

a transition to a ferromagnetic state is observed. These substances are apparently well described by the excitonic-ferromagnet model,^[1] so that it is possible to apply to them (of course, only qualitatively), the results obtained above. When the phases of CDW and SDW having the same period coincide, the summary magnetic moment of the sample is not equal to zero and a domain structure is produced. It is of interest to investigate such systems near the temperature of the transition to the ferromagnetic state, as an attempt to observe in them long-wave oscillations of the density and of the magnetic moment. A theoretical calculation with a two-component order parameter and at finite temperatures is a rather laborious task even in the homogeneous case, and will therefore be the subject of a separate paper.

Interest in the investigation of phase transitions in nonequilibrium system is stimulated by the search of means of raising the critical superconducting temperature. We have shown here that under the influence of a pump source the magnetic ordering due to collective effects of coexistence of singlet and triplet electron-hole pairings turns out to be inhomogeneous (modulated), with a period that is determined by the pump intensity. This effect can be observed in experiment by magnetic measurements.

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Susceptibility and Knight shift in one-dimensional disordered spin systems with isotropic antiferromagnetic interaction

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A one-dimensional model of classical spins with $n = 1, 2$, and 3 components (Ising, planar rotator, and Heisenberg models) and with random antiferromagnetic interaction J of the nearest neighbors is considered. In such a system, the average thermodynamic value of the spin at a site is different from zero in a magnetic field. The value of s is random, and its distribution is described by a function $f_s(x)$. An integral equation is obtained for $f_s(x)$ in weak magnetic field, assuming the distribution function $f_j(x)$ to be given. The moments of the distribution of s are calculated as functions of the type of function $f_j(x)$ and of the temperature. Conditions under which the susceptibility of the system χ increases as $T \rightarrow 0$ are analyzed. It is shown that if the susceptibility $\chi \rightarrow \infty$ as $T \rightarrow 0$, then the distribution of s becomes symmetrical as $T \rightarrow 0$, and the most probable value \bar{s} of s tends to be zero. The results are used to interpret the experimental data on the temperature dependence of the paramagnetic shift of the NMR in quasi-one-dimensional $\text{Qn}(\text{TCNQ})_2$ crystals.

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1. INTRODUCTION

This article is devoted to a theoretical investigation of the properties of one-dimensional spin systems with random exchange interaction. Interest in these systems is due to the experimental investigations of the quasi-

one-dimensional TCNQ salts with asymmetric cations^[1] and of magnetic polymers such as polymetalphosphines.^[2]

The class of magnetic polymers has not yet been investigated in great detail. All that is known is the temperature dependence of the susceptibility of two repre-

representatives of this class, containing Mn atoms (uncompensated spin $S=5/2$) and Cr atoms ($S=3/2$) in a temperature interval of the order of and larger than the exchange interaction. In the investigated temperature interval, the sample susceptibility can be described with good accuracy within the framework of the model of a classical system of spins with random antiferromagnetic Heisenberg interaction for the nearest-neighbor spins, and the variation of the exchange interaction is of the order of the average interaction. So strong a disorder of these systems is apparently to structure defects inherent in polymer compounds.

More widely studied was the class of quasi-one-dimensional disordered magnetic crystals. Typical representatives of this class are the charge-transfer salts $\text{Qn}(\text{TCNQ})_2$, $\text{Ad}(\text{TCNQ})_2$ and NMP-TCNQ . The crystals of these salts contain alternating parallel chains of TCNQ anions with uncompensated spin and of cations, the internal disorder being due to the random spatial orientation of the asymmetric cation molecule in the chain.^[1]

At temperatures below about 10–20 K, an increase of the paramagnetic susceptibility with decreasing T , $\chi \propto T^{-\alpha}$ with $0 < \alpha < 1$, was observed in TCNQ salts with Qn, Ad, and NMP. The increase of the total paramagnetic moment M of the crystal with increasing magnetic field H in strong fields $g\mu_B H \gg k_B T$ also follows a power law $M \propto H^{1-\alpha}$ (Ref. 3), and an analogous relation $C \propto T^{1-\alpha}$ was observed for the dependence of the heat capacity C on temperature in a zero magnetic field.^[4,5]

To explain the low-temperature anomalous magnetic properties of TCNQ salts with asymmetrical cations, a model of localized spins $S=1/2$, with a one-dimensional Heisenberg antiferromagnetic interaction, was proposed in Ref. 3. The Hamiltonian of this system is

$$\mathcal{H} = \sum_k (J_k S_k S_{k+1} - g\mu_B H S_k^z), \quad (1)$$

where S_k is the spin operator at site k and the quantities $J_k \geq 0$ are random. Within the framework of the Hamiltonian (1) it is easy to understand qualitatively the reason why the susceptibility χ increases with decreasing temperature, and the cause of the anomalous behavior of all the remaining thermodynamic characteristics of the system near the point $T=0$ and $H=0$, if it is assumed that the J_k can be arbitrarily small.^[5,6,7] By changing over in the Hamiltonian (1) from spin operators to Fermi operators and using the Landau Fermi-liquid approximation,¹⁾ we can express the thermodynamic quantities in terms of the fermion state density $\rho(\varepsilon)$ near the midpoint $\varepsilon=0$ of the fermion band. The assumption that the state density has an anomaly of the type $\rho(\varepsilon) = A\varepsilon^{-\alpha}$ as $\varepsilon \rightarrow 0$ permits a complete quantitative description of the functions $M(H, T)$ and $C(H, T)$, which agrees well with the experimental data^[3-5] (A and α are parameters of this semiphenomenological theory and are determined from the experimental data). There is thus no doubt at present that the Hamiltonian (1) with arbitrarily small values of J_k can provide a complete description of the low-temperature properties of TCNQ salts with asymmetric cations. The theory is as yet

