Energy bands of the Bethe lattice

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Energy bands are derived for the tight-binding model of particle motion on the Bethe lattice. The energy bands are used to calculate the density of states, which gives the standard answer. The bands are also used to calculate the ground state energy as a function of band filling.

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I. INTRODUCTION

The Bethe lattice is a special form of noncrystal. Each site has z neighbors, but there is only one way to get from one site to another. The standard model of particle motion has hopping between nearest neighbor sites using a tight-binding model. Brinkman and Rice[1] derived the density of states by examining the self-energy from hopping. Later Chen *et al.*[1,2] derived the same result using a transfer matrix. Here we introduce the idea of energy bands for the Bethe lattice, and use them to derive the same result for the density of states. Energy bands are also used to calculate other quantities such as the ground state energy as a function of filling.

The Bethe lattice continues to be a popular model. The earlier applications included localization,[3,4] alloys,[5] spin waves,[6,7] and spin glasses.[8] Recently it has been used to investigate properties of the Potts model,[9] the Blume-Capel model,[10] and the Hubbard model.[11]

For crystalline solids the particle motions are Bloch states that depend upon a wave vector $\mathbf{k}$. The energy states are derived from the tight-binding Hamiltonian. Neglecting spin it is[12]

$$H = t\sum_{j\delta} C^{\dagger}_{j+\delta} C_j , \tag{1}$$

which shows that all sites j can hop to all of the z neighboring sites $j+\delta$. For crystalline solids the energy bands are[12]

$$\varepsilon(\mathbf{k}) = t\sum_{\delta} \exp(i\mathbf{k}\cdot\boldsymbol{\delta}). \tag{2}$$

The Bethe lattice does not have the same type of energy band because it is not crystalline. However, we show that it has a band energy depending upon an angle θ,

$$\varepsilon(\theta) = A\cos(\theta), \quad A \equiv 2t\sqrt{z-1}. \tag{3}$$

The wave vector $\mathbf{k}$ for crystalline solids becomes a scalar which can be represented by an angle. The energy dispersion in Eq. (3) is precisely correct for a one-dimensional solid. In a chain $z=2$ and the energy dispersion is $\varepsilon(\theta)=2t\cos(\theta)$. However, we show that Eq. (3) is the correct dispersion relation for the Bethe lattice for any value of z. From now on we normalize all energies to the hopping parameter t which sets $t=1$.

In crystalline solids the ratio of surface to volume decreases rapidly as the number of sites N increases. That is not true of the Bethe lattice.[13–15] In the limit of large N the fraction of surface atoms approaches $f=(z-2)/(z-1)$, which is larger than one-half in most cases. The density of states for a finite value of N is dominated by surface effects, which does not change as N is increased. Instead, we follow Brinkman and Rice and consider the lattice with $N=\infty$. This density of states is a bulk value, which is different from that obtained in the limit of $N\to\infty$. The latter is dominated by surface effects.

II. MATRIX SOLUTION

The hopping is symmetric, in that it has the same phase for hopping to all of the neighbors. Consider a particle on a site which we call $j=0$. It is written as $|0\rangle$, which distinguishes it from the vacuum state $|0)$. The hopping to the z neighbors creates a symmetric state we call $|1\rangle$. A double hop to the second neighbors creates $|2\rangle$,

$$|0\rangle = C^{\dagger}_0|0), \tag{4}$$

$$|1\rangle = \frac{1}{\sqrt{z}}\sum_{\delta} C^{\dagger}_{\delta}|0), \tag{5}$$

$$|2\rangle = \frac{1}{\sqrt{z(z-1)}}\sum_{\delta}\sum_{\delta'\neq -\delta} C^{\dagger}_{\delta+\delta'}|0). \tag{6}$$

