Lattice Vibration of the Cayley Tree

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(Received November 2, 1977)

Vibrational properties of a Cayley-tree-type system are investigated: Normal modes and squared frequency spectral densities are calculated for infinite homogeneous monatomic and diatomic Cayley trees. Effect of an impurity is then investigated. Existence of a virtual localized mode is thereby discussed with emphasis. Eigenfrequencies and eigenfunctions of a spherical Cayley tree of finite size are also calculated. Then the spectral density of the infinite homogeneous Cayley tree and that of the spherical Cayley tree in the large limit size are compared, and the relation between these two systems is discussed.

§ 1. Introduction

Cayley-tree structure has been treated by many theoretists, especially in connection with the theory of cooperative phenomena. There are, however, still only very few papers on the vibrational properties of the Cayley tree. In 1961, Rubin and Zwanzig studied lattice dynamics of a rooted Cayley tree and found that its vibrational spectral density becomes very unusual in the limit of large size: It is dense within the interval \((m^{1/2} - 1, m^{1/2} + 1)\), but discontinuous at every frequency for which it does not vanish. Here \(m\) is the branching number.

Recently, Tsuchiya obtained the diagonal Green function of a homogeneous Cayley tree, or the Bethe lattice, and calculated therefrom the spectral density of squared frequency \(D(\omega^2)\). This density is smooth and has no singular points at all, contrary to the density obtained by Rubin and Zwanzig. Tsuchiya also considered the Bethe lattice with an impurity and found that there exists an impurity frequency above the band.

The purpose of the present paper is to study in more detail the vibrational properties of Cayley trees and, especially, to clarify the reason why the spectrum obtained by Rubin and Zwanzig and that obtained by Tsuchiya are at variance with one another. The systems studied are homogeneous monatomic and diatomic Bethe lattices and spherical Cayley trees of finite and infinite size. Here a Cayley tree is defined as a uniformly branching structure which has no closed loops. And an infinite homogeneous Cayley tree with translational invariance is called the Bethe lattice. At first, vibrational spectral densities and eigenfunctions of a monatomic and a diatomic Bethe lattice are calculated in §§ 2 and 3, respectively, by using lattice Green functions. The spectra obtained are smooth, except that it consists of two separate bands in the case of diatomic lattice. It is shown that, if the coordination number \(z\) is larger than 3, the eigenfunctions fall off in
a spherically symmetric way from a site appropriately chosen, as is expected naturally from the energy conservation.

Secondly, effects of an impurity at the origin is investigated in § 4, for monatomic Bethe lattice. It is shown that for $z \geq 3$ the impurity mode may lie either above or below the continuous frequency band. In the next section, § 5, it is shown that the pole of Green function which lies on the second Riemann sheet corresponds to a virtual localized mode, which is not normalizable but gives rise to a similar effect on the scattering cross section to that of a true impurity mode corresponding to a pole on the first Riemann sheet.

In § 6 the vibrational properties of finite and infinite spherical Cayley tree are discussed in detail, by paying attention to the intimate relation between the spherical Cayley tree and the rooted Cayley tree. It turns out that the difference between the spectrum of Rubin and Zwanzig and that of Tsuchiya originates from the fact that the effect of inhomogeneity, or effect of surface, which is essential in a Cayley tree in contrast to ordinary lattices, is eliminated in the treatment of homogeneous Bethe lattice.

Discussion is given finally in § 7.

§ 2. Homogeneous Bethe lattice

Consider an infinite Bethe lattice with translational invariance. Let $M$ be the mass of atom and $u_i$ be the displacement of the atom at the $i$-th site. We assume nearest neighbor coupling with force constant $K$. Coordination number is assumed to be $z$.

The lattice Green function $G_{fi}(\omega^p)$ connecting the $i$-th and the $f$-th site is then expanded as $^\wedge$.$^\wedge$.$^\wedge$.

$$G_{fi}(\omega^p) = G_t(\omega^p) \left[ \delta_{if} + (1 - \delta_{if}) \right] \times (V_{if} G_{fi} + \sum_{n_1 \neq f} V_{in_1} G_{ni} V_{nj} G_{jf}^{n_1} \sum_{n_1 \neq f, n_2 \neq f} V_{in_1} G_{ni} V_{nj} G_{nf}^{n_1} V_{nf} \times G_{nf}^{n_2} \cdots )], \tag{2.1}$$

where $G_t(\omega^p)$ is the diagonal Green function defined by

$$G_t(\omega^p) = \frac{1}{(\omega^p - \omega_i^2 - \Sigma(i))}, \tag{2.2}$$

where the self-energy part $\Sigma(i)$ is given by

$$\Sigma(i) = \sum_{n_1 \neq f} V_{in_1} G_{ni} V_{nj} + \sum_{n_1 \neq f, n_2 \neq f} V_{in_1} G_{ni} V_{nj} G_{nf}^{n_1} V_{nf} \cdots \tag{2.3}$$

and $G_{n_1n_2\cdots n_{i-1}}(\omega^p)$ is a $(n_i, n_i)$ matrix element of the operator $(\omega^p - (H_0 + V)^{n_1n_2\cdots n_{i-1})^{-1}$. Further, the operator $(H_0 + V)^{n_1n_2\cdots n_{i-1})$ is obtained from $(H_0 + V)$ by putting $\omega_i^p = \omega_i^p = \cdots = \omega_2^p = \infty$.

