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Low-energy density of states for disordered magnetic chains

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We extend earlier calculations of the low-energy density of states of a disordered magnetic chain to a third and intermediate class of random nearest-neighbor exchange interactions. In this intermediate class the probability of a zero-exchange interaction tends to a nonzero constant. We calculate the density of states for systems belonging to this intermediate class using the coherent-potential approximation and compare the results with those of exact numerical calculations on finite arrays. The existence of a logarithmic correction predicted earlier is established.

I. INTRODUCTION

In a recent paper Bernasconi, Schneider, and Wyss[1] derived, among other quantities, the density of states for a disordered one-dimensional chain where the disorder is characterized by random nearest-neighbor exchange interactions. The authors considered a model system which is equivalent to that described by the following infinite set of linearized equations of motion for the spin-raising operators associated with the Heisenberg Hamiltonian $-2\sum_n J_{n,n+1}\vec{S}_n\cdot\vec{S}_{n+1}$:

$$i\frac{dU_n}{dt}=2J_{n-1,n}S(U_{n-1}-U_n)+2J_{n,n+1}S(U_{n+1}-U_n) \quad . \tag{1}$$

Here $J_{n,n+1}=J_{n+1,n}$ are independent non-negative nearest-neighbor exchange interactions between sites n and $n+1$ distributed according to some given probability distribution $P(J)$, S is the spin, and $U_n=s_+^n/S^{1/2}$ is the (normalized) spin-raising operator at site n.

The authors of Ref. 1 solved the above set of equations for $\tilde{U}_n(\omega)$, the Laplace transform of $U_n(t)$, by considering an electrical network analog. The density of states $N(\epsilon)$ is then given by

$$N(\epsilon)=\frac{-1}{\pi}\mathrm{Im}[\langle\tilde{U}_0(-\epsilon+i0^+)\rangle] \quad , \tag{2}$$

where the average $\langle\cdots\rangle$ is defined with respect to the distribution of the $J_{n,n+1}$. The authors considered two classes of probability distributions for J: class (i); $P(J)$ such that

$$\int_0^\infty dJJ^{-1}P(J)<\infty \quad , \tag{3}$$

class (ii);

$$P(J)=\begin{cases}(1-\alpha)J^{-\alpha}, & 0<\alpha<1, \quad 0\leq J\leq 1\\ 0, & \text{otherwise} \quad .\end{cases} \tag{4}$$

Notice that as J goes to zero class (i) $P(J)$ goes to zero whereas class (ii) $P(J)$ go to infinity. Most distributions $P(J)$ of interest for physical problems belong to one of these classes.

At low energies it was found that systems belonging to class (i) show universal behavior resembling an ordered system in that $N(\epsilon)\approx\epsilon^{-1/2}$ whereas class (ii) systems show nonuniversal behavior with $N(\epsilon)\approx\epsilon^{-1/(2-\alpha)}$; i.e., $N(\epsilon)$ for a class (ii) systems depends on the parameter α characterizing the probability distribution for J.

In this paper we consider a disordered magnetic chain characterized by a probability distribution for J which is intermediate to classes (i) and (ii): class (iii); $P(J)$ such that

$$\lim_{J\to 0}P(J)=\text{const}=P_0\neq 0 \quad . \tag{5}$$

We solve for the density of states for systems belonging to class (iii) using the coherent-potential approximation (CPA) and compare the results with data obtained from exact numerical calculations on finite arrays.[2]

II. CPA APPROACH

The coherent-potential approximation, as developed by Tahir-Kheli,[3] and Foo and Bose,[4] can be used to calculate an analytic approximation to the density of states of a disordered magnetic chain characterized by a class (iii) distribution for J. Huber and Ching[5] have recently applied the CPA to systems belonging to classes (i) and (ii) and they have obtained a low-energy density of states for each class which is in excellent agreement with the exact results of Bernasconi *et al.*[1]

In the CPA we consider a magnetic chain to be described by an effective Hamiltonian which retains the symmetry of a perfectly ordered chain and is characterized by a coherent energy-dependent exchange interaction $J_c(\epsilon)$. The coherent exchange interaction is calculated by requiring that the net scattering from a single scatterer $J_{n,n+1}$ inserted in the chain must vanish. That is, we require the average $\langle T \rangle$ of the t matrix to be zero.

