Density of states of the Cayley tree

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Abstract
The density of states (DOS) for nearest-neighbor hopping on Cayley trees is studied with a simple tight-binding model. A Cayley tree characterized by the coordination number \( Z \) and size \( S \) has two types of energy states: linear chain states and confinement states. The former, which constitute the overwhelming majority in number, are degenerate by a power law of \( Z - 1 \) to the power of the number of shells constituting a tree, whereas the latter, the wavefunctions of which spread out all over the tree, are merely \( S + 1 \) non-degenerate states for site-centered trees or \( 2S \) non-degenerate states for bond-centered trees, independently of \( Z \). The polynomial equations that express the DOS of the confinement states are obtained, and the relation between the confinement states and the DOS of the Bethe lattice is discussed.

1. Introduction

Infinity distinguishes the bulk solid from clusters in solid-state physics. However, the presence of a surface separates the two realistically. Properties or states caused by surfaces have recently attracted attention, such as those of topological insulators [1] and graphene nanoribbons [2]. The properties of a crystal have typically been investigated using band calculations, whereas those of clusters or mesoscopic systems are performed mainly with cluster calculations. It is generally considered that the bulk properties conflict with the surface effects because the former can be obtained by removal of the latter. As for crystalline solids, the surface effects can be eliminated using periodic boundary conditions. In order to investigate the influence of surfaces and finite size, cluster calculations with increasing cluster size have often been utilized. Bulk properties may also be obtained from the results of cluster calculations for large-sized clusters because the surface in typical crystalline solids has less influence on the characteristics of the central portion as the cluster size is increased. From this perspective, the relationship between the Bethe lattice [3] and the Cayley tree [4] is extremely interesting [5]. The Bethe lattice is a pseudolattice that, strictly speaking, does not possess translational symmetries, whereas the Cayley tree is a finite-sized cluster of the Bethe lattice structure. In the Bethe lattice, to which periodic boundary conditions cannot be applied, the equivalence of every lattice site enables the density of states (DOS) to be obtained by Green’s function methods [6]. The exact expression of the DOS for long-range hopping interactions has been reported recently [7]. However, the Cayley tree is a peculiar model where the surface effects are significant because the surface approaches infinity as the size approaches infinity. Therefore, it is difficult to eliminate the surface effects from the Cayley tree. However, a formula for the DOS of the Cayley tree has been obtained by Derrida and Rodgers [8] in consideration of the Bethe lattice. The Cayley tree and Bethe lattice have played important roles as models in the field of condensed matter or statistical physics [9–16].

Here, with a focus on the surface effects, we prove specifically that the states of the Cayley tree can be classified into two types according to the degeneracy and that the Bethe lattice is not the thermodynamic limit of the Cayley tree with respect to the DOS. The site-centered Cayley tree and the bond-centered Cayley tree are investigated. The results for the DOS, which consists of the two types of states, are provided in analytical form. Furthermore, an approach to the bulk states from the DOS of Cayley trees is discussed.
2. Method

2.1. Models

Two kinds of Cayley trees that have the shell structure are considered, as shown in figure 1, where each site has a constant number of branches $Z$, which is referred to as the coordination number of the Bethe lattice. The site-centered and bond-centered Cayley trees dealt with in this study are represented as $(Z, S)_s$ and $(Z, S)_b$, respectively, characterized by both the coordination number $Z$ and size $S$.

We first consider the site-centered Cayley trees, as shown in figure 1(a). The number of sites in the $r$th shell of the tree is

$$N_{(r)} = Z(Z - 1)^{r - 1} \quad (r = 1, 2, \cdots, S);$$

therefore, the number of surface sites is

$$N_{(S)} = Z(Z - 1)^{S - 1}.$$  \hspace{1cm} (2)

The total number of sites is

$$N = 1 + \sum_{r=1}^{S} N_{(r)} = \frac{(Z - 1)N_{(S)} - 2}{Z - 2},$$

and the number of interior sites is

$$N_{I} = 1 + \sum_{r=1}^{S-1} N_{(r)} = \frac{N_{(S)} - 2}{Z - 2}.$$  \hspace{1cm} (4)

Therefore, the ratio of the number of surface sites to the number of interior sites is

$$\frac{N_{(S)}}{N_{I}} = \frac{(Z - 2)N_{(S)}}{N_{(S)} - 2} \xrightarrow{s \to \infty} \frac{Z - 2}{Z - 2},$$

and the ratio of the number of surface sites to the total number of sites is

$$\frac{N_{(S)}}{N} = \frac{(Z - 2)N_{(S)}}{(Z - 1)N_{(S)} - 2} \xrightarrow{s \to \infty} \frac{Z - 2}{Z - 1}.$$  \hspace{1cm} (6)