The dynamical equation of motion for the $i$-th atom is

$$(\omega^p - z \gamma) u_i - \sum_{\beta=1}^{z} \gamma u_{i+\beta} = 0, \tag{2.4}$$
where \( \rho \) runs over \( z \) nearest-neighbor sites and \( \gamma = K/M \). Therefore, the \( i \)-th site squared frequency \( \omega_i^2 \) determined by \( H_0 \) and the transfer part \( V \) are given by

\[
\begin{align*}
(H_0)\omega &= z\gamma \delta_{i,v}, \quad (V)\omega = -\gamma \sum_{p} \delta_{p,v,i+p}.
\end{align*}
\]

(2.5)

Thanks to the homogeneity of the system, we may replace \( i \) in (2.1) by 0 (the origin). We shall always do this in what follows:

From (2.1)\(~(2.4), if the site \( n \) is the \( n \)-th site from the origin, we can obtain the Green function \( G_{n0}(\omega^2) \) for \( \omega^2 > \omega_i^2 (\omega_i^2 = (\sqrt{z-1} + 1)^2 \gamma) \) through a continued-fraction expansion

\[
G_{n0}(\omega^2) = G_0(\omega^2) L(\omega^2)^n,
\]

(2.6)

\[
G_0(\omega^2) = \frac{1}{\omega^2 - z\gamma - z\gamma^2
\frac{\omega^2 - z\gamma - (z-1)\gamma^2
\frac{\omega^2 - z\gamma - (z-1)\gamma^2}{\omega^2 - z\gamma - (z-1)\gamma^2} \cdots}
\]

(2.7)

\[
L(\omega^2) = \frac{-\gamma}{\omega^2 - z\gamma - (z-1)\gamma^2
\frac{\omega^2 - z\gamma - (z-1)\gamma^2}{\omega^2 - z\gamma - (z-1)\gamma^2} \cdots}
\]

(2.8)

The spectral density \( D(\omega^2) \) of squared frequency can be calculated from the diagonal Green function (2.7). \( D(\omega^2) \) is given by

\[
D(\omega^2) = \frac{z\sqrt{(\omega^2 - \omega_i^2)(\omega^2 - \omega_0^2)}}{\omega^2 (2\gamma - \omega^2)} , \quad \omega_0^2 \leq \omega^2 \leq \omega_i^2 ,
\]

(2.9)

where \( \omega_0^2 = (\sqrt{z-1} - 1)^2 \gamma \). \( D(\omega^2) \) for \( \omega_0^2 \leq \omega^2 \leq \omega_i^2 \) is the one derived by Tsuchiya.\(^5\)\(^\\*\) However, it should be noted that \( \omega^2 = 0 \) and \( \omega^2 = 2\gamma \) corresponding to translational and out-of-phase vibrations, respectively, do not belong to spectra in \( D(\omega^2) \), as may be seen from \( \int_{\omega_0^2}^{\omega_i^2} D(\omega^2) d\omega^2 = 1 \).

By the help of off-diagonal Green function, the relation \( u_n(\omega^2) \sim_{\omega^2 \rightarrow \infty} \text{Im} G_{n0}(\omega^2 - \text{i}\varepsilon) \) and the dispersion relation \( \omega^2 = \gamma (z - 2\sqrt{z-1} \cos \theta) \), the eigenfunction \( u_n(\omega^2) \) in the continuous band \( |\omega^2 - z\gamma| \leq 2\sqrt{z-1}\gamma \) can be obtained as follows:

\(^5\) A similar spectral density for magnon in the Heisenberg model is seen in Ref. 10.)
\[ u_n(\omega^2) = \frac{1}{z \sin \theta} \left( \frac{1}{\sqrt{z-1}} \right)^n ((z-1) \sin (n+1) \theta - \sin (n-1) \theta) , \tag{2.10} \]

where normalization factor has been determined through
\[ (z-1)^{n/2} \sum_{n=1}^{\infty} u_n(\omega^2) D(\omega^2) d\omega^2 = \delta_{n,0} \tag{2.11} \]

If \( z \geq 3 \), all the eigenfunctions in the band fall off in a spherically symmetric way from a site appropriately chosen. This is naturally expected from the energy conservation and the symmetry of the lattice.

§ 3. Diatomic Bethe lattice

A diatomic Bethe lattice is composed of alternatingly arranged atoms \( \text{A} \) and \( \text{B} \) with masses \( m_\text{A} \) and \( m_\text{B} \). Let us assume that the nearest-neighbor force constant \( K \) and the coordination number \( z \) are the same as before. If the displacement at lattice site \( i \) occupied by \( \text{A} \) atom and the displacement at lattice site \( j \) occupied by \( \text{B} \) atom are denoted by \( u_i^\text{A} \) and \( u_j^\text{B} \), respectively, two sets of equations of motions are obtained:

\[ \omega^2 u_i^\text{A} = z \gamma_\text{A} u_i^\text{A} - \gamma_\text{A} \sum_{\rho} u_{i+\rho}^\text{A} , \]
\[ \omega^2 u_j^\text{B} = z \gamma_\text{B} u_j^\text{B} - \gamma_\text{B} \sum_{\rho} u_{j+\rho}^\text{B} , \]

