Scaling relation for phase transitions in a one-dimensional x-y model

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It is shown that in spin chains with interaction containing only transverse components (x-y model) the scaling relations are obeyed (as the exact solution predicts) near the magnetic-field transition point. The correlator of the longitudinal spin components is calculated and it is shown that as the critical point is approached the correlation radius tends to infinity. Critical exponents are found which differ, depending on the symmetry of interaction or, more particularly, on whether or not the total longitudinal spin chain is preserved. In the first case the singularity is a root singularity, the transition point separates states with zero and nonzero gaps, the correlator is independent of the distance in the scale-invariant region and vanishes at the transition point. In the second case (Ising model in a transverse field) the gap vanishes only at the transition point, the singularity is significantly weaker and is logarithmic, the correlation function at the transition point decreases in inverse proportion to the distance, and there is a region in which the scaling relation for magnetization is not valid because of the contribution of the regular part. The scaling relations differ somewhat from the usual ones,[1] since the transition occurs at zero temperature.

1. It is well known that near a second-order phase transition point (critical point) the behavior of a system is determined by the large-scale fluctuations for which the correlation radius tends to infinity as the transition point is approached. This leads to the fact that the characteristic sizes of dimension of length must disappear from the theory when the system is described in a sufficiently small neighborhood of the critical point, when the correlation radius becomes much larger than the interatomic distances. Scaling theory, which is based on this fact, establishes some general relations for the physical quantities near the transition point[1,2].

In view of the absence of a general microscopic theory of phase transitions it is very important to compare the predictions of scaling theory with the results of exactly solvable models[1,2]. Below we shall consider an exactly solvable model in one dimension, describing a spin system with nearest neighbor interaction which does not involve the longitudinal spin components (s^z)—the so-called x – y-model[3]. It is known[4-6] that a singularity of the thermodynamic functions (a magnetic field "phase transition) at zero temperature appears in such a system placed in a homogeneous magnetic field directed along the z axis, for some critical value of the field strength.

In the present paper we show that the exact solution implies that at the transition point the scaling relations are valid. The correlation function of the longitudinal spin components is calculated and it is shown that, as the critical point is approached, the correlation radius tends to infinity, which explains the validity of scaling transformations. We note that since there is no genuine long-range order in the system, this result is far from obvious. The scaling relations differ somewhat from the usual ones[1], since the transition occurs for zero temperature in a one-dimensional system.

2. We list the formulas which will be needed in the sequel. The Hamiltonian of the x – y model has the form

$$\mathscr{H}=-\sum_n J_{jk}s_n^j s_{n+1}^k-\mu H\sum_n s_n^z. \tag{2.1}$$

Here s_n is the spin operator ($s = 1/2$) at the n-th site of the chain, J_{jk} is the two-dimensional tensor of the interaction constants ($j, k = x, y$), H is the external magnetic field along the z-axis and μ is the magnetic moment. It is important that (2.1) can be diagonalized by a transformation from the spin operators s to the fermion creation-annihilation operators c and c^+. This reduces the system to an ideal gas of Fermi-oscillators[4] of energy ϵ_k:

$$\mathscr{H}=\sum_k (c_k^+c_k-1/2)\varepsilon_k, \quad -\pi\leqslant k\leqslant\pi. \tag{2.2}$$

The free energy of the spin chain in the x – y model, calculated from (2.2) is

$$\mathscr{F}=-T\sum_k \ln\{2\,\mathrm{ch}(\varepsilon_k/2T)\}, \tag{2.3}$$

which easily yields expressions for the magnetic moment $M = -\partial\mathscr{F}/\partial H$, susceptibility $\chi = -\partial^2\mathscr{F}/\partial H^2$, and specific heat $C = -T\partial^2\mathscr{F}/\partial T^2$.

In addition to the thermodynamic quantities we shall also be interested in the longitudinal spin correlation function

$$K(r)=\langle s_n^z s_{n+r}^z\rangle-\langle s_n^z\rangle\langle s_{n+r}^z\rangle. \tag{2.4}$$

The z-component of the spin entering here is related to the fermion operators as follows

$$s_n^z=1/2-a_n^+a_n,\quad a_n=\frac{1}{\sqrt{N}}\sum_k e^{ikn}a_k,\quad a_k=u_kc_k+v_k^*c_{-k}^+, \tag{2.5}$$

where u_k, v_k are the coefficients of the u – v-transformation[4], which we shall write out in the limiting cases which concern us.

