Numerical method for large-scale non-Hermitian matrices and its application to percolating Heisenberg antiferromagnets

Takamichi Terao
Department of Applied Physics, Hokkaido University, Sapporo 060, Japan

Kousuke Yakubo*
Department of Physics, University of California, Los Angeles, California 90024-1547

Tsuneyoshi Nakayama
Department of Applied Physics, Hokkaido University, Sapporo 060, Japan
(Received 18 February 1994)

A numerical method is developed for calculating the spectral density of states, eigenvalues, and eigenvectors of very large non-Hermitian matrices with real eigenvalues. We also present an efficient method to calculate the dynamic correlation function of the system described by non-Hermitian matrices. The effectiveness of the method is demonstrated by applying it to percolating classical Heisenberg antiferromagnets.

PACS number(s): 02.90.+p, 02.60.−x, 75.40.Mg, 75.50.Ee

I. INTRODUCTION

Eigenvalue analyses of very large matrices are important in many fields of physics [1], so efficient numerical algorithms, particularly suitable to advanced supercomputers, have been developed. It is becoming common to work with Hermitian matrices having a degree N of 10^6 or more. Among these, the forced oscillator method [2,3] is powerful enough to accurately compute the spectral densities of states, eigenvalues, and eigenvectors of very large matrices. This method is based on the principle that a linear mechanical system when driven by a periodic external force of frequency Ω will respond with large amplitudes in those eigenmodes close to this frequency. One can treat, in general, eigenvalue problems of very large $N\times N$ Hermitian matrices, by mapping them onto those of lattice dynamics. The algorithm [2,3] has been successfully applied to eigenvalue problems of large-scale *Hermitian* (or symmetric) matrices. Examples are fracton dynamics [4], photon localization [5], quantum-spin systems [6], electronic structures of amorphous systems [7], and $\pm J$ Ising spin glass [8].

It is highly desirable to extend the forced oscillator method (FOM) to be applicable to large-scale non-Hermitian matrices (with complex number elements). The eigenvalue analyses for *non-Hermitian* matrices are important in many areas of condensed matter physics such as antiferromagnets [9,10], spin glasses [11,12], electronic structures [13], and the master equation in nonequilibrium thermodynamics [14]. The standard method for treating an eigenvalue problem of $N\times N$ non-Hermitian matrices is the diagonalization techniques, such as the QR method or the Arnoldi method [15]. [The term QR method comes from the "QR decomposition" of a given matrix A as $A=QR$, where Q and R represent a unitary matrix Q and a right (or upper) triangular matrix R, respectively.] These have, however, a serious problem requiring a large amount of computer memory space, which makes it difficult to treat an eigenvalue problem of very large non-Hermitian matrices. Another difficulty arises due to the fact that, in general, eigenvalues of non-Hermitian matrices are sensitive to small changes in matrix elements [15]. This difficulty is due to the lack of orthogonality among eigenvectors for non-Hermitian matrices. From these mathematical difficulties, practical algorithms have not yet been developed for the analysis of large non-Hermitian matrices. The purpose of this paper is to extend the FOM [2,3] to be applicable to an eigenvalue problem of very large non-Hermitian matrices with real eigenvalues. We also present an efficient algorithm to calculate the dynamic correlation function $S(\mathbf{q},\omega)$. The advantage of the algorithm is that it is not necessary to perform the spatio-temporal Fourier transform of the correlation function $S(\mathbf{r},t)$. An application is made for percolating classical Heisenberg antiferromagnets.

In Sec. II, we present general arguments on the FOM [2,3] extended to non-Hermitian matrices. In Sec. III, the algorithm for calculating the dynamic correlation function, i.e., the dynamical structure factor $S(\mathbf{q},\omega)$, is given by illustrating classical Heisenberg antiferromagnets. Section IV presents calculated results obtained by applying the present algorithm to percolating classical Heisenberg antiferromagnets. Conclusions are given in Sec. V.

II. FORCED OSCILLATOR METHOD EXTENDED

A. Spectral density of states

We focus our attention, in the following general arguments, on an eigenvalue problem of a nonsymmetric matrix $\{D_{mn}\}$ with real number elements. The condition is not essential for our algorithm. In fact, the extension is

*Permanent address: Department of Applied Physics, Hokkaido University, Sapporo 060, Japan.

straightforward to the case of non-Hermitian matrices with complex elements [16]. A nonsymmetric (as well as non-Hermitian) matrix has two sets of eigenvectors called *right* eigenvector $|u(\lambda)\rangle$ defined by [1,17]

$$\omega_\lambda u_m(\lambda)=\sum_n D_{mn}u_n(\lambda)\ , \tag{1}$$

and *left* eigenvector $\langle v(\lambda)|$ given by

$$\omega_\lambda v_m(\lambda)=\sum_n v_n(\lambda)D_{nm}\ . \tag{2}$$

These eigenvectors belong to the same eigenvalue ω_λ. We can assume hereafter that all eigenvalues ω_λ are *positive* without loss of generality, because one can rewrite Eqs. (1) and (2) as

$$(\omega_\lambda+\omega_0)u_m(\lambda)=\sum_n (D_{mn}+\delta_{m,n}\omega_0)u_n(\lambda) \tag{3}$$

and

$$(\omega_\lambda+\omega_0)v_m(\lambda)=\sum_n v_n(\lambda)(D_{nm}+\delta_{m,n}\omega_0)\ , \tag{4}$$

where an appropriate amount of ω_0 should be added so that the minimum value of $\omega_\lambda+\omega_0$ is positive. Though left (or right) eigenvectors do not form orthogonal sets due to the nonsymmetricity of the matrix $\{D_{mn}\}$, biorthogonality conditions are present between them [1,17]. These are written as

$$\sum_\lambda |u(\lambda)\rangle\langle v(\lambda)|=\mathbf{I} \tag{5a}$$

and

$$\langle v(\lambda)|u(\lambda')\rangle=\delta_{\lambda,\lambda'}\ , \tag{5b}$$

where $\mathbf{I}$ is the unit matrix. The mapping of Eqs. (3) and (4) onto the equations of vibrational motion is done by [2,3]

$$\frac{d^2}{dt^2}x_m(t)=-\sum_n D'_{mn}x_n(t)\ , \tag{6}$$

$$\frac{d^2}{dt^2}y_m(t)=-\sum_n D'_{nm}y_n(t)\ , \tag{7}$$

where D'_{mn} is defined as $D'_{mn}=D_{mn}+\delta_{m,n}\omega_0$, and $x_m(t)$ and $y_m(t)$ denote the displacements of the site m. Since $|u(\lambda)\rangle$ forms a complete set of vectors [note that $|u(\lambda)\rangle$ does not form an orthogonal set, but they are *linearly independent*], the displacement $x_m(t)$ can be decomposed into a set of right eigenvectors $|u(\lambda)\rangle$ as

$$x_m(t)=\sum_\lambda P_\lambda(t)u_m(\lambda)\ , \tag{8}$$

where $P_\lambda(t)$ is the amplitude of the right eigenvector $|u(\lambda)\rangle$, and varies as $\sim\exp(-i\mu_\lambda t)$ $(\mu_\lambda^2\equiv\omega_\lambda+\omega_0)$ as seen from substituting Eq. (8) into (6). In the same way, the displacement $y_m(t)$ can be expanded by a set of left eigenvectors $\langle v(\lambda)|$ as

$$y_m(t)=\sum_\lambda Q_\lambda(t)v_m(\lambda)\ , \tag{9}$$

where $Q_\lambda(t)$ is the amplitude of the left eigenvector $\langle v(\lambda)|$, and varies as $\sim\exp(-i\mu_\lambda t)$.

The spectral density of states is calculated by the following procedure. The displacements $x_m(t)$ and $y_m(t)$ are set to be zero at $t=0$, then the periodic "forces" $F_m\cos(\Omega t)$ are imposed on each site m in Eqs. (6) and (7). Here F_m should be chosen as

$$F_m=F_0\cos(\phi_m)\ , \tag{10}$$

where ϕ_m is a random quantity taking a value within the range $0\le\phi_m<2\pi$, and F_0 is a constant.