This leads to a self-consistent constraint equation for $J_c(\epsilon)$,

$$0 = \langle T \rangle = \int_0^\infty \frac{dJP(J)[J - J_c(\epsilon)]}{1 - [J - J_c(\epsilon)]2f(\epsilon)} \quad , \tag{6}$$

where

$$2f(\epsilon) = \frac{-1}{J_c(\epsilon)} + \frac{\epsilon}{J_c[\epsilon^2 - 4\epsilon J_c(\epsilon)]^{1/2}} \quad . \tag{7}$$

From the complex root $J_c(\epsilon)$ of Eq. (6) we obtain the density of states,

$$N(\epsilon) = \frac{-1}{\pi} \mathrm{Im}\{[\epsilon^2 - 4\epsilon J_c(\epsilon)]^{-1/2}\} \quad . \tag{8}$$

Consider now a particular distribution belonging to class (iii):

$$P(J) = \begin{cases} P_0, & 0 \leq J \leq b \\ 0, & \text{otherwise} \quad . \end{cases} \tag{9}$$

From constraint Eq. (6) we have

$$0 = \int_0^b \frac{dJP_0[(J - J_c)2f - 1 + 1]}{1 - (J - J_c)2f} \quad , \tag{10}$$

$$0 = 1 + \frac{P_0}{2f} \int_0^b \frac{dJ}{J - (J_c + 1/2f)} \quad . \tag{11}$$

Integrating we have

$$\ln(b - \{J_c(\epsilon) + [2f(\epsilon)]^{-1}\}) - \ln(-\{J_c(\epsilon) + [2f(\epsilon)]^{-1}\}) = \frac{-2f(\epsilon)}{P_0} \quad . \tag{12}$$

The above equation can be solved numerically for the complex root $J_c(\epsilon)$ as a function of energy. The results are shown in Fig. 1.

For low energies, $\epsilon \lesssim 5 \times 10^{-3}$, Eq. (12) can be solved explicitly for $J_c(\epsilon)$,

$$J_c(\epsilon)^{-1} = P_0 \ln\epsilon \quad , \tag{13}$$

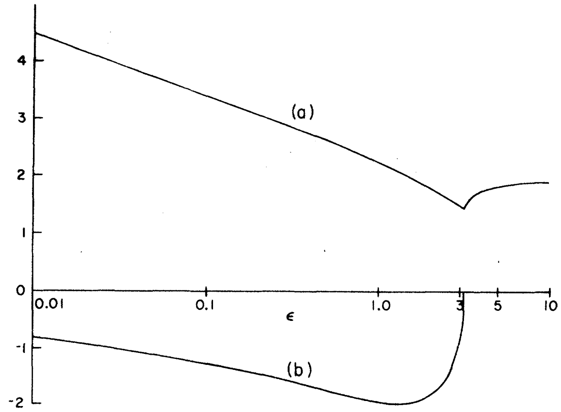

FIG. 1. Results of a numerical solution to constraint Eq. (12) for $J_c(\epsilon)$. (a) $[\mathrm{Re}(J_c)]^{-1}$; (b) $\mathrm{Im}(J_c) \times 10$. $\lim_{\epsilon\to\infty} \mathrm{Re}(J_c) = \frac{1}{2}$. $\mathrm{Im}(J_c) = 0$ for $\epsilon > 3.18$.

and hence at low energies we have

$$N(\epsilon) = \frac{1}{\pi} \left(\frac{P_0}{8}\right)^{1/2} \left(\frac{-\ln\epsilon}{\epsilon}\right)^{1/2} \quad . \tag{14}$$

Notice the anomalous logarithmic correction to the $\epsilon^{-1/2}$ behavior characteristic of the density of states of systems belonging to class (i). This $\ln\epsilon$ correction to the density of states had been predicted earlier by Bernasconi *et al.* on the basis of approximate calculations.[6] Equation (14) can be shown to be valid for all class (iii) systems in the low-energy limit provided the appropriate P_0 is used. It is interesting to note that for class (iii) systems the density of states at low energies depends on the particular $P(J)$ only through its limiting behavior near $J = 0$.