3. We first consider the phase transition in the isotropic x – y model: $J_{xx} = J_{yy} = J$, $J_{xy} = J_{yx} = 0$. In this case the dispersion law for the ϵ_k has the form

$$\varepsilon_k=|\mu H-J\cos k|, \tag{3.1}$$

and for $\mu H \leq J$ the spectrum (3.1) contains a nonanalytic point k_0:

$$k_0=\arccos(\mu H/J), \tag{3.1'}$$

where the excitation energy vanishes.

This singularity in the spectrum leads to square-root singularities[4] in the susceptibility both with respect to the field-strength and with respect to the temperature at the point $H = H_{cr} = J/\mu$, $T = 0$. We note that for nonzero temperature the singularities disappear from the physical quantities. The nominal magnetization is attained at the transition point (for $T = 0$). In dimensionless variables h, τ describing the deviations from the critical values of the field and temperature:

$$h = \frac{H_{cr} - H}{H_{cr}}, \quad \tau = \frac{T}{J}, \quad H_{cr} = \frac{J}{\mu}, \tag{3.2}$$

the critical point has the coordinates $h = 0$, $\tau = 0$. Omitting numerical coefficients we obtain, for small positive h and τ, from (2.3) and (3.1) the following formulas which define the critical exponents:

$$\begin{gathered} C \sim \tau^{-\alpha} \equiv \tau^{1/2}; \quad h/\tau \to 0; \\ M \sim \tau^{\beta} \equiv \tau^{1/2}, \quad h/\tau \to 0, \quad M \sim h^{1/\delta} \equiv h^{1/2}, \quad \tau/h \to 0; \\ \chi \sim \tau^{-\gamma} \equiv \tau^{-1/2}, \quad h/\tau \to 0, \quad \chi \sim h^{-\lambda} \equiv h^{-1/2}. \quad \tau/h \to 0. \end{gathered} \tag{3.3}$$

We now turn to a computation of the correlation function K(r). Using the coefficients of the u − v transformation, which in the isotropic case are equal to

$$u_k = \begin{cases} 0, & |k| < k_0 \\ 1, & |k| > k_0 \end{cases}, \quad v_k = -v_{-k} = \begin{cases} 1, & 0 < k < k_0 \\ 0, & k_0 < k \end{cases} \tag{3.4}$$

we obtain from (2.4), (2.5)

$$K(r) = -\frac{1}{\pi^2}\left[\int_0^{\pi} d\lambda \frac{\cos\lambda r}{\exp\{\varepsilon_\lambda T^{-1}\,\mathrm{sign}(\lambda - k_0)\} + 1}\right]^2. \tag{3.5}$$

For $T = 0$ the correlation function reduces to the simple expression

$$K(r, \tau = 0) = -\frac{1}{\pi^2}\frac{\sin^2 k_0 r}{r^2}. \tag{3.6}$$

From here it can be seen that the role of the correlation radius is played by the quantity $r_c = 1/k_0$. Far from the critical point this quantity is of the order of unity, i.e., the correlation radius is of the order of the interatomic distances. As the critical point is approached the correlation radius tends to infinity acord ing to (3.1′), behaving like $h^{-1/2}$:

$$r_c \sim h^{-1/2} \quad (\tau = 0). \tag{3.7}$$

At distances smaller than the correlation radius ($k_0 r \ll 1$) the correlation function does not depend on r and according to (3.6) decreases for distances $k_0 r \gg 1$. Thus, in the immediate vicinity of the critical point $H_{cr} = J/\mu$ one should expect the scaling relations to be valid in view of the fact that the correlation radius tends to infinity. We note, however, that since our system is one-dimensional, it will not exhibit a genuine long-range order. This manifests itself in the fact that at the same time as the correlation radius tends to infinity, the correlation function itself tends to zero.