As a next step, we calculate the quantity $\tilde{E}(t)$ defined by

$$\begin{aligned}\tilde{E}(t)&=\tfrac{1}{2}\left\{\sum_m \dot{x}_m(t)\dot{y}_m(t)+\sum_m\sum_n y_m(t)D'_{mn}x_n(t)\right\}\\&=\tfrac{1}{2}\sum_\lambda\{\dot{P}_\lambda(t)\dot{Q}_\lambda(t)+\mu_\lambda^2P_\lambda(t)Q_\lambda(t)\}\ ,\end{aligned} \tag{11}$$

where the biorthogonality condition Eq. (5b) is used. We introduce the quantities $\xi_\lambda(t)$ and $\eta_\lambda(t)$ defined by $\xi_\lambda(t)\equiv\dot{P}_\lambda(t)+i\mu_\lambda P_\lambda(t)$, and $\eta_\lambda(t)\equiv\dot{Q}_\lambda(t)+i\mu_\lambda Q_\lambda(t)$. After a time interval T, $\xi_\lambda(t)$ becomes, using Eqs. (3), (6), and (8),

$$\begin{aligned}\xi_\lambda(T)&=\frac{e^{i\mu_\lambda T}}{2}\sum_m F_m v_m(\lambda)\left[\frac{e^{i(\Omega-\mu_\lambda)t}}{i(\Omega-\mu_\lambda)}-\frac{e^{-i(\Omega+\mu_\lambda)t}}{i(\Omega+\mu_\lambda)}\right]_0^T\\&\approx\frac{e^{i\mu_\lambda T}}{2}\left\{\sum_m F_m v_m(\lambda)\right\}\frac{e^{i(\Omega-\mu_\lambda)T}-1}{i(\Omega-\mu_\lambda)}\ ,\end{aligned} \tag{12}$$

where the second term in the square brackets of Eq. (12) is neglected because the contribution from $\Omega\approx\mu_\lambda$ is dominant. In the same way, $\eta_\lambda(t)$ is obtained as

$$\eta_\lambda(T)\approx\frac{e^{i\mu_\lambda T}}{2}\left\{\sum_m F_m u_m(\lambda)\right\}\frac{e^{i(\Omega-\mu_\lambda)T}-1}{i(\Omega-\mu_\lambda)}\ . \tag{13}$$

Utilizing these quantities $\xi_\lambda(t)$ and $\eta_\lambda(t)$, the right-hand side of Eq. (11) is rewritten as $\frac{1}{2}\sum_\lambda\xi_\lambda^*(t)\eta_\lambda(t)$. Thus, one has

$$\begin{aligned}\tilde{E}(T)=\tfrac{1}{2}\sum_\lambda&\left\{\sum_m F_m v_m(\lambda)\right\}\\&\times\left\{\sum_n F_n u_n(\lambda)\right\}\frac{\sin^2\{(\mu_\lambda-\Omega)T/2\}}{(\mu_\lambda-\Omega)^2}\ .\end{aligned} \tag{14}$$

The averaged value of $\tilde{E}(T)$ over ϕ_m becomes

$$\begin{aligned}\langle\tilde{E}(T)\rangle&=\frac{F_0^2}{2}\sum_\lambda\frac{\sin^2\{(\mu_\lambda-\Omega)T/2\}}{(\mu_\lambda-\Omega)^2}\\&\qquad\times\left\langle\sum_m\sum_n v_m(\lambda)u_n(\lambda)\cos(\phi_m)\cos(\phi_n)\right\rangle\\&\approx\frac{F_0^2}{4}\sum_\lambda\frac{\sin^2\{(\mu_\lambda-\Omega)T/2\}}{(\mu_\lambda-\Omega)^2}\ ,\end{aligned} \tag{15}$$

where $\langle\cdots\rangle$ denotes the random phase average and the terms satisfying $m=n$ remain in the summation for m and n. For sufficiently large time T, the modes λ's con-

tributing to the sum in Eq. (15) are those belonging to eigenfrequencies μ_λ within the narrow range of $\mu_\lambda \approx \Omega$. For very large systems, it is not necessary to average over all possible ensembles $\{\phi_m\}$ explicitly. It suffices to choose a single configuration of $\{\phi_m\}$. Provided that the proper time interval T is used, Eq. (15) yields

$$\langle \tilde{E}(T,\Omega)\rangle \approx \frac{\pi T F_0^2}{8}\sum_\lambda \delta(\mu_\lambda-\Omega)=\frac{\pi T N F_0^2}{8}\tilde{\mathcal{D}}(\Omega)\ , \tag{16}$$

where $\tilde{\mathcal{D}}(\Omega)$ is the density of states for the mapped system. The spectral density $\mathcal{D}(\omega)$ for the original system is obtained as

$$\mathcal{D}(\omega)=\left|\frac{d\mu(\omega)}{d\omega}\right|\tilde{\mathcal{D}}(\mu)=\frac{4}{\pi T N F_0^2\sqrt{\omega+\omega_0}}\langle E(T,\mu)\rangle\ . \tag{17}$$

The calculated spectral density $\mathcal{D}(\omega)$ should be normalized unity by

$$\int_{-\infty}^{\infty}\mathcal{D}(\omega)d\omega=1\ . \tag{18}$$

The forced oscillator method enables us to calculate the density of states with an arbitrary resolution of frequency $\delta\omega$ by taking the proper time interval T. Let us describe the criterion for the choice of the time T to control the resolution $\delta\omega$. The frequency width of resonance $\delta\mu$ for the *mapped* system should be chosen as $\delta\mu \approx |d\mu(\omega)/d\omega|\delta\omega$, where $\delta\omega$ is the eigenvalue resolution required for the *original* system. Equation (15) indicates that the frequency width $\delta\mu$ is inversely proportional to the time T, as given by $\delta\mu \approx 4\pi/T$. Since $\mu_\lambda^2=\omega_\lambda+\omega_0$, the time interval T should be taken as $T\approx 4\pi/[|d\mu(\omega)/d\omega|\delta\omega]=8\pi\sqrt{\omega+\omega_0}/\delta\omega$ to gain the required resolution $\delta\omega$. In actual calculations, a small time step τ for time development must satisfy the condition $\mu_{\max}\tau<2$, where $\mu_{\max}$ is the maximum frequency of the mapped system. This means that a large ω_0 requires a small time step τ. This makes the CPU time large because the CPU time is proportional to computational steps ($=T/\tau$). In this point of view, the value of ω_0 should be chosen to perform efficient computations. In addition, the resolution $\delta\omega$ of the original system must satisfy the condition $\delta\omega \gg \Delta\omega$ [$\approx 1/N\mathcal{D}(\omega)$], where $\Delta\omega$ is the level spacing between adjacent eigenvalues $\{\omega_\lambda\}$ at the eigenvalue ω and $\mathcal{D}(\omega)$ is the spectral density of states per site. The condition $\delta\omega \ll \omega$ is also important to calculate accurately the spectral density of states at very small eigenvalues.

B. Eigenvalues and their eigenvectors

Let us describe the procedure to compute right and left eigenvectors. For right eigenvectors $|u(\lambda)\rangle$, the equation of motion with the external force $F_m\cos(\Omega t)$ is written as, using Eqs. (6) and (8),

$$\sum_\lambda\left\{\frac{d^2P_\lambda(t)}{dt^2}+\mu_\lambda^2P_\lambda(t)\right\}u_m(\lambda)=F_m\cos(\Omega t)\ . \tag{19}$$

By multiplying the left eigenvector $\langle v(\lambda')|$ and taking the sum for m in Eq. (19), one obtains the equation for the amplitude $P_\lambda(t)$, by using Eq. (5b),

$$\frac{d^2P_\lambda(t)}{dt^2}+\mu_\lambda^2P_\lambda(t)=\sum_m\{F_m v_m(\lambda)\}\cos(\Omega t)\ . \tag{20}$$

Equation (20) is solved with the initial condition $P_\lambda(t=0)=0$ as

$$P_\lambda(t)=\left\{\sum_m F_m v_m(\lambda)\right\}\times\frac{2\sin\{(\Omega+\mu_\lambda)t/2\}\sin\{(\Omega-\mu_\lambda)t/2\}}{\Omega^2-\mu_\lambda^2}\ , \tag{21}$$

and the amplitude of $x_m(t)$ after the time interval T yields, using Eq. (8),

$$x_m(T)=\sum_\lambda\left\{\sum_n F_n v_n(\lambda)\right\}\times\frac{2\sin\{(\Omega+\mu_\lambda)T/2\}\sin\{(\Omega-\mu_\lambda)T/2\}}{\Omega^2-\mu_\lambda^2}\times u_m(\lambda)\ . \tag{22}$$

