

Vibrational modes and spectrum of oscillators on a scale-free network

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We study vibrational modes and spectrum of a model system of atoms and springs on a scale-free network where we assume that the atoms and springs are distributed as nodes and links of a scale-free network. To understand the nature of excitations with many degrees of freedom on the scale-free network, we adopt a particular model that we assign the mass M_i and the specific oscillation frequency ω_i of the i th atom and the spring constant K_{ij} between the i th and j th atoms. We show that the density of states of the spectrum follows a scaling law $P(\omega^2) \propto (\omega^2)^{-\gamma}$, where $\gamma=3$ and that as the number of nodes N is increasing, the maximum eigenvalue grows as fast as \sqrt{N} .

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There has been notable progress in the study of the so-called scale-free network (SFN). SFN was discovered by the Faloutsos brothers and Albert, Jeong, and Barabási from studying the network geometry of the Internet [1,2]. They opened up an area in order to study very complex and growing network systems from physics to biology and economics [2]. The nature of SFN is characterized by a power-law behavior in a distribution function as a function of the number of nodes with k links, represented by $P(k) \propto k^{-\gamma}$ with $\gamma \approx 1-4$. This means that the system is scale-free, since there is no particular scale in the network geometry. In order to show how power-law distribution occurs in the SFN, Albert and Barabási first proposed a very simple model called the Albert-Barabási (AB)'s model [2].

The AB model [2] is constructed by the following process: Initially we put m_0 nodes as seeds in the system. Every time when a new node is added to the system, m new links appear such that the inserted node is linked to m nodes already existing in the system with the preferential attachment probability $\Pi_i(k_i) = k_i / \sum_{i=1}^{N-1} k_i$. Here k_i is the number of links at the i th node (called the degree of the i th node) and we assume $m \leq m_0$. The development of network in this model is described by a continuous equation for the degree of node: $dk_i/d\tau = m\Pi_i(k_i) = mk_i/2\tau$. By this, at time τ the system consists of $N(\tau)$ nodes and the $L(\tau)$ links with $L(\tau) = \frac{1}{2} \sum_{i=1}^{N(\tau)} k_i$. Then, the AB model exhibits power law with $\gamma=3$. Thus it has been concluded that the scale-free nature of the SFN is attributed to both the growth and the preferential attachment in the network.

Although researchers studied time evolution of an SFN so far, they regarded nodes and links in the network as meta-physical objects and correspondences such as agents and relationships in an area of science, respectively. Therefore they did not put any real physical meaning on the nodes and links in the SFNs, except some particular systems such as diffusion [3] and spins [4–8] on a SFN as well as the random

networks [9–11] and small world networks [12] have been studied. Therefore, even in the system of SFN, it seems worthwhile investigating excitations in a physical model such as vibrations, phonons, and electrons as well, although the problem might look too academic. Thus, as a prototype model, we would like to study vibrational modes and its spectrum of the system of oscillators on a SFN, where atoms and springs are regarded as nodes and links of the SFN.

We first adopt the AB model to construct a SFN. Let us now assume that *time evolution of the network is adiabatic to the temporal motion of the atoms and springs*. This guarantees that the vibrational model can be instantaneously solved, where the network is regarded as a static system consisting of $N(\tau)$ nodes and $L(\tau)$ links; the network adiabatically grows under its own time development.

