Netons: vibrations of complex networks

2003 J. Phys. A: Math. Gen. 36 6329

(http://iopscience.iop.org/0305-4470/36/23/304)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 6329–6336 PII: S0305-4470(03)58190-2

Netons: vibrations of complex networks

Beom Jun Kim[1], **H Hong**[2] **and M Y Choi**[2,3]

[1] Department of Molecular Science and Technology, Ajou University, Suwon 442-749, Korea
[2] Korea Institute for Advanced Study, Seoul 130-012, Korea
[3] Department of Physics, Seoul National University, Seoul 151-747, Korea

E-mail: beomjun@ajou.ac.kr

Received 9 September 2002, in final form 24 March 2003
Published 29 May 2003
Online at stacks.iop.org/JPhysA/36/6329

Abstract

We consider atoms interacting with each other through the topological structure of a complex network and investigate lattice vibrations of the system, the quanta of which we call *netons* for convenience. The density of neton levels, obtained numerically, reveals that unlike a local regular lattice, the system develops a gap of finite width, manifesting extreme rigidity of the network structure at low energies. Two different network models, the small-world network and the scale-free network, are compared: the characteristic structure of the former is described by an additional peak in the level density whereas a power-law tail is observed in the latter, indicating excitability of netons at arbitrarily high energies. The gap width is also found to vanish in the small-world network when the connection range $r = 1$.

PACS numbers: 89.75.Fb, 63.20.Dj

1. Introduction

A variety of network systems such as computer networks, neuronal networks, biochemical networks and social networks, possess complex topological structure, which can be described neither by regular networks nor by completely random networks [1]. Among various models for generating such complex networks, the Watts–Strogatz (WS) model [2] and the Barabási–Albert (BA) model [3] provide the two most representative networks. Both model networks are characterized by very small network diameters proportional to the logarithm of the network size, which is dubbed 'small-world behaviour' and commonly observed in various real networks. Other important properties of many real network systems include high clustering [2] and scale-free degree distributions [3]. While most existing studies of complex networks have focused on the geometrical and topological characterization, now there is an increasing number of studies paying attention to the dynamics defined on the networks.

Lattice vibrations and associated phonon excitations on local regular networks, e.g., one-dimensional (1D) chains or two-dimensional square lattices, have been a textbook example of the introductory solid-state physics. In the case of such regular networks, atoms located on vertices interact only with nearest neighbouring atoms, resulting in the standard linear phonon dispersion. On the other hand, when the interaction between atoms takes the form of the connection topology of a complex network, ingredients of a long-range nature enter into the system. For example, the WS network has both local edges and long-range shortcuts [2], which in this work are interpreted as the coexistence of local and long-range interactions. Existing studies on phonon excitations have mostly been performed on the local regular networks such as d-dimensional hypercubic lattices or on the fractal geometry [4]. Recently, the spectral properties of lattice vibrations have been studied in a small-world network similar to the WS network [5]. However, the effects of the local interaction range and the dependence of the spectral properties on the rewiring probability have not been investigated in detail.

The main purpose of this work is to study in detail the vibration spectra of both the WS network and the BA network, in comparison with those of regular lattices. We thus consider atoms located on vertices of a complex network and interacting with each other connected via edges of the network, and investigate lattice vibrations and phonon excitations, with emphasis on the effects of the network topology. The results of such study can have implications in the mechanical property of a system of long chains bent in a complicated way. For example, in a bundle of long flexible polymer chains, some monomers which are separated by a long distance along a chain can make new couplings, building shortcuts. Throughout this work, we refer to phonons in a complex network as *netons*, to manifest the qualitatively different characteristics due to the fact that the underlying geometric structure is not a usual periodic lattice. By means of numerical diagonalization of the dynamic matrix, neton excitation spectra are obtained and the corresponding density of neton levels is computed. It is revealed that the complex network, in general, has a finite gap in the level density, indicating the absence of low-energy excitations. The dependence of the gap width on the rewiring probability and the local interaction range is investigated in detail. The existence of the gap is also reflected by the vanishingly small specific heat at low temperatures. In the WS network three singularities are observed in the neton-level density: among them two are shown to be reminiscent of the van Hove singularity present in the local regular network, while the third one originates from the complex network structure. The BA network is also considered and the scale-freeness results in a power-law distribution of the level density, suggesting excitability of netons with arbitrarily high energies.

