Scaling properties of the dynamical structure factor of percolating Heisenberg antiferromagnets

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The scaling behavior of the dynamical structure factor $S(\mathbf{q},\omega)$ of percolating Heisenberg antiferromagnets is investigated in terms of a dynamic scaling argument and numerical calculations. It is found, based on the single-length-scaling postulate, that the asymptotic behavior of $S(\mathbf{q},\omega)$ can be characterized by only two exponents: the dynamic exponent z_a and a new exponent y. This theoretical prediction is confirmed by direct numerical calculations. The values of the exponents z_a and y are determined for the case of $d=2$ percolating Heisenberg antiferromagnets.

The spin dynamics of randomly diluted Heisenberg antiferromagnets (percolating Heisenberg antiferromagnets) has attracted much attention in recent years, because they should possess intriguing dynamical properties originating from their specific geometrical features.[1-6] With respect to the dynamics of elastic percolating systems, fracton excitations have played an important role distinguished from conventional vibrational modes (*phonons*). The dynamics of elastic or ferromagnetic percolating networks is described by equations of motion equivalent to the master equation for diffusing particles.[7] For these dynamical systems, Alexander and Orbach[8] pointed out that the spectral (or fracton) dimension $\tilde{d}$ is the key dimension to describe the dynamical properties of localized excitations in fractal structures, namely, dispersion relation, localization, and the density of states. The conjecture was given[8] that $\tilde{d}$ is equal to $\frac{4}{3}$ for any Euclidean dimension d. Large-scale simulations of the densities of states confirmed that $\tilde{d}$ definitely takes a value very close to $\frac{4}{3}$ for any Euclidean dimension $d(\geq 2)$.[9] The excitations belonging to this class are called *fractons.*

Recently, inelastic neutron-scattering experiments have been performed for three-dimensional percolating antiferromagnet, providing rich information on their dynamical properties.[6,10,11] The dynamical structure factor $S(q,\omega)$ for diluted antiferromagnets have been studied theoretically[12-14] and numerically.[5] The spin systems on a deterministic fractal has been studied by applying a dynamic scaling argument.[15] As shown in Ref. 16, the fracton dimension $\tilde{d}_a$ for antiferromagnetic fractons takes a value close to *unity* independent of the Euclidean dimension d, indicating that antiferromagnetic fractons belong to a different universality class from that of ferromagnetic or vibrational fractons. This is because antiferromagnetic fractons are governed by a different type of differential equation from that for elastic or ferromagnetic system. For this reason, the dynamical properties of antiferromagnetic fractons are interesting.

In this paper, we investigate this issue via the dynamical structure factor $S(\mathbf{q},\omega)$ of percolating Heisenberg antiferromagnets. At first, we predict the frequency and the wave-number dependence of the asymptotic behavior of $S(q,\omega)$ for percolating Heisenberg antiferromagnets, based on the single-length-scaling postulate. These results are confirmed by direct numerical calculations of the dynamical structure factor $S(\mathbf{q},\omega)$ and the localization length $\Lambda(\omega)$ for $d=2$ bond-percolating antiferromagnets at the percolation threshold. $Rb_2Mn_xMg_{1-x}F_4$ is an example of $d=2$ diluted Heisenberg antiferromagnets.[17]

We consider a percolating Heisenberg antiferromagnet, whose Hamiltonian is given by

$$\mathcal{H}=\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{1}$$

where $\mathbf{S}_i$ denotes the spin at the site i, and J_{ij} is the exchange coupling between nearest-neighbor spins. We choose J_{ij} as $J_{ij}=1$ if a bond between sites i and j is present on the percolating network, and $J_{ij}=0$ otherwise. The linearized equation of motion for spin deviation $S_i^+\equiv S_i^x+iS_i^y$ from the Néel state is expressed by, in units of $S/\hbar=1$ where S is the magnitude of single spin,

$$i\frac{\partial S_i^+}{\partial t}=\sigma_i\sum_j J_{ij}(S_i^+ + S_j^+)\ . \tag{2}$$

Here σ_i is a variable taking $+1$ for the site i belonging to the up-spin sublattice and -1 to the down-spin sublattice. This equation is rewritten in the matrix form,

$$\sum_j D_{ij}s_j(\lambda)=\omega_\lambda s_i(\lambda)\ , \tag{3}$$

where $\{s_i(\lambda)\}$ is the eigenvector belonging to the eigenfrequency ω_λ. The matrix element D_{ij} is defined by

$$D_{ij}=\sigma_i\left[J_{ij}+\delta_{ij}\sum_k J_{ik}\right]\ . \tag{4}$$

From this definition, one sees the matrix $[D_{ij}]$ is *asymmetric*, due to sign σ_i and the sign of the second term in the parentheses of the right-hand side, which is different from the symmetric ones for lattice vibrations or ferromagnetic spin waves.