This process can be extended to further neighbors. The first neighbor has z choices, but subsequent hops have only $z-1$ choices. A hop backward is not allowed since that goes to another state. In terms of these states, the Hamiltonian matrix becomes

$$H|0\rangle = \sqrt{z}|1\rangle, \tag{7}$$

$$H|1\rangle = \sqrt{z}|0\rangle + \sqrt{z-1}|2\rangle, \tag{8}$$

$$H|2\rangle = \sqrt{z-1}[|1\rangle + |3\rangle], \tag{9}$$

$$H|l\rangle = \sqrt{z-1}[|l-1\rangle + |l+1\rangle], \tag{10}$$

$$H=\begin{pmatrix} 0 & \sqrt{z} & 0 & 0 & \cdots \\ \sqrt{z} & 0 & \sqrt{z-1} & 0 & \cdots \\ 0 & \sqrt{z-1} & 0 & \sqrt{z-1} & 0 \\ 0 & 0 & \sqrt{z-1} & 0 & \sqrt{z-1} \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (11)$$

The Hamiltonian matrix has tridiagonal form, with all diagonal elements zero, and the off-diagonal elements are identical except those connecting the first state. Since the matrix has infinite dimension, its eigenvalue and eigenfunctions are

$$H\psi=E\psi, \quad (12)$$

$$E=A\cos(\theta), \quad A=2\sqrt{z-1}, \quad (13)$$

$$\psi(\theta)=\sqrt{\frac{2}{\pi}}\begin{bmatrix} \sin(\beta) \\ \sin(\theta+\gamma) \\ \sin(2\theta+\gamma) \\ \vdots \\ \sin(l\theta+\gamma) \\ \vdots \end{bmatrix}. \quad (14)$$

This ansatz eigenstate is inserted into the matrix equation. Note that $\beta\neq\gamma$ to account for the different matrix element to the first state. The eigenfunction satisfies all of the equations except those for the first two rows. These take more work, and determine $\beta(\theta)$ and $\gamma(\theta)$:

$$\sqrt{z}\sin(\theta+\gamma)=2\sqrt{z-1}\cos(\theta)\sin(\beta), \quad (15)$$

$$\sqrt{z}\sin(\beta)+\sqrt{z-1}\sin(2\theta+\gamma)$$

$$=2\sqrt{z-1}\cos(\theta)\sin(\theta+\gamma) \quad (16)$$

$$=\sqrt{z-1}[\sin(2\theta+\gamma)+\sin(\gamma)]. \quad (17)$$

Canceling the same factor from both sides of the last equation gives

$$\sqrt{z}\sin(\beta)=\sqrt{z-1}\sin(\gamma). \quad (18)$$

We multiply Eq. (15) by $\sqrt{z}$ and use Eq. (18) to eliminate $\sqrt{z}\sin(\beta)$, which gives an equation whose only unknown is $\gamma(\theta)$:

$$z\sin(\theta+\gamma)=2\sqrt{z-1}\cos(\theta)[\sqrt{z}\sin(\beta)]$$

$$=2(z-1)\cos(\theta)\sin(\gamma) \quad (19)$$

$$=(z-1)[\sin(\theta+\gamma)+\sin(\gamma-\theta)], \quad (20)$$

$$\sin(\theta+\gamma)=(z-1)\sin(\gamma-\theta). \quad (21)$$

This can be solved assuming that $z>2$,

$$\tan(\gamma)=\frac{z}{z-2}\tan(\theta), \quad (22)$$

$$\sin(\gamma)=\frac{z\sin(\theta)}{\sqrt{(z-2)^2\cos^2(\theta)+z^2\sin^2(\theta)}} \quad (23)$$

$$=\frac{z\sin(\theta)}{\sqrt{z^2-4(z-1)\cos^2(\theta)}}$$

$$=\frac{z\sin(\theta)}{\sqrt{z^2-A^2\cos^2(\theta)}}, \quad (24)$$

$$\sin(\beta)=\sqrt{\frac{z-1}{z}}\sin(\gamma)=\frac{\sqrt{z(z-1)}\sin(\theta)}{\sqrt{z^2-A^2\cos^2(\theta)}}. \quad (25)$$

Note that $z^2-A^2=(z-2)^2>0$ for values of $z>2$. The case $z=2$ is just a one-dimensional chain, which has a well-known trivial solution. The present theory is for $z>2$. These results complete the description of the eigenfunction.