2. The model

We build the WS network following [2]: first, a 1D regular network with only local connections of range r is constructed under the periodic boundary conditions. Next, each local edge (or link) is visited once, and with the rewiring probability P removed and reconnected to a randomly chosen vertex. After a whole sweep over the entire network, the average number of shortcuts in the system of size N is given by NPr. In the WS network built as above, an atom is put on every vertex whereas an edge connecting two vertices represents the coupling between the two atoms located at the two vertices. For simplicity, we assume that all atoms are identical, each having mass M and moving only along the direction of the chain. The equation of motion for the lth atom at the position x_l then reads

$$M\ddot{x}_l = C \sum_{m \in \Lambda_l} (x_m - x_l) \tag{1}$$

where Λ_l stands for the set of vertices connected to the lth vertex (via either local edges or shortcuts) and the interaction strength C is assumed to be the same for any pairs of the interacting atoms.

In the absence of shortcuts, equation (1) describes a 1D chain of atoms with only local connections up to the rth nearest neighbours. The analytic solution in this limit of $P = 0$ is easily found to take the form: $x_l \propto e^{i(kla-\omega t)}$, where a represents the interparticle spacing, ω is the eigenfrequency and the periodic boundary conditions, $x_{N+l} = x_l$, restrict the wavenumber k to take the value $k = 2\pi n/N$ with integer n. For simplicity, we set $a \equiv 1$, and obtain

$$\omega^2 = \frac{2C}{M}\sum_{j=1}^{r}(1 - \cos jk) \tag{2}$$

which leads to the dispersion relation

$$\omega \approx \sqrt{\frac{Cr(r+1)(2r+1)}{6M}}k \tag{3}$$

for small wavenumbers ($k \to 0$). Equation (3) shows that $\omega \propto k$ regardless of the local interaction range r. Such linear dependence of the frequency ω on the wavenumber k implies that the group velocity equals the phase velocity, both of which are frequency independent. Henceforth we measure the frequency ω in units of $\sqrt{C/M}$ for convenience.

In the presence of shortcuts ($P \neq 0$), the plane wave solution fails, owing to the lack of the translational symmetry. Substituting $x_l = \bar{x}_l e^{i\omega t}$ in equation (1), we write the equation of motion in the matrix form

$$\omega^2\mathbf{X} = \mathbf{D}\mathbf{X} \tag{4}$$

where $\mathbf{X}$ is the N-dimensional column vector with the components $\bar{x}_i$ ($i = 1, \ldots, N$). The $N \times N$ dynamic matrix $\mathbf{D}$ has the elements

$$D_{ij} = \begin{cases} |\Lambda_i| & \text{for } i = j \\ -1 & \text{for } j \in \Lambda_i \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where $|\Lambda_i|$ denotes the number of vertices connected directly to the ith vertex via local edges or shortcuts. It should be noted that D_{ij} lacks the translational symmetry due to the existence of shortcuts. We have performed numerical diagonalization of the dynamic matrix $\mathbf{D}$ for various network sizes $N = 100$, 200, 400 and 800, only to find insignificant difference between the two largest sizes. The eigenfrequencies found numerically for a given network realization are sorted in ascending order and an integer label n is attached from the lowest eigenfrequency ($n = 0$ for the smallest ω, $n = 1$ for the next smallest ω and so on). To obtain better statistics, we have also considered 1000–10 000 different network realizations, over which averages are taken.