In the case of the bond-centered Cayley trees, as shown in figure 1(b), the number of sites in the $r$th shell is

$$N_{(r)}^{(b)} = 2(Z - 1)^{r - 1} \quad (r = 1, 2, \cdots, S).$$

Therefore, the number of surface sites is

$$N_{(S)}^{(b)} = 2(Z - 1)^{S - 1}. \hspace{1cm} (8)$$
The total number of sites \( N^{(b)} \) and the number of the interior sites \( N_I^{(b)} \) are

\[
N^{(b)} = \sum_{r=1}^{S} N_r^{(b)} = \frac{(Z - 1)N_S^{(b)} - 2}{Z - 2}
\]  

(9)

and

\[
N_I^{(b)} = \sum_{r=1}^{S-1} N_r^{(b)} = \frac{N_S^{(b)} - 2}{Z - 2}.
\]

(10)

The expressions of \( N, N_I \), and their ratios are also available for the bond-centered trees by the substitution of equation (8) for equation (2).

For either Cayley tree, the surface sites are \( Z_2 \) times larger than the interior sites in large Cayley trees, and the surface then becomes dominant with larger \( Z \). This distinct characteristic of Cayley trees has been called a ‘peculiar surface’.

### 2.2. Calculations

We consider the simplest model for the hopping of a single quantum particle on sites in a Cayley tree, by only nearest-neighbor interactions. The tight-binding Hamiltonian is given by

\[
H = E_0 \sum_i |i \rangle \langle i | + t \sum_{\langle i,j \rangle} |i \rangle \langle j |,
\]

(11)

where \( E_0 \) is the on-site energy, \( t \) is the hopping energy (usually \( t < 0 \)) for the nearest-neighbor interaction, and \( |i, j \rangle \) denotes iteration over the nearest-neighbor sites. In matrix form:

\[
H = E_0 I + t A,
\]

(12)

where \( I \) and \( A \) are the identity matrix and the adjacency matrix in graph theory, respectively. In this study, we do not use the Green function or the recursion method but instead diagonalize the Hamiltonian matrix directly. A Cayley tree with size \( S \) consisting of \( N \) sites has \( N \) allowed energy states, which are obtained by diagonalization of the \( N \times N \) matrix \( H \). The calculations have been performed numerically for trees with various \( S \) and \( Z \). The determinant of \( H \) can be factorized into

\[
\det(H - EI) \propto \prod_{i=1}^{N} (E - E_i) = \prod_{j=1}^{N} (E - E_j)^{d_j} = 0
\]

(13)

using the energy level \( E_i \) along with the degeneracy \( d_j \), so that the DOS consists of sets of \( E_i \) and \( d_j \).

### 3. Results and discussion

The energy levels and their degeneracy of many Cayley trees were obtained through numerical calculations by diagonalization of the tight-binding Hamiltonian matrices. Data analysis revealed that most of the energy levels are degenerate and fixed, while the others are non-degenerate and unfixed. A fixed energy level depends on whether it can be found in the energy levels of any larger Cayley tree. First, the site-centered trees are analyzed. Next, the bond-centered trees are considered on the basis of the analytical results. Finally, the bulk states in the Cayley trees are discussed.

#### 3.1. Site-centered trees

A part of the numerical results from the tight-binding calculations for the site-centered trees is shown in table 1. Most of the energy levels of the \((3, 4)\) tree can be found in those of the \((3, 5)\) tree. The common energy levels in both trees are degenerate, while the others are non-degenerate. This characteristic is valid for any \((Z, S)\) and \((Z, S + 1)\) trees. The wavefunctions for the energy levels were investigated, examples of which are depicted in figures 2–5, and have revealed that a Cayley tree has two types of states: linear chain states that originate from the surface (figures 2–4) and interesting states that we have called confinement states afterward (figure 5).