For sufficiently large time T, only a few eigenmodes with eigenfrequencies μ_λ close to Ω have large amplitudes. One can accelerate the calculation by replacing the amplitude of the periodic force F_m at each site m by

$$F_m=x_m(T)\ . \tag{23}$$

Initial amplitude $x_m(t=0)$ at the site m is set to be zero again, and we follow the time developments of Eq. (6) with the external force $F_m\cos(\Omega t)$. After p iterations of this procedure, the amplitude $x_m(T)$ becomes

$$x_m^{(p)}(T)=\sum_\lambda\left\{\sum_n F_n v_n(\lambda)\right\}\left[\frac{2\sin\{(\Omega+\mu_\lambda)T/2\}\sin\{(\Omega-\mu_\lambda)T/2\}}{\Omega^2-\mu_\lambda^2}\right]^p u_m(\lambda)\ . \tag{24}$$

For sufficiently large p, only a single eigenmode λ_1 ($\mu_{\lambda_1}\approx\Omega$) survives such as

$$x_m^{(p)}(T)\approx C u_m(\lambda_1)\ , \tag{25}$$

where C is a constant. The eigenvalue μ_{λ_1} for the calculated right eigenvector $|u(\lambda_1)\rangle$ is obtained as follows. We define the quantities a_m, b_m, and δ_m given by [3]

$$a_m\equiv\sum_n D'_{mn}b_n\ , \tag{26}$$

where

$$b_m\equiv x_m^{(p)}(T)\ . \tag{27}$$

We introduce the quantity δ_m defined by

$$\delta_m\equiv a_m-\tilde{\mu}^2 b_m\ , \tag{28}$$

where $\tilde{\mu}$ is a quantity to be defined later. We see from Eqs. (26)–(28) that if the displacement $x_m^{(p)}(T)$ is equal to the eigenvector $u_m(\lambda_1)$ and $\tilde{\mu}=\mu_{\lambda_1}$, δ_m vanishes for any m. The normalized sum of the deviation δ^2, defined below, expresses the degree of convergence

$$\delta^2 \equiv \frac{\sum_m \delta_m^2}{\sum_m a_m^2} . \tag{29}$$

The quantity $\tilde{\mu}$ should be chosen as the deviation δ^2 to be minimized. By differentiating Eq. (29) with respect to $\tilde{\mu}^2$, the deviation δ^2 takes the minimum value

$$\delta^2 = 1 - \frac{\left[\sum_m a_m b_m\right]^2}{\left[\sum_m a_m^2\right]\left[\sum_m b_m^2\right]} , \tag{30}$$

when

$$\tilde{\mu}^2 = \frac{\sum_m a_m b_m}{\sum_m b_m^2} . \tag{31}$$

If the quantity δ is very small, $\tilde{\mu}$ becomes quite close to the eigenfrequency of the mapped system. Provided that the calculated $x_m^{(p)}(T)$ converges to the *right* eigenvector $|u(\lambda)\rangle$, the deviation δ approaches to zero. One can judge the convergence of the eigenvector from the magnitude of δ. In the same way, one can calculate the *left* eigenvector $\langle v(\lambda)|$ and its eigenvalue. The eigenvalue $\tilde{\omega}_\lambda$ of the original system is obtained by the relation $\tilde{\omega}_\lambda=\tilde{\mu}^2-\omega_0$. For the criterion of the time interval T for obtaining eigenvalues and eigenvectors, see Appendix A.

III. ALGORITHM CALCULATING DYNAMIC CORRELATION FUNCTION

This section describes an efficient method to calculate the dynamic correlation function of the system described by a nonsymmetric matrix $\{D_{mn}\}$. This algorithm enables us to treat very large systems compared with the direct diagonalization methods [15], without performing the Fourier transform of the spatio-temporal correlation function $S(\mathbf{r},t)$ of the system. The following is an application of the algorithm to classical Heisenberg antiferromagnets.

The Hamiltonian for Heisenberg antiferromagnets is given by

$$\mathcal{H} = \sum_{\langle mn \rangle} J_{mn}\mathbf{S}_m\cdot\mathbf{S}_n \tag{32}$$

where $\mathbf{S}_m$ denotes the spin vector at the site m, and J_{mn} the exchange coupling between nearest-neighbor sites m and n. The linearized equation of motion for spin waves is written, in units of $S/\hbar=1$,

$$i\frac{\partial}{\partial t}S_m^+(t)=\sigma_m\sum_n J_{mn}\{S_m^+(t)+S_n^+(t)\} , \tag{33}$$

where $S_m^+(t)$ is the spin deviation at the site m, and σ_m is a variable taking $+1$ at the site m belonging to the up-spin sublattice and -1 for the down sublattice. The equation of motion is transformed into a matrix form

$$\omega_\lambda u_m(\lambda)=\sum_n D_{mn}u_n(\lambda) , \tag{34}$$

where D_{mn} is the matrix element defined by $D_{mn}=\sigma_m J_{mn}$ for $m\neq n$, $D_{mm}=\sigma_m\sum_n J_{mn}$, and $u_m(\lambda)$ is the element of the eigenvector λ.

The dynamic structure factor for antiferromagnetic spin waves is defined by [18–20]

$$\begin{aligned} S(\mathbf{q},\omega) &= (n+1)\chi''(\mathbf{q},\omega) \\ &= (n+1)\pi\sum_\lambda \delta(\omega-\omega_\lambda)\left\{\sum_m e^{-i\mathbf{q}\cdot\mathbf{R}_m}\sigma_m v_m(\lambda)\right\} \\ &\quad\times\left\{\sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n}u_n(\lambda)\right\} , \end{aligned} \tag{35}$$

where $(n+1)$ is the Bose factor expressed by $1/(1-e^{-\beta\omega})$, $\chi''(\mathbf{q},\omega)$ is the imaginary part of generalized susceptibility, $\mathbf{R}_m$ is the positional vector of the site m, and $v_m(\lambda)$ is the element of left eigenvector of the matrix $\{D_{mn}\}$ (see Appendix B). Let us define the symbols $u'_m(\lambda)\equiv\sigma_m u_m(\lambda)$ and $v'_m(\lambda)\equiv\sigma_m v_m(\lambda)$ in Eq. (35). From the properties of matrix $\{D_{mn}\}$ defined in Eq. (34), $u_m(\lambda)$ and $v'_m(\lambda)$ are related with $v'_m(\lambda)=A_\lambda u_m(\lambda)$, where A_λ is a constant depending on the mode λ (see Appendix C). From this relation, one finds that the product $\{\cdots\}\{\cdots\}$ in Eq. (35) becomes a real quantity. Equation (35) is then rewritten as

$$\begin{aligned} S(\mathbf{q},\omega)=(n+1)\pi\sum_\lambda \delta(\omega-\omega_\lambda)\Bigg[&\left\{\sum_m \cos(\mathbf{q}\cdot\mathbf{R}_m)v'_m(\lambda)\right\}\left\{\sum_n \cos(\mathbf{q}\cdot\mathbf{R}_n)u_n(\lambda)\right\} \\ &+\left\{\sum_m \sin(\mathbf{q}\cdot\mathbf{R}_m)v'_m(\lambda)\right\}\left\{\sum_n \sin(\mathbf{q}\cdot\mathbf{R}_n)u_n(\lambda)\right\}\Bigg] . \end{aligned} \tag{36}$$