Let us introduce our vibrational model. Assume that q_i and ω_i are the displacement and the specific frequency of the i th atom of mass M_i , respectively. Define the Hamiltonian of the system:

$$H = \sum_{i=1}^{N(\tau)} \left(\frac{M_i}{2} \dot{q}_i^2 + \frac{M_i \omega_i^2}{2} q_i^2 \right) + \sum_{i,j=1(i \neq j)}^{N(\tau)} \frac{K_{ij}}{2} (q_i - q_j)^2, \quad (1)$$

where $\dot{q}_i = dq_i/dt$ the velocity of the i th atom and K_{ij} is the spring constant between the i th and j th atoms with $K_{ij} = K_{ji}$. By using the Euler-Lagrange equation, $d/dt(\partial H/\partial \dot{q}_i) = \partial H/\partial q_i$, we obtain $M_i(\ddot{q}_i + \omega_i^2 q_i) = \sum_{j=1}^{N(\tau)} K_{ji}(q_j - q_i)$, for $i = 1, \dots, N(\tau)$. And assuming $q_i(t) = q_i(\omega) e^{-i\omega t}$, we get

$$M_i(\omega_i^2 - \omega^2)q_i = \sum_{j=1}^{N(\tau)} K_{ji}(q_j - q_i), \quad (2)$$

for $i = 1, \dots, N(\tau)$. This is the eigenequation for our system.

Let us assume further that all springs are identical. This assumption might be an oversimplified one but it helps us to understand what is going on in the problem. We then have $K_{ij} = K_0 A_{ij}$, where A_{ij} is the ij th component of the adjacency matrix \hat{A} and K_0 the spring constant. The components of \hat{A} are non-negative such that $A_{ij} = 0$ or 1 according to whether or not a link between the i th and j th nodes exists in the

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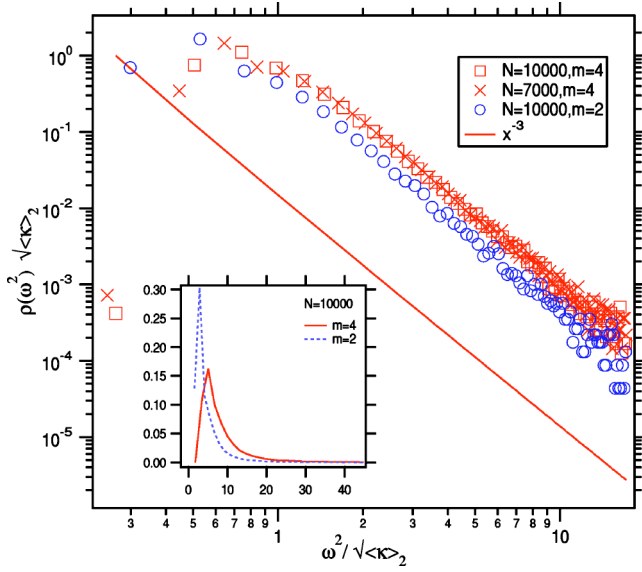


FIG. 1. (Color online) The tail behavior of the density of states, $\rho(\omega^2)\sqrt{\langle k \rangle_2}$ as a function of ω^2 , is shown in the logarithmic scales for the cases of the AB model with $m=2$ and $N=10^4$ (circles), with $m=4$ and $N=7 \times 10^3$ (crosses), and with $m=4$ and $N=10^4$ (squares), respectively. The line is a guide for showing $(\omega^2)^{-3}$. Here we have assumed that $\omega_0=K_0=M_0=1$ and $m_0=5$. $\langle k \rangle_2$ stands for the second order average degree of a node [13], which is defined by $\langle k \rangle_2 \equiv \sum_{i=1}^{N(\tau)} k_i^2 / \sum_{i=1}^{N(\tau)} k_i = \langle k^2 \rangle / \langle k \rangle$. The inset shows the density of states in the real scale for the cases of the AB model with $m=2$ and $m=4$ for $N=10^4$, respectively.

network. The degree $k_i(\tau)$ at the i th atom is given by $k_i(\tau) = \sum_{j=1}^{N(\tau)} A_{ji}$. From this, the last term in Eq. (2) becomes $\sum_{j=1}^{N(\tau)} K_{ji} q_j = K_0 k_i(\tau) q_i$. Hence, in this setting, we obtain

$$\Omega_i q_i = K_0 \sum_{j=1}^{N(\tau)} A_{ji} q_j, \quad (3)$$

for $i=1, \dots, N(\tau)$, where $\Omega_i \equiv M_i(\omega_i^2 - \omega^2) + K_0 k_i(\tau)$. We further assume that $M_i = M_0 = \text{const}$ and $\omega_i = \omega_0 = \text{const}$.