where \( \gamma_\text{A} = K/m_\text{A} \) and \( \gamma_\text{B} = K/m_\text{B} \) and \( \rho \) runs over the nearest-neighboring sites. In the method of renormalized perturbation, the diagonal Green functions \( G_\alpha^{\text{A}}(\omega^2) \) and \( G_\alpha^{\text{B}}(\omega^2) \) at \( \text{A} \) and \( \text{B} \) atom sites, respectively, are determined by the equations

\[ G_\alpha^{\text{A}}(\omega^2) = \frac{1}{\omega^2 - z \gamma_\alpha - \Sigma^\alpha(\omega^2)} \tag{3.1} \]

and

\[ \Sigma^\text{A}(\omega^2) = \frac{z \gamma_\text{A}}{\omega^2 - z \gamma_\text{B} - (1-1/z) \Sigma^\text{B}(\omega^2)} , \]
\[ \Sigma^\text{B}(\omega^2) = \frac{z \gamma_\text{A}}{\omega^2 - z \gamma_\text{B} - (1-1/z) \Sigma^\text{A}(\omega^2)} . \tag{3.2} \]

The self-consistent equations (3.2) have the solution

\[ \Sigma^\alpha(\omega^2) = \frac{X_\alpha X_\beta + \sqrt{(X_\alpha X_\beta - 4(1-z) \gamma_\alpha \gamma_\beta) X_\alpha X_\beta}}{2(z-1) X_\beta/z} , \tag{3.3} \]

where the abbreviation \( X_\alpha = \omega^2 - z \gamma_\alpha (\alpha = \text{A}, \text{B}) \) is used, and if \( \alpha \) takes \( \text{A} \), then \( \beta \) is \( \text{B} \) and vice versa. Similarly, it is possible to obtain the off-diagonal Green function \( G_\alpha^\text{B}(\omega^2) \) for \( \omega^2 > \omega^2_+ \) if the origin is occupied by an atom \( \text{A} \), as
Lattice Vibration of the Cayley Tree

\[ G_{2n}^a(\omega^2) = (L_A(\omega^2)L_B(\omega^2))^{\dagger}G_0^a(\omega^2), \]
\[ G_{2n+1}^a(\omega^2) = L_B(\omega^2)(L_A(\omega^2)L_B(\omega^2))^{\dagger}G_0^a(\omega^2), \]
where

\[ L_B(\omega^2) = -\frac{X_A X_B - \sqrt{(X_A X_B - 4(z-1)\gamma_A \gamma_B X_A X_B)}}{2\gamma_B(z-1)X_B}, \]
\[ L_A(\omega^2) = -\frac{X_A X_B - \sqrt{(X_A X_B - 4(z-1)\gamma_A \gamma_B X_A X_B)}}{2\gamma_A(z-1)X_A}. \]

If the origin is occupied by an atom \( B \), the corresponding Green functions \( G_{2n}^B(\omega^2) \) are obtained by only interchanging the suffices \( A \) and \( B \).

Vibrational spectral density of the diatomic Bethe lattice is given by

\[ D^a(\omega^2) = -\frac{1}{2\pi} \lim_{t \to +i0} \text{Im}(G_0^a(\omega^2 + i\varepsilon) + G_0^B(\omega^2 + i\varepsilon)). \]

In this case there exist two separate branches: acoustic and optical bands. The zeros of square roots of (3.3) give edges of each band. The top and bottom frequencies of the optical band, \( \omega_A^z \) and \( \omega_B^z \), respectively, and those of the acoustic band, \( \omega_A^z \) and \( \omega_+^z \), are obtained as

\[ \omega_{\pm}^z = \frac{z}{2} (\gamma_A + \gamma_B) \pm \sqrt{\left(\gamma_A - \gamma_B\right)^2 + 16(z-1)\gamma_A \gamma_B}/2, \]
\[ \omega_B^z = z\gamma_B \quad \text{and} \quad \omega_A^z = z\gamma_A, \]
if \( m_A > m_B \). The densities in each band are then given by

\[ D^a(\omega^2) = \frac{z}{4\pi} \frac{\sqrt{(\omega_+^2 - \omega^2)(\omega_+^2 - \omega_-^2)(\omega_B^2 - \omega^2)(\omega_A^2 - \omega^2)}}{\omega_+^2(\omega_A^2 + \omega_B^2 - \omega^2)} \left[ \frac{1}{\omega_A^2 - \omega^2} + \frac{1}{\omega_B^2 - \omega^2} \right] \]
\[ \text{for} \quad \omega_-^2 < \omega^2 < \omega_A^2, \]
\[ = \frac{z}{4\pi} \frac{\sqrt{(\omega_+^2 - \omega_-^2)(\omega_+^2 - \omega_A^2)(\omega_B^2 - \omega_A^2)(\omega_B^2 - \omega^2)}}{\omega_+^2(\omega_A^2 + \omega_B^2 - \omega^2)} \left[ \frac{1}{\omega_B^2 - \omega_A^2} + \frac{1}{\omega_B^2 - \omega^2} \right] \]
\[ \text{for} \quad \omega_B^2 < \omega^2 < \omega_+^2. \]