incapable, however, to state unequivocally how the distribution function of the quantities J_k must behave near $J_k=0$ if the Hamiltonian (1) is to yield the same power-law dependences of $\chi(T)$, $M(H, 0)$, and $C(0, T)$ that have been observed in experiment.^[3-6]

Theodorou and Morrel Cohen have proposed a microscopic model of an electron system with disorder (Hubbard model with random values of the electron energy at the sites), which is equivalent to a system of localized spins with interaction (1), if the analysis is confined to thermodynamic properties at low temperatures.^[6,7] Within the framework of this model, the randomness of the interaction of the spins J_k appears in natural fashion and the distribution function of the random quantities J_k can be calculated. The parameters J_k for different k turn out to be uncorrelated, their distribution functions are identical, and as $x \rightarrow 0$ the distribution function $f_j(x)$ takes the form $f_j(x) \propto x^\beta$, where the exponent β is positive or negative, depending on the parameters of the initial electron system. This model explains thus why the quantities J_k in the Hamiltonian (1) are random and why they can take on arbitrarily small values.

Shchegolev *et al.*^[10] have recently published experimental data on the paramagnetic shift and width of the NRM line in $\text{Qn}(\text{TCNQ})_2$. The paramagnetic NMR shift of the protons on the molecules is determined by the average electron spin per molecule, so that NMR measurements yield information on the distribution of the uncompensated spin at the sites on the chain. For a homogeneous system, the thermodynamic and quantum-mechanical mean value of the spin at the site $s_k = \langle S_k^z \rangle$ is the same for all sites and is proportional to the paramagnetic susceptibility χ and to the magnetic field H (the angle brackets denote here and below the thermodynamic and quantum-mechanical averaging, while averaging over the configuration will be designated by a bar over the symbol for the corresponding quantity). In a disordered system, the values of s_k at different sites are different and only the configuration mean value \bar{s}_k is proportional to χH (according to the ergodic hypothesis $\bar{s}_k = \sum_k s_k / N$, where N is the number of spins in the chain). We are interested in the distribution of the quantity s_k described by introducing the distribution function $f_s(x)$.

Let the NMR line shape $g(\nu)$ in the absence of inhomogeneous magnetization be determined by the function $g_0(\nu - \nu_0)$, where ν_0 is the center of the resonance line of the protons in the diamagnetic state at $s_k=0$ (usually $c_0(\nu - \nu_0)$ is a Gaussian distribution). Then, taking into account the inhomogeneity of the magnetization, we obtain for the line shape of the NMR on the protons

$$g(\nu - \nu_0) = \frac{1}{m} \sum_{i=1}^m \int_{-\infty}^{\infty} g_0(\nu - \nu_0 - \lambda_i x) f_i(x) dx, \quad (2)$$

where the constant λ_i is determined by the electron-proton hyperfine interaction on the molecule, and m is the number of protons on the molecule. Thus, measurements of the NMR line shape in an inhomogeneous system make it possible to determine from (2) the distribution function $f_s(x)$ if the function $g_0(\nu - \nu_0)$ is known.

Shchegolev *et al.* measured the temperature dependence of that frequency value $\tilde{\nu}$ at which the derivative of $g(\nu - \nu_0)$ with respect to frequency vanishes. The quantity $\tilde{\nu}$ is the most probable value of the frequency in the $g(\nu - \nu_0)$ distribution (the most probable value of a random quantity a will henceforth be designated \bar{a}). According to measurements made at $T > 8$ K, the quantity $\tilde{\nu}(T) - \nu_0$ is proportional to the susceptibility $\chi(T)$ and increases when the temperature decreases below 40 K, reaching a maximum at 8 K; below this temperature, $\tilde{\nu}(T) - \nu_0$ approaches zero with decreasing temperature. It follows from these data that if the distribution function $f_s(x)$ in (2) has a single peak (with center at $x = \bar{s}$), then the temperature dependence of $f_s(x)$ is such that $\bar{s}(T) \approx \bar{s}(T) = \chi(T)H$ at $T > 8$ K, but when the temperature is lowered ($T \rightarrow 0$) we have $\bar{s} \rightarrow 0$, whereas \bar{s} increases in proportion to $T^{-\alpha}$. Thus, measurements of the paramagnetic shift of the NMR in $\text{Qn}(\text{TCNQ})_2$ have shown that in this system the distribution function of s depends substantially on temperature, and the task of the theory is to determine this dependence within the framework of the Hamiltonian (1).

