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Low-temperature properties of the random Heisenberg antiferromagnetic chain

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The one-dimensional quantum spin-$\frac{1}{2}$ Heisenberg antiferromagnetic model with randomly distributed interaction strengths is solved approximately for several different distributions. Ground-state energy and low-temperature properties are evaluated. Universal qualitative features are found in the specific heat and the magnetic susceptibility, which display a power-law dependence on temperature. Such features hold for nonsingular distributions as well as for distributions with power-law divergence at the origin. The approximate method of solution is based on successive eliminations of spins coupled by the maximum coupling constant.

I. INTRODUCTION

In this paper we study some one-dimensional, quantum-mechanical Heisenberg antiferromagnetic systems with randomly distributed coupling constants. These systems are defined by the following Hamiltonian for a chain of L spins:

$$H = \sum_{r=1}^{L-1} K_r \vec{S}_r \cdot \vec{S}_{r+1} \quad , \tag{1.1}$$

where $\vec{S}_r$ are spin-$\frac{1}{2}$ operators. The nearest-neighbor coupling constants K_r are fixed in time and distributed randomly in space. The values of K_r follow a distribution function $P(K)$, $0 < K < J$. The "cutoff" J of the distribution $P(K)$ is taken to be equal to 1. The main results of this paper have been briefly reported earlier.[1]

There are several quasi-one-dimensional systems which provide experimentally accessible realizations of the model Hamiltonian defined in Eq. (1.1). The best known of these systems are the organic charge-transfer compounds *N*-methyl-phenazinium tetracyanoquinodimethanide (NMP-TCNQ), quinolinium-(TCNQ)$_2$, acridinium-(TCNQ)$_2$, and phenazine-TCNQ. Recent experimental[2-4] and theoretical[2,5,6] investigations of the low-temperature magnetic properties of these compounds strongly indicate that their magnetic behavior is that of a random-exchange Heisenberg antiferromagnetic chain. Other experimental systems which have been modeled by the random one-dimensional Heisenberg antiferromagnet include poly-(metal phosphinates)[7] and $(CD_3)_4NMn_xCu_{1-x}Cl_3$(TMMC:Cu).[8] Several approximate calculations of the thermodynamic and magnetic properties of this model have recently been made. These studies were partly motivated by experimental interest. Bulaevskii *et al.*[2] used a canonical transformation to map this model to one of interacting spinless fermions. Then they assumed that the excitation spectrum of the fermion system has a Landau Fermi-liquid character and that the density of states has a power-law singularity of the form $\rho(E) \sim |E|^{-\gamma}$ even if the distribution $P(K)$ is nonsingular at $K = 0$. With these assumptions, they were able to explain the low-temperature thermodynamic and magnetic properties of the TCNQ compounds, including the experimentally observed power-law divergence of the paramagnetic susceptibility as $T \to 0$. However, they were not able to give adequate theoretical justification for their assumptions. Their conclusions were criticized by Theodorou and Cohen[5] who argued that a power-law divergence of the susceptibility can only result from a distribution $P(K)$ which is singular at $K = 0$. Theodorou and Cohen studied the special case of a power-law distribution

$$P(K) \sim K^{c-1} \quad , \tag{1.2}$$

$0 < c < 1$, by using a cluster approximation[5,6] and found that both the paramagnetic susceptibility χ and the specific heat C at low temperatures exhibit power-law dependence on the temperature:

$$\begin{aligned} C &\sim T^c \quad , \\ \chi &\sim T^{c-1} \quad . \end{aligned} \tag{1.3}$$

This behavior is in agreement with the experimental results on the TCNQ compounds. However, some recent calculations by Alexander and Bernasconi[9] on the thermodynamics of a disordered Heisenberg ferromagnetic chain have cast doubts on the validity of the cluster approximation used by Theodorou and Cohen. Recently, Clark and Tippie[10] have studied a model called the exchange–coupled-pair model, which is equivalent to a disordered Heisenberg antiferromagnetic chain with every other coupling removed. This model can be solved exactly. For a power-law distribution of the exchange constants, their results are in agreement with those of Theodorou and Cohen. However, the connection of this model with the random exchange Heisenberg antiferromagnet is not clear. Classical models with fixed-length vectors replacing the spin operators in Eq. (1.1) were also studied previously.[5-7] Exact results were obtained for arbitrary $P(K)$.

Our interest here is to find out how the low-temperature properties of the quantum-mechanical system depend on the form of $P(K)$, in particular, to what extent a power-law singularity in $P(K)$ plays a role. We find that, for a general class of $P(K)$, including both singular and nonsingular cases, there are qualitatively universal properties. For small T, the specific heat C and the susceptibility χ behave approximately like

$$\begin{aligned} C &\propto T^{\gamma_c} , \\ \chi &\propto T^{\gamma_s - 1} , \end{aligned} \tag{1.4}$$

where the exponents γ_c and γ_s are not quite constant but are slowly varying functions of T (in fact, slowly decreasing functions of $\ln 1/T$). The exponents depend on $P(K)$, but not strongly. Also the magnetization M in a uniform external magnetic field h ($T << h \leq 1$) exhibits an approximate power-law dependence on h:

$$M \propto h^{\gamma_M} . \tag{1.5}$$

The exponent γ_M depends weakly on $P(K)$.

There are two important features of our results. First, the singular forms Eqs. (1.4) and (1.5) hold even when $P(K)$ is not singular. This is contrary to the view of some previous workers[5,6] that singular T dependence could not come from a nonsingular $P(K)$. Second, for a power-law distribution given by Eq. (1.2), the results (1.4) and (1.5) also hold and the exponents γ_c and γ_s are not constant as predicted by Eqs. (1.3).

The approach used here is based on successive elimination transformations, each of which eliminates a pair of neighboring spins with the maximum coupling constant. This elimination process lowers the cutoff J for the distribution $P(K)$. Of crucial importance is the fact that an elimination transformation also generates a new effective interaction between the two spins neighboring the eliminated pair. Thus the form of the distribution is modified as well, and one has a modified distribution $P(K,J)$ as a function of J. The elimination transformation is in the spirit of the Born-Oppenheimer approximation in molecular physics, where the electronic variables are eliminated to obtain effecitve interactions among the nuclear coordinates.[11] It is also similar to the renormalization-group transformation in studying scale invariance except that no cell-spin or scale-transformation concept is involved here.[12]

Upon carrying out the elimination transformations approximately, we find that, as J is lowered, $P(K,J)$ quickly approaches a power-law form

$$P(K,J) \rightarrow K^{\alpha-1} , \tag{1.6}$$

where the exponent $\alpha = \alpha(\ln 1/J)$ varies slowly with $\ln 1/J$. This approach to a power law is qualitatively universal, i.e., independent of the form of the initial distribution $P(K)$, and it accounts for the universal singular forms of Eqs. (1.4) and (1.5).

The outline of this paper is as follows. Section II is devoted to the derivation of the elimination transformation and the equation governing the change of $P(K,J)$ as a function of J. This is done in order to illuminate the basic ideas. In Sec. III we show how $P(K,J)$ approaches an approximate power-law form and how the exponent α varies with J. Generalization to nonzero temperatures is carried out in Sec. IV, where the free energy, the specific heat, and the zero-field susceptibility are obtained. We were not able to obtain an exact analytic solution of the equation for $P(K,J)$. Numerical solutions are presented to give quantitative support for the qualitative analyses. The presence of an external magnetic field causes many complications which are studied in Sec. V. The elimination transformations can also be carried out directly, one by one, for a computer-generated model with a prescribed $P(K)$. This numerical procedure bypasses the study of $P(K,J)$ and directly gets to the results; this is presented in Sec. VI. In Sec. VII, we compare our results to those previously obtained from the classical model and from other approximations. We conclude with a discussion of the accuracy of the approximate solution presented in this paper.

II. SUCCESSIVE ELIMINATION OF SPIN VARIABLES

Consider the Hamiltonian H defined by Eq. (1.1) with the distribution of coupling constant $P(K)$, $K \leq J$. The basic ingredient for our approximate analysis is to eliminate spin variables successively and thereby transform $P(K)$ into different distributions with lower values of J. The elimination procedure goes as follows.