#### 3.1.1. Linear chain states

The energy of an atomic cluster in a linear chain can be written as

\[
E = \alpha + 2 \beta \cos \theta,
\]

(14)

where \( \theta \) consists of the length \( n \) and the mode \( m \),

\[
\theta = \frac{m}{n + 1} \pi \quad (m = 1, 2, \cdots, n).
\]

(15)
Table 1. Numerical results of tight-binding calculations for (3, 4) and (3, 5) Cayley trees: energy ($\xi$) obtained from equation (19) and degeneracy ($D$), along with the analysis results of the type (L: linear chain state or C: confinement state) and the linear chain modes ($\theta$). The confinement states are non-degenerate.

| (3, 4) Cayley tree | (3, 5) Cayley tree |
|--------------------|--------------------|
| $\xi$              | $\xi$              |
| $D$                | $D$                |
| Type               | Type               |
| $\theta$           | $\theta$           |
| 1.811 291 364 3, 1  | 1.858 697 926 8, 1 |
| C                  | C                  |
| 1.618 033 988 7, 2 | 1.732 050 807 6, 2 |
| L                  | L                  |
| $4\pi$             | $2\pi$             |
| 1.414 213 562 4, 3 | 1.618 033 988 7, 3 |
| L                  | L                  |
| $\frac{4\pi}{3}$   | $\frac{2\pi}{3}$   |
| 1.104 184 583 1, 1 | 1.343 372 756 7, 1 |
| C                  | C                  |
| 1.000 000 000 0, 6 | 1.000 000 000 0, 14 |
| L                  | L                  |
| $\frac{2\pi}{5}$   | $\frac{2\pi}{7}$   |
| 0.618 033 988 7, 2 | 0.618 033 988 7, 3 |
| L                  | L                  |
| $\frac{4\pi}{3}$   | $\frac{2\pi}{3}$   |
| 0.000 000 000 0, 16 | 0.000 000 000 0, 32 |
| C, L               | L                  |
| $\frac{2\pi}{2}$   | $\frac{2\pi}{7}$   |
| $-$0.618 033 988 7, 2 | $-$0.618 033 988 7, 3 |
| L                  | L                  |
| $\frac{2\pi}{5}$   | $\frac{2\pi}{7}$   |
| $-$1.000 000 000 0, 6 | $-$1.000 000 000 0, 14 |
| L                  | L                  |
| $\frac{2\pi}{3}$   | $\frac{2\pi}{7}$   |
| $-$1.104 184 583 1, 1 | $-$1.343 372 756 7, 1 |
| C                  | C                  |
| $-$1.414 213 562 4, 3 | $-$1.414 213 562 4, 6 |
| L                  | L                  |
| $\frac{2\pi}{3}$   | $\frac{2\pi}{7}$   |
| $-$1.618 033 988 7, 2 | $-$1.618 033 988 7, 3 |
| L                  | L                  |
| $\frac{2\pi}{3}$   | $\frac{2\pi}{7}$   |
| $-$1.811 291 364 3, 1 | $-$1.858 697 926 8, 1 |
| C                  | C                  |

A Cayley tree with size $S$ comprises linear chains characterized by a depth $n$ from the surface, which ranges from $n = 1$ to $n = S$. Therefore, $\theta$ on the Cayley tree is expressed as

$$\theta_n(m) = \frac{m}{n + 1},$$  \hspace{1cm} (16)

and the energy is considered as $\alpha = E_0$ and $\beta = t\sqrt{Z - 1}$ from Mahan’s study [14],

$$E = E_0 + 2t\sqrt{Z - 1} \cos \theta_n(m),$$  \hspace{1cm} (17)

where $m = 1, 2, \ldots, n$, and $n = 1, 2, \ldots, S$. Considering $t < 0$ usually, this can be rewritten further as

$$\xi = -2 \cos \theta_n(m)$$  \hspace{1cm} (18)

by the introduction of a dimensionless energy

$$\xi = \frac{E - E_0}{|t|\sqrt{Z - 1}}.$$  \hspace{1cm} (19)

$\xi$ are used as values of energy in this study.

Figure 1(a) shows that waves with energy $\xi$, which satisfy the conditions for stationary waves $\lambda = 2(n + 1)/m$ using the wavelength $\lambda$ in units of topological distance between successive sites, travel on the linear chains from one site on the surface (the $S$th shell) through a site on the $(S - n)$th shell, which is inevitably an oscillating node, to other sites lying on the surface.