3. Results

Figure 1 shows the neton frequency ω versus the *quasi-wavenumber* $q \equiv 2\pi n/N$ at various values of the rewiring probability P for the local interaction range (a) $r = 1$ and (b) $r = 2$. Note that the quasi-wavenumber q becomes identical to the true wavenumber k only when $P = 0$. In general, the wavenumber k is not appropriate for the system in the presence of shortcuts ($P \neq 0$): it does not make a good quantum number for $P \neq 0$, where the translational symmetry is broken. For the range $r = 1$, figure 1(a) suggests that the linear dispersion relation $\omega \sim q$, which has been obtained analytically in equation (3) for $P = 0$, still appears

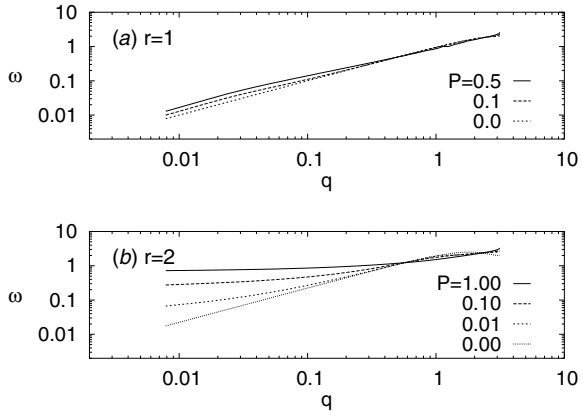

Figure 1. Frequency spectra of the WS network with size $N = 400$ and the local interaction range (*a*) $r = 1$; (*b*) $r = 2$. The neton frequency ω is plotted as a function of the quasi-wavenumber $q \equiv 2\pi n/N$, where n ($\geqslant 0$) is the integer labelling the eigenfrequency from the smallest one. In the absence of shortcuts ($P = 0$), the linear relation $\omega \sim q$ is shown for both $r = 1$ and $r = 2$. In the presence of shortcuts ($P \neq 0$), disclosed are very distinct frequency spectra between the two cases $r = 1$ and $r = 2$.

to hold at any value of P. In contrast, for the local interaction range $r = 2$, the dispersion $\omega(q)$ changes its functional form as P is raised from zero, reducing to the linear relation $\omega \sim q$ only in the limit of $P \to 0$ (see figure 1(*b*)). In particular, it is evident in figure 1(*b*) that for $P \neq 0$ there appears a nonzero minimum value of ω, below which the eigenfrequency does not exist. We have also examined the cases with range greater than 2 ($r > 2$) and confirmed that these features remain qualitatively the same. With regard to this, it is of much interest to note that the WS network has a finite clustering coefficient[4] only when $r \geqslant 2$ [2], which makes it plausible that the difference in the neton frequency spectrum between the cases $r = 1$ and $r = 2$, shown in figures 1(*a*) and (*b*), respectively, is a manifestation of the clustering effects. We have also considered numerically the decomposition property of the network and found that while the WS network with $r \geqslant 2$ does not decompose into distinct parts, for $r = 1$ the probability of decomposition is finite. However, it should be noted that those networks with $r = 1$ which are not decomposed still display the vanishing gap. Consequently, the vanishing gap in figure 1(*a*) for $r = 1$ has its origin not in the decomposition property but presumably in the clustering property of the network. Similar WS networks can also be built in a slightly different manner: instead of rewiring local connections with the total number of edges fixed, one may *add* shortcuts to the network without removing local connections. In this case, we have confirmed numerically that there exists a gap even for $r = 1$, which is in parallel to the observation that the XY model on the WS network with $r = 1$, constructed in such a way, has a finite-temperature transition, similar to that in the original WS network with $r > 1$ [6].

We next consider the neton-level density $g(\omega)$, which is given by [7]

$$g(\omega) \propto \int \mathrm{d}k\, \delta(\omega - \omega(k)) \tag{6}$$

[4] The clustering coefficient is defined to measure the extent to which two neighbouring vertices of a vertex are also neighbours of each other (see [2]).