Pick the pair of spins, $\vec{S}_1$ and $\vec{S}_2$, with the maximum coupling, i.e., $K = J$. If we ignore the influence of their neighbors $\vec{S}_1'$ and $\vec{S}_2'$ [see Fig. 1(a)], then the Hamiltonian for $\vec{S}_1, \vec{S}_2$ would be

$$H_0 = J\vec{S}_1 \cdot \vec{S}_2 . \tag{2.1}$$

The ground state $|s\rangle$ for H_0 is a singlet, and there are three excited states $|t\rangle$ forming a triplet. The energies are

$$\begin{aligned} E_s &= -\tfrac{3}{4}J , \\ E_t &= \tfrac{1}{4}J , \end{aligned} \tag{2.2}$$

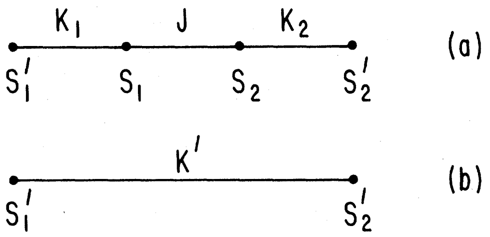

FIG. 1. Spins and coupling constants involved in the elimination transformation, which transforms (a) to (b).

respectively. $\vec{S}_1, \vec{S}_2$ are coupled to neighbors $\vec{S}_1'$ and $\vec{S}_2'$ via

$$\mathcal{H} = K_1 \vec{S}_1' \cdot \vec{S}_1 + K_2 \vec{S}_2 \cdot \vec{S}_2' \ . \tag{2.3}$$

Since J is the maximum value of the coupling constant, let us take into account the effect of $\mathcal{H}$ by perturbation expansion. Regarding $\vec{S}_1'$ and $\vec{S}_2'$ as fixed vectors, the ground-state energy E_s is modified to

$$E_s + \langle s|\mathcal{H}|s\rangle + \sum_t |\langle s|\mathcal{H}|t\rangle|^2 \frac{1}{E_s - E_t} \equiv E' + K' \vec{S}_1' \cdot \vec{S}_2' \ , \tag{2.4}$$

where we have dropped $O(\mathcal{H}^3)$ terms. A little algebra gives

$$\begin{aligned} E' &= -\tfrac{3}{4} J - \frac{3}{16J}(K_1^2 + K_2^2) \ , \\ K' &= \frac{K_1 K_2}{2J} \ . \end{aligned} \tag{2.5}$$

Now we remove the spins $\vec{S}_1, \vec{S}_2$ from the original Hamiltonian and add the effective coupling $K' \vec{S}_1' \cdot \vec{S}_2'$ and the constant E'. The new Hamiltonian should predict approximately the same ground-state properties as the original Hamiltonian. The spirit is the same as that of the Born-Oppenheimer approximation in molecular physics, where the electronic variables are eliminated to provide an effective coupling of nuclear coordinates

One can apply the procedure again, to eliminate the spins with the next strongest coupling. On applying the procedure many times, one alters the distribution $P(K)$: the cutoff value of J is lowered. The change of P when J is lowered to $J - dJ$ is obtained through

$$P(K,J-dJ) = \left\{ P(K,J) + dJ\, P(J,J) \int_0^J dK_1\, dK_2\, P(K_1,J) P(K_2,J) \times \left[\delta\left(K - \frac{K_1 K_2}{2J} \right) - \delta(K - K_1) - \delta(K - K_2) \right] \right\} [1 - 2dJ\, P(J,J)]^{-1} \ . \tag{2.6}$$

Note that $2dJ\, P(J,J)$ is the fraction of spins eliminated. It is convenient to introduce the variable

$$x \equiv K/J \ , \quad 0 \leq x \leq 1 \ , \tag{2.7}$$

and regard P as a function of x and J. Then Eq. (2.6) becomes

$$x \frac{\partial P}{\partial x} - J \frac{\partial P}{\partial J} = P(1,J) J^2 \int_0^1 dx_1\, dx_2\, P(x_1,J) P(x_2,J) \times \delta(x - \tfrac{1}{2} x_1 x_2) \ . \tag{2.8}$$

By solving this equation with a given initial distribution $P(x,1)$, one obtains the transformed distribution $P(x,J)$ for $J < 1$. We proceed to obtain the solution approximately and discuss the implications in the following section.

III. POWER-LAW SOLUTIONS AND THE GROUND-STATE ENERGY

An exact analytic solution to the transformation equation (2.8) would be very difficult, although numerical solution is straightforward. However, a great deal of qualitative and semiquantitative information can be obtained without numerical calculations. We shall present the numerical results at the end of the section.

A. Approximately universal power-law form and variations of exponents

It is clear from Eqs. (2.5) and (2.8) that the new coupling added is less than half of the ones eliminated, i.e.,

$$x < \tfrac{1}{2} x_1, \tfrac{1}{2} x_2 \tag{3.1}$$

in Eq. (2.8). Thus, $P(x,J)$ will grow fast for small x as J is lowered. One would expect $P(x,J)$ to become singular at $x = 0$, even if one starts with a nonsingular initial distribution $P(x,1)$. Such a singularity is most likely a power law of the form

$$P(x,J) \approx \frac{\alpha}{J} x^{-1+\alpha}, \quad \alpha > 0 \ , \tag{3.2}$$

where the prefactor, α/J, comes from the normalization requirement. One can see this by substituting

$P=1$ in the integrand of Eq. (2.8). The integral then gives $\ln(2/x)$, which indicates an increment of the exponent of a power of x.

One naturally asks the following questions: For J substantially less than 1, would $P(x,J)$ approach a universal form independent of $P(x,1)$? Is it a power law Eq. (3.2) with a universal exponent α, and how small does J have to be? It turns out that the only universal power law with a universal exponent is given by $\alpha=0$. The universal form can be approached only for unreasonably small J [i.e., for $\ln(1/J)\to\infty$] and is not useful for our purposes. Fortunately, the power law is approximately correct if we take into account a variation of α as a function of J, provided that α is small. The details are as follows.

Let us substitute the power-law form (3.2) in the Eq. (2.8). The integral is trivial. Equating the coefficients of $x^{\alpha-1}$ and $x^{\alpha-1}\ln x$ on both sides of the equation, one obtains,

$$\alpha+\frac{1}{\alpha}\frac{d\alpha}{d\eta}=-2^{\alpha}\alpha^2\ln 2\ , \tag{3.3a}$$

$$-\frac{d\alpha}{d\eta}=2^{\alpha}\alpha^2\ , \tag{3.3b}$$

$$\eta\equiv-\ln J\ . \tag{3.3c}$$

Clearly, α is overdetermined, indicating that the power-law form cannot be an exact solution even if α is allowed to vary with J. However, for small α, Eq. (3.3a) becomes

$$\begin{aligned}\frac{d\alpha}{d\eta}&=-\alpha^2(1+2^{\alpha}\alpha\ln 2)\\&=-\alpha^2 2^{\alpha}[1+\tfrac{1}{2}\alpha^2(\ln 2)^2+\cdots]\\&=-\alpha^2 2^{\alpha}[1+O(\alpha^2)]\ ,\end{aligned} \tag{3.4}$$

which is approximately the same as Eq. (3.3b). The difference is about 10% for $\alpha\sim\frac{1}{2}$ and 1% if $\alpha\sim\frac{1}{4}$. Thus, we expect that a power law with α determined by Eqs. (3.3) is approximately correct for small α. Integrating Eqs. (3.3), we obtain

$$\eta-\eta_1=-\int_{\alpha_1}^{\alpha}\frac{d\alpha}{\alpha^2}2^{-\alpha}\ , \tag{3.5}$$

where α_1 is the value of α at $\eta=\eta_1\equiv\ln 1/J_1$. Expanding $2^{-\alpha}$ and integrating, we obtain

$$\begin{aligned}\ln J_1/J&=\frac{1}{\alpha}-\frac{1}{\alpha_1}+\ln 2\ln\frac{\alpha}{\alpha_1}\\&\quad-\tfrac{1}{2}(\alpha-\alpha_1)(\ln 2)^2+O(\alpha^2,\alpha_1^2)\ .\end{aligned} \tag{3.6}$$

The limit $\ln 1/J\to\infty$ and $\alpha\to 0$ is of little interest since even for $1/J\sim 10^4$, $\ln 1/J$ is still not large. Figure 2 shows α as a function of $\ln 1/J$ as given by Eq. (3.5).

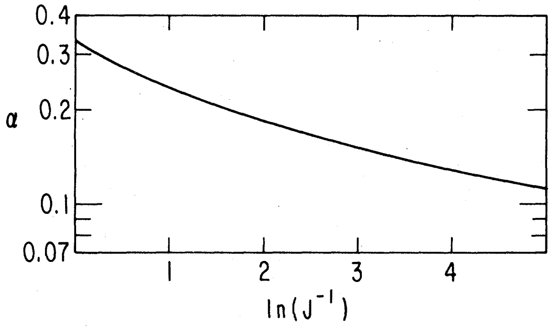

FIG. 2. α as a function of $\ln(J^{-1})$ as given by Eqs. (3.5). Other solutions are obtained by shifting the curve horizontally.

So far we have shown how the exponent α varies as J is lowered given a power-law form at $J=J_1$. What happens if $P(x,J_1)$ does not have a power-law form to start with? A study of Eq. (2.8) linearized around a given power law reveals that a perturbation which is less singular than this power-law form will decay as J decreases. However, if the perturbation is more singular, it will increase. This indicates qualitatively that the most singular part of $P(x,J)$ would grow at the fastest rate as J is lowered. The quantitative answer requires the full solution of the nonlinear equation. A numerical solution, to be presented in Sec. III C of this paper, shows that a power-law form quickly emerges as J is lowered even if $P(x,1)$ is nonsingular. The variation of α follows Eqs. (3.3).