The linear chain mode $\theta_n(m)$ corresponds to $d_n$-fold degenerate states, where

$$d_n = \begin{cases} (Z - 2)N_{(S-n)} & (1 \leq n < S) \\ Z - 1 & (n = S) \end{cases}$$  \hspace{1cm} (20)

because $d_n$ is the number of cases of linear chains that have nodes on the $(S - n)$ th shell. This is obviously $Z - 1$ for the case of $n = S$ when the central site is the node. For the case $n < S$, the shell consists of $N_{(S-n)}$ sites (nodes) from equation (1). Each of the sites has $Z - 1$ bonds toward the surface; the selection of one among them inevitably leads to $Z - 2$ cases. When $n$ becomes smaller, $d_n$ becomes larger. $d_n$ is the largest in the case of $n = 1$, where the shortest paths from the surface to the surface are allowed. From equations (16) and (18), the number of energy levels defined by $\theta_n(m)$ corresponds to that of irreducible fractions.
where \( k (2 \leq k \leq S + 1) \) and \( \ell (1 \leq \ell \leq k - 1) \) are integers. The number of pairs of \( n \) and \( m \) that satisfy equation (21) is

\[
\frac{\ell}{k} = \frac{m}{n + 1}.
\]
Figure 3. Typical wavefunctions of linear chain states with $\xi = \pm 1$ obtained by numerical calculation for the (3, 5) Cayley tree, which can be classified by penetration depth, $n$: $n = 5 \left( \theta_1(2) = \frac{3\pi}{5}, \theta_3(4) = \frac{4\pi}{5} \right)$ and $n = 2 \left( \theta_1(1) = \frac{\pi}{2}, \theta_2(2) = \frac{3\pi}{2} \right)$ in equation (16). The probability is depicted in the rightmost column. The amplitudes, nodes, etc, are the same as those defined in figure 2.

Figure 4. Typical wavefunctions of linear chain states with $\xi = 0$ obtained by numerical calculation for the (3, 5) Cayley tree, which correspond to three types of penetration depth, $n$, in equation (16), $n = 5 \left( \theta_3(3) = \frac{4\pi}{5} \right)$, $n = 3 \left( \theta_2(2) = \frac{3\pi}{2} \right)$, and $n = 1 \left( \theta_1(1) = \frac{\pi}{2} \right)$, although they are marginally mixed states. The probability is depicted in the rightmost column. The amplitudes, nodes, etc, are the same as those defined in figure 2.

$$L = \ln \left[ \frac{S + 1}{k} \right].$$ (22)
Accordingly, the energy level $\xi = -2 \cos(\ell \pi / k)$ is $D(\xi)$-fold degenerate:

$$D(\xi) = \sum_{n=1}^{S} \sum_{m=1}^{n} d_n \delta(\xi + 2 \cos(\ell \pi / k)) = \sum_{\ell=1}^{L} d_{\ell k-1}$$

$$= Z(Z-2) \sum_{\ell=1}^{L} N_{S-\ell k+1}$$

$$= \begin{cases} 
Z(Z-2)(Z-1)^{S-\ell k} (Z - 1)^{\ell k - 1} / (Z - 1)^{k - 1} & \text{for } L k - 1 < S \\
Z(Z-2)(Z-1)^{S-(L-1)k} (Z - 1)^{(L-1)k - 1} / (Z - 1)^{k - 1} + (Z - 1) & \text{for } L k - 1 = S 
\end{cases}$$  \(23\)

It is clear from $k = 2$ that the energy level $\xi = 0$ is the most degenerate. In the thermodynamic limit,

$$\frac{D(\xi)}{N} \to \frac{(Z-2)^2}{(Z-1)^k - 1}.$$  \(24\)

Consequently, the linear chain states are considered to be the so-called surface states because all the wavefunctions are localized in the region from the surface to depth $n$, avoiding the central portion of the tree.
Next, consider the total number of linear chain states, $N_L$:

$$N_L = \sum_{n=1}^{S} \sum_{m=1}^{n} d_n = \sum_{n=1}^{S} n d_n = \sum_{n=1}^{S-1} n d_n + S d_S$$

$$= Z(Z - 2) \sum_{n=1}^{S-1} n(Z - 1)^{S-n+1} + (Z - 1)S$$

$$= Z \left[ \left( \frac{Z - 1}{Z - 2} \right)^{S-1} - 1 \right] + (Z - 1)S$$

$$= N - S - 1,$$  \hspace{1cm} (25)

using the total number of states, $N$. The linear chain states are an overwhelmingly majority in number and increase in accordance with the power law of $Z - 1$, with the larger size; $N_L/N \to 1$ in the thermodynamic limit.