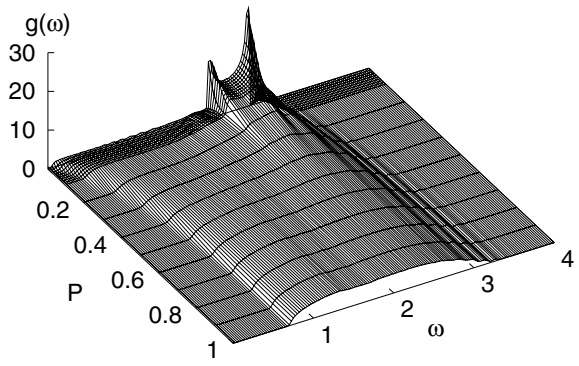

Figure 2. Neton-level density $g(\omega)$ of the WS network with size $N = 400$ and the local interaction range $r = 2$ as a function of the frequency ω and the rewiring probability P.

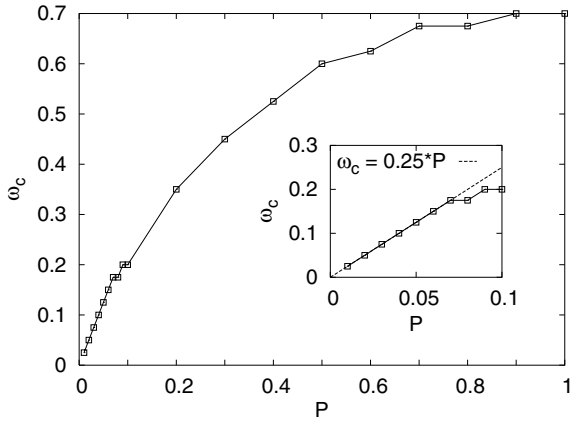

Figure 3. Dependence of the gap width ω_c on the rewiring probability P. The inset demonstrates that ω_c is well described by the relation $\omega_c \propto P$ for small P.

in one dimension. Using the mathematical identity $\delta(\omega - \omega(k)) = |\mathrm{d}\omega/\mathrm{d}k|^{-1}\delta(k - k_0)$ with $\omega(k_0) \equiv \omega$, we write equation (6) in the form

$$g(\omega) \propto \left|\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|^{-1}_{k_0}. \tag{7}$$

In the regular network ($P = 0$), equation (7), together with equation (3), gives the density $g(\omega)$ independent of ω, i.e., $g(\omega) \sim \omega^0$, in the low-frequency limit $\omega \to 0$.

In the presence of shortcuts, we use the box counting method to compute the neton-level density from the obtained eigenvalues of the dynamic matrix. The resulting density $g(\omega)$ is plotted in figure 2, which exhibits several characteristic features. First, as already found in figure 1(b), the density $g(\omega)$ develops a gap ω_c below which $g(\omega) = 0$. Figure 3 shows that the gap ω_c, well described by the linear relation $\omega_c \propto P$ for small P (see the inset of figure 3), keeps increasing as the rewiring probability P is raised and then appears to saturate for $P \gtrsim 0.7$. Such saturation behaviour has also been observed in the synchronization phenomena in the WS network [8]. The emergence of the gap implies that the WS network is very rigid against lattice vibrations at small energies. In other words, one cannot excite netons at sufficiently low energies. We also compute the specific heat of the WS network for $P = 0.1$, and compare

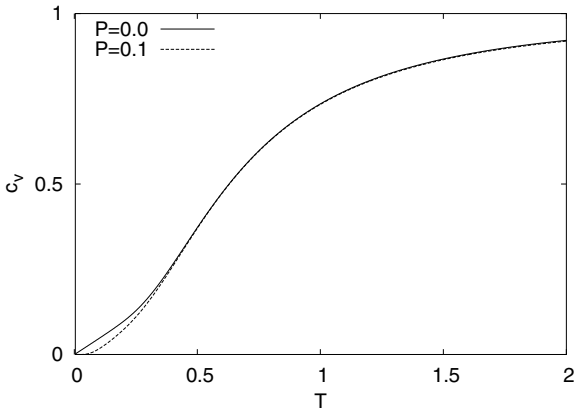

Figure 4. Specific heat c_v of the WS network with $N = 400$ and $r = 2$ at $P = 0$ and 0.1. The existence of a gap in the neton-level density at $P = 0.1$ is reflected by the exponentially small specific heat at low temperatures.