We consider two eigenvalue equations mapped to

$$\mu_\lambda^2 u_m(\lambda)=\sum_n D'_{mn}u_n(\lambda) \tag{37}$$

and

$$\mu_\lambda^2 v'_m(\lambda)=\sum_n(\sigma_m D'_{nm}\sigma_n)v'_n(\lambda) , \tag{38}$$

where D'_{mn} and μ_λ are defined by D_{mn} and ω_λ as described in Sec. II, and Eq. (38) is derived from Eq. (4) The corresponding equations of motion are

$$\frac{d^2}{dt^2}x_m(t)=-\sum_n D'_{mn}x_n(t) \tag{39}$$

and

$$\frac{d^2}{dt^2}z_m(t)=-\sum_n(\sigma_m D'_{nm}\sigma_n)z_n(t)\ . \tag{40}$$

By expanding the displacements $x_m(t)$ and $z_m(t)$ by eigenvectors, one has

$$x_m(t)\equiv\sum_\lambda P_\lambda(t)u_m(\lambda) \tag{41}$$

and

$$z_m(t)\equiv\sum_\lambda R_\lambda(t)v'_m(\lambda)\ , \tag{42}$$

where $P_\lambda(t)$ and $R_\lambda(t)$ are the amplitudes of the mode λ, and Eq. (41) is the same as Eq. (8). From Eqs. (40) and (42), $R_\lambda(t)$ varies as $\sim\exp(-i\mu_\lambda t)$ as well as the case for $P_\lambda(t)$. Equations for $P_\lambda(t)$ and $R_\lambda(t)$ with the external force $\sigma_m F_m\cos(\Omega t)$ become

$$\frac{d^2P_\lambda(t)}{dt^2}+\mu_\lambda^2P_\lambda(t)=\left\{\sum_m F_m v'_m(\lambda)\right\}\cos(\Omega t) \tag{43}$$

and

$$\frac{d^2R_\lambda(t)}{dt^2}+\mu_\lambda^2R_\lambda(t)=\left\{\sum_m F_m u_m(\lambda)\right\}\cos(\Omega t)\ . \tag{44}$$

As a next step, we introduce the quantity $\tilde{H}(t)$ defined by

$$\tilde{H}(t)\equiv\tfrac{1}{2}\sum_m\sigma_m\dot{x}_m(t)\dot{z}_m(t)+\tfrac{1}{2}\sum_m\sum_n\sigma_m z_m(t)D'_{mn}x_n(t)\ .$$

Using Eqs. (37), (41), (42), and the biorthogonality condition Eq. (5b), this becomes

$$\tilde{H}(t)=\tfrac{1}{2}\sum_\lambda\{\dot{P}_\lambda(t)\dot{R}_\lambda(t)+\mu_\lambda^2P_\lambda(t)R_\lambda(t)\}\ . \tag{45}$$

By defining $\xi_\lambda(t)\equiv\dot{P}_\lambda(t)+i\mu_\lambda P_\lambda(t)$ and $\zeta_\lambda(t)\equiv\dot{R}_\lambda(t)+i\mu_\lambda R_\lambda(t)$, Eq. (45) is expressed by the neat form $\tilde{H}(t)=\frac{1}{2}\sum_\lambda\xi^*_\lambda(t)\zeta_\lambda(t)$. As in the case of Eqs. (12) and (13), $\xi_\lambda(t)$ and $\zeta_\lambda(t)$ become

$$\xi_\lambda(t)\approx\frac{e^{i\mu_\lambda t}}{2}\left\{\sum_m F_m v'_m(\lambda)\right\}\frac{e^{i(\Omega-\mu_\lambda)t}-1}{i(\Omega-\mu_\lambda)} \tag{46}$$

and

$$\zeta_\lambda(t)\approx\frac{e^{i\mu_\lambda t}}{2}\left\{\sum_m F_m u_m(\lambda)\right\}\frac{e^{i(\Omega-\mu_\lambda)t}-1}{i(\Omega-\mu_\lambda)}\ . \tag{47}$$

Substituting Eqs. (46) and (47) into Eq. (45), one has

$$\tilde{H}(t,\Omega)=\tfrac{1}{2}\sum_\lambda\left\{\sum_m F_m v'_m(\lambda)\right\}\left\{\sum_n F_n u_n(\lambda)\right\}\times\frac{\sin^2\{(\mu_\lambda-\Omega)t/2\}}{(\mu_\lambda-\Omega)^2}\ . \tag{48}$$

In order to calculate Eq. (36), we put the external force $F_m=F_0\cos(\mathbf{q}\cdot\mathbf{R}_m)$ in Eq. (48). After sufficient time interval T, $\tilde{H}(T,\Omega)$ becomes

$$\tilde{H}^c_{\mathbf{q}}(T,\Omega)\equiv\frac{\pi TF_0^2}{4}\sum_\lambda\delta(\mu_\lambda-\Omega)\left\{\sum_m v'_m(\lambda)\cos(\mathbf{q}\cdot\mathbf{R}_m)\right\}\times\left\{\sum_n u_n(\lambda)\cos(\mathbf{q}\cdot\mathbf{R}_n)\right\}. \tag{49}$$

The time interval T should be chosen by the same way as the calculation of the spectral density of states described in Sec. II A. By setting external force $F_m=F_0\sin(\mathbf{q}\cdot\mathbf{R}_m)$, Eq. (48) yields

$$\tilde{H}^s_{\mathbf{q}}(T,\Omega)\equiv\frac{\pi TF_0^2}{4}\sum_\lambda\delta(\mu_\lambda-\Omega)\left\{\sum_m v'_m(\lambda)\sin(\mathbf{q}\cdot\mathbf{R}_m)\right\}\times\left\{\sum_n u_n(\lambda)\sin(\mathbf{q}\cdot\mathbf{R}_n)\right\}. \tag{50}$$

From Eqs. (49), (50), and (36), the dynamic structure factor $S(\mathbf{q},\omega)$ is given by

$$S(\mathbf{q},\omega)\approx(n+1)\left|\frac{d\mu(\omega)}{d\omega}\right|\frac{4}{TF_0^2}\{\tilde{H}^c_{\mathbf{q}}[T,\mu(\omega)]+\tilde{H}^s_{\mathbf{q}}[T,\mu(\omega)]\}\ . \tag{51}$$

For actual calculations, one can simplify Eqs. (37)–(51) using the following properties of the eigenvectors $|u(\lambda)\rangle$ and $\langle v(\lambda)|$ of antiferromagnetic spin waves.

From Eqs. (43) and (44), the formal solutions of $x_m(t)$ and $z_m(t)$ with the initial conditions $x_m(t=0)=z_m(t=0)=0$ are written as

$$x_m(t)=\sum_\lambda\left\{\sum_n F_n v'_n(\lambda)\right\}\times\frac{2\sin\{(\Omega+\mu_\lambda)T/2\}\sin\{(\Omega-\mu_\lambda)T/2\}}{\Omega^2-\mu_\lambda^2}\times u_m(\lambda)\ , \tag{52}$$

and

$$z_m(t)=\sum_\lambda\left\{\sum_n F_n u_n(\lambda)\right\}\times\frac{2\sin\{(\Omega+\mu_\lambda)T/2\}\sin\{(\Omega-\mu_\lambda)T/2\}}{\Omega^2-\mu_\lambda^2}\times v'_m(\lambda)\ . \tag{53}$$

Equations (52) and (53) lead to $x_m(t)=z_m(t)$ from the relations $v'_m(\lambda)=A_\lambda u_m(\lambda)$ and $v_m(\lambda)=A_\lambda u'_m(\lambda)$. Thus, it is sufficient to calculate only one part of Eqs. (39) and (40) with the external force $\sigma_m F_m\cos(\Omega t)$. The wave vectors $\mathbf{q}$ used in Eqs. (49) and (50) differ from each other by π/a [for example, $(\pi/a,\pi/a)$ for $d=2$], where a is a lattice constant. This is due to the difference between the magnetic Brillouin zone and the nuclear Brillouin zone for antiferromagnets [21]. This algorithm enables us to cal-

culate the ω dependence of $S(\mathbf{q},\omega)$ for fixed $\mathbf{q}$ as well as the wave number dependence for fixed ω by the same CPU time as that required for the density of states.

It is straightforward to extend this algorithm to other systems. For the dynamic structure factor of vibrational systems, one can define the formula [18,22]

$$S(\mathbf{q},\omega)=\frac{(n+1)}{\omega}\sum_{\lambda}\delta(\omega-\omega_\lambda)\left|\sum_{m}\{\mathbf{q}\cdot\mathbf{u}_m(\lambda)\}e^{-i\mathbf{q}\cdot\mathbf{R}_m}\right|^2, \tag{54}$$

where $\mathbf{u}_m(\lambda)$ is the atomic displacement of the vibrational eigenmode λ at the site m. Using this formula, one can calculate the ω and $\mathbf{q}$ dependence of $S(\mathbf{q},\omega)$ by the same procedure described in Eqs. (37)–(51).