We now consider the temperature dependence of the correlation radius. For $h = 0$ and small τ the integral (3.5) gets a considerable contribution from small λ and, as can be seen from (3.1) and (3.5), the quantity $r_c = \tau^{-1/2}$ becomes a characteristic distance, which one is entitled to consider as a correlation radius in this case. For $r \gg r_c$ the correlation function does not depend on r and has the form $K(r, h = 0) = -\tau/\pi^2$; for $r \gg r_c$ it decreases as the reciprocal square of the distance. Thus, the values of the critical exponents μ and ν which appear in the scaling relations, are

$$\begin{gathered} r_c \sim \tau^{-\mu} = \tau^{-1/2} \quad (h/\tau \to 0), \\ K(r) \sim r^{-\nu} = r^0 \quad (r \ll r_c,\ h, \tau \to 0). \end{gathered} \tag{3.8}$$

4. Let us compare the results we have obtained with scaling theory. We cannot use the results of[1] directly for the critical exponents, since those results have been obtained under the assumption that $T_c \neq 0$ and $K(r) \neq 0$ at $\tau = 0$, $h = 0$. However, for $T_c = 0$ the temperature factors in the expressions for the free energy and heat capacity contribute to the singular part. The vanishing of the correlation function at the transition point also leads to a change of the relations between the critical exponents. Indeed, the following expression for K(r) is a consequence of scale invariance[1]:

$$K(r) = r^{-2(d-x)} g(\tau r^y, h r^x),$$

where x, y are the coefficients of Kadanoff's scale transformation, g is an arbitrary function, which tends to a nonvanishing constant for $\tau \to 0$ and $h \to 0$, according to the condition $K(r) \neq 0$ at the transition point, whence $\nu = 2(d - x)$. In our case, on the contrary, such a behavior of g is impossible, and it follows from the condition $\nu = 0$ that $g(\tau r^y, 0) \sim (\tau r^y)^{2(d-x)/y}$, $\tau \to 0$, $r \ll r_c$, leading to the following asymptotic behavior of the correlation function

$$K(r \ll r_c) \sim \tau^{2(d-x)/y}, \quad \tau \to 0, \quad h = 0. \tag{4.1}$$

Taking these remarks into account, we are led to the following relations between the critical exponents:

$$\begin{aligned} &1)\ \alpha + \beta + \beta\delta = 1, && 3)\ \mu d = -\alpha, \\ &2)\ \beta\delta = \beta + \gamma, && 4)\ \gamma = \mu d - 2\beta + 1. \end{aligned} \tag{4.2}$$

The relations 1) and 3) of (4.2) differ from the usual ones[1] because of the vanishing transition temperature, and the relation 4) has been obtained making use of Eq. (4.1).

It is easy to see that in the case of the isotropic model the critical indices (3.3) and (3.8) satisfy the relations (4.2) and the model under consideration belongs to the systems for which scaling theory is valid.

5. In the isotropic x − y model considered above, the total spin (and accordingly, the Zeeman component) commutes with the Hamiltonian. Therefore the nominal magnetization was reached for a finite value of the magnetic field, equal to the critical field.

In the anisotropic x − y model ($J_{xx} \neq J_{yy}$) the total spin is no longer a constant of the motion. Therefore the value of the nominal magnetization in the ground state cannot correspond to finite values of the magnetic field and is reached asymptotically for $H \to \infty$. The transition point corresponds to an inflection point on the curve H(M), the singularity in the susceptibility is weakened considerably compared to the isotropic case and has a logarithmic character only.

We consider the simplest case $J_{xx} = 2J$, $J_{yy} = J_{xy} = 0$, i.e., the "Ising model in a transverse field." According to[4] the energy of the quasiparticles (2.2) is then equal to

$$\varepsilon_k = [(J - \mu H)^2 + 4\mu HJ \sin^2(k/2)]^{1/2}. \tag{5.1}$$

Both for $\mu H < J$ and for $\mu H > J$ there is a gap in the spectrum, a gap which vanishes at the critical point $H_{cr} = J/\mu$, which leads to the appearance of the singularities. Small values of k, for which

$$\varepsilon_k \approx J\sqrt{h^2 + k^2} \quad (k \to 0). \tag{5.2}$$

contribute to the singular parts of the thermodynamic quantities. For small h and τ we obtain with the help of (2.3) and (5.2) expressions which determine the critical exponents of the heat capacity and of the susceptibility (cf. (3.3)):

$$\begin{gathered} C \sim \tau, \quad h/\tau \to 0, \quad \alpha = 1; \\ \chi \sim \ln\tau, \quad h/\tau \to 0, \quad \gamma = 0; \quad \chi \sim \ln h, \quad \tau/h \to 0, \quad \lambda = 0. \end{gathered} \tag{5.3}$$