We have performed the calculation of spectrum of the oscillator system on a SFN with N nodes, directly diagonalizing the eigenequation of Eq. (3).

Figure 1 shows the tail behavior of the density of states. We find that the tail behavior is given by

$$P(\omega^2) \propto (\omega^2)^{-\gamma}, \quad (4)$$

where $\gamma=3$. This is coincident with the result in the weak coupling limit where the magnitude of spring constant K_0 is very small. In this limit, by a simple derivation using Eq. (3), we find $P(\omega^2 - \omega_0^2) \propto (\omega^2 - \omega_0^2)^{-\gamma}$ with $\gamma=3$. We may call this limit the *AB limit*, since the scaling behavior of the spectrum is the same as that of the network geometry itself. Thus we find that our vibrational model shares a common nature with the AB model of the SFN.

This is contrary to the conclusion previously obtained from the calculations of the spectrum of the adjacency matrix \hat{A} of the AB model [13–16]. There, it was shown that if the network has the tail behavior given by $P(k) \propto k^{-\gamma}$, then the

spectral tail for the eigenvalues λ of the adjacency matrix is given by $\rho(\lambda) \propto \lambda^{-\gamma'}$ where $\gamma' = 2\gamma - 1$. Hence if the AB model has $\gamma=3$, then $\gamma'=5$. This is different from our result of $\gamma'=3$.

The main reason for this phenomenon is explained as follows: In our vibrational model the Ω_i consists of the degree k_i of the node [see Eq. (3)]. Therefore, as the system grows, so does the magnitude of Ω_i . This can reduce the contributions of the higher terms in the perturbation series of \hat{A} . Hence the spectral behavior is dominated by the diagonal elements of eigenequation of Eq. (3). Here we note that while the adjacency matrix \hat{A} does not consist of diagonal elements at all, the eigenequation of Eq. (3) does consist of the diagonal elements that are the degrees of nodes. Since the distribution of the diagonal elements follows that of degrees of nodes, so does the distribution of the eigenvalues. Therefore this tendency is not affected by the magnitude of the coupling constant K_0 . Thus we are led to the same spectral behavior in the AB limit.

The physical meaning of the above results can be understood as follows: The main peak in the density of states is attributed to vibrational modes with frequency ω_0 . These modes are extremely localized within the least connected nodes in the SFN such that the total number of the localized modes provides the height of the peak. Since the number of modes is nothing but the number of degeneracy of the eigenequation, these localized modes are highly degenerate.

On the other hand, there is the power-law tail of $\rho(\omega^2) \propto (\omega^2)^{-3}$ as $\omega \rightarrow \infty$. This means that the larger the frequency of modes the fewer the number of modes. In other words, as the frequency is increasing, the number of modes is decreasing as power law. As the result, there appears only one mode with the maximum frequency (i.e., the maximum eigenvalue). The mode with the maximum frequency is extended over the entire system of the SFN. This situation means that in the SFN the lowest frequency modes can be very easily excited, while the maximum frequency mode is very hard to excite. Thus it is very hard for the high frequency modes to exist in the system of oscillators coupled in the SFN. This nature is very different from that of the standard systems of networks such as RN [9] and lattices [10], where there are a small number of degrees of nodes. This is the most prominent characteristic of our system.

The behavior of the maximum eigenvalue λ_{max} of the adjacency matrix \hat{A} is very important in the network theory [1,2,13–16]. In the standard networks such as the random networks [2,9], the maximum eigenvalue λ_{max} cannot grow as fast as the network grows [1,2,13–16]; and also, as in solid state physics, networks in most of the physical systems provide the so-called energy bands that are a spectrum with finite spectral regions [10]. This is due to the topology of the finite coordination number of atoms in the network of the lattice structure [10]. Therefore in order to elucidate the difference between the SFNs and other networks the growth of the maximum eigenvalue provides an important quantity.