By taking account of the dispersion relation \( (\omega^2 - z\gamma_A)(\omega^2 - z\gamma_B) - 4(z-1)\gamma_A \gamma_B \cos^2 \theta = 0 \), we can also show that

\[ \int_{\omega_-^2}^{\omega_+^2} D^a(\omega^2) d\omega^2 + \int_{\omega_B^2}^{\omega_+^2} D^a(\omega^2) d\omega^2 = 1 \]
\[ \text{(3.9)} \]
just in the same way as in a monatomic Bethe lattice. The above result is shown in Fig. 1 for several values of \( z \). We can also obtain the eigenfunctions in a diatomic Bethe lattice, by using the off-diagonal Green function. Analytic continuation from \( \omega^2 > \omega_+^2 \) into the interval \( \omega_B^2 < \omega^2 < \omega_+^2 \) leads to

\[ u_{2n}^a(\omega^2) \propto \lim_{t \to +i0} \text{Im} G_{2n+1}^a(\omega^2 + i\varepsilon). \]
Therefore, $u_{2n}^A(\omega^2)$ is given by

$$u_{2n}^A(\omega^2) = \left( \frac{1}{\sqrt{z-1}} \right)^{2n} \frac{(z-1) \sin(2n+1)\theta - \sin(2n-1)\theta}{z \sin \theta}. \quad (3 \cdot 10a)$$

In the same way we have $u_{2n+1}^B(\omega^2) \propto \lim_{x \to +\theta} \text{Im} G_{2n+1}^B(o^2 + i\epsilon)$ and consequently

$$u_{2n+1}^B(\omega^2) = - \frac{2\gamma_A \cos \theta \sqrt{z-1}}{\omega^2 - \gamma_B} \left( \frac{1}{\sqrt{z-1}} \right)^{2n+1} \frac{(z-1) \sin(2n+2)\theta - \sin 2n\theta}{z \sin \theta}. \quad (3 \cdot 10b)$$

In deriving (3·10a) and (3·10b), we have made use of the dispersion relation

$$\omega^2 = \gamma_A^2 + \gamma_B^2 + \sqrt{(\gamma_A^2 - \gamma_B^2)^2 + 16(z-1)\gamma_A \gamma_B \cos^2 \theta}$$

for $\frac{\pi}{2} < \theta < \pi$.

If another dispersion relation

$$\omega^2 = \frac{\gamma_A^2 + \gamma_B^2 + \sqrt{(\gamma_A^2 - \gamma_B^2)^2 + 16(z-1)\gamma_A \gamma_B \cos^2 \theta}}{2}$$

for $0 < \theta < \pi/2$ is used, the same expressions (3·10a) and (3·10b) are obtained for the acoustical branch $\omega_2 < \omega^2 < \omega_4$.  

§ 4. Impurity mode

If the mass $M$ and the coordination number $z$ at the origin are replaced by $M'$ and $p$, respectively, the Green function $G_{p0}^P(\omega^2)$ corresponding to (2·6) is obtained in just the same way as before:

$$G_{p0}^P(\omega^2) = G_p^P(\omega^2) \alpha L(\omega^2)^p, \quad \omega^2 > \omega_2^p \quad (4 \cdot 1)$$
where
\[ G_{\alpha}^p(\omega^5) = \frac{2(z-1)}{(z-1) - p\alpha} \omega^5 - p\alpha \gamma (z-2) + p\alpha \sqrt{(\omega^2 - \gamma^2)^2 - 4(z-1)^2}, \] (4.2)

\[ \alpha = M/M' \text{ and } L(\omega^5) \text{ is given by (2.8).} \] An impurity mode can be determined by utilizing the conditions that its frequency \( \omega_{\text{imp}}^5 \) gives a pole of the Green function \( G_{\alpha}^p(\omega^5) \) and that its amplitude is normalizable. For the present case the condition of normalizability is given by \( |L(\omega^5)| < 1/\sqrt{z-1} \). For \( z \geq 3 \), the impurity mode may lie either above or below the continuous band; the side in which it lies depends on the values of \( \alpha \) and \( p \).

The impurity frequency \( \omega_{\text{imp}}^5 \) and its eigenfunction \( u_{\alpha}^p \) are given by
\[ \omega_{\text{imp}}^5 = \frac{p\alpha \gamma (p\alpha - z + 2)}{p\alpha - z + 1} \] (4.3)

and
\[ u_{\alpha}^p(\omega_{\text{imp}}^5) = \frac{1}{\sqrt{M}} \left( \frac{\alpha((p\alpha - (z-1))^2 - (z-1))}{(p\alpha - (z-1))(p\alpha - (z-2))} \right)^{1/2} \lim_{\omega^5 \to \omega_{\text{imp}}^5} (\omega^5 - \omega_{\text{imp}}^5) G_{\alpha}^p(\omega^5) \]
\[ = \sqrt{M} \left( \frac{(p\alpha - (z-1))^2 - (z-1)}{(p\alpha - (z-1))(p\alpha - (z-2))} \right)^{1/2} \frac{1}{p\alpha - z + 1}, \] (4.4)

for \( p\alpha > z - 1 + \sqrt{z-1} \) and \( 0 < p\alpha < z - 1 - \sqrt{z-1} \). For this solution it is easy to show that
\[ M'u_{\text{imp}}^5(\omega_{\text{imp}}^5) + \sum_{n=1}^{\infty} M u_{\text{imp}}^5 (z-1)^{n-1} = 1. \] (4.5)

The impurity frequency \( \omega_{\text{imp}}^5 \) is determined by a pole of Green function \( G_{\alpha}^p(\omega^5) \). However, if one continues the function \( G_{\alpha}^p(\omega^5) \) analytically into the second Riemann sheet across the cut \( \omega^5 \leq \omega \leq \omega_{\text{imp}}^5 \), it turns out that \( G_{\alpha}^p(\omega^5) \) has also a pole on that sheet for \( z - 1 - \sqrt{z-1} < p\alpha < z - 1 + \sqrt{z-1} \). This pole will be examined in the next section.