We now analyze the behavior of the magnetization near the critical point. For the deviation $\mathscr{M}$ of the magnetic moment from its value at the critical point we obtain from (5.1) and (2.3)

$$\mathscr{M} \sim h \ln h, \quad \tau/h \to 0, \quad \delta = -1;$$
$$\mathscr{M} \sim h \ln \tau + \tau^2, \quad h/\tau \to 0. \qquad (5.4)$$

The expression for $\mathscr{M}$ as $h/\tau \to 0$ does not in general have the form required by the scale transformations, owing to the absence of a substantial contribution of the regular part of the magnetization for small h. One may not exclude this part of the magnetization, and for $h/\tau \to 0$ it yields the main contribution to $\mathscr{M}$. Such a power-law temperature behavior of $\mathscr{M}$ is a consequence of the vanishing of the energy gap at the critical point. Thus, the scaling relations are not applicable (in that part where they involve the exponent of the magnetization) for $h < \tau^2/\ln \tau$. Outside that region (in the (h, τ) plane) the scaling transformation is valid, and $\mathscr{M}$ can be represented in the form

$$\mathscr{M} \sim \tau \ln \tau f(h/\tau), \quad 1 \gg h/\tau \gg \tau/\ln \tau, \quad f(x) = x, \quad \beta = 1, \qquad (5.5)$$

which determines the exponent $\beta = 1$. Thus, it can be seen that the scaling relations (4.2) are valid if the thermodynamic quantities of the one-dimensional system 1) and 2) are satisfied (outside the region $h < \tau^2/\ln \tau$).

Let us now turn to the correlation functions.

Owing to the noncommutativity of the total spin with the Hamiltonian, the magnetic susceptibility has, as can be seen, the following form

$$\chi = \sum_r \overline{K}(r), \quad \overline{K}(r) = \int_0^{1/T} K(r,t)\,dt, \qquad (5.6)$$

where

$$K(r,t) = \langle s_n^z(t) s_{n+r}^z(0)\rangle - \langle s_n^z(t)\rangle\langle s_{n+r}^z(0)\rangle,$$
$$s_n^z(t) = e^{\mathscr{H}t} s_n^z e^{-\mathscr{H}t}. \qquad (5.7)$$

Comparing (5.6) with the corresponding formulas of the phenomenological scaling theory[1,7], we see that the role of the correlation function must in general be played by the quantity $\overline{K}(r)$. Using the expression (2.5) we obtain

$$K(r,t) = \frac{1}{N^2} \sum_{\lambda,\mu} \{[|u_\lambda|^2 n_\lambda e^{\varepsilon_\lambda t} + |v_\lambda|^2 (1-n_\lambda) e^{-\varepsilon_\lambda t}]$$
$$\times [|u_\mu|^2 (1-n_\mu) e^{-\varepsilon_\mu t} + |v_\mu|^2 n_\mu e^{\varepsilon_\mu t}] - u_\lambda^* v_\lambda v_\mu^* u_\mu [(1-n_\lambda) e^{-\varepsilon_\lambda t} - n_\lambda e^{\varepsilon_\lambda t}]\cdot$$
$$\times [n_\mu e^{\varepsilon_\mu t} - (1-n_\mu) e^{-\varepsilon_\mu t}]\} e^{i(\lambda-\mu) r}, \qquad (5.8)$$

where n_k is the Fermi distribution of quasiparticles of energy ϵ_k. For T = 0 this implies

$$\overline{K}(r) = \frac{2}{N^2} \int_0^\infty dt \sum_{\lambda,\mu} \{|v_\lambda|^2 |u_\mu|^2 + u_\lambda^* v_\lambda v_\mu^* u_\mu\} e^{-(\varepsilon_\lambda + \varepsilon_\mu) t} e^{i(\lambda-\mu) r}. \qquad (5.9)$$