III. EXACT NUMERICAL SOLUTIONS

Starting with the linearized equations of motion for the spin raising operators Eq. (1) and assuming a harmonic time dependence $\epsilon^{-i\omega t}$ for a finite magnetic chain with M spins we are led to the symmetric tridiagonal system of equations

$$U_n = A_{n,n} U_n + A_{n,n+1} U_{n+1} U_{n-1}, \quad 1 \leq n \leq M \quad , \tag{15}$$

where

$$\begin{aligned} A_{n,n} &= 2S(J_{n,n+1} + J_{n-1,n}) \quad , \\ A_{n,n+1} &= -2SJ_{n,n+1} = A_{n+1,n} \quad , \\ A_{n-1,n} &= -2SJ_{n-1,n} = A_{n,n-1} \quad . \end{aligned} \tag{16}$$

We can solve for the energy eigenvalue spectrum of the above system of equations by using Sturm-sequence techniques developed by Dean.[2] As outlined in Ref. 7 we consider the sequence

$$\mu_1(\epsilon)=\frac{2J_{1,2}-\epsilon}{2J_{1,2}}\ ,$$
$$\mu_n(\epsilon)=\frac{2J_{n,n+1}-2J_{n-1,n}-\epsilon}{2J_{n,n+1}}-\frac{J_{n-1,n}}{J_{n,n+1}\epsilon_{n-1}}\ ,\quad 2\le n\le M\ . \tag{17}$$

Here we are considering unit spins at M sites.

The Sturm-sequence property of Eq. (17) implies that the number of changes of sign in the sequence $\mu(\epsilon),\ldots,\mu_M(\epsilon)$, call it $n(\epsilon)$, is equal to the number of eigenvalues less than or equal to ϵ. Therefore $n(\epsilon_b)-n(\epsilon_a)$ is the number of eigenvalues in the interval $[\epsilon_a,\epsilon_b]$ and hence we have for the density of states

$$N\left[\frac{\epsilon_a+\epsilon_b}{2}\right]\simeq\frac{n(\epsilon_a)-n(\epsilon_b)}{M}\ . \tag{18}$$

We have carried out calculations in different energy regions for chains of up to 10^6 atoms assuming the distribution of Eq. (9) with $P_0=1$. The results for a chain with 50 000 sites are plotted as a histogram in Fig. 2. The solid line is the corresponding result obtained from the CPA by multiplying by the interval size $\Delta\epsilon=0.1$ and renormalizing to $M=50\,000$ sites. The Sturm-sequence results shown are the averages and standard deviation of fifteen calculations using different sets of the $J_{n,n+1}$.

IV. RESULTS AND CONCLUSIONS

In Fig. 3 we plot both the CPA and the Sturm-sequence results for $N(\epsilon)$ in the asymptotic region $\epsilon\lesssim 5\times10^{-3}$. The Sturm-sequence histogram has been converted to data points at the centers of the intervals in order to accommodate the $\ln\epsilon$ abscissa.

The equation of the best-fit line through the Sturm-sequence data points leads to the equation for the density of states

$$N(\epsilon)=\frac{M\Delta\epsilon}{\pi}\left[\frac{-\ln\epsilon}{(7.39\pm0.47)\epsilon}\right]^{1/2}\ , \tag{19}$$