We have described in this section the efficient method to calculate the dynamic structure factor for the system described by large-scale non-Hermitian matrix. This method enables us to calculate directly the dynamic structure factor without making the spatio-temporal Fourier transform of the correlation function.

IV. APPLICATION TO PERCOLATING HEISENBERG ANTIFERROMAGNETS

There is a growing interest in dynamic properties of spin-wave excitations on percolating Heisenberg antiferromagnets *(antiferromagnetic fractons),* because they show peculiar properties originating from geometrical disorder and self-similarity [23,24]. In a previous work, we have calculated the density of states (DOS) of percolating antiferromagnets [25], using *the equation of motion method* [21]. We have conjectured that the spectral dimension $\tilde{d}_a$, defined by the DOS, $\mathcal{D}(\omega)\sim\omega^{\tilde{d}_a-1}$, is equal to *unity* for any Euclidean dimension d, and antiferromagnetic fractons belong to a different universality class from that of vibrational or ferromagnetic fractons ($\tilde{d}\approx\frac{4}{3}$) [26,27].

Let us show that our algorithm mentioned above is quite efficient compared with the equation of motion method. We apply the external force $F_m\cos(\Omega t)$ to the system. The amplitude F_m is given by $F_{i\alpha}=\sigma_\alpha F_0\cos(\phi_i)$, where i denotes a unit cell and α the sublattice index, ϕ_i is chosen as a random quantity within the range $[0,2\pi]$. Note that this form of the external force is different from Eq. (10). The product $\{\cdots\}\{\cdots\}$ in Eq. (14) becomes

$$\begin{aligned}\left\{\sum_m F_m v_m(\lambda)\right\}\left\{\sum_n F_n u_n(\lambda)\right\}&=\sum_i\sum_\alpha F_{i\alpha}^2 v_{i\alpha}(\lambda)u_{i\alpha}(\lambda)\\&+\sum_i\sum_\alpha\sum_{\beta(\neq\alpha)}F_{i\alpha}F_{i\beta}v_{i\alpha}(\lambda)u_{i\beta}(\lambda)\\&+\sum_i\sum_{j(\neq i)}\sum_\alpha\sum_\beta F_{i\alpha}F_{j\beta}v_{i\alpha}(\lambda)u_{j\beta}(\lambda),\end{aligned} \tag{55}$$

where $m=i\alpha$ and $n=j\beta$. In Eq. (55), the third term vanishes by random phase averaging, and the second term becomes

$$\begin{aligned}&\sum_i\sum_\alpha\sum_{\beta(\neq\alpha)}F_{i\alpha}F_{i\beta}v_{i\alpha}(\lambda)u_{i\beta}(\lambda)\\&\quad=-F_0^2\sum_i\cos^2(\phi_i)\{v_{i\alpha=\uparrow}(\lambda)u_{i\alpha=\downarrow}(\lambda)\\&\qquad+v_{i\alpha=\downarrow}(\lambda)u_{i\alpha=\uparrow}(\lambda)\}.\end{aligned} \tag{56}$$

The value in the curly brackets of Eq. (56) vanishes using the relation between $u_n(\lambda)$ and $v_n'(\lambda)=\sigma_n v_n(\lambda)$ described in Appendix C. The averaged value of Eq. (55) yields

$$\begin{aligned}&\left\langle\left\{\sum_m F_m v_m(\lambda)\right\}\left\{\sum_n F_n u_n(\lambda)\right\}\right\rangle\\&\quad=\left\langle F_0^2\sum_i\sum_{\alpha=\uparrow,\downarrow}\cos^2(\phi_i)v_{i\alpha}(\lambda)u_{i\alpha}(\lambda)\right\rangle\\&\quad=\frac{F_0^2}{2}.\end{aligned} \tag{57}$$

In this way the same result as Eq. (15) is obtained. The following is the reason why the external force is chosen as $F_{i\alpha}=\sigma_\alpha F_0\cos(\phi_i)$. If we take F_m, given by Eq. (10), the left-hand side of Eq. (57) becomes

$$\begin{aligned}&\left\langle\left\{\sum_m F_m v_m(\lambda)\right\}\left\{\sum_n F_n u_n(\lambda)\right\}\right\rangle\\&\quad=A_\lambda\left\langle\sum_i\{\cos^2(\phi_{i\uparrow})|u_{i\uparrow}(\lambda)|^2-\cos^2(\phi_{i\downarrow})|u_{i\downarrow}(\lambda)|^2\}\right\rangle.\end{aligned} \tag{58}$$

The summand in the right-hand side of Eq. (58) includes both positive and negative terms, and this makes the convergence of the random phase average worse. When applying the forced oscillator method to the system described by a Hermitian matrix, this does not occur, because the corresponding summand to that in Eq. (58) has only positive terms. In the case of $F_{i\alpha}=\sigma_\alpha F_0\cos(\phi_i)$, the random phase average is given by, from Eq. (57),

$$\begin{aligned}&\left\langle\left\{\sum_m F_m v_m(\lambda)\right\}\left\{\sum_n F_n u_n(\lambda)\right\}\right\rangle\\&\quad=A_\lambda\left\langle\sum_i\cos^2(\phi_i)\{|u_{i\uparrow}(\lambda)|^2-|u_{i\downarrow}(\lambda)|^2\}\right\rangle.\end{aligned} \tag{59}$$

For antiferromagnetic spin waves, spin deviations at one sublattice have larger amplitudes than those on the other sublattice [28]. From this, the sign of $\{|u_{i\uparrow}(\lambda)|^2-|u_{i\downarrow}(\lambda)|^2\}$ tends to be definite, and this makes the convergence of the random phase average in Eq. (59) better. This choice of F_m makes the actual calculation quite efficient.

Now let us check the efficiency of the algorithm by calculating the DOS of $d=2$ antiferromagnetic spin waves excited on a *regular* system. The matrix $\{D_{mn}\}$ defined in Sec. III has positive and negative eigenvalues ω_λ, and the distribution of ω_λ is known to be symmetric around

$\omega=0$ [20]. In the following numerical calculations, we only consider the range of positive ω, and the definition of the density of states $\mathcal{D}(\omega)$ differs by a factor of 2 because the normalization condition [Eq. (18)] should be changed. The filled circles in Fig. 1 show the numerical results calculated for a 840×840 square lattice with periodic boundary conditions. The solid line in Fig. 1 is the exact DOS for $d=2$ antiferromagnetic magnons. We see that the calculated DOS is proportional to ω in the low frequency regime, and agrees well with the exact solution.

We have calculated, by applying the present method, the DOS for $d=2,3$ *percolating* classical Heisenberg antiferromagnets. The exchange coupling J_{mn} in Eq. (32) takes the value of unity when site m and n are connected, and $J_{mn}=0$ otherwise. The calculated DOS for a $d=2$ percolating antiferromagnet at $p_c(=0.50)$ is shown in Fig. 2 by filled squares. The bond-percolating (BP) network is formed on a 1100×1100 square lattice with periodic boundary conditions. This network has 657 426 spins. Least squares fitting for filled squares in Fig. 2 leads to $\tilde{d}_a=0.99\pm0.04$. The DOS for $d=3$ percolating antiferromagnets at $p_c(=0.25)$ are shown by filled triangles in Fig. 2. The BP networks of three realizations are formed on $100\times100\times100$ cubic lattices with periodic boundary conditions, and the largest network has 114 303 spins. The value of the spectral dimension calculated by least squares fitting for Fig. 2 is $\tilde{d}_a=0.98\pm0.04$. These values agree well with our previous conjecture, $\tilde{d}_a=1$ for any Euclidean dimension [25], for which the equation of motion method was employed. Our numerical method is more accurate than the equation of motion method, especially in the lower frequency regime.

