LINEAR NONUNIFORM SPIN CHAIN IN A TRANSVERSE MAGNETIC FIELD

R. O. ZAĬTSEV

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The magnetic susceptibility of a one-dimensional chain of spin 1/2 atoms located in a transverse magnetic field is calculated. The exchange interaction is anisotropic and depends on the cell number in a random fashion. Impurity atoms possess an extremely low mobility and hence the results can be expressed in terms of the distribution function of the square of the exchange interaction. It is shown that the special features of the magnetic susceptibility of an ideal chain become less pronounced, but under certain conditions new features arise which are related to the specifics of the spectra of one-dimensional disordered systems. No singularities in the specific heat are observed in this case.

INTRODUCTION

THE problem of the behavior of an ideal (impurity-free) chain of atoms with spin 1/2 was solved by Pikin and Tsukernik[1] for two limiting cases: 1) the interaction between the spin components that are transverse to the direction of the magnetic field differs from zero, and the interaction between the longitudinal component is equal to zero (x-y model in a transverse field), and 2) the magnetic field is transverse to the chain, and the spin projections along the chain interact (the one-dimensional Ising model in a transverse field). We assume that the exchange interaction is a random function of the number of the atom in the chain. This corresponds physically to a situation in which different spinless impurity atoms are placed randomly between the atoms and alter the value of the exchange integral. We assume that the relaxation times of the impurity atoms are so large that their distribution is thermodynamically not in equilibrium, but is determined by a certain specified distribution function. If the impurity atoms are different, then the distribution function of the square of the exchange interaction $G(\lambda)$ ($\lambda = J^2$) can be specified in place of the distribution function of these atoms.

In the limiting cases considered in[1], a connection can be established between the magnetic susceptibility and the function G. For special distribution laws $G(\lambda)$ it is possible to find an explicit expression for the magnetic susceptibility. Of greatest interest are fields of the order of J/μ (J^2 is the mean squared exchange interaction and μ is the Bohr magneton), when the susceptibility of the ideal lattice becomes infinite. In such fields, the susceptibility of a weakly non-ideal chain has a maximum that vanishes in the opposite limit of a strongly disordered system. The strongly disordered x-y model has a new singularity in weak fields and at low temperatures. This singularity is connected with the anomalously high density of states of the one-dimensional chain in the region of low frequencies[3].

1. x-y MODEL IN TRANSVERSE FIELDS

Using the notation of[1], we write down the Hamiltonian

$$\mathcal{H} = -\sum_k J_k(s_k^x s_{k+1}^x + s_k^y s_{k+1}^y) - \mu H\sum_k s_k^z. \qquad (1)$$

According to[1,2], the spin operators are expressed in terms of the fermion field operators a_k and a_k^+:

$$s_k^x + is_k^y = \prod_{m<k}(1-2a_m^+a_m)a_k, \quad s_k^x - is_k^y = a_k^+\prod_{m<k}(1-2a_m^+a_m),$$
$$s_k^z = {}^1/_2 - a_k^+a_k.$$

As a result, (1) is transformed into the Hamiltonian of an ideal Fermi gas with random parameters

$$\mathcal{H} = -{}^1/_2\sum_k J_k(a_k^+a_{k+1} + a_{k+1}^+a_k) - \mu H\sum_k({}^1/_2 - a_k^+a_k). \qquad (2)$$

We define in the usual manner the Green's function

$$G_{n,k}(\tau_1,\tau_2) = -\langle T(a_n(\tau_1)\bar{a}_k(\tau_2))\rangle.$$
$$a_k(\tau) = e^{\tau\mathcal{H}}a_k e^{-\tau\mathcal{H}}, \quad \bar{a}_k(\tau) = e^{\tau\mathcal{H}}a_k^+e^{-\tau\mathcal{H}}. \qquad (3a)$$

It is easily seen that the average magnetic moment at a given temperature is expressed in terms of the Green's function

$$M = \frac{\mu}{N}\sum_k\left\langle\frac{1}{2} - a_k^+a_k\right\rangle = \frac{\mu}{2N}\sum_k\langle a_ka_k^+ - a_k^+a_k\rangle$$
$$= -\frac{\mu}{2N}\sum_k[G_{k,k}(\tau+0,\tau) + G_{k,k}(\tau,\tau+0)]. \qquad (3b)$$