B. Ground-state energy

The ground-state energy can be evaluated in our approximation as follows. Let $N(J)$ be the fraction of spins which remain after lowering the cutoff from 1 to J. Then

$$\begin{aligned}\frac{dN(J)}{N(J)}&=2P(1,J)\,dJ\ ,\\N(J)&=\exp\left[-2\int_J^1 dJ\,P(1,J)\right]\ ,\end{aligned} \tag{3.7}$$

since $2P(1,J)dJ$ is the fraction of spins eliminated when changing J to $J-dJ$. Let $LE(J)$ be the constant term in the effective Hamiltonian, i.e., the accumulation of E' [see Eqs. (2.5)]. We then have

$$\begin{aligned}E(J-dJ)&=E(J)+dJ\,N(J)P(1,J)\\&\quad\times[-\tfrac{3}{4}J-\tfrac{3}{16}J(2\overline{x^2})]\ ,\\\overline{x^2}&\equiv J\int_0^1 dx\,P(x,J)x^2\ .\end{aligned} \tag{3.8}$$

The total ground-state energy per spin is obtained when all spins are eliminated; i.e.,

$$E=-\tfrac{3}{4}\int_0^1 dJ\,N(J)P(1,J)(1+\tfrac{1}{2}\overline{x^2})J\ . \tag{3.9}$$

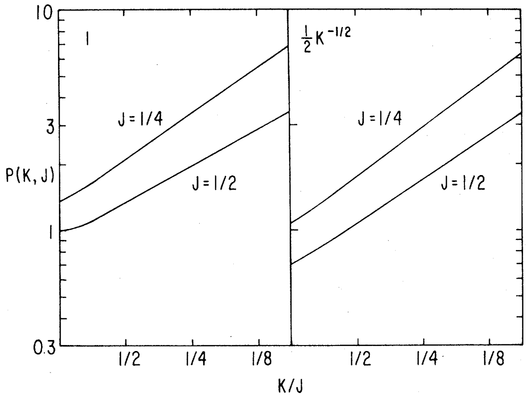

FIG. 3. Emergence of a power law $P(K,J)$ for $J=\frac{1}{2}$ and $\frac{1}{4}$, (a): $P(K,1)=1$, (b): $P(K,1)=\frac{1}{2}K^{-1/2}$ obtained by the numerical solution of Eq. (2.8).

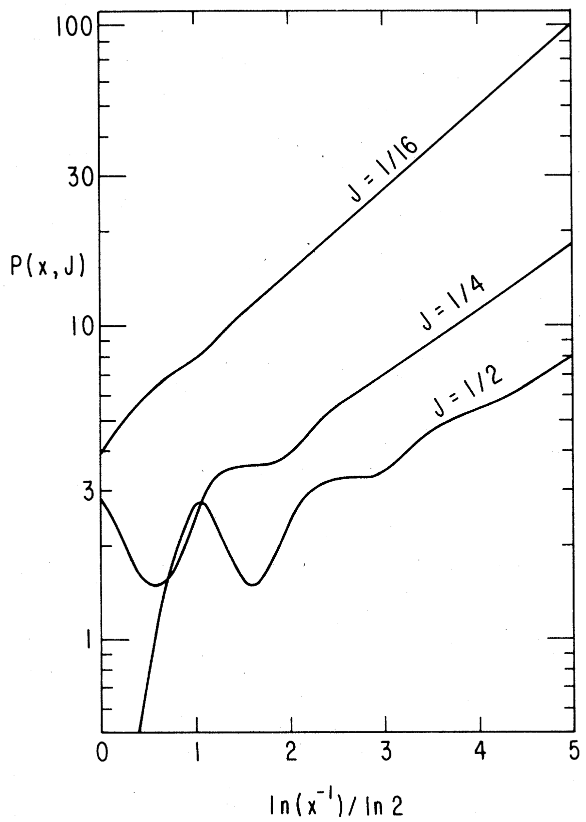

FIG. 4. Emergence of a power law $P(x,J)$ for $P(x,1)=2\theta(x-\frac{1}{2})$.

TABLE I. Ground-state energies per spin (E) for assorted distributions $P(K)$, $0<K<1$.

	E, calculated from	
$P(K)$	Numerical solutions of (2.8)	Direct elimination procedure
$2\theta(K-\frac{1}{2})$	−0.344	−0.341
1	−0.248	−0.246
$1.58e^{-K}$	−0.212	−0.210
$1.34e^{-K^2}$	−0.213	
$\frac{2}{3}K^{-1/3}$	−0.208	
$\frac{1}{2}K^{-1/2}$	−0.180	−0.178
$\frac{1}{3}K^{-2/3}$	−0.144	−0.142
$\frac{1}{5}K^{-4/5}$	−0.104	−0.103

If $P(x,1)$ has power law form with $\alpha=\alpha_1$, then E is easily evaluated using Eq. (3.6). One obtains

$$E=-\frac{3}{4}\alpha_1+\frac{33}{16}\alpha_1^2+\left(\frac{3}{32}+\frac{3}{4}\ln 2-\frac{33}{4}\right)\alpha_1^3+O(\alpha_1^4) \quad . \tag{3.10}$$

If $P(x,1)$ is not of a power-law form, a numerical solution is needed.

C. Numerical solution

The numerical solution of Eq. (2.8) is straightforward. We have obtained $P(x,J)$ starting from a variety of initial distributions. Figures 3 and 4 give the results. Table I gives the values for the ground-state energy per spin.

Since $P(x,J)$ is singular at $x=0$, our numerical solutions to Eq. (2.8) were not very accurate: the error is about 5%. A more sophisticated numerical program would improve the accuracy without difficulty. However, since great accuracy is of no interest at this moment, it was not attempted.

IV. THERMODYNAMIC PROPERTIES

A. Generalization of the elimination transformation

To study thermodynamic properties, we need to generalize our approximation to include the effects of a nonzero temperature $T\equiv 1/\beta$. Let us go back to Sec. II and consider the spins shown in Fig. 1(a). Again regard $\vec{S}_1'$ and $\vec{S}_2'$ as fixed vectors. Instead of calculating the ground-state energy of $\vec{S}_1$ and $\vec{S}_2$ as in Eq. (2.4), we now calculate the free energy to second order in $\mathcal{H}$ [see Eq. (2.3)] so obtaining

$$-\frac{1}{\beta}\ln \mathrm{Tr}_{\vec{S}_1,\vec{S}_2,\vec{S}_1',\vec{S}_2'} e^{-\beta(H_0+\mathcal{H})} = F_0 - \frac{1}{\beta}\ln \mathrm{Tr}_{\vec{S}_1',\vec{S}_2'} e^{-\beta\mathcal{H}_{\mathrm{eff}}} + O(\mathcal{H}^3) \; ,$$

$$F_0 = -\frac{1}{\beta}\ln\mathrm{Tr}_{\vec{S}_1,\vec{S}_2} e^{-\beta H_0} = -\tfrac{3}{4}J - \frac{1}{\beta}\ln(1+3e^{-\beta J}) \; , \tag{4.1}$$

$$\mathcal{H}_{\mathrm{eff}} = \langle\mathcal{H}\rangle_0 - \frac{1}{\beta}\int_0^\beta d\tau \int_0^\tau d\tau' \langle\mathcal{H}(\tau)\mathcal{H}(\tau')\rangle_0 + \tfrac{1}{2}\beta(\langle\mathcal{H}\rangle_0)^2 \; ,$$

where $\langle \cdots \rangle_0$ means averaging over $e^{-\beta H_0}$ and

$$\mathcal{H}(\tau) \equiv e^{\tau H_0}\mathcal{H}e^{-\tau H_0} \; . \tag{4.2}$$

For the H_0 and $\mathcal{H}$ defined in Eqs. (2.1) and (2.3), respectively, $\langle\mathcal{H}\rangle_0$ is zero. The second term in the expression for $\mathcal{H}_{\mathrm{eff}}$ can be written in terms of the matrix elements of $\mathcal{H}$ and the energies of the singlet and the triplet states [see Eqs. (2.2.)]:

$$-\frac{1}{\beta}\int_0^\beta d\tau\int_0^\tau d\tau' \langle\mathcal{H}(\tau)\mathcal{H}(\tau')\rangle_0 = -\frac{1}{1+3e^{-\beta J}}\sum_t |\langle s|H|t\rangle|^2 \frac{1-e^{-\beta J}}{J} - \frac{\beta e^{-\beta J}}{1+3e^{-\beta J}}\sum_{tt'}|\langle t|\mathcal{H}|t'\rangle|^2 \; . \tag{4.3}$$

Substituting Eq. (2.3) for $\mathcal{H}$ in Eq. (4.3) and working out the algebra, one obtains

$$-\frac{1}{\beta}\ln\mathrm{Tr}e^{-\beta(H_0+\mathcal{H})} = F' - \frac{1}{\beta}\ln\mathrm{Tr}_{\vec{S}_1'\vec{S}_2'}\exp(-\beta K'\vec{S}_1'\cdot\vec{S}_2') \; ,$$

$$F' = F_0 - \frac{3}{16J}(K_1^2+K_2^2)V(\beta J) \; , \tag{4.4}$$

$$K' = \frac{K_1K_2}{2J}W(\beta J) \; ,$$

where the functions V and W are defined by

$$V(y) = \frac{1-e^{-y}(1-y)}{1+3e^{-y}} \; ,$$
$$W(y) = \frac{1-e^{-y}(1+y)}{1+3e^{-y}} \; . \tag{4.5}$$

Equation (4.4) is the finite-temperature generalization of Eqs. (2.5). In the limit $T \to 0$ (i.e., $\beta \to \infty$), Eqs. (4.4) and (2.5) agree. The factor W for K' modifies the transformation equation for the distribution $P(x,J)$. Equation (2.8) becomes

$$x\frac{\partial P}{\partial x} - J\frac{\partial P}{\partial J} = P(1,J)J^2\int_0^1 dx_1\,dx_2\,P(x_1,J)P(x_2,J) \times \delta[x - \tfrac{1}{2}x_1x_2W(\beta J)] \; . \tag{4.6}$$

This completes our generalization of the theory of Sec. II to include finite-temperature effects.