In the case under consideration (the Ising model in a transverse field), using the general equations for the coefficients of the u – v transformation[4], we obtain

$$|u_\lambda|^2 = \frac{1}{2}\left(1 + \frac{\mu H - J\cos\lambda}{\varepsilon_\lambda}\right), \quad |v_\lambda|^2 = \frac{1}{2}\left(1 - \frac{\mu H - J\cos\lambda}{\varepsilon_\lambda}\right),$$
$$u_\lambda^* v_\lambda = i\frac{J\sin\lambda}{2\varepsilon_\lambda}. \qquad (5.10)$$

At distances which are large compared to the interatomic distances, $r \gg 1$, we have an explicit expression for the quantities $K(r, t)$

$$K(r,t) \approx \left(\frac{h}{2\pi}\right)^2 [K_1^2(h\sqrt{(Jt)^2 + r^2}) - K_0^2(h\sqrt{(Jt)^2 + r^2})], \quad \tau = 0, \; r \gg 1 \qquad (5.11)$$

in terms of the modified Bessel functions $K_\nu(z)$ (Bessel functions of imaginary argument), which have the following expressions in terms of the Hankel functions

$$K_\nu(z) = {}^1/_2 \pi i e^{i\pi\nu/2} H_\nu^{(1)}(iz).$$

From here, making use of the asymptotic behavior of the functions $K_0(z)$ and $K_1(z)$[8], it is easy to see that for $r \gg r_c = 1/h$, the "correlation" $\overline{K}(r)$ decreases exponentially with the distance, and for $r \ll r_c$ the principal contribution to $\overline{K}(r)$ comes from the singularity of the function $K_1(x)$, which for small x behaves like $1/x$:

$$K_1(x) = \frac{1}{x} + \frac{x}{2}\ln x + \ldots \quad (x \ll 1).$$

We finally arrive at the following behavior of the correlation function $\overline{K}(r)$: it decreases exponentially with the distance for $r \gg r_c = 1/h$ and behaves like r^{-1} if $r \ll r_c$:

$$\overline{K}(r) \propto \begin{cases} 1/r^\nu = 1/r, & 1 \ll r \ll r_c \\ r^{1/2} e^{-2hr}, & r \gg r_c \end{cases}; \quad r_c = 1/h, \quad \tau = 0. \qquad (5.12)$$

From here it can be seen that r_c plays the role of a correlation length, which tends to infinity like h^{-1} for $h \to 0$. In distinction from the isotropic model $\overline{K}(r)$ does not vanish at the transition point:

$$\overline{K}(r) \sim 1/r, \quad 1 \ll r, \quad h = \tau = 0, \qquad (5.13)$$

and its slow decrease leads to the logarithmic singularity of χ. From the general expression (5.8) it is not hard to see that the dependence of the correlation radius on τ for $h = 0$ has the form

$$r_c \sim 1/\tau^\mu = 1/\tau \quad (h = 0). \qquad (5.14)$$

Such a dependence on τ is determined by the linear character of the dispersion law of ϵ_k for small k at h = 0 (5.2), in the same manner as the square root variation of the correlation length in the isotropic case was determined by the quadratic dependence of ϵ on k at the critical point.

In connection with the fact that at the transition $\overline{K}(r) \neq 0$ the usual scaling relation for the exponent ν[1] holds (cf. supra, Sec. 4)

$$\gamma = \mu(d - \nu). \qquad (5.15)$$

Thus, the relations of scaling theory for the anisotropic chain differ from (4.2) in that the equality 4) is replaced by (5.15). As can be seen from what was said above, these relations are valid also in the case of the Ising model in a transverse field, in agreement with the fact that the correlation radius tends to infinity.

We call attention to the difference of the character of the transition with respect to the magnetic field in the isotropic and anisotropic x – y models. In the first case the transition point separates states (phases) with vanishing and nonzero gaps, which can be used to characterize each of the phases (i.e., as an order parameter). In the second case the gap vanishes only at one point (the critical point).

In conclusion we note that in the x – y model the scale invariance of the pair-correlation functions leads automatically to scale invariance of the "many-particle" correlations of the form $\langle s_n^z s_m^z \ldots s_p^z \rangle$, since the latter can always be reduced to products of pair-correlations. This is a consequence of the quadratic nature of the Hamiltonian of the x – y model when expressed in terms of Fermi-operators. Thus the model we have discussed belongs to the systems to which scaling is applicable.

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122