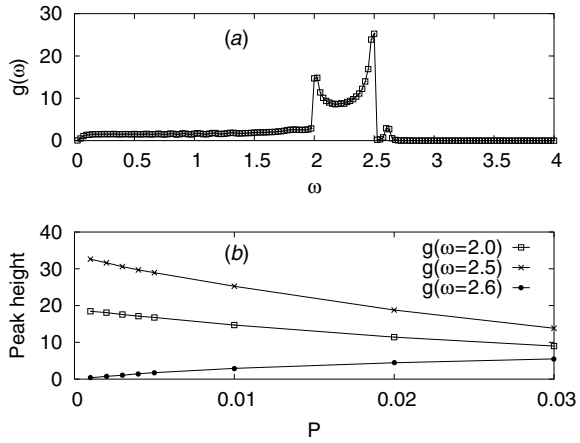

Figure 5. (*a*) Neton-level density $g(\omega)$ in the WS network with size $N = 400$ for $r = 2$ and $P = 0.01$. (*b*) Heights of the three peaks in (*a*) versus P. Of the three, two peaks are reminiscent of the local regular network and consequently their heights decrease with P. In contrast, the height of the third peak increases with P, suggesting that it has its origin in the complex network structure.

it with that of the local regular network ($P = 0$) in figure 4. As expected, the presence of a finite gap in the neton-level density gives rise to exponentially small specific heat at low temperatures. This is in contrast to the local regular network, where thermal excitations of phonons are gapless and, accordingly, the specific heat is described by the well-known Debye form with power-law dependence on the temperature, i.e., $c_v \propto T$ in one dimension.

The second interesting feature observed in the neton-level density in figure 2 is the emergence of sharp peaks at small P. Figure 5(a) shows in detail the density $g(\omega)$ at $P = 0.01$, displaying three peaks. It is well known that a local regular network ($P = 0$) (i.e., a regular lattice) has van Hove singularities whenever $\mathrm{d}\omega/\mathrm{d}k$ vanishes (see equation (7)). For example, in the local regular network with the second-nearest behaviour interaction ($r = 2$), the positions of the van Hove singularities are easily obtained: the eigenfrequency $\omega = \sqrt{2(2 - \cos k - \cos 2k)}$ given by equation (2), combined with the

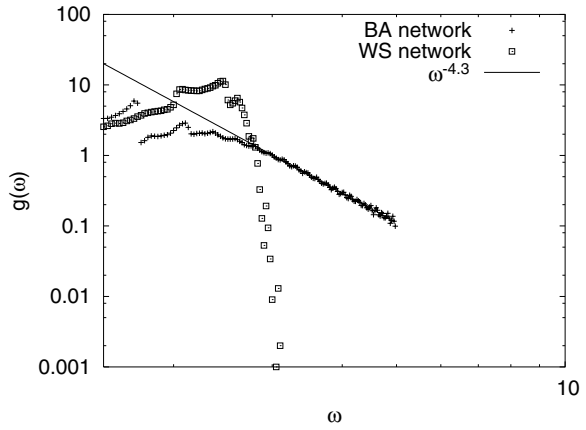

Figure 6. Neton-level density $g(\omega)$ in the BA network with size $N = 200$ and $M = 3$ is compared with that in the WS network with $N = 400$, $r = 2$ and $P = 0.1$. The log–log plot of $g(\omega)$ versus ω discloses the power-law tail at high frequencies in the BA network.

condition $\mathrm{d}\omega/\mathrm{d}k = 0$, leads to two singularities at $\omega = 2$ and $\omega = 5/2$; this allows us to conclude that the first two peaks in figure 5(a) are remnants of the van Hove singularities present in the local regular network. On the other hand, the third peak at $\omega \approx 2.6$ cannot be explained in terms of the singularity of the local regular network. In order to probe the origins of the peaks, we measure how the peak heights change as the rewiring probability P is varied and plot the results in figure 5(b). The first peak and the second one at $\omega = 2$ and at $\omega = 2.5$, respectively, are observed to have heights which decrease with P. This again confirms that these two peaks originate from the local regular network, thus becoming weaker as the network loses its local structure. The height of the third peak, in contrast, is found to grow as P is increased, which clearly indicates that the third peak provides a feature generic to the WS network structure.