As was numerically studied by many authors [1,2,14–16], the maximum eigenvalue λ_{max} of the adjacency matrix \hat{A} in the AB model is proportional to $\sqrt{k_{max}}$ such that λ_{max}

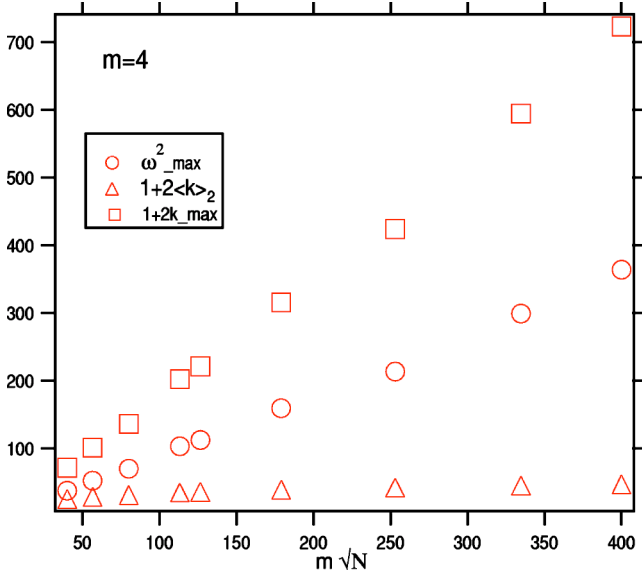


FIG. 2. (Color online) The behavior of the maximum eigenvalue in the spectrum. The maximum eigenvalue ω_{max}^2 (circles), the maximum degree of nodes $\omega_0^2+2\langle k \rangle_2$ (triangles), and the second order average degree $\omega_0^2+2k_{max}$ of nodes (squares) are shown, respectively. The calculations have been carried out for the AB model with $m=4$ and N is up to $N=10^4$.

$\propto \sqrt{k_{max}}$. Here k_{max} means the maximum degree of a node in the network such that $k_{max} = \max_i \{k_i\}$, and the numerical studies showed that $k_{max} \propto \sqrt{N}$. Therefore we obtain $\lambda_{max} \propto N^{1/4}$.

In spite of such efforts, the growth of the maximum eigenvalue of a physical model on the SFN is not so well-known. This is because the eigenvalues of the adjacency matrix are different from those of the eigenequation of a physical system. In this sense, the problem to investigate the growth behavior of the maximum eigenvalue is not a trivial one. Thus, in order to see this point, let us consider the maximum eigenvalue ω_{max} of our vibrational system of oscillators.

We have performed calculations of the maximum eigenvalue (i.e., vibrational mode) ω_{max} in our model of oscillators on the AB-SFN, where $m=4$ and N is developed up to $N=10^4$. In Fig. 2, the maximum eigenvalue ω_{max}^2 , the maximum degree of a node k_{max} , and the second order average degree $\langle k \rangle_2$ are shown, respectively. Here we have obtained the following relation:

$$\omega_0^2 + 2\langle k \rangle_2 \leq \omega_{max}^2 \leq \omega_0^2 + 2k_{max}. \quad (5)$$

This looks similar to the result in the previous literature [1,2,14–16]:

$$\omega_{max}^2 \propto \omega_0^2 + \sqrt{k_{max}}, \quad (6)$$

which is not supported by our numerical calculations, however. Therefore, as the spectral tail of our vibrational model is different from that of the AB-model as discussed in the previous section, so is the growth behavior of the maximum eigenvalue of our vibrational model. This is an important property of our physical model with the AB-SFN.