We write down the equations of motion for the operators a and a:

$$\dot{a}_k(\tau) = {}^1/_2J_ka_{k+1}(\tau) + {}^1/_2J_{k-1}a_{k-1}(\tau) - \mu Ha_k(\tau),$$
$$-\dot{\bar{a}}_k(\tau) = {}^1/_2J_k\bar{a}_{k+1}(\tau) + {}^1/_2J_{k-1}\bar{a}_{k-1}(\tau) - \mu H\bar{a}_k(\tau). \qquad (4)$$

It is convenient to make the canonical transformation

$$a_k(\tau) = e^{-\mu H\tau - ik\pi/2}b_k(\tau), \quad \bar{a}_k(\tau) = e^{\mu H\tau + ik\pi/2}\bar{b}_k(\tau).$$

For the operators b we have the following equations:

$$\dot{b}_k(\tau) = -{}^1/_2iJ_kb_{k+1}(\tau) + {}^1/_2iJ_{k-1}b_{k-1}(\tau),$$
$$\dot{\bar{b}}_k(\tau) = -{}^1/_2iJ_k\bar{b}_{k+1}(\tau) + {}^1/_2iJ_{k-1}\bar{b}_{k-1}(\tau). \qquad (5)$$

We introduce the notation $\overline{J_k^2} = 4E^2$, $\lambda_k = J_k^2/4E^2$ (the bar denote averaging with a specified distribution function). Then the solution of (5) takes the form

$$b_k(\tau) = \sum_\nu e^{-E\omega_\nu\tau}\psi_\nu(k)c_\nu, \qquad (6)$$
$$\bar{b}_k(\tau) = \sum_\nu e^{E\omega_\nu\tau}\psi_\nu^*(k)c_\nu^+;$$

c_ν and c_ν^+ are the annihilation and creation operators in the state ν; $\psi_\nu(k)$ and ω_ν are the eigenfunctions and eigenvalues of the system of equations

$$\omega_\nu \psi_\nu(k) = i\lambda_k^{1/2}\psi_\nu(k+1) - i\lambda_{k-1}^{1/2}\psi_\nu(k-1),$$
$$\lambda_k^{1/2} = \operatorname{sign} J_k \sqrt{\lambda_k}, \quad \bar{\lambda}_k = 1. \tag{7}$$

The system (7) coincides with the system of equations for the one-dimensional chain of elastically coupled atoms, which was investigated in detail by Dyson[3]. Assume for simplicity that the number of cells N is odd. Then the system (7) has one zero root, and the remaining roots enter in pairs[3], viz., to each positive eigenvalue there corresponds a negative eigenvalue with complex conjugate eigenfunctions (altogether $(N-1)/2$ pairs of roots). The function $N(\zeta)$ is the fraction of the roots ω_ν for which $\omega_\nu^2 < \zeta$. The quantity $N'(\zeta)\cdot 2\sqrt{\zeta}$ give the density of states.

We express the magnetic moment in terms of $N(\zeta)$. We substitute in the definition (3b) the operators a expressed in terms of the ψ-functions, and then go over in the usual manner[4] to the Fourier representation in terms of the discrete frequencies $\omega_n = \pi T(2n+1)$. As a result we obtain

$$M = -\frac{\mu T}{2N}\sum_{\omega_n, k}[G_{\omega_n}(k,k) + G_{-\omega_n}(k,k)] = -\frac{\mu T}{N}\operatorname{Re}\sum_{\omega_n,\nu}\frac{1}{i\omega_n - \mu H - E\omega_\nu}.$$

We make use of the fact that the roots enter in the summation in pairs, and the zeroth root has a negligible statistical weight at $N \gg 1$. Then

$$M = -\frac{2\mu T}{N}\sum_{\omega_n,\nu,\omega_\nu>0}\operatorname{Re}\frac{i\omega_n - \mu H}{(i\omega_n - \mu H)^2 - (E\omega_\nu)^2}.$$

We assume that $N \gg 1$, after which we can change from summation to integration, using the characteristic function $N(\zeta)$. After summing over the frequencies ω_n we obtain

$$M = \mu\int_0 [n_0(\omega E - \mu H) - n_0(\omega E + \mu H)]\,\omega N'(\omega^2)\,d\omega,$$
$$n_0(\omega) = 1/(e^{\omega/T}+1). \tag{8}$$

Formula (8) becomes much simpler if it is assumed that the temperature is equal to zero ($T \ll \{\mu H, E\}$):

$$M = \frac{\mu}{2}N\left[\left(\frac{\mu H}{E}\right)^2\right]. \tag{9}$$

Dyson[3], and also Bellman[5], obtained an integral equation connecting the function $N(\zeta)$ with the distribution function of the quantities λ. A solution of this equation was obtained by Dyson for the following distribution function:

$$G(\lambda) = \frac{n^n\lambda^{n-1}e^{-n\lambda}}{(n-1)!}, \quad \bar{\lambda} = 1;$$

where n are integers. For large n we obtain a Gaussian distribution with unity mean value and variance $1/\sqrt{n}$.