Finally, we examine neton excitations in the BA network [3]. In more detail, we first grow the BA network, following [3]: starting from M vertices initially (at time $t = 0$), we attach a vertex with M edges at every time step. Once the BA network is built, we then put an atom on each vertex, assuming that the network is embedded in a 1D chain. The frequency spectrum is obtained in the same way as that of the WS network, with the dynamic matrix still given by equations (4) and (5). Similar to the WS network, the emergence of a gap is revealed. As the number M becomes larger, the gap grows and the peaks tend to smear out. Another interesting observation in the BA network is the slow decay of the density $g(\omega)$ at large frequencies, which is to be compared with the vanishingly small density at high frequencies found in the WS network. The log–log plot of the density $g(\omega)$ versus the frequency ω, displayed in figure 6, reveals that the BA network exhibits power-law decay which is well scaled as $g(\omega) \sim \omega^{-4.3}$. In contrast, $g(\omega)$ in the WS network shows very rapid decay, which is presumably of exponential form. The observed power-law decay of $g(\omega)$ in the BA network implies that netons may be excited with arbitrarily high energies. It is of interest to compare this with the behaviour of the adjacency matrix of the BA network [9]. Although the adjacency matrix $\mathbf{A}$, with $A_{ii} = 0$ and $A_{ij} = -D_{ij}$ for $i \neq j$, and the dynamic matrix $\mathbf{D}$ have different diagonal components, both show similar scale-free distributions at large eigenvalues.

4. Conclusion

In summary, we have investigated the phonon spectra in the monatomic chain where atoms interact with each other through the edges of complex networks. The density of phonon levels in the complex network, i.e., neton levels, has been found to develop a gap, which indicates that netons may not be excited up to the critical frequency, and accordingly, a finite amount of energy is required to generate lattice vibrations. This robustness of a complex network has also been shown to yield exponentially small specific heat at low temperatures, in contrast to the power-law temperature dependence in the local regular network. The characteristic structure of the WS network has been described by the emergence of a peak in the level density in addition to those originating from the van Hove singularities. In the BA network, on the other hand, the level density has been found to decay algebraically at high frequencies, which suggests excitability of arbitrarily high-energy netons.

Acknowledgments

This work was supported in part by the Korea Science and Engineering Foundation through grant no R14-2002-062-01000-0 (BJK) and in part by the Ministry of Education of Korea through the BK21 project (MYC).

References

[1] For reviews, see, e.g.
The special issue on complex systems 1999 *Science* **284** 79
Watts D J 1999 *Small Worlds* (Princeton, NJ: Princeton University Press)
Newman M E J 2000 *J. Stat. Phys.* **101** 819
Strogatz S H 2001 *Nature* **410** 268
Dorogovtsev S N and Mendes J F F 2002 *Adv. Phys.* **51** 1079
Albert R and Barabási A-L 2002 *Rev. Mod. Phys.* **74** 47
[2] Watts D J and Strogatz S H 1998 *Nature* **393** 440
[3] Barabási A-L and Albert R 1999 *Science* **286** 509
Barabási A-L, Albert R and Jeong H 1999 *Physica* A **272** 173
Albert R, Jeong H and Barabási A-L 1999 *Nature* **401** 130
[4] Alexander S and Orbach R L 1982 *J. Physique. Lett.* **43** L625
[5] Monasson R 1999 *Eur. Phys. J* B **12** 555
[6] Hong H, Choi M Y and Kim B J 2002 *Phys. Rev.* E **65** 047104
[7] See, e.g., Ashcroft N W and Mermin I 1976 *Solid State Physics* (New York: Saunders)
[8] Hong H, Choi M Y and Kim B J 2002 *Phys. Rev.* E **65** 026139
[9] Goh K-I, Kahng B and Kim D 2001 *Phys. Rev.* E **64** 051903