The dynamical structure factor $S(q,\omega)$ averaged over all possible realizations of percolating networks is characterized by a function of $q(=|\mathbf{q}|)$ due to the spherical symmetry of the systems. Based on the single-length-scaling postulate (SLSP) as in the case of elastic vibrations,[18-20] $S(q,\omega)$ for antiferromagnetic fractons is given by the following scaling form, with the characteristic

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length $\Lambda(\omega)$:

$$S(q,\omega)=q^{-y}F[q\Lambda(\omega)] , \tag{5}$$

where $F(x)$ is a scaling function, and y is a new exponent characterizing $S(q,\omega)$. In the long-wavelength limit $q\xi \ll 1$, where ξ is the correlation length, Christou and Stinchcombe[21] have obtained, using a Green's-function technique, an analytic expression of $S(q,\omega)$ of percolation antiferromagnets which satisfies the dynamical scaling hypothesis. Their result suggests that $S(q,\omega)$ takes a Lorentzian form with respect to frequency ω. In view of the matching long-wavelength modes ($q\xi \ll 1$) with antiferromagnetic fractons ($q\xi \gg 1$) at the magnon-fracton crossover, where the wavelength of fracton $2\pi/q \approx \xi$ (see also Ref. 5), the frequency dependence of $S(q,\omega)$ should take a Lorentzian form even in the short-wavelength fracton regime. The Lorentzian form of $S(q,\omega)$ is written as

$$S(q,\omega)=G(q)\frac{\Gamma(q)}{[\omega-\omega_c(q)]^2+\Gamma^2(q)} , \tag{6}$$

where $\Gamma(q)$ and $G(q)$ denote the width of the line shape and the q-dependent function, respectively. The characteristic frequency $\omega_c(q)$ represents the peak position of $S(q,\omega)$ in the frequency space. The SLSP [Eq. (5)] requires that both $\omega_c(q)$ and the linewidth $\Gamma(q)$ obey the same power law as $\omega_c(q)=\omega_0 q^{z_a}$ (the dispersion relation) and $\Gamma(q)=\Gamma_0 q^{z_a}$, respectively, where z_a is the dynamic exponent for percolating antiferromagnets. This exponent is related to the fracton dimension $\tilde{d}_a$ as $z_a=D_f/\tilde{d}_a$ (D_f is the fractal dimension).[8] By comparing Eq. (6) with Eq. (5), one obtains $G(q)=G_0 q^{z_a-y}$ where G_0 is a constant, namely, $S(q,\omega)$ becomes

$$S(q,\omega)=G_0\frac{\Gamma_0 q^{2z_a-y}}{(\omega-\omega_0 q^{z_a})^2+\Gamma_0^2 q^{2z_a}} . \tag{7}$$

Equation (7) predicts that $S(q,\omega)$ takes the power law as $\omega^{-2}q^{-y+2z_a}$ for $q\Lambda(\omega) \ll 1$, and q^{-y} for $q\Lambda(\omega) \gg 1$.

We have performed numerical calculations to confirm the above predictions for the asymptotic properties of $S(q,\omega)$, and determined the value of the exponents z_a and y. The dynamical structure factor $S(q,\omega)$ is related to the generalized susceptibility $\chi(\mathbf{q},\omega)$

$$S(\mathbf{q},\omega) \propto \langle n(\omega)+1 \rangle \mathrm{Im}[\chi(\mathbf{q},\omega)] , \tag{8}$$

where $\langle n(\omega)+1 \rangle = 1/(1-e^{-\hbar\omega/k_B T})$ is the Bose factor.[12] The generalized susceptibility $\chi(\mathbf{q},\omega)$ is defined by the spatial-Fourier transform of the two-point susceptibility $\chi_{ij}(\omega) \equiv S_i^+(\omega)/h_j^+(\omega)$. The symbols $S_i^+(\omega)$ and $h_j^+(\omega)$ represent the temporal-Fourier transform of $S_i^+(t)$ and the transverse field $h_j^+(t)$, respectively. In the following calculations, the Bose factor is neglected because we consider $T=0$ and $p=p_c$, at the multicritical point.[22] We define the matrix $[N_{ij}(\omega)]$ as $N_{ij}(\omega) \equiv \sigma_i(\omega\delta_{ij}-D_{ij})$, satisfying $\sum_j N_{ij}(\omega)S_j^+(\omega)=-h_i^+(\omega)$. Thus, $\chi_{ij}(\omega)$ can be obtained from the inverse of the matrix $N_{ij}(\omega)$ by $\chi_{ij}(\omega)=-[N^{-1}(\omega)]_{ij}$.[23] The spatial Fourier transform $\chi(\mathbf{q},\omega)$ can be written, using eigenvectors $\{s_i(\lambda)\}$ calculated by numerical diagonalization of the matrix $[D_{ij}]$,