The above can be confirmed by the numerical results of the tight-binding calculations. There are the energy levels and their degeneracy identical to the values due to equations (18) and (23) of the linear chain states in the numerical results for the $(3, 4)$ and $(3, 5)$ Cayley trees listed in table 1. For example, the energy levels $\xi = \pm \sqrt{2}$ of the $(3, 5)$ tree can also be found in the $(3, 4)$ tree. These linear chain states that correspond to the depth $n = 3$ ($\theta_S(1) = \pi/4$ or $\theta_S(3) = 3\pi/4$ from equation (16)) are localized within the shells from the fifth shell to the second shell (nodes), as shown in figure 2. The linear chain states exhibit $\Delta \xi = \pm \sqrt{2} = d_S = 6$-fold degeneracy from equation (23) with $k = 4$ or equation (20) with $n = 3$. In regard to the linear chain states of $\xi = \pm 1$ and 0, as shown in figures 3 and 4, respectively, $\xi = \pm 1$ ($k = 3$) is 14-fold degenerate (the breakdown is $D(\pm 1) = d_0 + d_3 = 3 \cdot 2^3 + 2 = 14$) or $\xi = 0$ ($k = 2$) is 32-fold degenerate ($D(0) = d_0 + d_1 + d_2 = 3 \cdot 2^3 + 3 \cdot 2^1 + 2 = 32$), in accordance with equation (23). Furthermore, $D(\xi = \pm \sqrt{2}/2)$ is 3 for $k = 5$, and $D(\xi = \pm \sqrt{3})$ is 2 for $k = 6$. The $N_L$ linear chain states can be found in all the states $N$ that obey equation (25); $N_L/N = 41/46$ and 88/94 for the $(3, 4)$ and $(3, 5)$ trees, respectively.

Figures 2–4 show that the probability distributions of the states that belong to the same energy level are distributed along the radial axis of the tree with explicit nodes on the sites, while each wavefunction is localized anisotropically with respect to the center of the tree. We emphasize that the linear chain states are a type of surface state because the probabilities for their existence inside the $(S - n)$ th shell are zero.

3.1.2. Confinement states

Next, we focus on the remaining states obtained by elimination of the linear chain states from all the states. The number of remaining states is identical to the number of shells in a Cayley tree,

$$N_C = N - N_L = S + 1$$  \hspace{1cm} (26)

from equation (25). There are very few states because the linear chain states are in an overwhelmingly majority, so that

$$\frac{N_C}{N} = \frac{(S + 1)(Z - 2)}{Z(Z - 1)^3 - 2},$$  \hspace{1cm} (27)

$N_C/N \sim S/Z^3 \to 0$ when $Z \to \infty$ or in the thermodynamic limit.

We have investigated the wavefunctions of the remaining states. Figure 5 shows the wavefunctions of the $(3, 5)$ tree, which each have a peak intensity at the central site and spread out isotropically all over the tree in conformity with the spherical symmetry. The wavefunctions also maintain radial symmetry in other trees with large $Z$. The wavefunctions spread out over the tree; that is, their spread is restricted by the size of the tree. We will hereinafter refer to the states other than the linear chain states as confinement states. Explicit nodes cannot be found in the confinement states essentially, whereas there are nodes on the sites in the linear chain states that are localized to a region near the surface. We emphasize that the states are non-degenerate, independently of $Z$.

We have estimated a polynomial equation of $\xi$ for the confinement states by removal of the terms of the linear chain states from equation (13):

$$\sum_{m=0}^{M} C_m(Z, S)\xi^{S+1-2m} = 0,$$  \hspace{1cm} (28)

where the coefficient is defined as

$$C_m(Z, S) = (-1)^m \left[ 1 + \left( \frac{1}{Z - 1} \right)^m \frac{m}{Z + 1 - m} \right] \frac{(S + 1 - m)}{m},$$  \hspace{1cm} (29)
using a binomial coefficient, and \( M \) denotes the integer

\[
M = \text{Int} \left\{ \frac{S + 1}{2} \right\} = \begin{cases} 
\frac{(S + 1)/2}{S/2} & \text{for } S = \text{odd} \\
S/2 & \text{for } S = \text{even}
\end{cases} \tag{30} 
\]

Equation (28) is Sturm’s problem in algebra, excluding the root \( \xi = 0 \) when \( S \) is even, because \( C_0(Z, S) = 1 \). There are certainly \( S + 1 \) distinct real roots in the range between \(-2\) and \(+2\). The roots, that is, the energies of the confinement states, are distributed symmetrically with respect to \( \xi = 0 \). Thus, all the confinement states are non-degenerate, and one of their energies is always located at \( \xi = 0 \) for even \( S \), as shown in figure 6. There are also cases where the energy of the confinement state is coincidentally identical to that of the linear chain state, which will be discussed later, e.g., \( \xi = 0 \) for even \( S \) and \( \xi = \pm \sqrt{3} \) for the \((3, 9)\) tree. Thus, the energies for the confinement states of a large Cayley tree can be obtained without performing large matrix calculations. For example, the energies of large-sized trees in figure 6 are obtained using equation (28). The \((3, 81)\) tree, which consists of \(7.3 \times 10^{24}\) sites, requires an enormous matrix. Figure 7 shows that the DOS of the confinement states (c-DOS) is almost the same, independently of \( Z \), because the term including the fraction \( 1/(Z - 1) \) in equation (29) does not contribute significantly to the c-DOS.