So far, however, we do not know any method of calculating $f_s(x)$ for quantum Heisenberg models with random interaction. We shall therefore investigate in the present article the behavior of the function $f_s(x)$ for models of classical spins with antiferromagnetic interaction in all those cases in which χ is seen to increase as $T \rightarrow 0$. The results enable us to draw qualitative conclusions concerning the temperature dependence of $f_s(x)$ in the quantum model. It can furthermore be assumed that a classical spin system provides a fair approximation for the description of magnetic polymer^[2] with spins as high as 5/2 and 3/2. And once the temperature dependence of the NMR line shape in magnetic polymers is eventually experimentally studied,^[2] then these data can be compared with the theoretical results obtained below for a classical disordered Heisenberg model.

2. EQUATION FOR THE SPIN DISTRIBUTION FUNCTION AT THE SITES IN ISOTROPIC CLASSICAL MODELS

We consider a spin-interaction model with $n = 1, 2, 3$ components in a magnetic field $H \rightarrow 0$. The Hamiltonian of the system is

$$\begin{aligned} \mathcal{H} &= \sum_{k=-\infty}^{+\infty} (J_k S_k^z S_{k+1}^z - h S_k^z), \quad n=1, \\ \mathcal{H} &= \sum_{k=-\infty}^{+\infty} (J_k S_k S_{k+1} - h S_k^z), \quad n=2, 3, \end{aligned} \quad (3)$$

where $h = g\mu_B H$. In the case $n=1$ (the Ising model) we have $S_k^z = \pm 1$, and the unit vector S_k specifies the direction in the two-dimensional space (x, z) in the planar-resonator model ($n=2$) and the direction in three-dimensional space in the Heisenberg model ($n=3$).²⁾

The random quantities J_k with different k will be assumed independent, we assume the distribution functions for them to be the same and equal to $f_J(x)$. In a weak magnetic field the thermodynamic mean value of

the spin s_k at the site k is given by

$$s_k = \langle S_k^z \rangle = \frac{h}{T} \sum_{p=-\infty}^{+\infty} \langle S_k^z S_{k+p}^z \rangle = \frac{h}{Tn} \sum_{p=-\infty}^{+\infty} \langle S_k S_{k+p} \rangle. \quad (4)$$

Our task is to determine the distribution functions of the quantities s_k . For an infinite chain these functions are the same for all s_k and we designate them $f_s(x)$. According to the ergodic hypothesis the function $f_s(x)$ describes also the distribution of s_k over the chain. In all the considered isotropic models, the correlation functions $\langle S_k S_{k+p} \rangle$ are defined by the relations^[12,13]

$$\langle S_k S_{k+p} \rangle = (-1)^p \prod_{m=k}^{k+p-1} u_m, \quad u_m = u \left(\frac{J_m}{T} \right),$$

$$u(x) = \frac{d}{dx} \ln(e^x + e^{-x}) = \text{th } x, \quad n=1,$$

$$u(x) = \frac{d}{dx} \ln \left(\int_0^\pi e^{x \cos \theta} d\theta \right) = \frac{d}{dx} \ln I_0(x), \quad n=2,$$

$$u(x) = \frac{d}{dx} \ln \left(\int_0^\pi e^{x \cos \theta} \sin \theta d\theta \right) = \text{cth } x - \frac{1}{x}, \quad n=3,$$

where $I_0(x)$ is a Bessel function of imaginary argument. From (4) and (5) we obtain

$$s_k = \frac{h}{Tn} \sigma_k, \quad \sigma_k = \xi_k + \eta_k - 1,$$

$$\begin{aligned} \xi_k &= 1 - u_{k+1} + u_{k+1}u_{k+2} - u_{k+1}u_{k+2}u_{k+3} + \dots, \\ \eta_k &= 1 - u_{k-1} + u_{k-1}u_{k-2} - u_{k-1}u_{k-2}u_{k-3} + \dots \end{aligned} \quad (6)$$

From the definition of the random quantities u_k it follows that all are independent and have the same distribution function $f_u(x)$. From (6) we get for an infinite chain

$$\xi_k = 1 - u_k \xi_{k+1}, \quad (7)$$

and an analogous relation holds for η_k . The random quantities u_{k+1} and ξ_{k+1} in (7) are independent. The quantities ξ_k and ξ_{k+1} have in an infinite system the same distribution function $f_\xi(x)$. For this function we get from (7) the integral equation

$$\begin{aligned} f_\xi(x) &= \int_{-\infty}^{+\infty} dx_1 dx_2 f_u(x_1) f_\xi(x_2) \delta(1 - x - x_1 x_2) \\ &= T \int_0^\infty \frac{dx_1}{u(x_1)} f_J(x_1 T) f_\xi \left(\frac{1-x}{u(x_1)} \right). \end{aligned} \quad (8)$$

The quantities ξ_k and η_k are independent, and for the distribution function $f_\sigma(x)$ of the quantity σ we get

$$f_\sigma(x) = \int_{-\infty}^{+\infty} dx_1 f_\xi(x - x_1 + 1) f_\xi(x_1), \quad (9)$$

and $f_s(x) = Tnh^{-1} f_\sigma(xTn/h)$. Equations (8) and (9) determine the function $f_\sigma(x)$ in terms of the specified distribution function $f_J(x)$. Since the series for ξ_k is of alternating sign and each succeeding term of the series is smaller than the preceding one, it follows that $0 \leq \xi_k \leq 1$ and analogously $0 \leq \eta_k \leq 1$. Thus, $-1 \leq \sigma_k \leq +1$, i.e., the function $f_\sigma(x)$ differs from zero in the interval $[-1, +1]$.