$$\begin{aligned}\chi(\mathbf{q},\omega)&=\frac{-1}{V}\sum_i\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_i}\{N^{-1}(\omega)\}_{ij}e^{-i\mathbf{q}\cdot\mathbf{R}_j}\\&=\frac{-1}{V}\sum_\lambda\frac{1}{\omega-\omega_\lambda}\left\{\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}\tilde{s}_i(\lambda)\right\}\\&\quad\times\left\{\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}s_j(\lambda)\right\} ,\end{aligned} \tag{9}$$

where $\tilde{s}_i(\lambda)$ is defined by $\sum_i\sigma_i\tilde{s}_i(\lambda)s_i(\lambda')=\delta_{\lambda,\lambda'}$, and $S(\mathbf{q},\omega)$ is written as

$$\begin{aligned}S(\mathbf{q},\omega)&=\lim_{\delta\to+0}\mathrm{Im}[\chi(\mathbf{q},\omega+i\delta)]\\&=\frac{\pi}{V}\sum_\lambda\delta(\omega-\omega_\lambda)\left\{\sum_i e^{-i\mathbf{q}\cdot\mathbf{R}_i}\tilde{s}_i(\lambda)\right\}\\&\quad\times\left\{\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}s_j(\lambda)\right\} ,\end{aligned} \tag{10}$$

where $\mathbf{R}_i$ denotes the positional vector of site i.

We have treated $d=2$ bond-percolating Heisenberg antiferromagnets at the percolation threshold ($p_c=0.50$) with periodic boundary conditions. The ensemble average has been taken over 54 percolating networks formed on 62×62 square lattices. We have calculated the eigenvalues and the eigenvectors of matrix $\{D_{ij}\}$ by a direct diagonalization technique. At first, we have calculated the frequency dependence of localization length $\Lambda(\omega)\sim\omega^{-1/z_a}$. The localization length $\Lambda(\omega)$ is obtained from the eigenvectors $\{s_i(\lambda)\}$ by the Thouless criterion for localization[24]

$$\{\Lambda(\omega)\}^{-D_f}=\frac{\langle\sum_i|s_i(\lambda)|^4\rangle_\omega}{\langle\{\sum_i|s_i(\lambda)|^2\}^2\rangle_\omega} , \tag{11}$$

where $\langle \cdots \rangle_\omega$ denotes the average over all eigenmodes λ with frequencies close to ω. The calculated result of $\Lambda(\omega)$ is shown in Fig. 1. The filled circles and the vertical bars represent the averaged values and the deviations of the localization length $\Lambda(\omega)$, respectively. Our result indicates $z_a=1.83\pm0.08$, which implies $\tilde{d}_a=1.03\pm0.04$

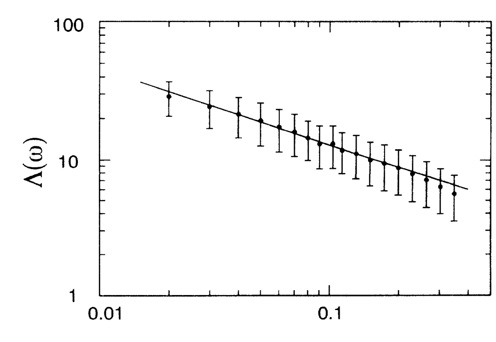

FIG. 1. The frequency dependence of the localization length $\Lambda(\omega)$ for $d=2$ bond-percolating antiferromagnets at p_c on 62×62 square lattices. The ensemble average is taken over 54 samples.