The general form of the function $N(\zeta)$ is given in Dyson's paper[3] (formulas (63)–(78)). We write down directly the value of the magnetic moment at fixed n in the limiting cases of weak and strong fields.

$T \ll \mu H \ll E/\sqrt{n}$—weak fields:

$$M = \frac{\mu(\pi^2 - 6t_{n-1})}{12[(\ln nz + s_{n-1} + \gamma)^2 + \pi^2]}, \quad \chi = \frac{\mu(\pi^2 - 6t_{n-1})}{3H|\ln nz|^3},$$
$$z = (\mu H/E)^2 = (2\mu H)^2/\overline{J^2}, \quad s_n = \sum_{k=1}^n k^{-1}, \quad t_n = \sum_{k=1}^n k^{-2} \tag{10}$$

$T \ll E/\sqrt{n} \ll \mu H$—strong fields:

$$M = \frac{\mu}{2}\left\{1 - \frac{2(nz)^{2n-1}(\ln nz - s_{n-1} + \gamma)e^{-nz}}{[(n-1)!]^2}\right\},$$
$$\chi = 2\mu(nz)^{2n}e^{-nz}\ln nz / H[(n-1)!]^2. \tag{11}$$

The magnetic susceptibility of the disordered chain diverges because such a chain "has a much larger fraction of low-lying frequencies than an ideal chain"[3]. With increasing field, the susceptibility decreases. In strong fields it is exponentially small, and the magnetic moment differs exponentially little from its maximum value. At $(\mu H)^2 \sim \overline{J^2}$, there is no singularity in the susceptibility.

It is of interest to calculate the susceptibility for finite temperatures but in weak fields: $\mu H \ll \{E, T\}$. To this end, we expand (8) in powers of μH:

$$\chi = \frac{2\mu^2}{T}\int_0^\infty n_0(E\omega)[1 - n_0(E\omega)]N'(\omega^2)\,\omega\,d\omega. \tag{12}$$

When $\mu H \ll E \ll T$ we obtain the Curie law: $\chi = \mu^2/4T$. At $\mu H \ll T \ll E$ the integration is cut off at $\omega \sim T/E$, so that we have $\chi \approx \mu^2 T^{-1} N[(T/E)^2]$. At $(\mu H)^2 \ll T^2 \ll E^2/n$ we have

$$\chi \sim \frac{\mu^2(\pi^2 - 6t_{n-1})}{6T\{[\ln(nT^2/E^2) + s_{n-1} + \gamma]^2 + \pi^2\}}; \tag{13}$$

at $T^2 \ll E^2 \ll nT^2$ we get

$$\chi \sim \mu^2/\pi(\overline{J^2})^{1/2}.$$

Thus, the disordered chain reveals a strong paramagnetism at low temperatures; the susceptibility of an ideal chain is constant.

It can be shown that at low temperatures the specific heat of a nonideal chain vanishes like $\ln^{-3}(E^2/T^2)$, and the entropy vanishes like $\ln^{-2}(E^2/T^2)$.

In the limit of large n and not too weak fields, $n(\mu H)^2 \gg \overline{J^2}$, we obtain the magnetic moment and the susceptibility of an ideal spin chain having a root singularity at $(\mu H)^2 = \overline{J^2}$[1].

2. ONE-DIMENSIONALISING CHAIN IN A TRANSVERSE FIELD

The Hamiltonian of the system is

$$\mathscr{H} = -2\sum_k J_k s_k^x s_{k+1}^x - \mu H\sum_k s_k^z. \tag{14}$$

Changing over again to Fermi operators, we obtain

$$\mathscr{H} = -\tfrac{1}{2}\sum_k J_k(a_k^+ a_{k+1} + a_{k+1}a_k) - \tfrac{1}{2}\sum_k J_k a_k^+ a_{k+1}^+$$
$$+ \tfrac{1}{2}\sum_k J_k a_k a_{k+1} - \mu H\sum_k(\tfrac{1}{2} - a_k^+ a_k).$$