We note the electronic property of the site-centered Cayley tree. If the c-DOS is half-filled, then the tree is metallic when \( S \) is even, whereas it has an energy gap when \( S \) is odd. In contrast, taking into account the linear chain states at \( \xi = 0 \), any tree is supposed to be metallic, independently of \( S \). However, no hopping electrons are ever present on the central site of the tree in the linear chain states, most of which, corresponding to the states with a penetration depth \( n = 1 \), have only paths between nearest-neighbor sites on the surface.

### 3.2. Bond-centered trees

Both the bond-centered and site-centered Cayley trees have two types of states: the linear chain states and the confinement states. An example of the numerical results from tight-binding calculations for the bond-centered trees is shown in table 2. The corresponding wavefunctions are depicted in figures 8 and 9.

#### 3.2.1. Linear chain states

The linear chain states characterized by depth \( n \), from the surface and the mode \( m \), are \( d_n^{(b)} \)-fold degenerate, where

\[
\theta_n = (Z - 2) \Lambda_{(S-n)}^{(b)} \tag{31}
\]
Figure 7. Comparison between the DOS of confinement states for Cayley trees with $S = 81$ and the DOS of Bethe lattices. The former, which are obtained by Gaussian broadening with HWHM = 0.05 for $\xi$, are almost unchanged, whereas the latter change shape in accordance with the coordination number $Z$. The blue line in the top panel represents the DOS of the confinement states for the $(3, 40)$ bond-centered tree, which are close to those of the $(3, 81)$ site-centered tree.

Table 2. Numerical results of tight-binding calculations for the $(3, 4)$ Cayley tree (energy, $\xi$, and degeneracy, $D$), along with the analysis results of the type (L: linear chain state or C: confinement state), the linear chain modes ($\theta$) and their degeneracy given by equation (16) and equation (31), respectively. The confinement states are non-degenerate.

| $\xi$         | $D$ | Type | $\theta$ | $\sum d$ |
|--------------|-----|------|----------|----------|
| 1.711 888 669 3 | 1   | C    | 1        | 1        |
| 1.564 704 283 3 | 1   | C    | 1        | 1        |
| 1.414 213 562 4 | 2   | L    | $\frac{3\pi}{4}$ | 2        |
| 1.000 000 000 0 | 4   | L    | $\frac{2\pi}{3}$ | 4        |
| 0.812 370 958 9 | 1   | C    | 1        | 1        |
| 0.459 555 344 9 | 1   | C    | 1        | 1        |
| 0.000 000 000 0 | 10  | L    | $\frac{2\pi}{\sqrt{2}}$ | $2 + 8$ |
| $-0.459 555 344 9$ | 1   | C    | 1        | 1        |
| $-0.812 370 958 9$ | 1   | C    | 1        | 1        |
| $-1.000 000 000 0$ | 4   | L    | $\frac{7\pi}{4}$ | 4        |
| $-1.414 213 562 4$ | 2   | L    | $\frac{\pi}{4}$ | 2        |
| $-1.564 704 283 3$ | 1   | C    | 1        | 1        |
| $-1.711 888 669 3$ | 1   | C    | 1        | 1        |
The energy level \( \xi = -2 \cos(\ell \pi / k) \) is \( D^{(b)}(\xi) \)-fold degenerate:

\[
D^{(b)}(\xi) = \sum_{n=1}^{S-1} \sum_{m=1}^{n} d_{n}^{(b)} \delta(\xi + 2 \cos(\ell \pi / k)) = \sum_{\ell=1}^{L} d_{2k-1}^{(b)}
\]

\[
= (Z - 2) \sum_{\ell=1}^{L} N_{S-\ell k+1}^{(b)}
\]

\[
= 2(Z - 2)(Z - 1)^{S-\ell k-1} (Z - 1)^{Lk} - 1
\]

\[
= 2(Z - 2)(Z - 1)^{S-\ell k-1} (Z - 1)^{Lk} - 1
\]  

(32)

where

\[
L = \text{Int}\left[\frac{S}{k}\right] \quad (2 \leq k \leq S).
\]  

(33)

In the thermodynamic limit,

\[
\frac{D^{(b)}(\xi)}{N_{S}^{(b)}} \rightarrow \frac{(Z - 2)^2}{(Z - 1)^{S-\ell k - 1}}
\]  

(34)

This is also the same as equation (24). The validity of equation (32) can be confirmed by the degeneracy in Table 2: \( D(\xi = 0) = 10 \) for \( k = 2 \), \( D(\xi = \pm 1) = 4 \) for \( k = 3 \), and \( D(\xi = \pm \sqrt{2}) = 2 \) for \( k = 4 \).