We have calculated an antiferromagnetic fracton eigenmode by the method described in Sec. II B. This eigenmode is calculated for $d=2$ BP antiferromagnet at the percolation threshold (p_c) formed on a 100×100 square lattice, and the number of spins is 6885. Figure 3 shows the eigenmode belonging to the eigenvalue $\omega=0.049\,341\,266\,562$. The magnitude of spin deviation

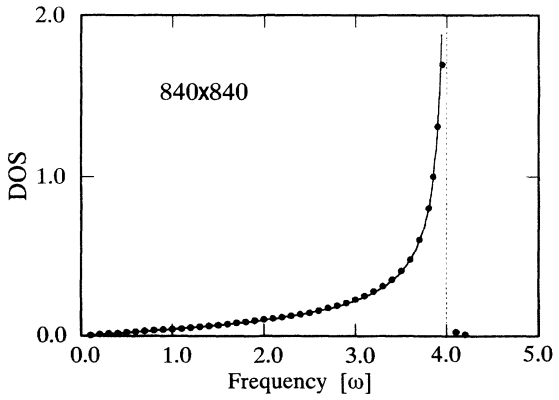

FIG. 1. The density of states of spin waves for a regular square lattice per one site. The solid line shows the exact solution. Filled circles are calculated results for a 840×840 square lattice.

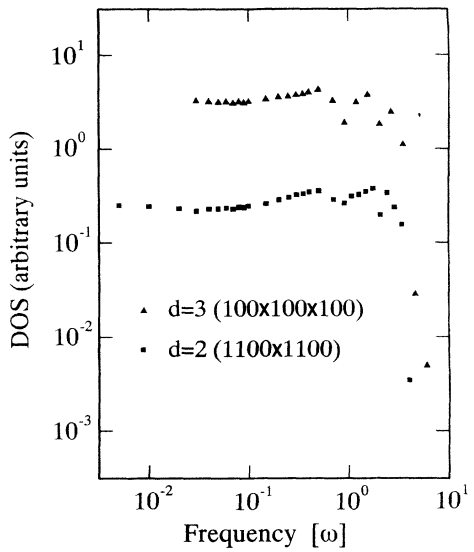

FIG. 2. The density of states of antiferromagnetic fractons for $d=2,3$ BP networks at the percolation threshold p_c. Filled squares indicate calculated results for $d=2$. Filled triangles show the results for $d=3$.

S_m^+ on each spin is shown by arrows in Fig. 3. One sees that the fracton is strongly localized. The deviation δ defined in Eq. (30) takes a value $\delta\approx1.0\times10^{-8}$, suggesting that the eigenmode is very pure, as described in Sec. II B.

Let us show the results for $S(\mathbf{q},\omega)$ calculated by the numerical method described in Sec. III. Uemura and Birgeneau [29] have performed inelastic neutron scattering experiments on $Mn_xZn_{1-x}F_2$. They have observed the crossover between the sharp spin-wave peak at small

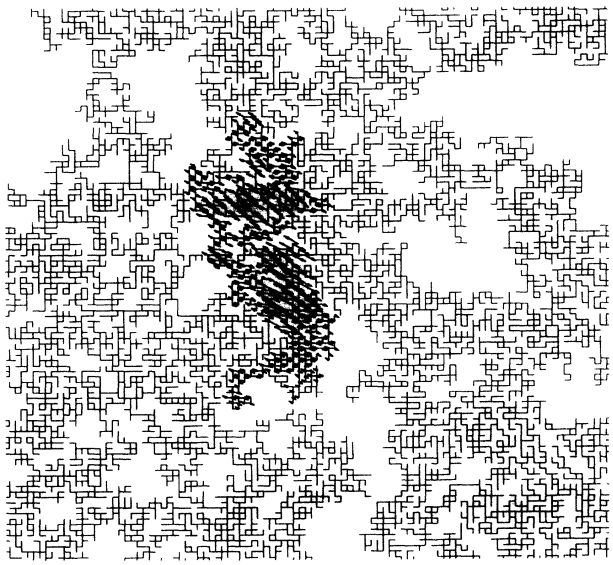

FIG. 3. Antiferromagnetic fracton eigenmode excited on $d=2$ BP network formed on a 100×100 square lattice. The eigenfrequency is $\omega=0.049\,341\,266\,562$. Arrows for very small magnitude are omitted in this figure.

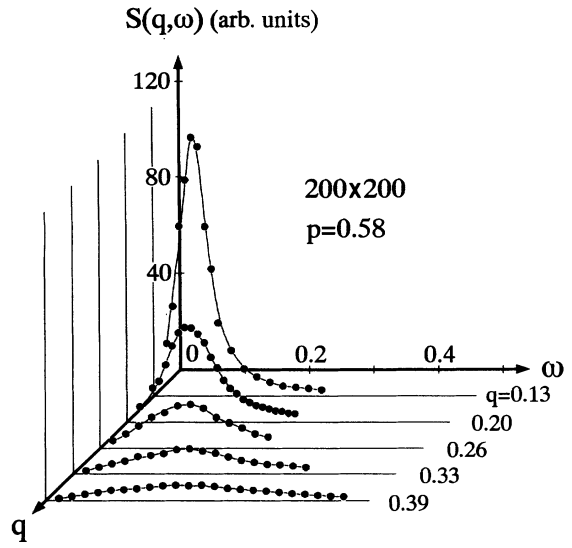

FIG. 4. The ω dependence of $S(\mathbf{q},\omega)$ for $d=2$ BP networks at $p=0.58$ formed on 200×200 square lattice. The results were obtained by averaging over six realizations of BP networks.

wave vectors and the broad fracton response at large wave vectors, and a double-peak feature at the crossover which reflects magnon and fracton components. Chen and Landau [30] have performed numerical simulations for site-diluted bcc antiferromagnets, and they found a double peak structure at the crossover region at $p=0.50$. Takahashi and Ikeda, and Ikeda *et al.* [31] have studied $d=3$ diluted antiferromagnets $RbMn_xMg_{1-x}F_3$. Most of their studies are performed at the percolation concentration p, far from the percolation threshold p_c.

The ω dependence of $S(\mathbf{q},\omega)$ for $d=2$ BP antiferromagnets at $p=0.58$ is shown in Fig. 4. The ensemble average is taken over six realizations of BP networks formed on 200×200 square lattices. The largest network has 37 449 spins. The correlation length of this system is $\xi\approx29a$ (a is a lattice constant) and the crossover frequency ω_ξ is estimated to be $\omega_\xi\approx0.12$ from the data corresponding to $q=2\pi/\xi\approx0.22(a=1)$ in Fig. 4. We have calculated $S(\mathbf{q},\omega)$ along the $\mathbf{q}=[1,0]$ direction from the magnetic zone center. These results indicate, for small wave vectors ($q<\xi^{-1}$), the appearance of sharp asymmetric peaks at low energies with tails extending towards higher energies. These sharp asymmetric line shapes are contributed from both magnons and fractons. As q increases, peak widths increase very rapidly and peak positions shift to higher energies beyond $\omega\approx\omega_\xi$. This indicates that magnons cross over to fractons at $\omega\approx\omega_\xi$, and the q dependence becomes irrelevant at higher ω, reflecting strongly localized properties of antiferromagnetic fractons.

V. CONCLUSIONS

We have extended the forced oscillator method to be applicable to eigenvalue problems for very large nonsymmetric (or non-Hermitian) matrices. This method has the following advantages: (i) it requires computer memory space of the order of N for large sparse matrices, (ii) it is very suitable to parallel and vector supercomputers, (iii) the algorithm is simple and efficient compared with other conventional techniques, (iv) it is possible to calculate the spectral density of states within an arbitrary range of eigenvalues and with a given resolution, and (v) one can calculate quite accurately the specific eigenvalue and its eigenvector, and judge the accuracy.

We have described an efficient numerical method to calculate the dynamic correlation function for the systems described by very large non-Hermitian matrices. This method enables us to calculate directly without making the spatiotemporal Fourier transform of the correlation functions $S(\mathbf{r},t)$.

We have demonstrated the efficiency of the FOM by calculating the DOS, eigenvectors, and $S(\mathbf{q},\omega)$ for percolating classical Heisenberg antiferromagnets. We hope that the present work is useful to study dynamical systems described by very large non-Hermitian matrices, and also stimulates experimental researches on fracton dynamics of percolating antiferromagnets.

