Numerical computation of the density of states for disordered magnetic chains

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Using the negative eigenvalue theorem we compute the density of magnon states for a disordered magnetic chain of 5×10^8 spins. Good agreement is obtained with the asymptotic expansion of the coherent potential approximation for a half-Gaussian distribution of nearest-neighbor interactions.

The authors of several recent papers[1-4] have derived and/or computed the density of magnon states for a disordered one-dimensional chain where the disorder is characterized by random nearest-neighbor interactions. A general model for such a system is the following set of equations:

$$c_n\frac{dP_n}{dt}=w_{n-1,n}(P_{n-1}-P_n)+w_{n,n+1}(P_{n+1}-P_n) \quad . \tag{1}$$

The above equations can also be used to characterize the diffusion and hopping conduction of classical particles, tight-binding electronic states, lattice vibrations of a harmonic chain, and an electrical network.[4] For the electrical network problem, the $w_{n,n+1}$ are line conductances, the c_n are capacitances, and the P_n represent node potentials.

Huber and Ching[2] have used a coherent potential approximation (CPA) to derive an asymptotic formula for the density of states, $\rho(\lambda)$, for Eq. (1) in a system where the w's were distributed continuously with a probability density which was finite at $w=0$. They obtained the result

$$\rho(\lambda)=\frac{1}{\pi}\left[\frac{-P_0\ln\lambda}{8\lambda}\right]^{1/2} , \tag{2}$$

where P_0 denotes the probability density at $w=0$. The parameter λ refers to the eigenvalues of (1) and is equal to the square of the frequency in the magnon problem (see below). Bernasconi, Schneider, and Wyss[5] used an alternative method to arrive at the same expression, which has been shown to be in agreement with the exact result.[6]

Recently, W. R. Schneider derived an analytic formula for the density of states in a system where the interaction constants were distributed according to

$$P(w)=P_0, \quad 0\le w\le P_0^{-1} ,$$
$$=0, \quad w>P_0^{-1} . \tag{3}$$

He obtained the result[7]

$$\rho(\lambda)=\frac{1}{\pi}\left[\frac{-P_0\ln\lambda}{8\lambda}\right]^{1/2}\times\left[1+\frac{1}{2}\frac{\ln(-\ln\lambda)}{-\ln\lambda}+\frac{1}{2}\frac{\ln(2/P_0)}{-\ln\lambda}+\cdots\right] . \tag{4}$$

In this paper we are interested in the determination of the asymptotic density of states for a half-Gaussian distribution

$$P(w)=\frac{2}{\sqrt{2\pi}}e^{-w^2/2}, \quad w\ge0 . \tag{5}$$

For a general distribution the CPA yields

$$\rho(\lambda)=\frac{1}{\pi}\left[\frac{-P_0\ln\lambda}{8\lambda}\right]^{1/2}\times\left[1+\frac{1}{2}\frac{\ln(-\ln\lambda)}{-\ln\lambda}+\frac{1}{2}\frac{\ln(2/A)}{-\ln\lambda}+\cdots\right] . \tag{6}$$

The first two terms of (6) are the same as in Eq. (4). In the CPA they are present for all continuous distributions which are finite at $w=0$. The third term depends on the form of the distribution:

$$\ln A=-\lim_{b\to0}\left[P_0^{-1}\int_b^\infty P(w)w^{-1}dw+\ln b\right] . \tag{7}$$

For the distribution given by Eq. (3) one has $A=P_0$ so that in this case the CPA reproduces the first three terms of the asymptotic expansion. With the half-Gaussian one obtains

$$A=\exp[-(\ln2-\gamma)/2]=0.9437 , \tag{8}$$

where, γ, 0.5772, is Euler's constant.

Equation (6) is difficult to test numerically due to the slow logarithmic variation in the asymptotic region. Previous numerical calculations[2,3] have not been able to compute the density of states of systems large enough to have an adequate statistical distribution of eigenvalues in the asymptotic regime. In this paper we will extend the calculations of Ref. 3 to systems which are sufficiently large to allow a direct test of the asymptotic expansion obtained from the CPA.

The model for our system of disordered spins is a set of classical planar rotators characterized by the interaction energy:

$$V=-\tfrac{1}{2}\sum_{ij}J_{ij}\cos(\theta_i-\theta_j) . \tag{9}$$

This classical model has dynamical behavior equivalent to that described by the linearized equations of motion for the anisotropic Heisenberg Hamiltonian

$$H=-\tfrac{1}{2}\sum_{ij}J_{ij}\vec{S}_i\vec{S}_j+\frac{1}{2I}\sum_i(S_i^z)^2 . \tag{10}$$

In the above equation S_i is the spin operator at site r_i on a regular (periodic) chain, the constant I plays the role of the moment of inertia in the rotator analog, and J_{ij} is the value of the exchange integral between sites r_i and r_j. The exchange integrals are assumed to have a random Gaussian distribution about zero with standard deviation 1 and are

nonzero only for nearest neighbors:

$$P(J)=\frac{1}{\sqrt{(2\pi)}}\exp(-J^2/2)\ . \tag{11}$$

The ground state of the classical planar rotators is obtained by minimizing the total interaction energy. The state of minimum total interaction energy is characterized by each spin pointing in the direction of the local field due to its nearest neighbors. The constraint equation for the ground state of the chain is $\cos(\theta_i^0-\theta_j^0)=\mathrm{sgn}(J_{ij})$, where the angles $\{\theta_i^0\}$ are the equilibrium configuration spin angles.