For low temperatures, i.e., $T \ll 1$, we expect the factor $W(\beta J)$ in Eq. (4.6) to have no qualitative effect on the solutions obtained in Sec. III. When J is lowered we again expect a power-law form of $P(x,J) \propto x^{-1+\alpha}$ to emerge with α satisfying an equation similar to Eqs. (3.3). Indeed, by a similar calculation one obtains

$$-\frac{d\alpha}{d\eta} = \alpha^2(2/W)^\alpha\{1+O[\alpha^2(\ln W)^2]\} \; , \tag{4.7}$$
$$\eta \equiv -\ln J \; .$$

The power law holds if we drop the $O[\alpha^2(\ln W)^2]$ term in Eqs. (4.7). Since $W(\beta J) < 1$, the exponent α would decrease faster than it does in the $T=0$ case. The quantity $1/W$ does become much larger than 1 for $J \ll T$:

$$\frac{1}{W} \approx 8T^2/J^2 \tag{4.8}$$

according to Eqs. (4.5). However, for $\alpha\ln(1/W)$ to become large, one needs

$$J \lesssim Te^{-1/2\alpha} \; , \tag{4.9}$$

which is a severe condition for small α. Note that $\alpha\ln(1/W)$ cannot be much larger than unity since α decreases as J is lowered and $\alpha < (\ln 1/J)^{-1}$ always. Thus, we expect only slight modification of the results obtained in Sec. II for $P(x,J)$, as long as $J > Te^{-1/2\alpha}$. Numerical calculations have verified this expectation.

B. Free energy and the specific heat

The quantity F' in Eqs. (4.4) gives the free energy of the eliminated pair of spins. Following the same argument for calculating the ground-state energy in Sec. III, we obtain the free energy per spin as

$$F = \int_0^1 dJ\,N(J)P(1,J)\{-T\ln(1+3e^{-J/T}) - \tfrac{3}{4}J[1+\tfrac{1}{2}\overline{x^2}V(J/T)]\} \; , \tag{4.10}$$

where $N(J)$ and $\overline{x^2}$ are defined by Eqs. (3.7) and (3.8), respectively. Equation (4.10) reduces to the ground-state energy Eq. (3.9) for $T \to 0$ [$V(\infty)=1$, see Eqs. (4.5)].

We are interested in the T dependence of the specific heat C for $T \ll 1$. In particular, we want to find out to what extent C follows a nonintegral power law in T. The power-law variation in T is expected in view of the power-law form of $P(x,J)$. The reasoning goes as follows. For J below some value J_1, $P(x,J) \approx (\alpha/J)x^{\alpha-1}$. Therefore, by Eqs. (3.7)

$$N(J) \approx N(J_1)\exp\left[-2\int_J^{J_1} dJ\,\alpha/J\right] , \tag{4.11}$$

for $J < J_1$. If α is approximately constant, then

$$N(J) \propto J^{2\alpha} , \tag{4.12}$$

which would then produce a term proportional to $T^{1+2\alpha}$ in Eq. (4.10) for the free energy and $T^{2\alpha}$ for C. Since α does vary with J, the T dependence cannot be strictly a simple power law. Let us study Eq. (4.10) more closely.

Using the fact that

$$N(J)P(1,J) = \frac{1}{2}\frac{dN(J)}{dJ} , \tag{4.13}$$

[see Eq. (3.9)], we rewrite Eq. (4.10) as

$$F = F^{(0)} - F^{(1)} + F^{(2)} , \tag{4.14}$$

$$\begin{aligned} F^{(0)} &= -\tfrac{1}{2}T\ln(1+3e^{-1/T}) - \tfrac{3}{8}\left[1-\int_0^1 dJ\,N(J)\right] ,\\ F^{(1)} &= \tfrac{1}{2}\int_0^1 dJ\,N(J)f(J/T) ,\\ &\qquad\qquad f(J/T) \equiv (1+\tfrac{1}{3}e^{J/T})^{-1} ,\\ F^{(2)} &= -\tfrac{3}{8}\int_0^1 dJ\,N(J)P(1,J)\overline{x^2}JV(J/T) . \end{aligned} \tag{4.15}$$

Let us concentrate on $F^{(1)}$ first. Because of the factor $f(J/T)$, the integral is effectively cut off near $J \sim T$. For small T, let us assume that $P(x,J)$ has already approached a power-law form $(\alpha/J)x^{\alpha-1}$ so that

$$\begin{aligned} &dN(J)/dJ = 2\alpha N(J)/J ,\\ &N(J) = N(T)\exp\left[-2\int_{\ln(1/T)}^{\eta} d\eta'\,\alpha(\eta')\right] , \end{aligned} \tag{4.16}$$

where $\eta \equiv -\ln J$. Therefore we obtain

$$\begin{aligned} F^{(1)} &= \tfrac{1}{2}TN(T)\\ &\quad\times\int_{-\infty}^{\infty} d\xi\,g(\xi)\exp\left[-2\int_0^{\xi} d\xi'\,\alpha(\xi'+\ln 1/T)\right]\\ &\quad+O(e^{-1/T}) , \end{aligned} \tag{4.17}$$

where we have written $J = e^{-(\xi+\ln 1/T)}$ and

$$g(\xi) \equiv e^{-\xi}f(e^{-\xi}) . \tag{4.18}$$

The ξ integral of Eq. (4.17) turns out to be approximately a constant. Thus the temperature variation of $F^{(1)}$ comes essentially from $TN(T)$:

$$\ln F^{(1)} \approx \ln T + \ln N(T) + \text{const} . \tag{4.19}$$

The derivative of $\ln N(T)$ with respect to $\ln T$ is just 2α [see Eqs. (4.16)]. Thus

$$1+\gamma \equiv \frac{d\ln F^{(1)}}{d\ln T} \approx 1+2\alpha(\ln 1/T) \tag{4.20}$$

gives the slope of $F^{(1)}$ vs T on a log-log plot. Since $\alpha(\eta)$ is a slowly varying function of η, we conclude that

$$F^{(1)} \approx \text{const}\times T^{1+\gamma} , \tag{4.21}$$

with $\gamma \approx 2\alpha$ approximately remaining constant over a range of T. The other terms $F^{(0)}$ and $F^{(2)}$ in Eqs. (4.14) and (4.15) do not have a rapid T variation.

One might expect that the specific heat

$$C = -Td^2F/dT^2 \tag{4.22}$$

would behave like $T^{2\alpha}$ in view of Eqs. (4.20) and (4.21). However, the T dependence of $\alpha(\ln 1/T)$, even though slight, modifies this conclusion considerably. Differentiating $T^{1+2\alpha}$ twice and taking into ac-

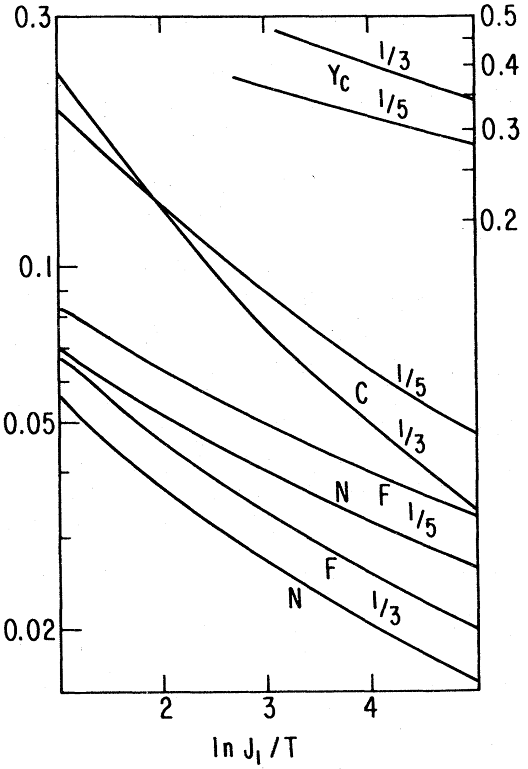

FIG. 5. Evaluation of $F^{(1)}/T$, N, and the specific heat C, assuming $d\alpha/d\eta = -\alpha^2 2^\alpha$ and $P(x,J) = \alpha x^{\alpha-1}/J$ for $J < J_1$ for $\alpha = \frac{1}{3}$ and $\frac{1}{5}$ at $J = J_1$.

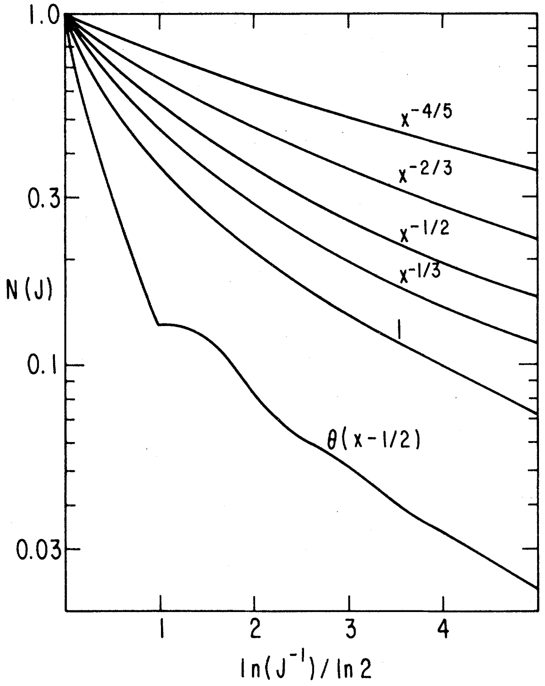

FIG. 6. Behavior of $N(J)$ via the numerical solution of Eqs. (4.6).

count the fact that $d\alpha/d\eta \approx -\alpha^2$, we obtain

$$C \propto T^{\gamma_c} ,\qquad \gamma_c \approx 3\alpha . \tag{4.23}$$

This estimate of γ_c is very crude. One can do a better calculation, without solving Eq. (4.6), by evaluating Eq. (4.17). This means assuming a power-law solution but doing the algebra more accurately. This can be done easily on a desk calculator. Figure 5 shows the results. While $\ln(F^{(1)}/T)$ and $\ln N(T)$ are nearly parallel, the specific-heat curve is steeper. The relationships $\gamma \approx 2\alpha$ and $\gamma_c \approx 3\alpha$ are only qualitatively correct.