III. DENSITY OF STATES

The Green's function in the Matsubara formalism, at nonzero temperature, in the θ representation is

$$\mathcal{G}(\theta,ip_n)=\frac{1}{ip_n-\varepsilon(\theta)}. \quad (26)$$

Transforming to the spatial representation, we define $\mathcal{G}_{0l}$ as the probability of starting at site 0 and propagating to a site l away,

$$\mathcal{G}_{0l}(ip_n)=\int_0^\pi d\theta g_{0l}(\theta)\mathcal{G}(\theta,ip_n), \quad (27)$$

$$g_{00}(\theta)=\frac{2}{\pi}\sin^2[\beta(\theta)], \quad (28)$$

$$g_{0l}(\theta)=\frac{2}{\pi}\sin[\beta(\theta)]\sin[l\theta+\gamma(\theta)]. \quad (29)$$

The factors on the right come from the appropriate element of the eigenfunction $\psi(\theta)$. The last formula applies for $l>0$. The retarded function is obtained by the analytical continuation $ip_n\rightarrow E+i\eta$ where η is infinitesimal. The density of states is proportional to the imaginary part of the retarded Green's function $G_{00}(E)$,

$$\rho(E)=-\frac{1}{\pi}\mathrm{Im}\{G_{00}(E)\} \quad (30)$$

$$=\int_0^\pi d\theta g_{00}(\theta)\delta[E-A\cos(\theta)] \quad (31)$$

$$=\frac{g_{00}}{A|\sin(\theta)|}=g_{00}(\theta)\frac{d\theta}{dE}, \quad (32)$$

$$\rho(E)=\frac{z}{2\pi}\frac{\sqrt{A^2-E^2}}{z^2-E^2}. \quad (33)$$

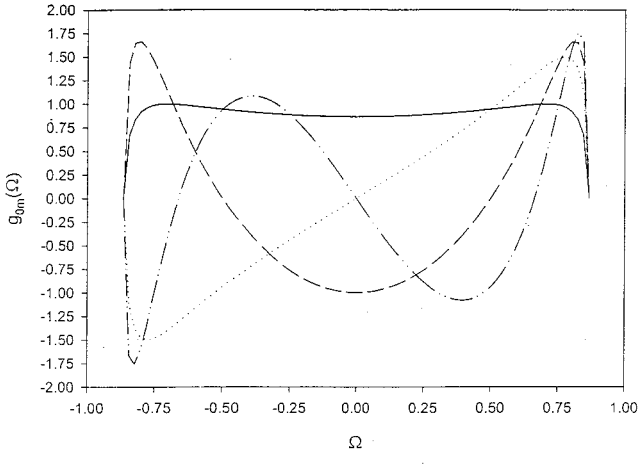

FIG. 1. Curves of $\rho_{0l}(\Omega)$ for $-A/z \leqslant \Omega = E/z \leqslant A/Z$ for the case of $z=4$ and $l=0,1,2,3$. The lines for a value of l has l nodes.

The last expression is the density of energy states of the Bethe lattice, in agreement with Brinkman and Rice.[1] Note that $g_{00}(\theta)$ is the density of states in θ space. This concept is used below to calculate the ground state energy.

The density of states is normalized to one electron,

$$\int dE\rho(E) = \frac{z}{2\pi}\int_{-A}^{A} dE \frac{\sqrt{A^2-E^2}}{z^2-E^2} = 1. \tag{34}$$

A similar expression can be derived for the probability that an electron starts on site 0 and ends on l,

$$\rho_{0l}(E) = \frac{2}{\pi}\int_0^{\pi} d\theta \sin[\beta(\theta)]\sin(l\theta+\gamma)\,\delta[E-A\cos(\theta)] \tag{35}$$

$$= \frac{\sqrt{z}}{\pi}\frac{\sin(l\theta+\gamma)}{\sqrt{z^2-E^2}}, \tag{36}$$

where the angle θ and $\gamma(\theta)$ are evaluated using Eq. (24) and $\theta = \cos^{-1}(E/A)$. Figure 1 shows curves for $\rho_{0l}(\Omega)$, $l=0,1,2,3$, for the case that $z=4$. Here $\Omega = E/z$ and spans the range of $-A/z \leqslant \Omega \leqslant A/Z$. For $z=4$ then $A/z = \sqrt{3}/2$. The value of l in the figure is simply the number of nodes.