The total number of linear chain states is

\[
N_{L}^{(b)} = \sum_{n=1}^{S-1} n d_{n} \sum_{n=1}^{S-1} n d_{n} = 2(Z - 2) \sum_{n=1}^{S-1} n (Z - 1)^{S-n+1}
\]

\[
= 2 \left\{ \left( Z - 1 \right)^{S-1} - 1 \right\} \left( \frac{Z - 1}{Z - 2} \right) - (S - 1)
\]

\[
= N_{S}^{(b)} - 2S.
\]  

(35)

The linear chain states of the bond-centered trees also have an overwhelmingly majority in number, with \( N_{L}^{(b)}/N_{S}^{(b)} \rightarrow 1 \) in the thermodynamic limit.

3.2.2. Confinement states

The confinement states of both the bond-centered and site-centered trees are non-degenerate, whereas the number

\[
N_{L}^{(b)} = N_{S}^{(b)} - N_{L}^{(b)} = 2S
\]  

(36)

from equation (35). Furthermore, a polynomial equation for the confinement states of the bond-centered trees has been estimated in the same way as that for the site-centered trees:

\[
\xi = \pm 1.4142135624 \quad (2)
\]

\[
\xi = \pm 1.000000000 \quad (4)
\]

\[
\xi = 0.000000000 \quad (10)
\]

Figure 8. Probabilities of linear chain states obtained by numerical calculation for the bond-centered (3, 4)\(_{b}\) Cayley tree. The amplitudes are normalized by the respective maximum values. Sites depicted by transparent circles denote nodes. The numerals in parentheses following the energy values indicate the degeneracy. The linear chain states, which are localized to a region near the surface, have nodes on the sites.
However, the coefficients are a little more complicated than equation (29),

$$C_m(Z, S) = (-1)^m \left( Q_{2(Z-m)-1}(m+2) + \frac{1}{Z-1} Q_{2(Z-m)-1}(m+1) \right).$$

Figure 9. Wavefunctions of confinement states obtained by numerical calculation for the bond-centered (3, 5) Cayley tree. The wavefunctions of $\xi_1, \xi_3, \xi_5$, and $\xi_7$ spread out over the tree in a radial distribution, while those of $\xi_2, \xi_4, \xi_6$, and $\xi_8$ spread antisymmetrically across the center of the tree. The confinement states have no explicit nodes. The amplitudes are normalized by the maximum or minimum values of the respective wavefunctions.
3.3. Searching for bulk states

We have no choice but to consider that the confinement states correspond to the so-called bulk states if a Cayley tree is able to have bulk states, because the confinement states are obtained by elimination of the linear chain states, which will be discussed later, e.g., $\xi = \pm \sqrt{2}$ for the $(3, 6)_b$ and $(3, 10)_b$ trees.

We compare the DOS of the bond-centered tree to that of the site-centered tree. Roughly speaking, the bond-centered tree can be interpreted as a pair of the site-centered trees. This is directly reflected in the number of the confinement states, $N_{\text{conf}} / N_c \sim 2$, as well as the degeneracy of the linear chain states, $D(\xi) / D(\xi) \sim N(\xi) / N \sim N_{\text{conf}} / N_c = 2 / Z$. However, it can be seen from figure 7 that both large trees are not much different in the c-DOS. We also note the electronic property of the bond-centered Cayley tree that has the half-filled DOS. The c-DOS of the bond-centered tree has an energy gap around $\xi = 0$, while the linear chain states are the most degenerate at $\xi = 0$; however, the electrons in the states avoid the central portion of the tree, as evident from figure 8.