The numerical solution to Eq. (4.6) without any assumption gives the results shown in Figs. 6 and 7. We see that the simple power-law calculation shown in Fig. 5 gives good qualitative answers.

C. Magnetic susceptibility

The presence of a magnetic field $\vec{h}$ makes the problem much more complicated. The elimination transformation studied above would generate randomly distributed magnetic fields and other types of interactions. We shall consider these complications in Sec. V. Here we shall study only the susceptibility

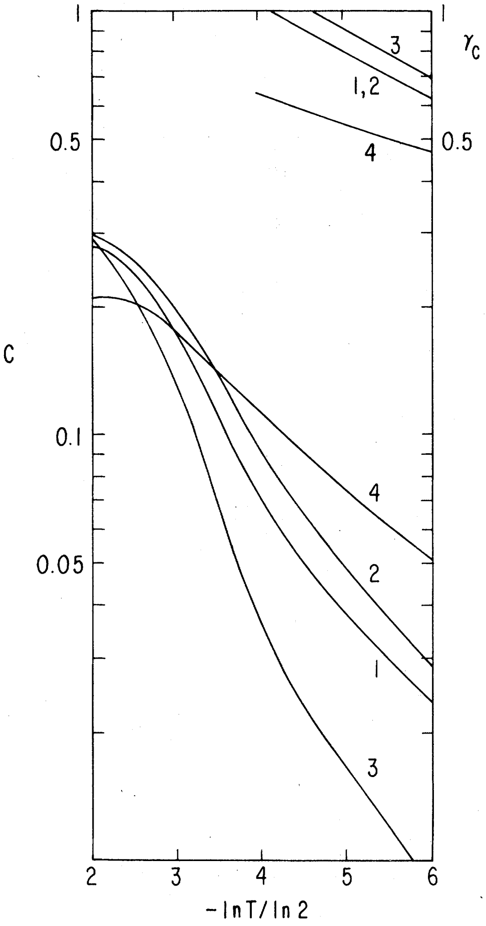

FIG. 7. Specific heat $C \propto T^{\gamma_c}$ calculated via the numerical solution of Eqs. (4.6). Labels 1, 2, 3, and 4 refer to $P(x,1) \propto 1$, e^{-x}, $\theta(x-\frac{1}{2})$, and $x^{-2/3}$, respectively.

for $h \rightarrow 0$. Let the total spin be

$$\vec{S} = \sum_{r=1}^{L} \vec{S}_r . \tag{4.24}$$

The field $\vec{h}$ adds a term $-\vec{h}\cdot\vec{S}$ to the Hamiltonian. Since $\vec{S}$ commutes with the original Hamiltonian, one easily verifies that the susceptibility per spin is

$$\chi = \langle S^2 \rangle / 3TL , \tag{4.25}$$

where the average is evaluated at $h=0$.

The next question is how χ is modified by the elimination transformation. Again we consider the spins in Fig. 1(a) and write

$$\vec{S} \equiv \vec{S}' + \vec{S}_1 + \vec{S}_2 ,$$
$$\langle S^2 \rangle = \langle (\vec{S}_1 + \vec{S}_2)^2 \rangle + 2\langle (\vec{S}_1 + \vec{S}_2)\cdot \vec{S}' \rangle + \langle S'^2 \rangle . \tag{4.26}$$

We then carry out the averaging over the $\vec{S}_1, \vec{S}_2$ variables keeping all other spins as fixed vectors. Some algebra gives

$$\langle S^2\rangle = 2f(J/T) - \frac{2}{3T}f(J/T)\langle(K_1\vec{S}_1' + K_2\vec{S}_2')\cdot\vec{S}\,'\rangle + O(K_1^2, K_2^2, K_1K_2) + \langle S'^2\rangle \ , \tag{4.27}$$

where $f(y) = (1 + e^y/3)^{-1}$ appeared in Eqs. (4.15), and K_1, K_2, $\vec{S}_1'$, $\vec{S}_2'$ were defined earlier [see Fig. 1(a)]. We have kept only first-order terms in K_1 and K_2.

Let $\chi(J)$ be the susceptibility for the remaining spins after the cutoff is lowered to J. The connection between $\chi(J)$ and $\chi(J-dJ)$ can be obtained from Eq. (4.27). Since $\chi = \langle S^2\rangle/3TL$, we have

$$\chi(J) = dJ\, N(J) P(1,J) \times \left[\frac{2}{3T}f(J/T) - \frac{4}{3T}f(J/T)\bar{x}J\chi(J)/N(J)\right] + \chi(J - dJ) \ . \tag{4.28}$$

We have made the approximation

$$\begin{aligned}\langle(K_1\vec{S}_1' + K_2\vec{S}_2')\cdot\vec{S}\,'\rangle &\approx 2\langle K\rangle\langle\vec{S}_1'\cdot\vec{S}\,'\rangle \\ &\approx 2\langle K\rangle\langle S'^2\rangle/LN(J) \\ &\approx 2\langle K\rangle 3T\chi(J)/N(J) \ ,\end{aligned}$$

where

$$\langle K\rangle = J\int dx\, P(x,J)Jx \equiv J\bar{x}(J) \ . \tag{4.29}$$

Integrating the differential relation (4.28), we obtain the susceptibility

$$\chi = \chi(1) = \frac{2}{3T}\int_0^1 dJ\, \tilde{N}(J)P(1,J)f(J/T) \ ,$$

$$\tilde{N}(J) \equiv \exp\left[-2\int_J^1 dJ'\, P(1,J') \times \left(1 + \frac{2J'}{3T}f(J'/T)\bar{x}(J')\right)\right] \ . \tag{4.30}$$

The factor $\tilde{N}(J)$ would reduce to $N(J)$ if the last term involving $\bar{x}$ is ignored. We can obtain the T dependence of χ qualitatively following the same steps in calculating the free energy above. Again assume that $P(x,J)$ has reached a power-law form $x^{\alpha-1}$ for $J < J_1$. For $T < J_1$, we then have

$$\bar{x}(J) \approx \alpha(\ln 1/J)/[1 + \alpha(\ln 1/J)] \ , \tag{4.31}$$

which is small for small α. In parallel to Eq. (4.19), we obtain from Eqs. (4.30)

$$\ln\chi \approx -\ln T + \ln\tilde{N}(T) + \text{const} \ . \tag{4.32}$$

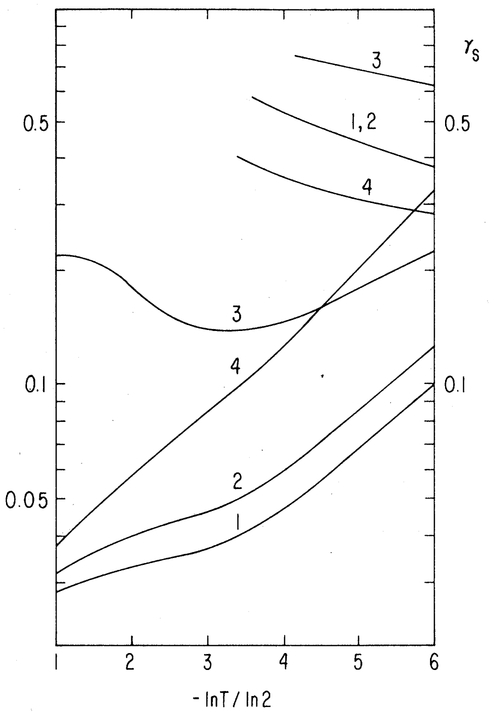

FIG. 8. Susceptibility $\chi \propto T^{\gamma_s - 1}$, obtained by the numerical solution of Eqs. (4.6). The labels 1, 2, 3, and 4 are the same as in Fig. 7.

The slope of χ vs T on a log-log plot is

$$\begin{aligned}-1 + \gamma_s &\equiv \frac{d\ln\chi}{d\ln T} \\ &\approx -1 + 2\alpha(\ln 1/T)[1 + O(\alpha)] \ .\end{aligned} \tag{4.33}$$

Since $\alpha(\eta)$ is slowly varying in η, the susceptibility follows power law

$$\chi \propto T^{\gamma_s - 1} \ , \tag{4.34}$$

with $\gamma_s \approx 2\alpha(\ln 1/T)$. Quantitative results obtained from numerical solutions of Eq. (4.6) are shown in Fig. 8. The universal power-law T dependence is evident at low temperatures. A more complete calculation of χ will be discussed in Sec. VI.