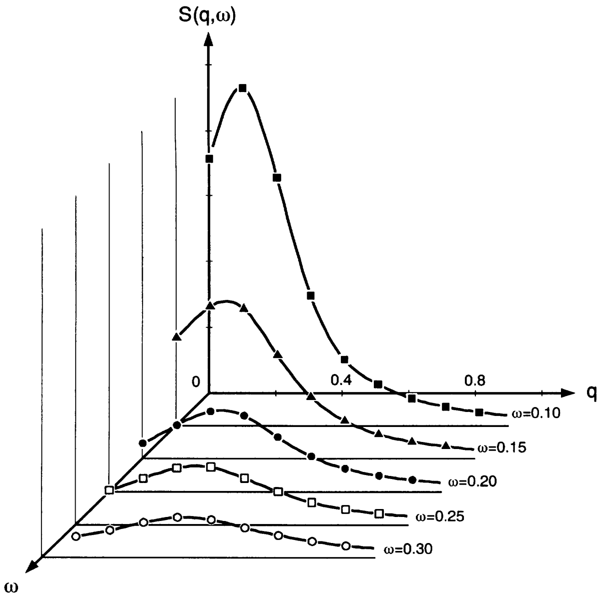

FIG. 2. The frequency and the wave-number dependence of $S(q,\omega)$ for $d=2$ bond-percolating antiferromagnets at p_c on 62×62 square lattice.

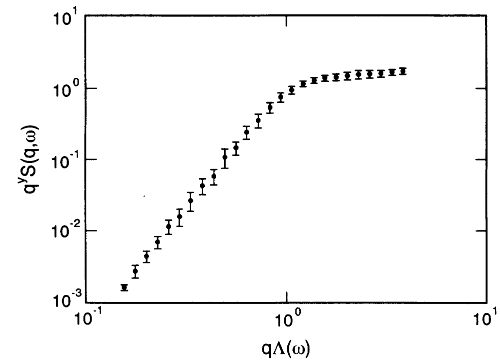

FIG. 3. The scaling function $F[q\Lambda(\omega)]\equiv q^yS(q,\omega)$ as a function of $q\Lambda(\omega)$. The filled circles and the vertical bars represent the averaged values and the statistical errors of $F[q\Lambda(\omega)]$, respectively.

from the relation $\tilde{d}_a=D_f/z_a$, where $D_f=91/48$ for $d=2$. The value of $\tilde{d}_a$ agrees well with our previous work.[16] As shown in Fig. 1, the localization length $\Lambda(\omega)$ ranges from 6 to 30 lattice spacing. So the finite-size effect is negligible in the high-frequency regime, except $\Lambda(\omega)\approx 30$.

Second, we have calculated the dynamical structure factor $S(q,\omega)$ using the eigenvectors $\{s_i(\lambda)\}$ on the same networks with those of the localization length $\Lambda(\omega)$. The frequency and the wave-number dependence of $S(q,\omega)$ obtained numerically are shown in Fig. 2 in a linear scale. Each solid line is only a guide to the eye. These results indicate that the linewidth increases rapidly as increasing peak position. The value of the exponent y in Eq. (5) is evaluated by the least-squares fitting from the q dependence of $S(q,\omega)$ with fixed values of $q\Lambda(\omega)$, as $y=3.0\pm 0.3$. Figure 3 is a plot of calculated values for the scaling function $F[q\Lambda(\omega)]=q^yS(q,\omega)$ as a function of $q\Lambda(\omega)$ using the above value of y. Filled circles represent the average value over data within a narrow range of scaling variables $q\Lambda(\omega)$. The vertical error bars indicate the width of the distribution. The universal curve in Fig. 3 exhibits that antiferromagnetic fractons satisfy the SLSP. The profile of the scaling function $F[q\Lambda(\omega)]$ in Fig. 3 indicates that the frequency dependence of $S(q,\omega)$ behaves asymptotically as $S(q,\omega)\propto\omega^{-1.9\pm 0.1}$ for $q\Lambda(\omega)\ll 1$ and the wave-number dependences as $S(q,\omega)\propto q^{0.5\pm 0.1}$ for $q\Lambda(\omega)\ll 1$ and $S(q,\omega)\propto q^{-2.8\pm 0.1}$ for $q\Lambda(\omega)\gg 1$. Taking into account the values of $z_a=1.83\pm 0.08$ and $y=3.0\pm 0.3$, these results satisfy our theoretical predictions [see below Eq. (7)] with respect to the frequency and the wave-number dependence for $S(q,\omega)$.

In conclusion, we have investigated scaling properties of the dynamical structure factor $S(q,\omega)$ of percolating Heisenberg antiferromagnets at p_c. We have predicted the asymptotic form of $S(q,\omega)$ based on the single-length-scaling postulate. The numerical results of the frequency and the wave-number dependence of $S(q,\omega)$ on $d=2$ bond-percolating antiferromagnets agree well with the scaling predictions. The values of the exponents z_a and y have been determined numerically. We hope that these findings stimulate further neutron-scattering experiments.

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