Let go back to Eq. (3) to consider the origin of the in-

equality, Eq. (5). From the Hadamard-Gerschgorin's theorem [10] we can derive an inequality

$$|\Omega_i| \leq K_0 \sum_{j=1}^{N(\tau)} |A_{ji}| \frac{|q_j|}{|q_i|}. \quad (7)$$

Since $|q_j|/|q_i| \leq 1$ and $|A_{ji}| = A_{ji}$, we can derive $|\Omega_i| \leq K_0 \sum_j A_{ji} = K_0 k_i(\tau)$, which then yields a theorem.

Theorem 1.

$$\left| \omega^2 - \omega_i^2 - \frac{K_0}{M_i} k_i(\tau) \right| \leq \frac{K_0}{M_i} \sum_j |A_{ji}| = \frac{K_0}{M_i} k_i(\tau). \quad (8)$$

Thus there exists at least one atomic site (i.e., node) that satisfies Eq. (8) for all eigenvalues ω . This implies that ω^2 is included within a disk of radius $K_0 k_i(\tau)/M_i$ and its center $\omega_i^2 + K_0 k_i(\tau)/M_i$.

Since in our model all K_{ij} (i.e., A_{ij}) are non-negative, by applying the Perron-Frobenius's theorem [10] to Eq. (8) we can derive $|\omega^2 - \omega_i^2| \leq 2K_0 k_i(\tau)/M_i$. Hence the maximum frequency ω_{max}^2 satisfies another theorem.

Theorem 2.

$$2 \frac{K_0}{M_0} \min_i \{k_i(\tau)\} \leq \omega_{max}^2 - \omega_0^2 \leq 2 \frac{K_0}{M_0} \max_i \{k_i(\tau)\}. \quad (9)$$

We assumed that $M_i \equiv M_0 = \text{const}$ and $\omega_i = \omega_0 = \text{const}$. Hence this theorem verifies our numerical results in the previous section.

Therefore the upper limit of the spectrum (i.e., spectral edge) grows as fast as the network grows. This is a remarkable fact for excitations in the SFN models and this nature is very different from that of Anderson localization where only mobility edge may appear in the spectrum and the band edge cannot grow as fast as the system size grows [10].

The above Theorems seem good enough to consider the standard networks such as periodic lattice systems or the random networks [10] or the small world networks [12] that the distribution of the degrees of node is limited. Because in these systems there exist finite lower and upper limits of the degrees of node such that the error width is bounded as

$$\Delta(\omega_{max}^2 - \omega_0^2) \geq \max_i \left[2 \frac{K_0}{M_i} k_i(\tau) \right] - \min_i \left[2 \frac{K_0}{M_i} k_i(\tau) \right]. \quad (10)$$

Next, we confirm that the above theorems can be applied even for the SFN, although in the SFNs there exist various orders of nodes without any bound but with a power-law distribution. Denote by $\vec{k}_i = (A_{i1}, \dots, A_{iN(\tau)})^t$ the i th column vector of $\hat{\mathbf{A}}$. The vector represents the way of links between the i th node and other nodes; it defines the degree k_i of the i th node such that $k_i \equiv \vec{k}_i^t \cdot \vec{k}_i = \sum_j A_{ij}$. Therefore let us call \vec{k}_i vectors the *link vectors*. Using this representation, we can rewrite the adjacency matrix as $\hat{\mathbf{A}} = (\vec{k}_1, \dots, \vec{k}_{N(\tau)}) = (\vec{k}_1^t, \dots, \vec{k}_{N(\tau)}^t)^t$. From this, we can derive that $\hat{\mathbf{A}}^2 = (\vec{k}_1^t \cdot \vec{k}_j)$, which is nothing but the Gramian matrix among the link vectors, \vec{k}_i , such that $\text{Tr}(\hat{\mathbf{A}}^2) = \sum_{i=1}^{N(\tau)} \vec{k}_i^t \cdot \vec{k}_i = \sum_{i=1}^{N(\tau)} k_i = 2L(\tau)$.