Ground state energy

Two different methods are presented for the calculation of the ground state energy at zero temperature. The first uses the energy band picture derived in the previous section. The partition function for fermions is ($\beta = 1/k_B T$)

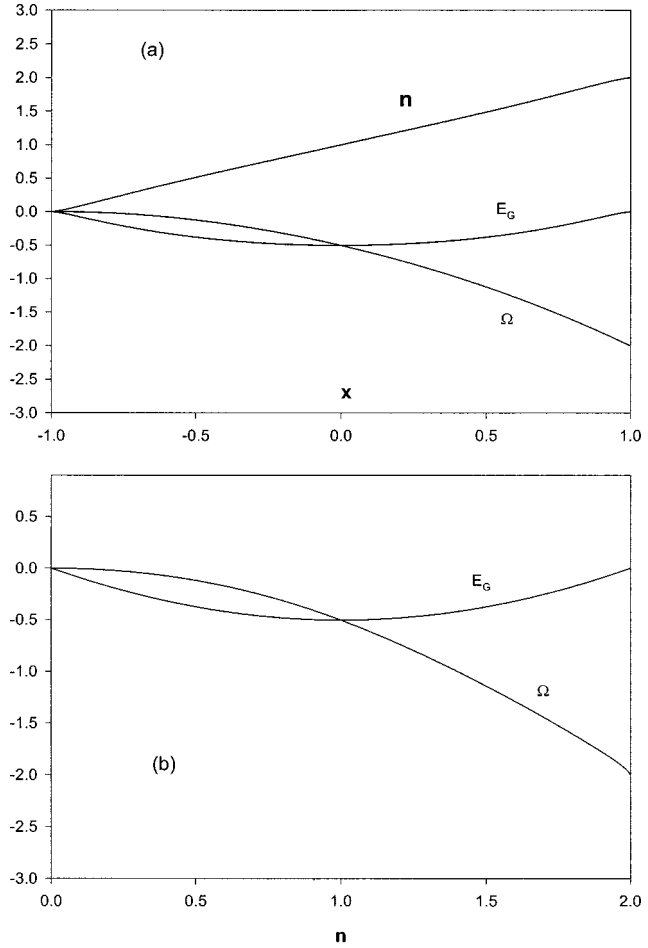

FIG. 2. (a) $n(\mu)$, $E_G(\mu)/(A)$, and $\Omega(\mu)/(NA)$ as functions of $x=\mu/A$. (b) $E_G(n)/(A)$ and $\Omega(n)/(NA)$.

$$Z = e^{-\beta\Omega} = \Pi_\theta[1+e^{-\beta[\varepsilon(\theta)-\mu]}]^2, \tag{37}$$

$$\Omega = -2k_B T\sum_\theta \ln[1+e^{-\beta[\varepsilon(\theta)-\mu]}], \tag{38}$$

$$= -2Nk_B T\int_0^{\pi} d\theta g_{00}(\theta)\ln[1+e^{-\beta[\varepsilon(\theta)-\mu]}] \tag{39}$$

$$= -2Nk_B T\int_{-A}^{A} dE\rho(E)\ln[1+e^{-\beta[E-\mu]}]. \tag{40}$$

The factor of 2 is for spin degeneracy. The summation over θ has been converted to an integral by using $g_{00}(\theta)$ as the density of θ states. In the last equation the integral has been converted to energy space using Eq. (32). At zero temperature,

$$\lim_{T\to 0}\Omega = -2N\int_{-A}^{\mu} dE\rho(E)[\mu-E] = NE_G - \mu N_e, \tag{41}$$