To calculate the moments of the distribution it is convenient to introduce the characteristic function $\varphi_\sigma(t)$ for the quantity σ ($\varphi_\sigma(t)$ is the Fourier transform of the function $f_\sigma(x)$). It follows from (8) and (9) that

$$\varphi_0(t) = \varphi^2(t),$$

$$\varphi(t) = T \int_0^{\infty} f_s(xT) \varphi[-tu(x)] \exp\left\{i \frac{t}{2}[1-u(x)]\right\} dx. \quad (10)$$

Expanding the functions $\varphi(t)$ and $\varphi_0(t)$ in (10) in powers of t , we obtain the coefficients of the series of $\varphi_0(t)$ in t , and the k -th order derivative of $\varphi_0(t)$ with respect to t at $t=0$ yields the value of $i^k \sigma^k$. For the first two moments of s we obtain from (10)

$$\chi = \frac{s}{h} = \frac{1-\bar{u}}{Tn(1+\bar{u})}, \quad \bar{u} = T \int_0^{\infty} f_s(xT) u^k(x) dx, \quad (11)$$

$$\bar{s}^2 = (\bar{s})^2 + \frac{2k^2[\bar{u}^2 - (\bar{u})^2]}{T^2 n^2 (1-\bar{u}^2)(1+\bar{u})^2}.$$

3. TEMPERATURE DEPENDENCE OF THE SUSCEPTIBILITY AND THE SPIN DISTRIBUTION FUNCTION IN CLASSICAL ISOTROPIC MODELS

In this part we determine, within the framework of the classical model, that for of the function $f_J(x)$ near $x=0$ which leads to the appearance of a singularity of the magnetic susceptibility as $T \rightarrow 0$. At the same time we find the form of f_s for those $f_J(x)$ distributions at which χ increases at $T \rightarrow 0$. We confine ourselves to the class functions $f_J(x)$ with a power-law asymptotic behavior as $x \rightarrow 0$, i.e., to functions of the type $f_J(x) \sim x^{-\alpha}$ as $x \rightarrow 0$ ($\alpha < 1$), and obtain those values of α at which the susceptibility increases without limit when the temperature drops to zero. Later on, a quantitative analysis will be made of the temperature dependences of χ and $f_s(x)$ for a distribution function $f_J(x)$ of the form

$$f_J(x) = (1-c)\delta(x-I_0) + cp(x), \quad (12)$$

$$p(x) = \begin{cases} (1-\alpha)I_1^{\alpha-1}x^{-\alpha}, & 0 \leq x \leq I_1, \\ 0, & x > I_1 \text{ or } x < 0, \end{cases}$$

where $\alpha < 1$ and $\delta(x)$ is the delta function. The first term of $f_J(x)$ describes the homogeneous interaction in the chain, and the second represents "defects" with concentration c , where $1 \geq c > 0$. The growth of χ as $T \rightarrow 0$ is determined by the second term of $f_J(x)$, since this term describes the distribution of the weak interactions. If $\alpha > 0$, the function $f_J(x)$ is singular at $x \rightarrow 0$, and if $\alpha = 0$ the distribution of J is homogeneous at small J . As $\alpha \rightarrow 1$ or $I_1 \rightarrow 0$, we have $p(x) \rightarrow \delta(x)$, i.e., in a chain with probability c there is no interaction at all between neighboring spins. This limiting case corresponds to the "piecewise" model, which we shall use as the starting point for the understanding of the causes of the growth of χ as $T \rightarrow 0$ and of the specifics of the $f_0(x)$ distribution at low temperatures.

The "piecewise" model. As $I_1 \rightarrow 0$ or $\alpha \rightarrow 1$, the distribution (12) takes the form

$$f_J(x) = (1-c)\delta(x-I_0) + c\delta(x), \quad (13)$$

i.e., the entire system breaks up in random fashion into noninteracting subsystems ("pieces") and the interaction within the subsystems is homogeneous and is equal to I_0 .

At $T \geq I_0$ the average spin \bar{s} coincides with the corresponding value in the homogeneous chain, accurate to terms of order of c as $c \rightarrow 0$, the variance Ds is small

to the extent that the concentration c is small, and in this temperature region $Ds(\bar{s})^2 \sim c \ll 1$.