where in this case the number sites is $M=10^6$ and

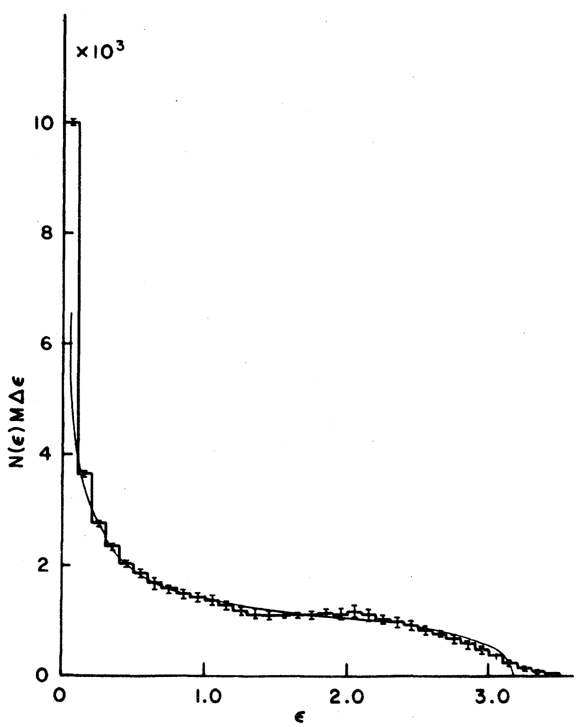

FIG. 2. Histogram of the density of states of a disordered magnetic chain with $M=50\,000$ sites. The histogram is the average of 15 calculations of $N(\epsilon)M\Delta\epsilon$ with the error bars being the standard deviation of $[n(\epsilon+\Delta\epsilon)-n(\epsilon)]$ for each interval. The solid line is the corresponding CPA result multiplied by $M\Delta\epsilon$ where the interval size is $\Delta\epsilon=0.1$.

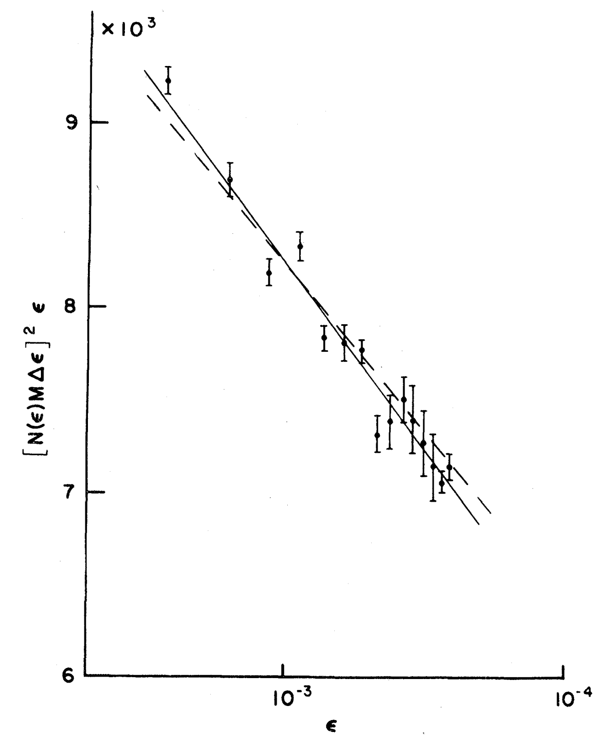

FIG. 3. Low-energy density of states of a disordered magnetic chain with 10^6 sites. The Sturm-sequence histogram results have been converted to data points at the centers of energy intervals. The 50% error bars are obtained from the standard deviations of twenty-two calculations of $[N(\epsilon)M\Delta\epsilon]^2\epsilon$ with different sets of $J_{n,n+1}$. The solid line is the best-fit line through the Sturm-sequence data points. The dashed line is the corresponding asymptotic CPA result.

the interval size is $\Delta\epsilon = 2.5 \times 10^{-4}$. The corresponding result for the CPA is

$$N(\epsilon) = \frac{M\Delta\epsilon}{\pi}\left[\frac{-\ln\epsilon}{8\epsilon}\right]^{1/2}, \qquad (20)$$

from which we see that there is good agreement between the CPA and the exact numerical result. One should note that the CPA is only an approximate theory and therefore we need not necessarily expect perfect agreement with the exact numerical calculation in any limit. Another reason for the slight discrepancy in the denominators in Eqs. (19) and (20) may be that we are not at low enough energies for the analytic asymptotic form of the density of states given in Eq. (14) to hold. The difficulty with pushing the exact calculation to lower energies lies with the problem that as the energy intervals become smaller the number of sites in the magnetic chain must be increased in order to have appreciable statistics in any particular interval. We are eventually limited by computer time as to the maximum size of the chain.

The most important result of this paper is the demonstration of the existence of a logarithmic correction in the low-energy density of states of systems with a class (iii) distribution for J. As noted, the presence of such a correction had been predicted earlier[6] on the basis of approximate calculations. It has been confirmed by our numerical experiment. As in the case of class (i) and class (ii) systems the CPA yields a remarkably good approximation to $N(\epsilon)$ at low energies.

Note added in proof. Equation (14) has also been derived in a recent article by Alexander *et al.* [S. Alexander, J. Bernasconi, R. Orbach, and W. R. Schneider, Rev. Mod. Phys. 53, 175 (1981)].

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