$$N_e = 2N\int_{-A}^{\mu} dE\,\rho(E)$$

$$= \frac{N}{\pi}\left[z\theta_\mu - (z-2)\tan^{-1}\left(\frac{z}{z-2}\tan(\theta_\mu)\right)\right], \quad (42)$$

$$\mu = -A\cos(\theta_\mu). \quad (43)$$

The fractional concentration is $n = N_e/N$. The chemical potential spans the range $-A \leq \mu \leq A$ as the band goes from empty to full. At $n=0$, $\mu=-A$, $\theta_\mu = 0$. At half filling, $\mu = 0$, $\theta_\mu = \pi/2$, and $n=1$. As the band fills up, $\mu \to A, \theta_\mu \to \pi$, and $n \to 2$. The ground state energy per site is

$$E_G = -2\int_{-A}^{\mu} E\,dE\,\rho(E)$$

$$= -\frac{z}{\pi}\left[\sqrt{A^2-\mu^2} - (z-2)\tan^{-1}\left(\frac{\sqrt{A^2-\mu^2}}{z-2}\right)\right]. \quad (44)$$

These formulas are plotted in Fig. 2 for the case that $z=4$. In Fig. 2(a), the graph gives $n(\mu)$, $\Omega/(AN)$, and E_G/A as functions of $-1 \leq x = \mu/A \leq 1$. The figure shows that $n(\mu)$ is quite linear except near the end points. In Fig. 2(b) are shown Ω/AN and E_G/A as functions of n.

In order to check this result, we provide another method of finding the ground state energy of the Bethe lattice. It uses the results of Brinkman and Rice that the hopping term gives rise to the self-energy of the electron. The contribution of the self-energy to the ground state energy is determined by a coupling-constant integral $d\eta$. The grand canonical potential Ω is given by[12]

$$\beta\Omega = \beta\Omega_0 + \sum_{j\sigma n}\int_0^t \frac{d\eta}{\eta}\mathcal{G}_\eta(ip_n)\Sigma_\eta(ip_n), \quad (45)$$

$$\beta\Omega_0 = 2N\ln(1+e^{\beta\mu}), \quad (46)$$

$$\mathcal{G}_\eta = \frac{1}{ip+\mu-\Sigma_\eta}, \quad (47)$$

$$\Sigma_\eta = \frac{2z\eta^2}{ip+\mu+\sqrt{(ip+\mu)^2-4(z-1)\eta^2}}. \quad (48)$$

The summation over $(j\sigma)$ equals $2N$.

$$\beta\delta\Omega = 2N\sum_n \int_0^t \frac{d\eta}{\eta}\mathcal{G}_\eta(ip_n)\Sigma_\eta(ip_n), \quad (49)$$

$$\mathcal{G}_\eta(ip_n)\Sigma_\eta(ip_n) = \frac{2z\eta^2}{(ip+\mu)[(ip+\mu)+\sqrt{(ip+\mu)^2-4(z-1)\eta^2}]-2z\eta^2}. \quad (50)$$

The summation over ip_n is done first. It is converted into a contour integral $ip_n \to z'$. If $A^2 = 4(z-1)$ then there is a branch cut along the real axis in the range $-A\eta \leq z'+\mu \leq A\eta$. Integrating around the branch cut gives, after some algebra,

$$\delta\Omega = \frac{zN}{\pi}\int_0^t \frac{d\eta}{\eta}\int_{-A\eta}^{A\eta} d\varepsilon\,\varepsilon\, n_F(\varepsilon-\mu)g_\eta(\varepsilon), \quad (51)$$

$$g_\eta(\varepsilon) = \frac{\sqrt{A^2\eta^2-\varepsilon^2}}{z^2\eta^2-\varepsilon^2}. \quad (52)$$