At $T \rightarrow 0$, it is easy to calculate $\bar{\sigma}$, $\bar{\sigma}^2$, and $\bar{\sigma}^4$ and reconstruct completely the function $f_0(x)$ for an arbitrary concentration c :

$$\chi = \frac{\bar{s}}{h} = \frac{c}{Tn(2-c)} + \frac{4(1-c)}{(2-c)^2} \chi_0, \quad \chi_0 = \frac{n-1}{4nI_0}, \quad \bar{\sigma}^2 = \bar{\sigma}^2 = \frac{2(1-c)+c^2}{(2-c)^2}, \quad (14)$$

$$f_0(x) = \frac{1}{(2-c)^2} [(1-c)^2 \delta(x+1) + 2(1-c)\delta(x) + \delta(x-1)],$$

where the susceptibility χ_0 of a homogeneous chain is referred to a single site. The results (14) admit of a simple interpretation. The pieces with even numbers of spins as $T \rightarrow 0$ yield a mean value $\bar{\sigma} \approx 4(1-c)(2-c)^{-2} n \chi_0 T \rightarrow 0$ at each site, and the probability that the node belongs to an even piece is $2(1-c)(2-c)^{-2}$. Odd pieces have one unpaired spin and as $T \rightarrow 0$ they yield a susceptibility growth that follows the Curie law. At each site of an odd piece, regardless of its length, we have $|\sigma| = 1$ and the sign of σ at the neighboring sites of the odd piece is opposite, being positive on the terminal sites. This result for the piecewise model follows directly from (6) if it is recognized that $u(x) \rightarrow 1$ as $x \rightarrow \infty$, so that ξ_k (as well as η_k) is a sum of the finite series $1 - 1 + 1 - \dots$, which is equal to 0 or 1, depending on the location of the node k . It follows from this picture that the entire asymmetry of the distribution of the quantity s relative to the point $s=0$ is connected with one end-point spin of the odd pieces; at $c \ll 1$ the asymmetry is small to the extent that c is small, and $\bar{s} = ch/2Tn$, so that $(\bar{s})^2/Ds \sim c^2 \ll 1$.

Thus, in the piecewise model the variance of the distribution of s increases like T^{-2} as $T \rightarrow 0$, and at $c \ll 1$ the distribution of s becomes symmetric with respect to the point $s=0$. As the temperature decreases from I_0 to 0, the value of \bar{s} in this model changes from \bar{s} to 0.

Singular distribution of J , low temperatures. We proceed now to investigate the form of the distribution $f_s(x)$ at $T \ll I_1$ and $0 < \alpha < 1$. From (11) we get, accurate to terms of higher order in the temperature,

$$\chi = \frac{\bar{s}}{h} = a_1 \frac{c}{2n} (1-\alpha) I_1^{\alpha-1} T^{-\alpha} + (1-c) \chi_0, \quad (15)$$

$$\bar{\sigma}^2 = \frac{T^2 n^2}{h^2} \bar{s}^2 = \frac{2a_2}{2a_1 - a_2}, \quad a_n = \int_0^{\infty} x^{-n} [1-u(x)]^n dx.$$

It is seen from (15) that $\bar{\sigma} = Tn\bar{s}/h \rightarrow 0$ as $T \rightarrow 0$, but the limiting value of $\bar{\sigma}^2$ differs from zero, is independent of the concentration c , and depends only on the parameter α (when α changes from 1 to 0, the limiting value of $\bar{\sigma}^2$ decreases from 1/2 to 0 at $n=2$ or 3 and from 1/2 to $\ln 2 - 1/2$ for $n=1$). It is easy to verify that, regardless of the value of c , all the odd moments of the distribution of σ vanish in the limit as $T \rightarrow 0$, and all the even moments tend to limits that depend only on α . When α changes from unity to zero, the ratio $\bar{\sigma}^4/(\bar{\sigma}^2)^2$ changes from 2 to infinity at $n=2$ and 3 to approximately four at $n=1$. Consequently, in the limit as $T \rightarrow 0$, regardless of the concentration c , the distributions of σ and s become symmetrical, and $\bar{s} \rightarrow 0$. From the continuity in the parameter α it follows that the three peaks in the distribution of σ remain, at least for α values close to unity.

The form of the distribution $f_\sigma(x)$ at $\alpha \leq 1$ and $T \rightarrow 0$ is shown qualitatively in the figure.

To understand the behavior of the susceptibility and of the function $f_s(x)$ as functions of the temperature in the case of singular $f_j(x)$ distributions, we can use the "cluster" concepts of Theodorou and M. Cohen.^[6,7] We define a cluster as a group of spins $m, m+1, \dots, m+p$ with interactions $J_m, J_{m+1}, \dots, J_{m+p-1} > T$ and with interactions $J_{m-1}, J_{m+p} < T$ at the boundary of the cluster (pieces are particular cases of clusters, differing only that the breakdown into clusters depends on the temperature, and in the piecewise model the breakdown into pieces is constant at $T < I_0$). A contribution to the susceptibility is made by clusters with odd numbers of spins. The effective concentration of such clusters is

$$c'(T) \approx c \int_0^T \frac{p(x) dx}{2} = \frac{c I_1^{\alpha-1} T^{1-\alpha} (1-\alpha)}{2}.$$

Each odd cluster gives a susceptibility $1/T$, and we obtain for the singular part of χ an expression that differs from the exact expression (15) by only a numerical factor. Inside the cluster there is a strong antiferromagnetic spin correlations $\langle S_m S_{m+k} \rangle \approx (-1)^k$ for $1 \ll k \leq p$, but this correlation becomes weak for spins from different clusters. The distribution of the average spin s_k over the cluster is therefore similar to that in the piecewise model, i.e., $s_k \approx (-1)^{m+k} h / T n$. As $T \rightarrow 0$, the effective cluster concentration decreases like $T^{1-\alpha}$ and, in accordance with the results for the piecewise model, when the temperature decreases the asymmetry of the distributions of s and σ with respect to the point 0 vanishes, regardless of the value of c .