The equations of motion for the spin angles ϕ, which characterize the deviation of the spins from their equilibrium orientations, take the form

$$I\ddot{\phi}_i=-\sum_j A_{ij}\phi_j\ , \tag{12}$$

where the matrix elements A_{ij} are given by

$$A_{ij}=\delta_{ij}\sum_k|J_{ik}|-(1-\delta_{ij})|J_{ij}|\ , \tag{13}$$

from which it is evident that A_{ij} has the same structure as the dynamical matrix associated with Eq. (1) for $c_n=1$. We note that the exchange energies appear in the dynamical equation only as absolute values. Therefore the "effective" probability distribution for $P(J)$ is a half-Gaussian, and the limiting value of the probability distribution at $J=0$ is $P_0=(2/\pi)^{1/2}$.

We also derived the equations of motion for an XY model Hamiltonian. The result is similar to Eq. (13) above, but with the moment of inertia I replaced by $1/A_{ii}$. This case was found to have a low-energy eigenvalue spectrum similar to that associated with Eq. (12).[8]

The numerical computation of the density of states entails calculating eigenvalues, or at least the distribution of the eigenvalues, of the matrix A. Huber and Ching[2] computed the eigenvalue distribution for chains of 500 spins by directly diagonalizing the dynamical matrix. Their results are in good agreement with the CPA result at moderately low energy. Grassl, Zhao, and Huber[3] used a negative eigenvalue algorithm to compute the eigenvalue distribution for chains of 10^6 spins and were able to compute the density of states down to an energy as low as $\lambda=5\times10^{-4}$.[3] At this energy,

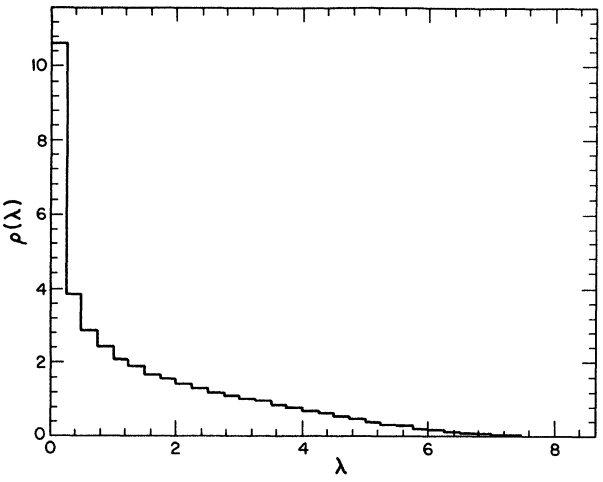

FIG. 1. Distribution of eigenvalues for disordered linear chain of 5×10^8 spins.

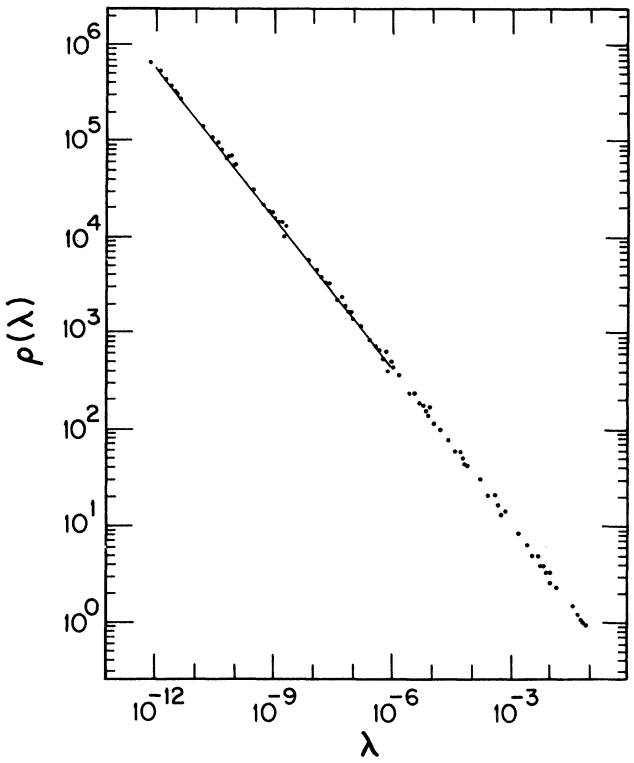

FIG. 2. Low-energy eigenvalue distribution for disordered linear chain of 5×10^8 spins. Solid line is a least-squares fit discussed in the text.

the second and third terms in Eq. (6) still account for approximately 15% of the density of states. Neither of the above studies was able to investigate systems large enough to test the accuracy of Eq. (6) at the level of 1–2%.

Our most recent calculations have involved the eigenvalue distribution for a chain of 5×10^8 spins. Using the negative eigenvalue theorem we were able to extend the computation of the density of states down to an energy of $\lambda=10^{-12}$, and at this energy the second and third terms of Eq. (6) contribute approximtely 7.4%, with the third term being only 1.4%. The entire eigenvalue distribution is shown in Fig. 1, and the low-energy distribution is displayed in Fig. 2. The eigenvalue histogram in Fig. 2 was fit to an expression of the form

$$\frac{1}{\pi}\left[\frac{-P_0\ln\lambda}{8\lambda}\right]^{1/2}\{1-(\alpha/2\ln\lambda)[\ln(-\ln\lambda)+\ln(2/A)]\}\ ,$$

where A is given by Eq. (8), $P_0=(2/\pi)^{1/2}$, and α is a fitting parameter. For λ in the interval $10^{-12}\leq\lambda\leq10^{-6}$ we found $\alpha=0.970$, in good agreement with the CPA value, $\alpha=1$. The difference in the two numbers could reflect the presence of higher-order terms in the asymptotic expansion.

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