§ 5. Virtual localized mode

From the isotropic property of off-diagonal Green functions (2.6) and (4.1), we find a pseudo-linear chain which gives the same Green function as that of the Bethe lattice. The equations of motion of this pseudo-linear chain can be derived by assuming that the atoms at the same distance from the origin have the same displacement, and come out to be
\[ -M'\omega^5 u_0 = pKu_1 - pKu_0, \]
\[ -M\omega^5 u_n = Ku_{n-1} - (m+1)Ku_n + mKu_{n+1} \text{ for } n \geq 1, \] (5.1)

where \( m = z - 1 \).

To make the set of equations hermitian, new displacements \( \{v_\alpha\} \) are introduced
Then \((5\cdot1)\) is transformed into
\[
(\omega^2 - \alpha \gamma p) v_0 + \alpha \gamma p \frac{1}{\sqrt{m}} v_1 = 0 ,
\]
\[
\gamma \sqrt{m} v_{n-1} + (\omega^2 - (m + 1) \gamma) v_n + \gamma \sqrt{m} v_{n+1} = 0 .
\]  
(5\cdot3)

We can solve Eq. \((5\cdot3)\) by means of Tchebycheff polynomials. In the scattering form, the solution is, as is easily verified by substitution,
\[
v_n = e^{-i\omega n} - S(\theta) e^{i\omega n} ,
\]  
(5\cdot4)

where
\[
S(\theta) = \frac{D(\theta)}{D(\theta)} = \frac{m e^{i\theta} + (m - \alpha p) e^{-i\theta} + (\alpha p - (m + 1)) \sqrt{m}}{m e^{-i\theta} + (m - \alpha p) e^{i\theta} + (\alpha p - (m + 1)) \sqrt{m}} ,
\]  
(5\cdot5)

\[
\omega^2 = \gamma (m + 1 - 2 \sqrt{m} \cos \theta) .
\]  
(5\cdot6)

The first term of the right-hand side of \((5\cdot4)\) represents an incoming wave, while the second term represents the scattering wave. The function \(S(\theta)\) is usually called scattering matrix.

We define \(S(X)\) and \(D(X)\) as the analytic continuation of \(S(\theta)\) and \(D(\theta)\), respectively, across the real axis for \(\text{Im}(X) \geq 0\). As \(D(X)\) is analytic on the whole \(X\)-plane, a pole of \(S(X)\) corresponds to a zero of \(D(X)\). For \(p\alpha > \sqrt{m} + m\), we have \(D(X_\nu = \pi + i \eta_\nu) = 0\) for \(\eta_\nu > 0\), and the corresponding frequency is
\[
\omega_\nu^2 = \gamma (m + 1 - 2 \sqrt{m} \cos X_\nu) = \frac{\gamma \alpha p (\alpha p - (m - 1))}{\alpha p - m} .
\]
For \(0 < p\alpha < m - \sqrt{m}\), we have \(D(X'_\nu = i \eta'_\nu) = 0\) for \(\eta'_\nu > 0\); the corresponding frequency remains the same as above. These poles of scattering matrix \(S(X)\) in the upper half-plane of \(X\) correspond to the poles of the Green function in the first Riemann sheet and are associated with localized modes.

On the other hand, for \(m < \alpha p < m + \sqrt{m}\) and \(m - \sqrt{m} < \alpha p < m\), we have \(D(X_\nu = \pi - i \eta_\nu) = 0\) and \(D(X'_\nu = - i \eta'_\nu) = 0\) for \(\eta_\nu, \eta'_\nu > 0\), respectively. The corresponding frequency is given by
\[
\omega_\nu^2 = \gamma \frac{\alpha p (\alpha p - z + 2)}{\alpha p - z + 1} .
\]
These poles of \(S(X)\) in the lower half-plane of \(X\) can be identified with the poles of the Green function in the second Riemann sheet and represent a virtual localized mode. Such a mode cannot be normalized, in contrast with a true localized mode. The scattering cross section \(\sigma(\omega^2)\) may be calculated by comparing our solution
with the solution of the equations of motion:

\[ \gamma \sqrt{m} v_{n-1} + (\omega^2 - (m + 1) \gamma) v_n + \gamma \sqrt{m} v_{n+1} = 0, \quad n \geq 0 \]

with

\[ v_{-1} = 0. \quad (5.7) \]

The result is

\[ \sigma(\omega^2) = \left| S(\theta) - \left( \frac{e^{i\theta}}{e^{-i\theta}} \right)^2 \right| = \frac{p \alpha - m \left( \omega^2 - \omega_0^2 \right) \left( \omega_2^2 - \omega_0^2 \right) \left( \omega^2 - \alpha p \gamma / (p \alpha - m) \right)^2}{\omega^2 \left( \omega_0^2 - \omega_0^2 \right)} \]

for \( \omega_2^2 < \omega^2 < \omega_0^2 \). \quad (5.8)

As is well known, the localized mode and virtual localized mode cannot be distinguished by the scattering experiment. The frequencies \( \omega_0^2 \) and \( \omega_2^2 \) for localized and virtual localized modes are depicted as the function of \( \alpha \) and \( p \) in Fig. 2.