Homogeneous distribution of J , low temperatures. It remains now to consider regular distributions with $\alpha \leq 0$. In the Ising model, these distributions do not lead to a growth of χ as $T \rightarrow 0$, while in the continuous Heisenberg and planar-rotator models this growth takes place only if $\alpha = 0$.³⁾

From (10) we obtain for $n=2$ and 3 and for $\alpha = 0$

$$\bar{s} = \frac{c}{h} = \frac{c}{2} I_1^{-1} g\left(\frac{I_1}{T}\right) + (1-c) \chi_0, \quad \bar{\sigma}^2 = \frac{s^2 n^2 T^2}{h^2} = \frac{a_2}{g(I_1/T) - a_2/2}, \quad (16)$$

$$g(x) = \int_0^x dt [1 - u(t)] = \begin{cases} \frac{1}{2} \ln(2\pi x), & n=2 \\ \ln(2x), & n=3 \end{cases}$$

It is seen from (16) that \bar{s} increases logarithmically with decreasing temperature, and the value of s is distributed approximately in the interval from $-h/nT \ln^{1/2}(I_1/T)$ to $+h/nT \ln^{1/2}(I_1/T)$. In contrast to the singular distributions with $\alpha > 0$, however, now $\bar{\sigma}^2$ tends to zero as $T \rightarrow 0$ like $a_2 \ln^{-1}(I_1/T)$. It is easy to verify

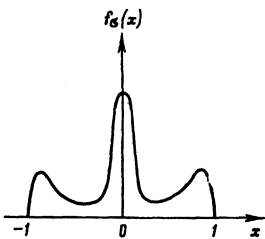


FIG. 1. Qualitative picture of the distribution $f_s(x)$ as $T \rightarrow 0$ and at values of α close to unity.

that all even moments $\overline{\sigma^{2n}}$ tend to zero like $b_n \ln^{-1}(I_1/T)$ (for, example, $b_4 = 3/2 a_2 + 1/8 a_4$) and the ratio $\overline{\sigma^4}/(\overline{\sigma^2})^2$ increases like $\ln(I_1/T)$ as $T \rightarrow 0$. Thus, in the limiting case $\alpha = 0$ the distribution of s has only one peak at $s = 0$.

At $\alpha = 0$, the Ising model and the continuous models give different results for the behavior of χ as $T \rightarrow 0$. In addition, the cluster argument of Theodorou and Cohen provides a qualitatively correct description of the situation in the Ising model for all values of α ; it describes correctly the situation in the continuous models at $\alpha > 0$, but predicts incorrectly the behavior of χ as $T \rightarrow 0$ in the case $\alpha = 0$ for the continuous models. What is the reason?

In all classical models, long range-order sets in as $T \rightarrow 0$, since $u(x) \rightarrow 1$ as $x \rightarrow \infty$. The approach to this long-range order, however, is different in the Ising model and in the continuous models, because $1 - u(x) \sim 2e^{-2x}, 1/2x$, and $1/x$ as $x \rightarrow \infty$ and at $n=1, 2$, and 3, respectively. In the Ising model the magnetic excitations are connected with complete breakdown of the antiferromagnetic correlation of the neighboring spins, and for such excitations there is a gap equal to the exchange interaction of the corresponding spins. The quantities χ and $1 - u$ are therefore exponentially small as $T \rightarrow 0$. Excitations of this type, which we shall call "breaks", exist also in the continuous models. But the latter have, besides breaks, also gapless excitations of the spin-wave type, for which the spin rotation at neighboring sites is small. The asymptotic behavior of the type x^{-1} in the continuous models is due precisely to the spin waves. In the homogeneous model, the contributions of the two types of excitation are approximately equal at $T \approx I_0$, but at $T \ll I_0$ only the spin-wave excitations remain and lead to a nonzero susceptibility χ_0 as $T \rightarrow 0$.

The disordered character of the exchange interaction, which admits of arbitrarily small J , facilitates the appearance of breaks, and the antiferromagnetic correlation of the neighboring spins is violated in those places where $J < T$, i.e., at the boundaries of the clusters. Small J , however, facilitate also the appearance of spin-wave excitations, increasing their density of states at low energies. The cluster argument of Theodorou and Cohen takes into account only excitations of the break type. In the Ising model only this type of excitation exists, and therefore the cluster argument predicts correctly the condition $\alpha > 0$ at which χ increases as $T \rightarrow 0$ in the Ising model. In the continuous models, for the singular distribution functions (12), the behavior of the susceptibility at low temperatures is determined mainly by the breaks, and the cluster argument again yields the correct asymptotic form of χ as $T \rightarrow 0$. At $\alpha = 0$, however, the growth of χ as $T \rightarrow 0$ in the continuous models is determined only by the spin-wave excitations, since the contribution from the break yields $\chi \rightarrow \text{const} \neq 0$ as $T \rightarrow 0$. In this situation, the cluster argument^[6,7] can not predict correctly the behavior of the susceptibility at low temperatures.