V. EFFECTS OF A MAGNETIC FIELD

As mentioned in the last section, the presence of a uniform external magnetic field $\vec{h}$ in the z direction introduces several complications in the calculation. To first order in perturbation theory, the elimination transformation studied above generates additional magnetic fields acting on the spins $\vec{S}_1'$ and $\vec{S}_2'$. These magnetic fields are functions of J, K_1, and K_2, and are, therefore, randomly distributed. Also, the second-order term in perturbation theory generates a random Ising interaction of the form $LS'_{1z}S'_{2z}$. Thus, in order to treat the effect of eliminating a bond correctly, one has to take into account both the random magnetic field and the Ising interaction. We, therefore, write the Hamiltonian for the four spins shown in Fig. 1(a) as

$$\begin{aligned}
&\mathcal{H}_{\text{total}} = H_0 + \mathcal{H} \;, \\
&H_0 = J\vec{S}_1\cdot\vec{S}_2 + LS_{1z}S_{2z} - h_1S_{1z} - h_2S_{2z} \;, \\
&\mathcal{H} = K_1\vec{S}_1\cdot\vec{S}'_1 + K_2\vec{S}_2\cdot\vec{S}'_2 + M_1S_{1z}S'_{1z} \\
&\qquad + M_2S_{2z}S'_{2z} - h_3S'_{1z} - h_4S'_{2z} \;.
\end{aligned} \tag{5.1}$$

The four eigenstates of H_0 have the following energies:

$$\begin{aligned}
E_1 &= -\tfrac{1}{4}(J+L) - \tfrac{1}{2}x \;, \\
E_2 &= -\tfrac{1}{4}(J+L) + \tfrac{1}{2}x \;, \\
E_3 &= \tfrac{1}{4}(J+L) + \tfrac{1}{2}(h_1+h_2) \;, \\
E_4 &= \tfrac{1}{4}(J+L) - \tfrac{1}{2}(h_1+h_2) \;,
\end{aligned} \tag{5.2}$$

where

$$x = [J^2 + (h_1-h_2)^2]^{1/2} \;.$$

Substituting Eqs. (5.1) for $\mathcal{H}$ in Eqs. (4.1) and using Eqs. (5.2), one obtains

$$-\frac{1}{\beta}\ln \operatorname{Tr} e^{-\beta(H_0+\mathcal{H})} = F' - \frac{1}{\beta}\ln \operatorname{Tr}_{\vec{S}'_1\vec{S}'_2} \exp[-\beta(K'\vec{S}'_1\cdot\vec{S}'_2 + L'S'_{1z}S'_{2z} - h'_1S'_{1z} - h'_2S'_{2z})] \;, \tag{5.3}$$

where

$$\begin{aligned}
F' = &-\frac{1}{\beta}\ln[e^{-\beta E_1}+e^{-\beta E_2}+e^{-\beta E_3}+e^{-\beta E_4}] - [(K_1+M_1)^2+(K_2+M_2)^2] \\
&\times\left[\tfrac{1}{32}\beta\left(\frac{(h_1-h_2)^2}{x^2}(e^{-\beta E_1}+e^{-\beta E_2}) + e^{-\beta E_3}+e^{-\beta E_4}\right) + \frac{J^2}{16x^2}(e^{-\beta E_1}-e^{-\beta E_2})\Big/(E_2-E_1)\right]Z_0^{-1} \\
&-\tfrac{1}{16}(K_1^2+K_2^2)\left(\frac{e^{-\beta E_1}-e^{-\beta E_3}}{E_3-E_1} + \frac{e^{-\beta E_1}-e^{-\beta E_4}}{E_4-E_1} + \frac{e^{-\beta E_2}-e^{-\beta E_3}}{E_3-E_2} + \frac{e^{-\beta E_2}-e^{-\beta E_4}}{E_4-E_2}\right)Z_0^{-1} \\
&+\tfrac{1}{32}\beta(K_1+M_1)^2\left(\frac{h_1-h_2}{x}(e^{-\beta E_1}-e^{-\beta E_2}) - e^{-\beta E_3}+e^{-\beta E_4}\right)^2 Z_0^{-2} \\
&+\tfrac{1}{32}\beta(K_2+M_2)^2\left(\frac{h_1-h_2}{x}(e^{-\beta E_1}-e^{-\beta E_2}) + e^{-\beta E_3}-e^{-\beta E_4}\right)^2 Z_0^{-2} \;,
\end{aligned} \tag{5.4a}$$

$$K' = \frac{JK_1K_2}{4x}\left(\frac{e^{-\beta E_1}-e^{-\beta E_3}}{E_3-E_1} + \frac{e^{-\beta E_1}-e^{-\beta E_4}}{E_4-E_1} - \frac{e^{-\beta E_2}-e^{-\beta E_3}}{E_3-E_2} - \frac{e^{-\beta E_2}-e^{-\beta E_4}}{E_4-E_2}\right)Z_0^{-1} \;, \tag{5.4b}$$

$$\begin{aligned}
L' = &(K_1+M_1)(K_2+M_2)\left[\tfrac{1}{4}\beta\left(\frac{(h_1-h_2)^2}{x^2}(e^{-\beta E_1}-e^{-\beta E_2}) - e^{-\beta E_3}-e^{-\beta E_4}\right) + \frac{J^2}{2x^2}(e^{-\beta E_1}-e^{-\beta E_2})\Big/(E_2-E_1)\right]Z_0^{-1} \\
&+\tfrac{1}{4}\beta(K_1+M_1)(K_2+M_2)\left((e^{-\beta E_3}-e^{-\beta E_4})^2 - \frac{(h_1-h_2)^2}{x^2}(e^{-\beta E_1}-e^{-\beta E_2})^2\right)Z_0^{-2} - K' \;,
\end{aligned} \tag{5.4c}$$

$$h'_1 = h_3 + \tfrac{1}{2}(K_1+M_1)\left(e^{-\beta E_3}-e^{-\beta E_4} - \frac{h_1-h_2}{x}(e^{-\beta E_1}-e^{-\beta E_2})\right)Z_0^{-1} \;, \tag{5.4d}$$

$$h'_2 = h_4 + \tfrac{1}{2}(K_2+M_2)\left(e^{-\beta E_3}-e^{-\beta E_4} + \frac{h_1-h_2}{x}(e^{-\beta E_1}-e^{-\beta E_2})\right)Z_0^{-1} \;, \tag{5.4e}$$

$$Z_0 = e^{-\beta E_1}+e^{-\beta E_2}+e^{-\beta E_3}+e^{-\beta E_4} \;. \tag{5.4f}$$

For $L = M_1 = M_2 = h_1 = h_2 = h_3 = h_4 = 0$, one obtains $L' = h'_1 = h'_2 = 0$, and Eqs. (5.4a) and (5.4b) for F' and K'

reduce, as they should, to the corresponding equations given in Eqs. (4.4). The Eqs. (5.4) are too complicated for an analytic treatment. However, one can use a computer to directly carry out the elimination transformations one by one and numerically calculate the free energy from Eqs. (5.4a)–(5.4f). Once the free energy as a function of the magnetic field is known, all magnetic properties can be calculated. The results obtained from this procedure will be presented in the next section.

One comment on the transformation Eqs. (5.4a)–(5.4f) is appropriate. When the external magnetic field $\vec{h}$ is small compared to the cutoff J, the perturbation expansion used in deriving Eqs. (5.4a)–(5.4f) is in terms of $\langle K\rangle/J$, ($\langle K\rangle$ is a typical value of K_1 or K_2) which is small. For $h >> J$, the expansion parameter is $\langle K\rangle/h$, which is also small. However, for $h \simeq J$, two energy levels of H_0 cross, and $\langle K\rangle/T$ becomes the expansion parameter. For $h << T$ (as, for example, in the calculation of the zero-field susceptibility), this does not cause any problem, because $\langle K\rangle/T \lesssim h/T$ is still very small. But, for $h >> T$ (as, for example, in the calculation of the magnetization in high fields), $\langle K\rangle/T$ may become quite large and the perturbation expansion may break down. For this reason, our results for strong magnetic fields may not be as reliable as those for weak or zero fields.

VI. CALCULATION OF THERMODYNAMIC AND MAGNETIC PROPERTIES BY DIRECT APPLICATION OF THE ELIMINATION TRANSFORMATIONS

The successive elimination of spin variables described in the previous sections can be directly carried out by using a computer. This numerical procedure bypasses the study of the evolution of the distribution function of the coupling constants and directly leads to the free energy. We have used this procedure to calculate the ground-state energy and various thermal and magnetic properties for several distributions of the exchange constants. Owing to the reasons mentioned in the last section, this is the only way we have been able to calculate the magnetic properties. The calculations of the ground-state energy, the free energy, and the specfic heat provide useful checks on the results obtained in Secs. III and IV by numerically solving Eqs. (2.8) and (4.6). The calculational procedure goes as follows.