![Graph showing the variation of squared frequencies](https://example.com/graph.png)

Fig. 2. The variation of squared frequencies \( \omega_0^2 \) (solid curve) and \( \omega_2^2 \) (dashed curve) for a localized and a virtual localized modes as the function of \( \alpha \) and \( p \).

§ 6. Spherical Cayley tree

In the case of the \( N+1 \)-th order spherical Cayley tree, the potential is given by

\[ V = \frac{K}{2} \left[ \sum_{i=1}^{s} (u_{y} - u_{i})^2 + \sum_{i=1}^{s} \sum_{t=1}^{m} (u_{i} - u_{i,t})^2 + \ldots \right. \]

\[ \left. + \sum_{i=1}^{s} \sum_{t=1}^{m} \sum_{y=1}^{m} (u_{i,t} - u_{t})^2 + \sum_{i=1}^{s} \sum_{t=1}^{m} \sum_{y=1}^{m} (u_{i} - u_{i,t,y})^2 \right], \quad (6.1) \]
Here, \( u_0 \) is the displacement of the atom at the origin and \( u_{i_1 i_2 \ldots i_N} (1 \leq s \leq N+1) \) is the displacement of the atom at the point labelled by \( (i_1 i_2 \ldots i_N) \), which we call the point of the \( s \)-th shell. As before, \( z \) is the coordination number and \( m \) is the branching number. They are related by \( z = m + 1 \). For convenience, all atoms on the surface, i.e., in the \( N+1 \)-th shell, are held fixed. In the expression (6·2), \( i \) and \( j \) run over all atoms on the spherical Cayley tree.

The system under consideration is a modification of that examined by Rubin and Zwanzig, a rooted Cayley tree. The root, which is held fixed, is called 0. Starting from the root, the tree is constructed by a branching process. If we repeat the process \( N \) times, we obtain an \( N \)-th order tree. Displacements of atoms on the surface, or in the \( N+1 \)-th shell, are held fixed. The spherical and rooted Cayley trees are shown in Fig. 3.

![Diagram of Cayley trees](https://example.com/cayley_trees.png)

Fig. 3. (a) The \( N+1 (=3) \)-th order spherical Cayley tree with branching number \( m (=2) \). 1, 2 and 3 in the Figure represent, respectively, the first, the second and the third shells. (b) The \( N (=3) \)-th order rooted Cayley tree with branching number \( m (=2) \). The 0-th atom usually fixed is called the root, and the shell is defined in the same way as that of the spherical Cayley tree.

The allowed frequencies can be found by seeking the roots of secular equation. The secular equation for a spherical Cayley tree is given by

\[
D_{s+1}(\omega^2) = \det [\omega^2 \delta_{ij} - \bar{r}_{ij}] = 0, \tag{6·3}
\]

where the order of the determinant \( D_{s+1}(\omega^2) \) is

\[
\frac{(m+1) m^2 - 2}{m-1} \times \frac{(m+1) m^2 - 2}{m-1} \quad \text{and} \quad \bar{r}_{ij} = K_{ij}/M.
\]

According to Rubin and Zwanzig, we can get non-linear recurrence equations for the secular determinants \( D_{s+1}(\omega^2) \) as

\[
D_{s+1}(\omega^2) = x D_{s}^{m+1}(\omega^2) - (m+1) \gamma^2 D_{s}(\omega^2) - D_{s-1}^{m}(\omega^2), \tag{6·4a}
\]
Lattice Vibration of the Cayley Tree

\[ D_n(\omega^2) = x D_{n-1}(\omega^2) - m \gamma^2 D_{n-1}(\omega^2)^{m-1} D_{n-2}(\omega^2) \quad \text{for } n \geq 2, \]  
\[ D_1(\omega^2) = \omega^2 - (m+1) \gamma, \quad D_0(\omega^2) = 1, \]  
where the \( D_n(\omega^2) \)'s are the secular determinants of the \( n \)-th order rooted Cayley tree and \( x = \omega^2 - (m+1) \gamma \). In order to get the linear recurrence formula, we put

\[ D_{N+1}(\omega^2) = D_N(\omega^2) \{ D_N(\omega^2) D_{N-1}(\omega^2) \cdots D_1(\omega^2) \}^{m-1} Q_{N+1}(\omega^2) \]  
(6.5a)

and

\[ D_n(\omega^2) = \{ D_{n-1}(\omega^2) D_{n-2}(\omega^2) \cdots D_1(\omega^2) \}^{m-1} P_n(\omega^2). \]  
(6.5b)

Then, \{ \( D_{n-1} D_{n-2} \cdots D_1 \) \} \( m-1 \) can be factored out from each term, leaving the linear recurrence formulas

\[ Q_{N+1}(\omega^2) = x P_N(\omega^2) - (m+1) \gamma^2 P_{N-1}(\omega^2), \]  
(6.6a)

\[ P_n(\omega^2) = x P_{n-1}(\omega^2) - m \gamma^2 P_{n-2}(\omega^2). \]  
(6.6b)