Continuous models in the entire temperature range. We have investigated above the behavior of systems with $1 > \alpha \geq 0$ at low temperatures. We consider now the

behavior of the continuous models in the entire temperature range.

At $c \ll 1$ the behavior of the system in the temperature region $T \geq I_0$ does not differ from the behavior of a homogeneous system. For temperatures $I_1 \ll T \ll I_0$ we obtain

$$\chi = \chi_0 + \frac{c}{2T} \cdot \frac{Ds}{(\bar{s})^2} = \frac{2c}{(c+4T\chi_0)(c+2T\chi_0)^2}. \quad (17)$$

It follows from (17) that the susceptibility is practically constant and is equal to χ_0 at $T > cI_0$, after which it begins to increase monotonically at $I_1 < T < cI_0$ in accord with the Curie law, this growth slows down at $T \approx I_1$, and at $T \ll I_1$ we get $\chi \sim T^{-\alpha}$ at $\alpha > 0$ and $\chi \sim \ln(I_1/T)$ at $\alpha = 0$. The relative variance $Ds/(\bar{s})^2$ is of the order of c when $T \gg I_0 c^{1/2}$, it increases with decreasing temperature in the region from $I_0 c^{1/2}$ to $I_0 c$, then remains practically constant at $2c^{-2}$ from $I_0 c$ to I_1 , and with further decrease of temperature the ratio $Ds/(\bar{s})$ increases like $T^{2\alpha-2}$ at $\alpha > 0$ and like $1/T^2 \ln^3(I_1/T)$ at $\alpha = 0$.

At $c \approx 1$, the growth of $Ds/(\bar{s})^2$ with decreasing temperature begins at a temperature on the order of I_1 , and \bar{s} differs little from \bar{s} only at temperatures $T \gg I_1$.

4. DISCUSSION

We now formulate briefly the results for classical models, and discuss the degree to which these results can be valid for the quantum Heisenberg model of spins $1/2$.

1. In the classical models, the singularity of $f_j(x)$ as $x \rightarrow 0$ leads to a singular behavior of the same type in the temperature dependence of χ as $T \rightarrow 0$. In the continuous classical models the susceptibility increases logarithmically as $T \rightarrow 0$ if $f_j(x)$ is constant or decreases as $x \rightarrow 0$ not faster than logarithmically (not faster than $|\ln x|^{-\beta}$ with $1 > \beta > 0$). In all the remaining cases there is no increase of susceptibility as $T \rightarrow 0$.

At present we do not know of corresponding exact conclusion for the Heisenberg spin $1/2$ model (the results for the quantum XY model are given in Ref. 3). Theodorou and Cohen^[6,7] have advanced the hypothesis that the cluster argument is suitable also for the prediction of the behavior of the susceptibility in the Heisenberg quantum model, and accordingly the susceptibility increases as $T \rightarrow 0$ only in the case when the distribution function $f_j(x)$ is singular. There are grounds, however, for doubting the correctness of this conclusion for the Heisenberg quantum model. In fact, the energy at which the short-range antiferromagnetic correlation is destroyed for the spins k and $k+1$ in the Heisenberg quantum model depends not only on the exchange interaction J_k of the spins k and $k+1$, but also on the structure of the interactions of the other spins of the chain in the vicinity of the sites k and $k+1$. There are therefore no grounds for assuming that the cluster argument is suitable for the description of the loss of short-range order in a chain (i.e., of excitations of the break type).⁴⁾ In addition, for a spin- $1/2$ chain we have no understanding whatever of the relative role of excitations of the spin-wave type, whose contribution to the suscep-

tibility is not accounted for by the cluster argument. Yet we have verified, with continuous classical models with $\alpha = 0$ as an example, that the growth of the susceptibility as $T \rightarrow 0$ can be due only to these excitations.

2. In the classical models, the second moment of the distribution of s increases with decreasing temperature like T^{-2} when the susceptibility has a power-law increase, and increases like $1/T^2 \ln(I_1/T)$ if χ increases logarithmically. In the limit as $T \rightarrow 0$ the distribution of s becomes symmetric about $s = 0$, so that when the temperature decreases the most probable value of s changes from the mean value \bar{s} to zero. We note that the results $\bar{s}(T) \rightarrow 0$ and the growth of $\bar{s}(T)$ as $T \rightarrow 0$ can occur only if $(\bar{s}^2)^{1/2}$ increases faster than \bar{s} with decreasing temperature.

The last conclusion is general and is valid also in the Heisenberg quantum model. Therefore if experiments yields $\bar{s}(T) \rightarrow 0$ and $\chi(T) \rightarrow \infty$ as $T \rightarrow 0$, then the second moment of the NMR line should increase with decreasing temperature faster than $\chi(T)$. We note that in the piecewise model for the quantum case we have $\bar{s}^2 \sim T^{-2}$ as $T \rightarrow 0$, and in another mode of disorder this growth will of course not be faster than T^{-2} .