One starts with a large number of spins arranged regularly on a line. The computer is used to generate the nearest-neighbor coupling constants according to a given distribution. One then searches for the pair of spins which have the largest coupling constant and eliminates that pair. The new couplings for the two spins neighboring the eliminated pair are calculated according to the prescription given above. One then searches for the pair with the next-largest coupling constant, and this process is continued until all the spins have been eliminated. Each application of the elimination transformation generates a contribution $F'(E')$ to the free energy (ground-state energy). The sum of all these contributions gives the total free energy (ground-state energy). In the calculation of the ground-state energy, Eqs. (2.5) are used. The free energy at finite temperatures is calculated by using Eqs. (4.4). The specific heat is obtained by fitting the free energy per spin $F(T)$ to a function of the form

$$F(T)=F(0)-\exp[A+B\ln T+C(\ln T)^2+D(\ln T)^3+E(\ln T)^4] \ , \qquad (6.1)$$

and then differentiating it twice with respect to T. In choosing the form (6.1) we have been guided by the approximate analytic results of Sec. IV B [see Eqs. (4.20) and (4.21)]. In the calculation of the magnetic properties, one starts with $h_r=h$, $L_r=0$ for all r, and the K_r's distributed according to the given probability distribution. One then uses Eqs. (5.4) to calculate the new couplings and the free-energy increment generated by the elimination transformation. The zero-field magnetic susceptibility $\chi(T,0)$ is obtained by calculating the free energy per spin $F(T,h)$ for several very small values of h ($h/T << 1$), and then fitting it to a function of the form

$$F(T,h)=F(T)-\tfrac{1}{2}\chi(T,0)h^2+\chi'(T)h^4 \ . \qquad (6.2)$$

The magnetization $M(T,h)$ in high fields ($h >> T$) is obtained by calculating $F(T,h)$, and also $F(T,h+\Delta h)$, $\Delta h/h << 1$, for several values of Δh, and then fitting the free-energy difference to a polynomial in Δh:

$$F(T,h+\Delta h)-F(T,h)=-M(T,h)\Delta h-\tfrac{1}{2}\chi(T,h)(\Delta h)^2+\chi''(T,h)(\Delta h)^3 \qquad (6.3)$$

The results of our calculations are shown in Table I and in Figs. 9 through 13. These results were obtained by performing the elimination transformations on a chain of 1000 spins with periodic boundary condition, and then averaging over 10 different configurations for each distribution of the coupling constants. The numerical uncertainty (estimated from variations from one configuration to another) is $\lesssim 3\%$ in the calculations of the ground-state energy, the free energy, the specific heat, and the susceptibility, and is $\lesssim 10\%$ in the calculations of the exponents γ_c and γ_s and the magnetization. Because of the rather large uncertainties in the calculated values of the magnetization, we did not calculate the variation of the exponent γ_M with h. Better accuracy can be

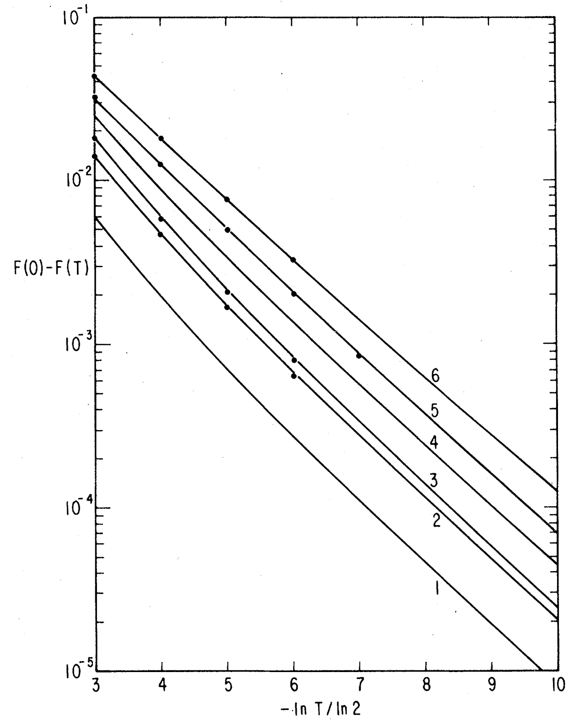

FIG. 9. Free energies (with ground-state energy subtracted off) calculated by the direct elimination procedure. The dots represent results obtained from numerical solutions of Eqs. (4.6). The labels 1, 2, 3, 4, 5, and 6 refer to $P(x,1) \propto \theta(x-\frac{1}{2})$, 1, e^{-x}, $x^{-1/2}$, $x^{-2/3}$, and $x^{-4/5}$, respectively.

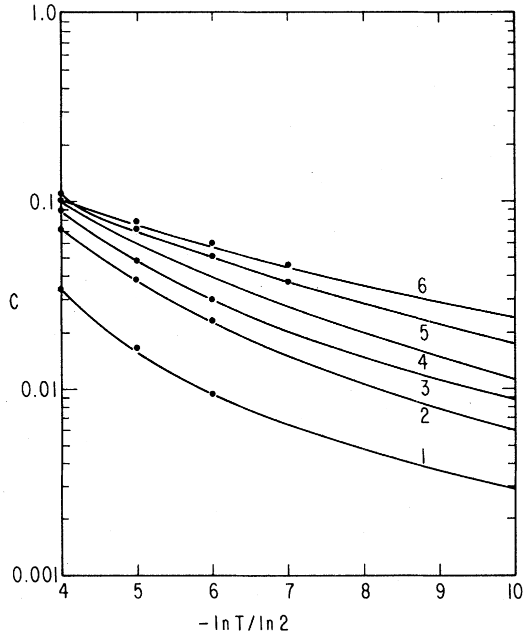

FIG. 10. Specific heat C calculated by the direct elimination procedure. The dots represent results obtained from numerical solutions of Eqs. (4.6). The labels 1–6 are the same as in Fig. 9.

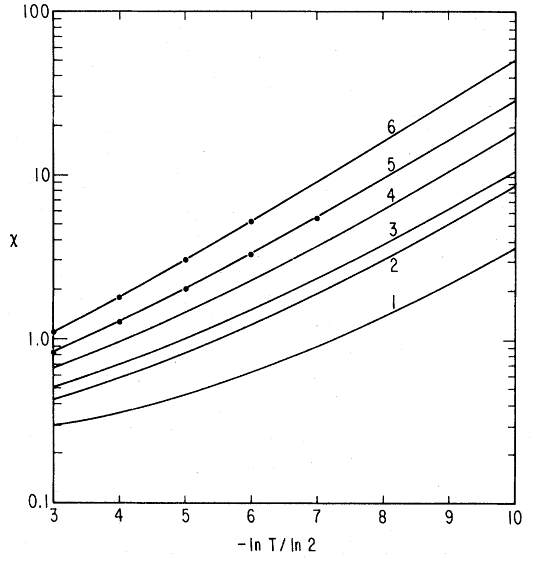

FIG. 11. Zero-field susceptibility χ calculated by the direct elimination procedure. The dots represent results obtained from numerical solutions of Eqs. (4.6). The labels 1–6 are the same as in Fig. 9.

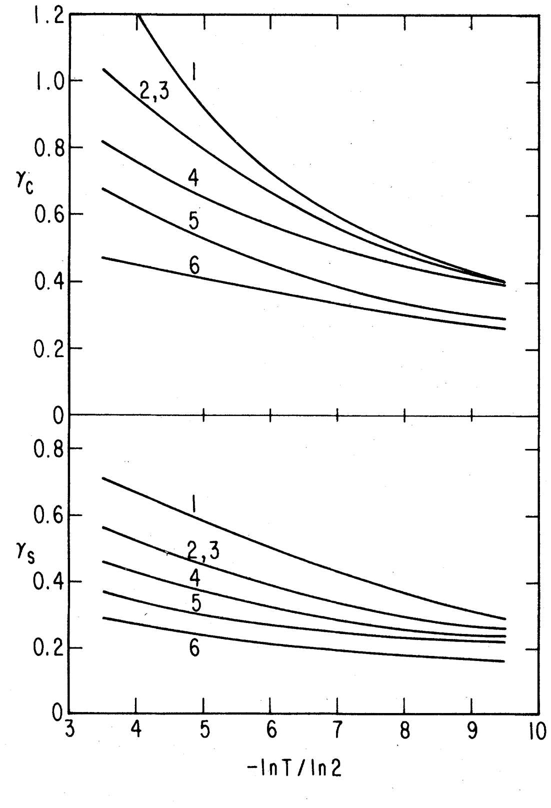

FIG. 12. Specific-heat exponent γ_c and the susceptibility exponent γ_s as functions of temperature for assorted distributions. The labels are the same as in Fig. 9.

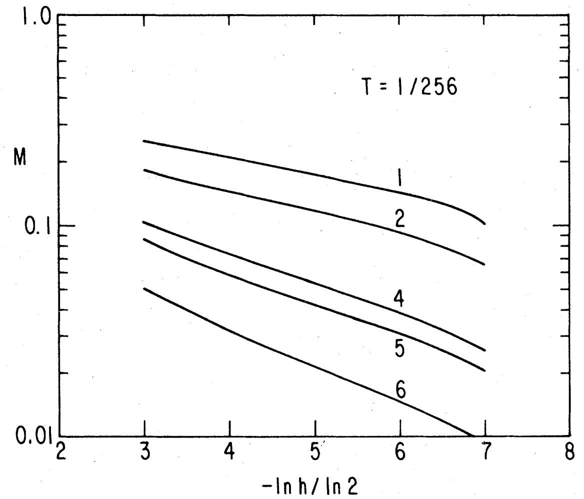

FIG. 13. High-field magnetization M as a function of the magnetic field h for assorted distributions. The labels are the same as in Fig. 9.

obtained either by taking larger samples or by averaging over more configurations.

It is evident from Table I and Figs. 9 and 10 that the results obtained from numerical solutions of Eqs. (2.8) and (4.6) are in good agreement with those obtained from the direct elimination procedure. The calculation of the zero-field susceptibility described in Sec. IV C neglects terms of order K_1^2, K_2^2, K_1K_2, and treats the effects of the random magnetic field in an approximate way, whereas the direct elimination procedure treats everything correctly to second order in perturbation theory. The terms neglected in the first calculation are expected to be unimportant for initial power-law distributions because the perturbation expansion for such distributions should converge very rapidly. That this is indeed the case is clear from Fig. 11, which shows that the values of the susceptibility obtained from the two calculations are in excellent agreement with each other for the power-law distributions 5 and 6. For the nonsingular distributions 1, 2, and 3, the values of χ obtained from the direct elimination procedure are somewhat higher than those obtained from the other method.