ACKNOWLEDGMENTS

This work was supported in part by a Grant-in-Aid for Scientific Research on the Special Projects, "Computational Physics as a New Frontier in Condensed Matter Research," from the Japan Ministry of Education, Science, and Culture (MESC). One of the authors (T.T.) thanks JSPS and the MESC for financial support.

APPENDIX A

This appendix provides the criterion for the proper time interval T for obtaining eigenvalues and eigenvectors. In principle, large T makes the frequency width of resonance $\delta\omega$ small, but the required CPU time becomes large at the same time to be proportional to $p\times T$, where p is the number of iterations introduced in Eq. (24). In Ref. [3], the optimization conditions (the choice of T and p) are given, in addition to the method to judge the mode mixing ratio for the eigenvalue problem of Hermitian matrices. We present here similar formulas to Eqs. (15)–(27) in Ref. [3] for non-Hermitian matrices. These are much more complicated due to the absence of orthonormality condition among the eigenvectors.

Let us introduce the deviation δ' defined by

$$\delta'^2\equiv\frac{\sum_m \delta_m\tilde{\delta}_m}{\sum_m a_m\tilde{a}_m}, \tag{A1}$$

where quantities a_m and δ_m are defined in Eqs. (26) and (28). $\tilde{a}_m$ and $\tilde{\delta}_m$ are defined by $\tilde{a}_m\equiv\sum_n D'_{nm}\tilde{b}_n$ and $\tilde{\delta}_m\equiv\tilde{a}_m-\tilde{\mu}^2\tilde{b}_m$, respectively, where $\tilde{b}_m\equiv y_m^{(p)}(T)$ is the displacement $y_m(t)$ introduced in Eq. (9) after the p iteration. Note that δ' is different from δ defined by Eq. (29). Equation (A1) is rewritten as $\delta'^2=(\tilde{\Gamma}_4-2\tilde{\mu}^2\tilde{\Gamma}_2+\tilde{\mu}^4\tilde{\Gamma}_0)/\tilde{\Gamma}_4$, where $\tilde{\Gamma}_0\equiv\sum_m b_m\tilde{b}_m$, $\tilde{\Gamma}_2\equiv\sum_m a_m\tilde{b}_m$,

and $\tilde{\Gamma}_4 \equiv \sum_m a_m \bar{a}_m$, respectively. One can show $\tilde{\Gamma}_n = \sum_\lambda \mu_\lambda^n P_\lambda(T) Q_\lambda(T)$, corresponding to the formula Eq. (20) in Ref. [3]. Under the assumption that the displacement $x_m^{(p)}(T)$ [and $y_m^{(p)}(T)$] consists primarily of two modes ($\lambda = 1,2$) after p iterations, one finds

$$\tilde{\mu}^2 = \frac{\mu_1^2 P_1 Q_1 + \mu_2^2 P_2 Q_2}{P_1 Q_1 + P_2 Q_2} \tag{A2}$$

and

$$\delta'^2 = \frac{P_1 P_2 Q_1 Q_2 (\mu_1^2 - \mu_2^2)}{(P_1 Q_1 + P_2 Q_2)(\mu_1^4 P_1 Q_1 + \mu_2^4 P_2 Q_2)} , \tag{A3}$$

as in the case of Eqs. (18)–(22) in Ref. [3]. Provided that the level spacing $\Delta\mu \equiv |\mu_1 - \mu_2| \ll \mu_1$ and $P_1 \gg P_2$ ($Q_1 \gg Q_2$), the quantity δ' becomes

$$\delta' \approx \frac{2\Delta\mu}{\tilde{\mu}} \left[\frac{P_2 Q_2}{P_1 Q_1} \right]^{1/2} . \tag{A4}$$

Equation (A4) corresponds to Eq. (23) in Ref. [3]. Equation (A4) leads to, using Eq. (21) and the formula for $Q_\lambda(t)$,

$$\log\delta' \approx p \ln \left| \frac{h(\Omega,\mu_2;T)}{h(\Omega,\mu_1;T)} \right| + \ln \left| \frac{2\Delta\mu}{\tilde{\mu}} \left[\frac{\left\{\sum_m F_m v_m(\lambda_2)\right\}\left\{\sum_n F_n u_n(\lambda_2)\right\}}{\left\{\sum_m F_m v_m(\lambda_1)\right\}\left\{\sum_n F_n u_n(\lambda_1)\right\}} \right]^{1/2} \right| , \tag{A5}$$

where

$$h(\Omega,\mu_\lambda;T) \equiv 2\sin\{(\Omega+\mu_\lambda)T/2\} \times \sin\{(\Omega-\mu_\lambda)T/2\}/(\Omega^2-\mu_\lambda^2) .$$

The second term of the right-hand side of Eq. (A5) is independent of the time interval T. The relation between the required values of p and T for fixed $\delta' = \delta_0'$, is given by

$$p \approx \ln \left| \frac{\tilde{\mu}\delta_0'}{2\Delta\mu} \left[\frac{\left\{\sum_m F_m v_m(\lambda_1)\right\}\left\{\sum_n F_n u_n(\lambda_1)\right\}}{\left\{\sum_m F_m v_m(\lambda_2)\right\}\left\{\sum_n F_n u_n(\lambda_2)\right\}} \right]^{1/2} \right| \times \left[\ln \left| \frac{h(\Omega,\mu_2;T)}{h(\Omega,\mu_1;T)} \right| \right]^{-1} . \tag{A6}$$

Equation (A6) indicates that the time interval T should be taken to satisfy $|\sin\{(\Omega-\mu_1)T/2\}| \approx 1$ [and $|\sin\{(\Omega-\mu_2)T/2\}| \approx 0$] in order to make the value of p small. One can choose the magnitude of $\Omega-\mu_1$ to be the same order as the level spacing $\Delta\mu$, and the time interval T as $T \sim \pi/\Delta\mu$ from this condition.

APPENDIX B

Proof of Eq. (35): Equations of motion for antiferromagnetic spin waves are written as

$$i\frac{\partial}{\partial t} S_m^+(t) = \sum_n D_{mn} S_n^+(t) - \sigma_m h_m^+(t) , \tag{B1}$$

where $h_m^+(t) \equiv h_m^x(t) + i h_m^y(t)$ is the transverse magnetic field applied at the site m.

Introducing the temporal Fourier transforms $S_m^+(\omega)$ and $h_m^+(\omega)$, Eq. (B1) is rewritten as

$$\sum_n G_{mn}(\omega) S_n^+(\omega) = -h_m^+(\omega) , \tag{B2}$$

where $G_{mn}(\omega) \equiv \sigma_m(\delta_{m,n}\omega - D_{mn})$. By defining the two-point susceptibility $\chi_{mn}(\omega) \equiv S_m^+(\omega)/h_n^+(\omega)$ and its spatial Fourier transform $\chi(\mathbf{q},\omega)$ [20], one has $\chi_{mn}(\omega) = -\{\mathbf{G}(\omega)^{-1}\}_{mn}$ and

$$\chi(\mathbf{q},\omega) \equiv \sum_m \sum_n e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} \chi_{mn}(\omega) = -\sum_m \sum_n e^{i\mathbf{q}\cdot\mathbf{R}_m} \{\mathbf{G}(\omega)^{-1}\}_{mn} e^{-i\mathbf{q}\cdot\mathbf{R}_n} . \tag{B3}$$

By introducing the quantity C_λ defined by

$$e^{-i\mathbf{q}\cdot\mathbf{R}_m} = \sum_\lambda C_\lambda u_m'(\lambda) ,$$

one has

$$C_\lambda = \sum_m v_m'(\lambda) e^{-i\mathbf{q}\cdot\mathbf{R}_m} .$$

Using this, Eq. (B3) is calculated as

$$\chi(\mathbf{q},\omega) = -\sum_m \sum_n e^{i\mathbf{q}\cdot\mathbf{R}_m} \{\mathbf{G}(\omega)^{-1}\}_{mn} e^{-i\mathbf{q}\cdot\mathbf{R}_n} = -\sum_\lambda C_\lambda \sum_m e^{i\mathbf{q}\cdot\mathbf{R}_m} \sum_n \{\mathbf{G}(\omega)^{-1}\}_{mn} u_n'(\lambda)$$
$$= -\sum_\lambda \frac{C_\lambda}{\omega-\omega_\lambda} \left\{\sum_m e^{i\mathbf{q}\cdot\mathbf{R}_m} u_m(\lambda)\right\} = -\sum_\lambda \frac{1}{\omega-\omega_\lambda} \left\{\sum_m e^{-i\mathbf{q}\cdot\mathbf{R}_m} v_m'(\lambda)\right\} \left\{\sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n} u_n(\lambda)\right\} .$$