3.3. Searching for bulk states

We have no choice but to consider that the confinement states correspond to the so-called bulk states if a Cayley tree is able to have bulk states, because the confinement states are obtained by elimination of the linear chain states that originate from the surface. However, figure 7 shows that the c-DOS is not in agreement with the DOS of the Bethe lattice (Bethe-DOS) [6, 7, 14] obtained by Green’s function methods. The difference is evident, even if the site-centered tree with the size $S = 81$ cannot be considered as the thermodynamic limit. Assuming the energy levels of the confinement states are in ascending order, $\xi_1 < \cdots < \xi_i < \cdots < \xi_{S+1}$ for the site-centered tree, the wavefunction of a confinement state with energy $\xi_i$ has $i - 1$ implicit nodes, independently of $Z$, as shown in figure 10. This suggests the radial nodes of $s$ orbitals of the hydrogen atom or associated Laguerre polynomials, which is likely to reflect the spherical shape and size of the tree. Two peaks near the edges of the c-DOS in figure 7 indicate that many of the confinement states near $\xi_1$ and $\xi_{S+1}$ ($\xi_{S+2}$ for the bond-centered tree) are caused by confinement in the finite size. The lowest energy $\xi_1$ and highest energy $\xi_{S+1} = -\xi_1$ ($\xi_{S+2}$ for the bond-centered tree) are caused by confinement in the finite size.
the bond-centered tree) of every Cayley tree are outside of the energy range of the linear chain states. We consider that the non-degenerate energy level \(\xi_1\), which corresponds to the ground state of the Cayley tree, does not always correspond to the bulk state or the Perron–Frobenius uniform mode on the Bethe lattice [15, 16].

In this study, we have not introduced the assumption that the surface effects decay with distance from the surface. The result is the c-DOS due to confinement in finite size. If the assumption, instead of periodicity, is able to bring the bulk states, then the Bethe-DOS must be a proper subset of the c-DOS, in other words, the bulk states can be distinguished from the confinement states, because the confinement states are non-degenerate as long as the tree remains finite in size. There is a clue to determine the bulk states among the confinement states, because the linear chain states are determined: \(\xi = 0, -\sqrt{2}, \text{ and } -\sqrt{3}\) correspond to \(n = 1, 3, 5\), respectively, from equation (16). The wavefunction with \(\xi = 0\) of the (3, 2) tree is the same as the central part of that of the (3, 4) tree, which is the same as the central part of that of the (3, 6) tree. The wavefunction with \(\xi = -\sqrt{3}\) of the (3, 3) tree is the same as the central part of that of the (3, 9) tree. The wavefunction with \(\xi = -\sqrt{2}\) of the (3, 6) tree is the same as the central part of that of the (3, 10) tree. Circles and lines representing sites and bonds on large shells are omitted for simplicity. The amplitudes are normalized by the maximum or minimum values of the respective wavefunctions.

![Figure 11](image)

**Figure 11.** Examples of the wavefunctions of the central states that are rare states of the confinement states (see text). The explicit nodes on sites at depth \(n\) from the surface that define the linear chain states are determined: \(\xi = 0, -\sqrt{2}, \text{ and } -\sqrt{3}\) correspond to \(n = 1, 3, 5\), respectively, from equation (16). The wavefunction with \(\xi = 0\) of the (3, 2) tree is the same as the central part of that of the (3, 4) tree, which is the same as the central part of that of the (3, 6) tree. The wavefunction with \(\xi = -\sqrt{3}\) of the (3, 3) tree is the same as the central part of that of the (3, 9) tree. The wavefunction with \(\xi = -\sqrt{2}\) of the (3, 6) tree is the same as the central part of that of the (3, 10) tree. Circles and lines representing sites and bonds on large shells are omitted for simplicity. The amplitudes are normalized by the maximum or minimum values of the respective wavefunctions.
wavefunction with $\xi_c$ of the $(Z, S_m)$ tree corresponds to the central part of that of the $(Z, S_{m+1})$ tree. Therefore, we call these central states. There is a possibility that the central states constitute the bulk states because we consider that the angle $\theta$ representing the energy of the Bethe-DOS in equation (3) in [14] corresponds to equation (16) in this paper, although the central states are only some of the confinement states that constitute a very small minority of all the states of the Cayley tree. However, this is a mere conjecture. There remain some questions regarding the central states and the bulk states. Further investigation and consideration including the comparison with the DOS obtained by Derrida and Rodgers [8] are thus required to clarify the relation between the confinement states and the bulk states.

4. Conclusion

We have investigated and analyzed the DOS of Cayley trees. The DOS consists of two types of states: linear chain states, where paths from the surface to the surface are formed by avoiding the central part or site, and confinement states due to quantum confinement in finite size. The former are degenerate states that occupy the overwhelming majority in number, while the latter are non-degenerate states, the number of which is identical to merely one or two times as many as the number of shells that constitute the Cayley tree. It is the confinement states that must have some relationship with the DOS of the Bethe lattice.

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