In the Matsubara representation, the equations of motion are

$$\dot{a}_k(\tau) = \tfrac{1}{2}J_{k-1}a_{k-1}(\tau) + \tfrac{1}{2}J_k a_{k+1}(\tau) + \tfrac{1}{2}J_k\bar{a}_{k+1}(\tau) - \tfrac{1}{2}J_{k-1}\bar{a}_{k-1}(\tau) - \mu H a_k(\tau),$$
$$-\dot{\bar{a}}_k(\tau) = \tfrac{1}{2}J_{k-1}\bar{a}_{k-1}(\tau) + \tfrac{1}{2}J_k\bar{a}_{k+1}(\tau) + \tfrac{1}{2}J_k a_{k+1}(\tau) - \tfrac{1}{2}J_{k-1}a_{k-1}(\tau) - \mu H\bar{a}_k(\tau). \tag{15}$$

It is convenient to solve (15) by the Gor'kov method[6]. We introduce the two-component quantity $\psi_{k\alpha}$: $\psi_{k1} = a_k(\tau)$, $\psi_{k2} = -\bar{a}_k(\tau)$. The Green's function is defined by

$$G_{k\alpha;\,n\beta}(\tau_1,\tau_2) = -\langle T(\psi_{k\alpha}(\tau_1)\bar{\psi}_{n\beta}(\tau_2))\rangle.$$

The magnetic moment is expressed in terms of the Green's function in analogy with (3):

$$M=-\frac{\mu}{2N}\sum_{k}\mathrm{Sp}[\tau^zG_{kk}(\tau+0,\tau)]=-\frac{\mu T}{2N}\sum_{\omega_n}\mathrm{Sp}[\tau^zG_{\omega_n}].$$

We can verify with the aid of (15) that the Green's functions $\tau^Z G_{\omega n}(k, p)$ is the inverse of the following matrix of order 2N:

$$\begin{vmatrix} A & u_1 & 0 & 0 & \cdot & \cdot & 0 & 0 & 0 \\ v_1 & A & u_2 & 0 & \cdot & \cdot & 0 & 0 & 0 \\ 0 & v_2 & A & u_3 & \cdot & \cdot & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdot & \cdot & A & u_{N-2} & 0 \\ 0 & 0 & 0 & 0 & \cdot & \cdot & v_{N-2} & A & u_{N-1} \\ 0 & 0 & 0 & 0 & \cdot & \cdot & 0 & v_{N-1} & A \end{vmatrix} \quad (16)$$

$$A=-\mu H+i\omega_n\tau^z,\; u_k={}^1/_2J_k(1+\tau^x),\; v_k={}^1/_2J_k(1-\tau^x).$$

The matrix (16) is the sum of a unit matrix multiplied by $-\mu H$ and a matrix B that is independent of the field.

The logarithmic derivative of the determinant of the matrix (16) is expressed in terms of the eigenvalues of the matrix B:

$$\frac{\partial(\ln\Delta)}{\partial H}=\frac{\partial}{\partial H}\sum_{k=1}^{2N}\ln(-\mu H+b_k)=\mu\sum_{k=1}^{2N}\frac{1}{\mu H-b_k}, \quad (17)$$

b_k are the eigenvalues of the matrix B and Δ is the determinant of the matrix (16). Since the right-hand side of (17) is proportional to the trace of the matrix inverse to (16), we obtain

$$M=\frac{T}{2N}\sum_{\omega_n}\frac{\partial\ln\Delta}{\partial H}. \quad (18)$$

We denote by C_k the determinant of the matrix (16) with the first $2k-2$ rows and columns crossed out. The determinant D_k is of order $2(N-k)+1$. Its first row has three nonzero elements: $d_{11} = i\omega_n$ and $d_{12} = d_{13} = J_k$. The first column has the following nonzero elements: $d_{11} = i\omega_n$, $d_{21} = J_k/2$, and $d_{31} = -J_k/2$. The remaining part of the determinant is the matrix (16) with the first 2k rows and columns crossed out. It is easy to verify that C_k and C_k are connected by the following system of recurrence relations:

$$C_k=[(\mu H)^2+\omega_n^2]C_{k+1}-i\omega_nJ_k^2D_{k+1},$$
$$D_k=i\omega_nC_{k+1}+J_k^2D_{k+1};$$

$C_{N+1} = 1$ and $D_{N+1} = 0$ by definition.

We introduce the quantity $x_k = iC_k/D_k$; we then obtain

$$\frac{C_k}{C_{k+1}}=(\mu H)^2+\omega_n^2+\frac{\omega_nJ_k^2}{x_{k+1}}, \quad \ln\Delta=\sum_{k=1}^{N}\ln\frac{C_k}{C_{k+1}},$$

$$x_k=\frac{[\omega_n^2+(\mu H)^2]x_{k+1}+\omega_nJ_k^2}{\omega_nx_{k+1}+J_k^2}. \quad (19)$$

Relations (19) enable us to establish a connection between the distribution function $G(\lambda)$ of the random quantities $\lambda_k = J_k^2$ and the distribution function with respect to the variable x. We note that these equations occur in the two-dimensional Ising model with random anisotropy[7].