We observe that

\[ P_0(\omega^2) = D_0(\omega^2) = 1, \quad P_1(\omega^2) = D_1(\omega^2) = \omega^2 - (m+1) \gamma. \]  
(6.7)

Starting with (6.7) and tracing back to (6.6a) and (6.6b), we know that \( Q_{N+1}(\omega^2) \) and \( P_n(\omega^2) \) are polynomials of the \( N+1 \)-th and \( n \)-th degree in \( \omega^2 \), respectively. These can be calculated by referring to the property of Tchebycheff polynomials. The result is

\[ P_n(\omega^2) = (m^{1/2} \gamma)^n \sin (n+1) \theta / \sin \theta, \]  
(6.8)

\[ Q_{N+1}(\omega^2) = (m^{1/2} \gamma)^N \sin \left( \frac{(N+2) \theta}{\sin \theta} - \frac{1}{m} \frac{\sin N \theta}{\sin \theta} \right), \]  
(6.9)

where \( \theta \) is defined by the dispersion relation

\[ \omega^2 = \gamma (m+1 - 2 \sqrt{m} \cos \theta). \]  
(6.10)

From (6.5a) and (6.5b), the determinant \( D_{N+1}(\omega^2) \) is expressed in terms of \( Q_{N+1}(\omega^2) \) and \{ \( P_n(\omega^2) \) \} as

\[ D_{N+1}(\omega^2) = Q_{N+1}(\omega^2) P_N(\omega^2)^N \prod_{r=1}^{N-1} \{ P_r(\omega^2) \}^{(m-1)(m+1)m^{N-r-1}}. \]  
(6.11)

Thus it is seen that one can locate the eigenfrequencies by seeking the zeros of the polynomials \( Q_{N+1}(\omega^2) \) and \( P_n(\omega^2) \) (\( n = 1, 2, \ldots, N \)). Thereby the multiplicity of these zeros should naturally be taken into account.

Except the zeros of \( Q_{N+1}(\omega^2) \), the \( n \) zeros of \( P_n(\omega^2) \) are easily found to be

\[ \theta_k^{(n)} = \frac{k \pi}{n+1}, \quad 1 \leq k \leq n. \]  
(6.12)

The corresponding frequencies are obtained from (6.10) as
K. Wada, T. Fujita and T. Asahi

\[ \omega(n, k) = \gamma(m + 1 - 2m^{1/2} \cos \theta_k^{(m)}) , \quad 1 \leq k \leq n , \quad 1 \leq n \leq N. \]

The above result is the same one as that given by Rubin and Zwanzig. Thus the spectral density \( D'(\omega^2) \) of the spherical Cayley tree is given, in the limit of large size, by

\[
D'(\omega^2) = \lim_{N \to \infty} \left[ -\frac{1}{\pi} \lim_{\varepsilon \to 0} \log \frac{d}{d\omega^2} \log D'_N(\omega^2 + i\varepsilon) / T_N \right]
\]

\[
= \lim_{N \to \infty} \left( -\frac{1}{\pi} \right) \lim_{\varepsilon \to 0} \left( \frac{Q'_{N+1}(\omega^2 + i\varepsilon)}{Q'_{N+1}(\omega^2 + i\varepsilon)} + \frac{mP'_N(\omega^2 + i\varepsilon)}{P_N(\omega^2 + i\varepsilon)} \right)
\]

\[
+ \sum_{n=1}^{N-1} \sum_{k=1}^{n} \frac{(m-1) (m+1) m^{N-r-1}}{(n, k)^2 + i\varepsilon} / T_n,
\]

where \( T_n = ((m+1)m^{N-2})/m-1 \) is the total number of sites. We could not find a closed form for (6.14). However, for practical purpose it is enough to know the spectra of \( P_1(\omega^2) \), \( P_2(\omega^2) \), \( \ldots \), and \( P_{10}(\omega^2) \), because for \( m \geq 2 \) they cover more than 99% of the whole spectrum. The spectral densities for a Bethe lattice and for a spherical Cayley tree are shown in Fig. 4.

Fig. 4. The spectral density of squared frequency \( D'(\omega^2) \) for a spherical Cayley tree in the large limit size. \( D'(\omega^2) \) for \( m = 2 \) is shown in (a) and \( D'(\omega^2) \) for \( m = 3 \) is shown in (b) and they cover about 99.4% and 99.99% of the whole spectra, respectively. The corresponding spectral density \( D(\omega^2) \) of the Bethe lattice is depicted in the right-hand corner of each figure for comparison.
Finally let us calculate the eigenfunctions of the spherical Cayley tree. Consider an \( n \)-th order rooted Cayley tree with fixed surface atoms. We assume that in this tree the atoms in the same shell have the same displacements and denote the displacements in the \( k \)-th shell by \( \tilde{u}_k \). Then we have a set of equations

\[-M\omega^2\tilde{u}_k = K\tilde{u}_{k-1} - (m + 1) K\tilde{u}_k + m K\tilde{u}_{k+1}, \quad k = 1, 2, \ldots, n\]  \tag{6·15}

with \( \tilde{u}_0 = \tilde{u}_{n-1} = 0 \). The eigenfunction of this system is given by

\[\tilde{u}_k = c \left( \frac{1}{\sqrt{m}} \right)^k \sin k\theta, \]  \tag{6·16}

where \( c \) is a constant. The eigenfrequencies are determined by

\[ \left( \frac{1}{\sqrt{m}} \right)^{n+1} \sin (n + 1)\theta = 0, \quad \omega^2 = \gamma (m + 1 - 2\sqrt{m} \cos \theta). \]  \tag{6·17}