Here the relation $\mathbf{G}(\omega)|u(\lambda)\rangle=(\omega-\omega_\lambda)|u'(\lambda)\rangle$ is used. The dynamic structure factor $S(\mathbf{q},\omega)$ is given as $S(\mathbf{q},\omega)=(n+1)\chi''(\mathbf{q},\omega)$, where $\chi''(\mathbf{q},\omega)=\lim_{\delta\to+0}\mathrm{Im}[\chi(\mathbf{q},\omega+i\delta)]$. Then, one has

$$\chi''(\mathbf{q},\omega)=\pi\sum_\lambda\delta(\omega-\omega_\lambda)\left\{\sum_m e^{-i\mathbf{q}\cdot\mathbf{R}_m}v'_m(\lambda)\right\}\times\left\{\sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n}u_n(\lambda)\right\}. \tag{B4}$$

APPENDIX C

Proof of $v'_m(\lambda)=A_\lambda u_m(\lambda)$: Eq. (34) yields

$$\mathbf{DU}=\mathbf{U}\Lambda\ , \tag{C1}$$

and the corresponding equation for left eigenvectors leads to

$$(\mathbf{U}^{-1})\mathbf{D}=\Lambda(\mathbf{U}^{-1})\ . \tag{C2}$$

Here we have defined

$$\Lambda=\begin{bmatrix}\omega_1 & & 0\\ & \omega_2 & \\ 0 & & \ddots\end{bmatrix},$$

$$\mathbf{U}\equiv(|u(\lambda_1)\rangle,|u(\lambda_2)\rangle,\ldots)\ ,$$

and, from Eq. (5),

$$\mathbf{U}^{-1}=\begin{bmatrix}\langle v(\lambda_1)|\\ \langle v(\lambda_2)|\\ \vdots\end{bmatrix}.$$

Since $\hat{\sigma}\mathbf{D}\hat{\sigma}=\mathbf{D}^T$ from the definitions of $\mathbf{D}$ and $(\hat{\sigma})_{mn}\equiv\delta_{m,n}\sigma_m$, Eq. (C2) becomes

$$(\hat{\sigma}\mathbf{D}\hat{\sigma})(\mathbf{U}^{-1})^T=(\mathbf{U}^{-1})^T\Lambda\ .$$

Hence,

$$\mathbf{D}(\mathbf{U}^{-1}\hat{\sigma})^T=(\mathbf{U}^{-1}\hat{\sigma})^T\Lambda\ , \tag{C3}$$

where $(\mathbf{U}^{-1}\hat{\sigma})^T=(|v'(\lambda_1)\rangle,|v'(\lambda_2)\rangle,\ldots)$. From Eqs. (C1) and (C3), one has

$$|v'(\lambda)\rangle=A_\lambda|u(\lambda)\rangle\ , \tag{C4}$$

where A_λ is a constant depending on λ. The constant A_λ can be determined by Eq. (5b), using the condition $\sum_n u_n(\lambda)v_n(\lambda)=A_\lambda\sum_n\sigma_n\{u_n(\lambda)\}^2=1$.

[1] See, for example, *Large Scale Eigenvalue Problems,* edited by J. Cullum and R. A. Willoughby (North-Holland, Amsterdam, 1986).

[2] M. L. Williams and H. J. Maris, Phys. Rev. B **31**, 4508 (1985).

[3] K. Yakubo, T. Nakayama, and H. J. Maris, J. Phys. Soc. Jpn. **60**, 3249 (1991).

[4] See, for example, T. Nakayama, K. Yakubo, and R. Orbach, Rev. Mod. Phys. **66**, 381 (1994).

[5] T. Nakayama, M. Takano, and K. Yakubo, Phys. Rev. B **47**, 9249 (1993).

[6] K. Fukamachi and H. Nishimori, Phys. Rev. B **49**, 651 (1994).

[7] H. Tanaka and T. Fujiwara, Phys. Rev. B **49**, 11 440 (1994).

[8] K. Hukushima, K. Nemoto, and H. Takayama (unpublished).

[9] G. J. Hu and D. L. Huber, Phys. Rev. B **33**, 3599 (1986).

[10] D. L. Huber and W. Y. Ching, Phys. Rev. B **47**, 3220 (1993).

[11] L. R. Walker and R. E. Walstedt, Phys. B **22**, 3816 (1980).

[12] I. Avgin and D. L. Huber, Phys. Rev. B **48**, 13 625 (1993).

[13] See, for example, R. Haydock, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1980), Vol. 35.

[14] N. G. van Kampen, *Stochastic Process in Physics and Chemistry* (North-Holland, Amsterdam, 1992).

[15] See, for example, J. H. Wilkinson and C. Reinsch, *Linear Algebra* (Springer-Verlag, Berlin, 1971); F. Chatelin, *Valeurs Propres de Matrices* (Masson, Paris, 1988).

[16] The eigenvalue problem for a $N\times N$ matrix with complex elements, $\mathbf{D}x_\lambda=\omega_\lambda x_\lambda$, can be decomposed into that for a $2N\times2N$ matrix with real elements as

$$\begin{bmatrix}\mathbf{D}_R & -\mathbf{D}_I\\ \mathbf{D}_I & \mathbf{D}_R\end{bmatrix}\begin{bmatrix}x_\lambda^R\\ x_\lambda^I\end{bmatrix}=\omega_\lambda\begin{bmatrix}x_\lambda^R\\ x_\lambda^I\end{bmatrix},$$

where $\mathbf{D}\equiv\mathbf{D}_R+i\mathbf{D}_I$, $x_\lambda\equiv x_\lambda^R+ix_\lambda^I$. The $2N\times2N$ matrix of order $2N$ has a doubly degenerate eigenvalue ω_λ and its eigenvectors are given by $(x_\lambda^R,x_\lambda^I)^T$ and $(-x_\lambda^I,x_\lambda^R)^T$. See also Ref. [15].

[17] See, for example, L. E. Reichl, *A Modern Course in Statistical Physics* (University of Texas Press, Austin, 1980).

[18] W. Marshall and S. W. Lovesey, *Theory of Thermal Neutron Scattering* (Oxford University Press, Oxford, 1971).

[19] W. J. L. Buyers, D. E. Pepper, and R. J. Elliott, J. Phys. C **5**, 2611 (1972).

[20] S. Kirkpatrick and A. B. Harris, Phys. Rev. B **12**, 4980 (1975).

[21] R. Alben and M. F. Thorpe, J. Phys. C **8**, L275 (1975); **9**, 2555 (1975).

[22] S. Alexander, E. Courtens, and R. Vacher, Physica A **195**, 286 (1993).

[23] R. Orbach and K. W. Yu, J. Appl. Phys. **61**, 3689 (1987).

[24] G. Polatsek, O. Entin-Wohlman, and R. Orbach, Phys. Rev. B **39**, 9353 (1989).

[25] K. Yakubo, T. Terao, and T. Nakayama, J. Phys. Soc. Jpn. **62**, 2196 (1993).

[26] S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).

[27] T. Nakayama, Physica A **191**, 386 (1992).

[28] F. Keffer, H. Kaplan, and Y. Yafet, Am. J. Phys. **21**, 250 (1953).
[29] Y. J. Uemura and R. J. Birgeneau, Phys. Rev. Lett. **57**, 1947 (1986); Phys. Rev. B **36**, 7024 (1987).
[30] K. Chen and D. P. Landau, J. Appl. Phys. **73**, 5645 (1993).
[31] M. Takahashi and H. Ikeda, Phys. Rev. B **47**, 9132 (1993); H. Ikeda, J. A. Fernandez-Baca, R. M. Nicklow, M. Takahashi, and K. Iwasa (unpublished).