For this reason, we present the main results without proof. The distribution function $\nu(x)$ satisfies the equation

$$\nu(x)=\int_{-\infty}^{+\infty}dx'\int_0^\infty d\lambda\,\delta\left[x-\omega_n-\frac{(\mu H)^2x'}{\omega_nx'+\lambda}\right]G(\lambda)\nu(x'). \quad (20)$$

The susceptibility has a maximum under the condition

$$\ln(\mu H_c)^2=\int_0^\infty G(\lambda)\ln\lambda\,d\lambda. \quad (21)$$

For example, for a binary solid solution we have

$$G(\lambda)=c_1\delta(\lambda-\lambda_1)+c_2\delta(\lambda-\lambda_2), \quad c_1+c_2=1;$$

$c_{1,2}$ are the concentrations of atoms with exchange integrals respectively equal to $J_{1,2} = \sqrt{\lambda_{1,2}}$. Substituting this expression in (21), we obtain $\mu H_c = J_1^{c_1}J_2^{c_2}$.

An asymptotic solution of (20) could be obtained for the following distribution[7]

$$G(\lambda)=\begin{cases} n\lambda_0^{-n}\lambda^{n-1}, & 0<\lambda<\lambda_0 \\ 0, & \lambda>\lambda_0 \end{cases}, \quad \overline{J^2}=\bar\lambda=\frac{n\lambda_0}{1+n}; \quad (22)$$

λ_0 is the maximum value of the squared exchange interaction.

In the limit $n \gg 1$ we have with the aid of (21) $\mu H_c(n) = \sqrt{\lambda_0}e^{-1/2n}$.

The anomalous part of the susceptibility near the maximum is given by

$$\chi=\frac{\mu^2}{2\pi\sqrt{\lambda_0}}\left\{\int_0^\infty\left[\frac{\partial^2}{\partial\delta^2}\ln K_\delta(x)-\frac{1}{1+x}\right]dx+\ln(8n^2/e^3)\right\}, \quad (23)$$

$\delta = 4n^2\mu\lambda_0^{-1/2}[H - H_c(n)]$, and $K_\delta(x)$ is a Bessel function. As $\delta \to 0$ we get

$$\chi=\chi_{max}=\mu^2\ln n/\pi\sqrt{\lambda_0},\; n\gg1. \quad (24)$$

The susceptibility has no singularity in the limit as $\mu H \to 0$. This can be easily shown by expanding relations (18)—(20) in powers of $(\mu H)^2$ and noting that at $H = 0$ we have $\nu(x) = \delta(x-\omega_n)$.

CONCLUSION

The properties of a one-dimensional chain with impurities differ strongly from the properties of an ideal chain. The susceptibility singularities of the ideal chain become smeared out and turn into maxima whose widths increase with increasing fluctuations of the exchange interaction. For example, from (24) we have at $n \gg 1$

$$\chi_{max}\sim\frac{\mu^2}{\pi(\overline{J^2})^{1/2}}\ln\left[\frac{\overline{J^2}}{\overline{\Delta J^2}}\right], \quad \Delta H\sim\frac{\bar J}{\mu}\left[\frac{\overline{\Delta J^2}}{\overline{J^2}}\right]^2$$

ΔH is the "broadening" of the $\chi(H)$ curve.

A one-dimensional x-y chain has certain additional interesting properties. At low temperatures, the reciprocal susceptibility behaves like $T\ln^2(\bar J/T)$, at zero temperature the susceptibility increases with decreasing field like $H^{-1}\ln^{-3}(\bar J/\mu H)$. This phenomenon is connected with the anomalously large ($\sim\omega^{-1}|\ln^{-3}\omega|$) density of states of the one-dimensional disordered chain[3].

It must be noted that no one has yet succeeded in calculating the susceptibility of a chain with interaction of the type

$$\sum_k g_k(s_k^xs_{k+1}^y+s_{k+1}^xs_k^y).$$

An ideal chain has in this case a logarithmic singularity in weak fields and at low temperatures, precisely where the non-ideal x-y chain has a singularity. It can be shown that in this case, too, there exist recurrence relations for the calculation of the determinant Δ (see formula (18)). The distribution function $\nu(x)$, however, obeys a more complicated equation.

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