The factor $g_\eta(\varepsilon)$ is the density of states for a system with bandwidth $A\eta < \varepsilon < A\eta$. Note that the chemical potential does not scale with the coupling constant. The order of the two integrals can be interchanged, which gives

$$\delta\Omega = \frac{zN}{\pi}\int_{-At}^{At} d\varepsilon\, n_F(\varepsilon-\mu)H(\varepsilon), \quad (53)$$

$$H(\varepsilon) = \varepsilon\int_{|\varepsilon|/A}^{t}\frac{d\eta}{\eta}g_\eta(\varepsilon) \quad (54)$$

$$= \mathrm{sgn}(\varepsilon)\left[\tan^{-1}\left(\frac{\sqrt{(At)^2-\varepsilon^2}}{|\varepsilon|}\right) - b\tan^{-1}\left(\frac{\sqrt{(At)^2-\varepsilon^2}}{b|\varepsilon|}\right)\right], \quad (55)$$

where $b = (z-2)/z$. The function $H(\varepsilon)$ has a discontinuity at $\varepsilon = 0$, where the term in square brackets is $\pi(1-b)/2 = \pi/z$. At zero temperature the occupation factor $n_F(\varepsilon-\mu)$ is replaced by a step function $\Theta(\mu-\varepsilon)$ and the integral can be evaluated. Its derivative with respect to μ gives the occupation number:

$$n = \frac{2}{1+e^{-\beta\mu}} - \frac{z}{\pi}H(\mu), \quad (56)$$

$$\delta\Omega = -\frac{z}{\pi}N\left[\sqrt{(At)^2-\mu^2}-|\mu|\tan^{-1}\left(\frac{\sqrt{(At)^2-\mu^2}}{|\mu|}\right)\right.$$
$$+b|\mu|\tan^{-1}\left(\frac{\sqrt{(At)^2-\mu^2}}{b|\mu|}\right)$$
$$\left.-t(z-2)\tan^{-1}\left(\frac{\sqrt{(At)^2-\mu^2}}{t(z-2)}\right)\right]. \quad (57)$$

The expression for the particle density $n(\mu)$ is identical to that found in the band model, although it appears slightly different. The first term in n is from Ω_0, which gives

$$\frac{1}{N}\frac{\partial(\beta\Omega_0)}{\partial(\beta\mu)}=\frac{2}{1+e^{-\beta\mu}}\rightarrow 2\Theta(\mu). \quad (58)$$

At zero temperature this term becomes a step function that is zero for $\mu<0$ and 2 for $\mu>0$. $H(\mu)$ is also a step function, and the two steps cancel. The combined contribution to $n(\mu)$ from Ω_0 and $\delta\Omega$ yields a smooth curve when plotted as a function of μ. The final curve is identical to that found from the band model.

The change in the ground state energy $\delta\Omega$ has a cusp at half filling, which is caused by the discontinuity of $H(\varepsilon)=-H(-\varepsilon)$ at $\varepsilon=0$. In calculating the ground state energy, the function Ω_0 is included. It has the form

$$\frac{\Omega_0}{N}=-2k_BT\ln(1+e^{\beta\mu})\rightarrow -2\mu\Theta(\mu). \quad (59)$$

At zero temperature it becomes proportional to the chemical potential when μ is positive. This term eliminates the cusp in $\delta\Omega$ and the final curve becomes identical to Ω found from the band model. The coupling-constant integral, using the Brinkman-Rice self-energy, gives the same ground state energy and particle density, as a function of the chemical potential, as found earlier using the band model.

The ground state energy per particle E_G/n can be evaluated. In the limit of $n\rightarrow 0$ it goes to $-A$. Of course, this result is expected from the band model. In a system of few particles they occupy the lowest energy state, which is the bottom of the band.

A similar result can be found for the ferromagnetic state in which all electrons have the same spin. In that case only one particle is on a site, and the factor of 2 is removed from $N_e(\mu)$ and $E_G(\mu)$. In this case $0\leqslant n\leqslant 1$ as $-A\leqslant\mu\leqslant A$.

IV. DISCUSSION

The concept of energy bands is introduced into the hopping energy of the Bethe lattice. The energy bands are used to calculate the density of states and ground state energy. The former result agrees with Refs. 1 and 2.

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