VII. DISCUSSION

A. Comparison with results from the classical model

The model studied above is strictly quantum mechanical. It is instructive to compare our results with those derived from the corresponding classical model, which include some exact analytic results. There are qualitative differences, which we discuss below. The comparison will further illuminate the physical picture.

The classical model is defined by the Hamiltonian Eq. (1.1) with the spin operators replaced by classical vectors. It is customary to choose the length of each spin vector to be $[\frac{1}{2}(\frac{1}{2}+1)]^{1/2}=(\frac{3}{4})^{1/2}$. Since the susceptibility is known exactly[7,13] for the classical model, let us start with it:

$$\chi_{\mathrm{cl}}=\frac{1}{4T}\frac{1+\langle u\rangle}{1-\langle u\rangle}\ , \tag{7.1}$$

$$u(K/T)\equiv\frac{4T}{3K}-\coth\frac{3K}{4T}\ , \tag{7.2}$$

where $\langle u\rangle$ is averaged over $P(K)$, the distribution of K. In reading the literature, we often detect the tacit belief that χ_{cl} is nonsingular for nonsingular $P(K)$. This belief is, however, incorrect. For example, take $P(K)=1$, $0<K<1$. We obtain

$$\langle u\rangle=\frac{4T}{3}\ln\left[\frac{3/4T}{\sinh(3/4T)}\right]$$

$$\approx -1+\frac{4T}{3}\ln(3/2T)+O(e^{-1/T})\ , \tag{7.3}$$

which gives a logarithmic singularity in χ_{cl} for $T\rightarrow 0$. Evidently, χ_{cl} has a logarithmic singularity as long as $P(0)$ is nonzero:

$$\lim_{T\rightarrow 0}\chi_{\mathrm{cl}}=\tfrac{1}{6}P(0)(\ln 1/T+\mathrm{const})\ . \tag{7.4}$$

Although χ_{cl} is singular, it is not as singular as the power law T^{γ_s-1} obtained above in the quantum-mechanical case. To understand this discrepancy qualitatively, let us try to apply the method of eliminating spins to the classical model.

The singularities in the susceptibility and the specific heat appeared in the quantum-mechanical case because a singular $P(x,J)$ was generated as J was lowered even though the initial $P(x,1)$ had no singularity. We shall present strong evidence, although not a rigorous proof, that $P(x,J)$ would not be as singular for the classical model.

Again return to Fig. 1(a) and derive the effective coupling constant K' upon eliminating the spins $\vec{S}_1$ and $\vec{S}_2$. For the classical model, the algebra is much easier. Instead of Eqs. (4.4), we obtain

$$K'_{\mathrm{cl}}=-\frac{u(J/T)}{4T}K_1K_2\ , \tag{7.5}$$

where u is the same function as given by Eq. (7.2). This is very different from the quantum-mechanical Eqs. (4.4). While, for Eqs. (4.4), one finds $K'\rightarrow\frac{1}{2}K_1K_2/J$ in the $T\rightarrow 0$ limit, in the classical case we have $K'\rightarrow(1/4T)K_1K_2$, which diverges as $T\rightarrow 0$. This divergence excludes the generation of a power-law singularity in $P(x,J)$. Therefore, no power-law singularity in C and χ are expected in the subsequent calculation using $P(x,J)$. This argument is not rigorous because a large $K'_{\rm cl}$ implies the breakdown of the approximate transformation which requires the generation of small K'.

Theodorou and Cohen[5,6] used the exact result that $\chi_{\rm cl}$ is only weakly divergent for a nonsingular $P(K)$ to argue that a power-law divergence in the susceptibility of the quantum-mechanical model could result only from a singular $P(K)$. Their argument was based on the *assumption* that $\chi_{\rm cl}$ should always be an upper bound for the quantum-mechanical χ. This assumption is, however, incorrect, as is easily checked by explicitly calculating χ and $\chi_{\rm cl}$ for the four-spin system shown in Fig. 1(a). One finds that when $K_1K_2/2JT$ and T/J are small, one has $\chi > \chi_{\rm cl}$. The physical reason is that the quantum-mechanical states are discrete. For small T/J, the spins $\vec{S}_1$, and $\vec{S}_2$ are frozen in a singlet state, and $\vec{S}_1'$ and $\vec{S}_2'$ become essentially free. This does not happen for the classical case where the excitation energy has a continuous spectrum.

B. Comparison with results from other approximations

The Fermi-liquid approximation of Bulaevskii *et al.*[2] predicts the following behavior for the susceptibility, the specific heat, and the magnetization:

$$\begin{aligned} &\chi \propto T^{\gamma-1}, \quad T \ll 1 \;, \\ &C \propto T^{\gamma}, \quad T \ll 1 \;, \\ &M \propto h^{\gamma}, \quad T \ll h \ll 1 \;. \end{aligned} \tag{7.6}$$

The exponent γ does not depend upon the temperature or the magnetic field. These predictions are in good agreement with the experimental results[2-4] for the TCNQ compounds. In our notation, this would correspond to $\gamma_s = \gamma_c = \gamma_M = \gamma$. Our results indicate that both γ_s and γ_c are slowly varying functions of $\ln(1/T)$, although for initial power-law distributions $P(K) \sim K^{c-1}$, $0 < c < 1$, with c close to zero, the temperature dependence is very weak. We also find that γ_c is always greater than γ_s and γ_M is close to γ_s. Bulaevskii *et al.*[2] did not give any prescription for relating the exponent γ to the distribution $P(K)$ of the coupling constants.

Theodorou and Cohen[5,6] used a cluster approximation to study the special cases of singular power-law distributions, $P(K) \sim K^{c-1}$, $0 < c < 1$. They found that

$$\begin{aligned} &\chi \propto T^{c-1}, \quad T \ll 1 \;, \\ &C \propto T^{c}, \quad T \ll 1 \;. \end{aligned} \tag{7.7}$$

In our notation, this corresponds to $\gamma_s = \gamma_c = c$. We find that at relatively high temperatures, $\gamma_s > c$. As the temperature is lowered, γ_s approaches c and becomes less than c at very low temperature. The behavior of γ_c is found to be qualitatively similar to that of γ_s. Another important difference between the conclusions of Theodorou and Cohen and ours is that, while they claim that a singular $P(K)$ is essential for a singular power-law temperature dependence of χ, we find that the approximate power-law form is a universal feature exhibited by both singular and nonsingular distributions.

C. Accuracy of the approximations

There are some difficult unanswered questions about the accuracy of the elimination transformations used in our calculation. Note that improving them means keeping higher-order terms in the perturbation expansion which would generate more complicated forms of interaction such as next-nearest neighbor and longer ranged ones. As a rudimentary check, we solved the four-spin problem of Fig. 1(a) with $K_1 = K_2$ exactly and also by the elimination process. The agreement was found to be quite good if $K/J \lesssim 0.5$. We thus expect our approximation to be quite good as long as $P(K)$ is not peaked near the maximum of K. We also used the elimination transformation to calculate the ground-state energy of the uniform antiferromagnetic chain which has the Hamiltonian of Eq. (1.1) with all the K_r's equal to K. Equation (2.5) was used to eliminate two of every three spins and the ground-state energy was calculated by accumulating the constant term E' generated by each application of the elimination transformation. The result was

$$E/K = -0.45 \;, \tag{7.8}$$

which is quite close to the exact result[14]

$$E/K = -0.44314 \;. \tag{7.9}$$

Since the perturbation expansion should be better in the random case (because both K_1 and K_2 are less than J), we expect our approximate solution to be quite accurate.

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[1] S. Ma, C. Dasgupta, and C. K. Hu, Phys. Rev. Lett. 43, 1434 (1979).

[2] L. N. Bulaesvkii, A. V. Zvarykina, Yu. S. Karimov, R. B. Lyubovskii, and I. F. Shchegloev, Zh. Eksp. Teor. Fiz. 62, 725 (1962) [Sov. Phys. JETP 35, 384 (1972)].

[3] L. J. Azevedo and W. G. Clark, Phys. Rev. B 16, 3252 (1977).

[4] I. F. Schegolev, Phys. Status Solidi 12, 9 (1972).

[5] G. Theodorou and M. H. Cohen, Phys. Rev. Lett. 37, 1014 (1976).

[6] G. Theodorou, Phys. Rev. B 16, 2264, 2273 (1977).

[7] J. C. Scott, A. F. Garito, A. J. Heeger, P. Nannelli, and H. D. Gillman, Phys. Rev. B 12, 356 (1975).

[8] Y. Endoh, G. Shirane, R. J. Birgeneau, and Y. Ajiro, Phys. Rev. B 19, 1476 (1979).

[9] S. Alexander and J. Bernasconi, J. Phys. C 12, L1 (1979).

[10] W. G. Clark and L. C. Tippie, Phys. Rev. B 20, 2914 (1979).

[11] We do not have a clear-cut small parameter like the electron-nuclear mass ratio in the Born-Oppenheimer approximation. What appear in our procedure are the ratios of weak coupling constants and strong coupling constants.

[12] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).

[13] M. E. Fisher, Am. J. Phys. 32, 343 (1964).

[14] L. Hulthen, Ark. Mat. Astron. Fys. A 26, 11 (1938).