We see that this gives the same set of eigenfrequencies as \( P_n(\omega^2) \) gives. In fact, we can construct the eigenfunctions of the original spherical Cayley tree as follows: Consider a spherical Cayley tree of \( N-n \) shells. If we attach to each site in the outermost shell of this tree an \( n \)-th order rooted Cayley tree, we obtain the original \( N+1 \)-th order spherical Cayley tree. Then each of the displacements \( \tilde{u}_0 \) of these attached rooted Cayley trees corresponds to the displacement \( u_{i_1i_2\cdots i_{N-n}} \) at a site in the \( N-n \)-th shell of the original spherical Cayley tree. Next, choose the set of the \( \tilde{u}_i \)'s in such a way that the sum relation \( \sum_{i_1i_2\cdots i_{N-n}} u_{i_1i_2\cdots i_{N-n}} = 0 \) is fulfilled for the displacements at the sites which branch from a site \( (i_1i_2\cdots i_{N-n}) \). Further, put the remaining displacements in the spherical Cayley tree equal to zero. Then \( \tilde{u}_0 \) corresponds to \( u_{i_1i_2\cdots i_{N-n}} \) and \( m-1 \) independent eigenfunctions can be determined within the above restriction, if we make the linear combinations of the eigenfunction given by \( 6·16 \) in the \( n \)-th order rooted Cayley tree.

Since there are \( (m + 1) m^{N-n-1} \) lattice points on the \( N-n \)-th shell and at each point \( m-1 \) independent eigenfunctions may be chosen for one frequency \( \omega^2 = \omega^2(n, k) \), the total multiplicity becomes \( (m + 1) m^{N-n-1}(m-1) \). For \( P_x(\omega^2) \)-mode, the restriction has the form \( \sum_{i_1i_2\cdots i_{N-n}} u_{i_1} = 0 \); the multiplicity is therefore \( m \). For \( Q_{N+1}(\omega^2) \)-modes also, we can proceed in just the same way. The assumption of the same displacement in the same shell leads us to a set of equations

\[ (\omega^2 - (m + 1) \gamma) \tilde{u}_0 + \gamma (m + 1) \tilde{u}_1 = 0, \]

\[ \gamma \tilde{u}_{k-1} + (\omega^2 - (m + 1) \gamma) \tilde{u}_k + m \gamma \tilde{u}_{k+1} = 0, \quad k = 1, 2, \ldots, N \]

\[ \tilde{u}_{N+1} = 0. \]  \tag{6·18}

The solution is easily found to be

\[ u_k = c (1/\sqrt{m})^k \left[ \sin (k-1)\theta - m \sin (k+1)\theta \right]. \]  \tag{6·19}
The eigenfrequencies determined by the formula $u_{N,1} = 0$ are identical with those given by $Q_{N+1}(\omega^i) = 0$. In this case we can take (6·19) as the eigenfunction of the total system. Note that in the limit of large $N$, this eigenfunction becomes the eigenfunction of a homogeneous Bethe lattice.

§ 7. Discussion

We have seen that an infinite homogeneous Cayley tree (the Bethe lattice) and a spherical Cayley tree in the large limit size behave in a quite different manner; for example, their vibrational spectral densities are at variance with each other. Referring to the argument given in the preceding section, this can be explained as follows: In the spherical Cayley tree in the large limit size, the fraction of points on the surface of the tree is $(m-1)/m$. Therefore, contrary to the usual lattices, the surface effects appear even in the thermodynamic limit. In the Bethe lattice, on the other hand, the assumption of homogeneity forces us to neglect the effect of inhomogeneity such as surface effects. This is the reason why Rubin and Zwanzig obtained an unusual spectrum while Tsuchiya got a smooth and even spectrum. Only the modes of the spherical Cayley tree for which $Q_{N+1}(\omega^i) = 0$ and which range from the origin to the surface, change into the eigenmodes of the Bethe lattice. This explains therefore the fact that if the defects are put at the center of a spherical Cayley tree, this tree in the large limit size gives the same defect mode as the Bethe lattice gives.

We have seen that the pole of the Green function in the second Riemann sheet gives rise to a virtual localized mode. The virtual localized mode contributes to the scattering cross section in just the same amount as a localized mode does. The virtual mode does not, however, contribute to the spectral density, because it cannot be normalized. It is worth while noting that the solutions corresponding to $\omega^i = 0$ and $\omega^i = 2\pi k$, which represent uniform translation and out-of-phase vibration, respectively, belong to virtual localized modes in the case of a homogeneous Bethe lattice.

We have also seen that loopless properties of the Bethe lattice make the system one-dimensional-like and make it easy to calculate exactly the lattice Green functions by the method of renormalized perturbation. However, it is also possible to extend our discussions to the decorated Bethe lattices such as the cactus tree.

Acknowledgement

One of the authors (K.W.) wishes to express his sincere thanks to Professor J. Hori for critical reading of the manuscript.

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