3. In the classical models the distribution of s has three peaks in the limit as $T \rightarrow 0$ if $\chi \sim T^{-\alpha}$ and α is not very small. As $\alpha \rightarrow 0$ only one peak of the distribution of s remains at $s = 0$.

Arguments can be advanced that the distribution of s as $T \rightarrow 0$ in a spin- $1/2$ system will have only one peak near the value $s = 0$. We consider the piecewise model for the Hamiltonian (1). For an odd piece the average value of the unpaired spin at the site (in a magnetic field) decreases from the edge of the chain towards its middle, and alternates in sign⁵⁾ (thus, for a piece of three spins we have $s_1 = s_3 = h/6T$ and $s_2 = -h/12T$). Therefore even in an odd piece, if large enough, the most probable is a value of s close to zero.

Thus, on the basis of the Heisenberg Hamiltonian for a spin- $1/2$ system with random exchange interaction, we can apparently explain the temperature dependence of the paramagnetic shift of the NMR in $\text{Qn}(\text{TCNQ})_2$ obtained in Ref. 10. It is undoubtedly of interest to measure also the second moment of the NMR line in this compound and to determine on the basis of these data the value of \bar{s}^2 as a function of temperature.

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Note added in proof (20 June 1978). It is shown in Ref. 15 that in a disordered system of fermions with interaction the energy conservation law and the localized character of the wave functions restricts the decay of the quasiparticles, and their damping decreases more rapidly than $(\epsilon - \epsilon_F^2)^2$ when the quasiparticle energy ϵ approaches ϵ_F , if $\rho(\epsilon)$ near ϵ_F is singular. It can be assumed that in this situation, too, the damping of the quasiparticles near ϵ_F is small enough.

¹The question of the applicability of the Fermi-liquid approximation to our system remains open from the theoretical point of view. This approximation does not hold for ordinary ordered one-dimensional systems of fermions with spins, since a charge-density-wave instability and a superconducting instability or a spin-density-wave instability alter the ground state of the system.^{18,91} In a system of spinless fermions there is no spin-density-wave instability or a superconducting instability with momentum $q=0$. In a strongly disordered system we have also no charge-density-wave instability or a superconducting instability with momenta $q \neq 0$. Thus, a system of spinless interacting Fermi particles, equivalent to the Heisenberg Hamiltonian of spin-1/2 particles with random interaction, constitutes a normal Fermi liquid. In the case of a normal three-dimensional homogeneous Fermi liquid the damping of the quasi-particles near the Fermi level is small because of the constraints imposed on the decay by the energy and momentum conservation laws (see Note Added in Proof).

²We know now of magnetic crystals that can be described within the framework of a one-dimensional model of spins with $n=1, 2$, and 3.¹¹¹ It is not clear as yet, however, whether exchange interaction with sufficiently strong disorder can be realized in real compounds in the situations $n=1$ and 2.

³The conclusion that χ increases as $T \rightarrow 0$ in the Heisenberg model as $\alpha=0$ is cited in Ref. 2. It follows from (11) that the growth of χ as $T \rightarrow 0$ in the continuous models ($n=2, 3$) occurs when $f_J(x)$ decreases as $x \rightarrow 0$, but not faster than logarithmically, i.e., not faster than $|\ln x|^{-\beta}$ with $1 > \beta > 0$.

⁴If we consider two neighboring clusters with strong interaction I_0 within the clusters and weak interaction $J_k \ll I_0$ for spins k and $k+1$ on their boundary, then the energy required to destroy the antiferromagnetic order for the spins k and $k+1$ is proportional to J_k only if each cluster has an odd number of spins, and furthermore in this case the proportionality coefficient depends on the number of spins in the clusters. In all the remaining situations the interaction energy of the clusters is proportional to J_k^2 . Under these conditions all the excitations of the quantum

chain can be delocalized, as is the case in the quantum XY model (see Ref. 7). The cluster interpretation cannot be used to describe excitations of the delocalized type.

⁵This result is connected with the fact that in a one-dimensional spin-1/2 system there is no order even at $T=0$.¹¹⁴¹

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Scattering of light in smectic A

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It is shown that because of an anomalous momentum dependence, fluctuations of the deviation of layers (the Landau-Peierls mode) lead to strong fluctuations of the modulus of the order parameter. This produces additional scattering of light, which can be observed at small scattering angles when there is zero momentum transfer in the plane of a layer.

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A smectic liquid crystal of type A is a system with one-dimensional periodicity. In it, as in a nematic, the molecules are oriented along a certain axis; and in addition, there is a density wave along this axis because of ordering of the centers of mass of the molecules. A smectic A is usually represented as a system of layers with a thickness of the order of the length of a molecule, in each of which elongated, rod-shaped mo-

lecules are arranged with their long axes along the normal to the layer. Fluctuations of the displacement of the layers in such a system, with one-dimensional periodicity, were considered by Landau and Peierls.¹¹ Let the layers be perpendicular to the z axis, and let u be the displacement of a layer from the equilibrium position. Then the free energy F of such a system, in the approximation quadratic with respect to u , has the