)}$ (after division by $y + 1$) is a polynomial of degree $(N-1)/2$ in $y + y^{-1}$. Its zeros for $N = 3, 5$ are easy to find. The corresponding values of the complex magnetic field are

5)In the closed chain, application of the transformation[10] would not lead to an expression quadratic in a^+ and a, because of the product $s_N^+ s_1^-$.

$$H_k = \pi i T \quad \pm J + \pi i T \quad (N = 3),$$

$$H_k = \pi i T, \ \pm 2J \sin\frac{\pi}{10} + \pi i T, \quad \pm J + \pi i T \quad (N = 5). \qquad (21)$$

For $T \to 0$ they coincide with those values of the field H_k^0 (see (17)) at which occurs the reorganization of the ground state of the system discussed above, accompanied by a spin inversion. In contrast to the open chain, at these singular points there occurs no vanishing of the energy of an elementary excitation; that is, there are no "critical modes."

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