We now rewrite Eq. (3) as $\Omega_i \vec{q} = K_0 \hat{\mathbf{A}} \vec{q}$. Hence $\Omega_i^2 \vec{q}$

$= K_0^2 \hat{\mathbf{A}}^2 \vec{q}$. Let us now use the Hadamard-Gerschgorin theorem or the Perron-Frobenius theorem [10] for $K_0^2 \hat{\mathbf{A}}^2$. We can derive an inequality $|\Omega_i^2| \leq K_0^2 \sum_{j=1}^{N(\tau)} |(\hat{\mathbf{A}}^2)_{ji}| |q_j| / |q_i|$. Since $|q_j| / |q_i| \leq 1$ and $|(\hat{\mathbf{A}}^2)_{ji}| = (\hat{\mathbf{A}}^2)_{ji} = \vec{k}_j \cdot \vec{k}_i$, we can derive $|\Omega_i^2| \leq K_0^2 \sum_j |(\hat{\mathbf{A}}^2)_{ji}| = K_0^2 \sum_j \vec{k}_j \cdot \vec{k}_i = K_0^2 \vec{k}_{tot} \cdot \vec{k}_i$, where $\vec{k}_{tot} = \sum_{i=1}^{N(\tau)} \vec{k}_i = (k_1, k_2, \dots, k_N)$. Then we have $|\omega^2 - \omega_i^2 - K_0 k_i(\tau) / M_i|^2 \leq (K_0 / M_i)^2 \vec{k}_{tot} \cdot \vec{k}_i$. Therefore it then yields a theorem.

Theorem 3.

$$\left| \omega^2 - \omega_i^2 - \frac{K_0}{M_i} k_i(\tau) \right| \leq \frac{K_0}{M_i} \sqrt{\vec{k}_{tot} \cdot \vec{k}_i}. \quad (11)$$

Thus there exists at least one atomic site that satisfies Eq. (11) for all eigenvalues ω . This implies that ω^2 is included within a disk of radius $(K_0 / M_i) \sqrt{\vec{k}_{tot} \cdot \vec{k}_i}$ and its center $\omega_i^2 + K_0 k_i(\tau) / M_i$. Since $|\omega^2 - \omega_i^2| - |K_0 k_i(\tau) / M_i| \leq |\omega^2 - \omega_i^2 - K_0 k_i(\tau) / M_i|$, we obtain $|\omega^2 - \omega_i^2| \leq (K_0 / M_i) (k_i(\tau) + \sqrt{\vec{k}_{tot} \cdot \vec{k}_i})$. Therefore for the maximum frequency we obtain

$$\omega_{max}^2 \leq \omega_i^2 + \max_i \left[\frac{K_0}{M_i} (k_i(\tau) + \sqrt{\vec{k}_{tot} \cdot \vec{k}_i}) \right]. \quad (12)$$

The right-hand side of Eq. (12) is comparable with that of Eq. (9). In this way, the Theorems work for the SFN systems as well.

In conclusion, we have studied the system of oscillators connected by springs in the geometry of the AB model. We have found that the power-law behavior of the distribution of eigenvalues is the same as that of the distribution of degrees of nodes in the AB model as well. Second, we have found numerically that the asymptotic behavior of the maximum eigenvalue ω_{max} of the system is bounded as in Eq. (5). This results in the \sqrt{N} growth of the maximum eigenvalue as $N \rightarrow \infty$. We have also proved the above numerical results by applying mathematical theorems. Thus we conclude that when we apply a certain physical model to the geometry of an SFN, the physical property is strongly dominated by the geometrical property of the SFN. In this sense, not only the network geometry but also the physical model are important in the study of the SFN. The applications of the present model to other systems such as an electronic model might be straightforward. Therefore we expect that the physical nature of this model may share with that of such other systems.

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