Long-range correlations in Bethe lattices

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We show that the long-range correlations in Bethe lattices contain pathological features that cause great difficulties when calculating physical properties that depend on them.

The Bethe lattice[1] is a mathematical artifact widely used in calculating properties of disordered systems.[2,3] Its use is justified because it preserves the local coordination Z of the atoms and does not assume long-range order. In addition, it is easy to handle mathematically.

When calculating local properties, such as the density of states or the *local* response at defect sites, this approximation gives reasonable results in spite of the unphysical nature of the network.[3] When trying to calculate properties, however, that involve correlations between distant atoms, such as infrared spectrum and Raman and neutron scattering responses, the Bethe lattice fails to give satisfactory answers.[4]

Under these circumstances, extreme care has to be taken in defining a Bethe lattice, and the existence of a surface in the network is of paramount importance for determining the character of long-range correlations.

Let us examine the problem in its simplest form by considering an s-like tight-binding Hamiltonian with a hopping integral V between neighboring atoms. The equations of motion for the Green's functions[5] are

$$\begin{aligned} &Eg_{0,0}=1+ZVg_{0,1}\ , \\ &Eg_{0,1}=Vg_{0,0}+(Z-1)Vg_{0,2}\ , \\ &\cdots\ , \\ &Eg_{0,n}=Vg_{0,n-1}+(Z-1)Vg_{0,n+1}\ , \\ &\cdots\ . \end{aligned} \tag{1}$$

These equations are valid for all the atoms in a shell n. When the lattice has a surface, the equation set terminates at the last shell N (i.e., the surface) which has a different equation

$$Eg_{0,N}=Vg_{0,N-1} \tag{2}$$

for free ends.

In any large physical system, the number of surface atoms is negligible in comparison with the number of atoms in the volume, but in the Bethe lattice this is not so. The ratio between the number of sites in the surface and the total number of sites tends to $(Z-2)/(Z-1)$ as $N\rightarrow\infty$, which is not zero for $Z>2$.

If we ignore Eq. (2), as is usually done, and assume an infinite network, we find the solution of Eq. (1) by defining

$$g_{0,n}=tg_{0,n-1}\ , \tag{3}$$

where the transfer function t is simply

$$t=\frac{E\pm[E^2-4V^2(Z-1)]^{1/2}}{2V(Z-1)} \tag{4}$$

and

$$g_{0,0}=(E-ZVt)^{-1}\ . \tag{5}$$

The sign of the square root is uniquely determined by the analytical properties of the Green's function. The band is confined to the energy range $-2V(Z-1)^{1/2}<E<2V(Z-1)^{1/2}$, so that the spectral limits ($|E|=ZV$) are not attained for $Z>2$.

The infrared spectrum and neutron and Raman cross sections are related to the imaginary part of quantities like[6]

$$\sum_J g_{0,J}\ , \tag{6}$$

which in the Bethe lattice can be calculated by use of (3) and (5).

The sum of the first r terms of the Bethe lattice described by (1) is

$$\begin{aligned} \Sigma_r &= g_{0,0}+Zg_{0,1}+Z(Z-1)g_{0,2}+\cdots+Z(Z-1)^{r-1}g_{0,r} \\ &= g_{0,0}\left[1+\frac{Z}{(Z-1)}\sum_{l=1}^{r}[(Z-1)t]^l\right] \\ &= \frac{1-ZV(Z-1)^r(1-t)g_{0,r}}{E-ZV}\ , \end{aligned} \tag{7a}$$

which has the limiting form

$$\Sigma_\infty=1/(E-ZV)\ . \tag{7b}$$

However, the finite sum (7a) does not converge uniformly to the limiting form (7b), and, as an example, we show in Fig. 1 the result for the imaginary part of (7a) for $N=50$ on the linear chain $Z=2$. It will be seen that there are N oscillations with a period $1/N$.

The imaginary part of (7b) is a δ function at $E=ZV$

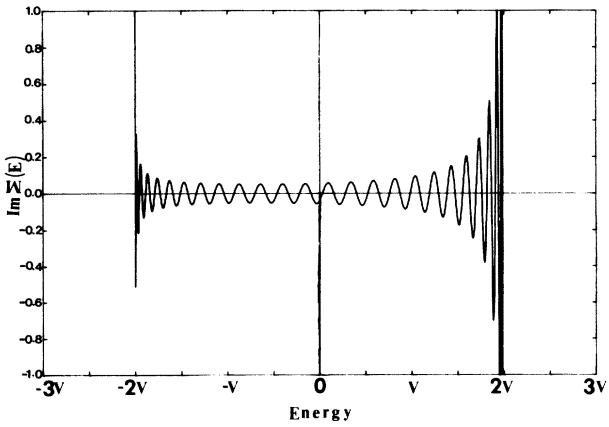

FIG. 1. Imaginary part of $\Sigma_N(E)$ in units of 4π [Eq. (7a)] for $N=50$ on the one-dimensional infinite chain ($Z=2$).

where there is *not* an eigenstate of the Hamiltonian for $Z > 2$ if boundaries are included via Eq. (2).

We shall show below that the surface effects described by Eq. (2) cannot be neglected.

Note that, although the modulus of the argument of the sum in (7a) can be greater than one, the sum is correct. In fact, the sum (6) can be done exactly for the finite system with free ends. Writing the equations of motion in a convenient way we get

$$\begin{aligned} &Eg_{0,0}=1+ZVg_{0,1}\ , \\ &ZEg_{0,1}=ZVg_{0,0}+ZV(Z-1)g_{0,2}\ , \\ &Z(Z-1)Eg_{0,2}=ZV(Z-1)g_{0,1}+ZV(Z-1)^2g_{0,3}\ , \\ &\cdots\ , \\ &Z(Z-1)^{N-1}Eg_{0,N}=ZV(Z-1)^{N-1}g_{0,N-1}\ . \end{aligned} \tag{8}$$

Summing up (8) we obtain a finite sum Σ_N similar to (7):

$$E\Sigma_N=1+ZV\Sigma_N-ZV(Z-1)^Ng_{0,N}\ , \tag{9}$$

or

$$\Sigma_N=\frac{1-ZV(Z-1)^Ng_{0,N}}{E-ZV}\ . \tag{10}$$

There are several important results which follow from this equation:

(i) There is no δ function at $E=ZV$ because at this energy the numerator of (10) is exactly zero for all N. This can be seen by solving (1) for $g_{0,N}$ as a set of linear equations:

$$g_{0,N}(E)=\frac{\det\begin{pmatrix} E & -ZV & 0 & 0 & \cdots & 1 \\ -V & E & -(Z-1)V & 0 & \cdots & 0 \\ 0 & -V & E & -(Z-1)V & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & -V & 0 \end{pmatrix}}{\det\begin{pmatrix} E & -ZV & 0 & 0 & \cdots & 0 \\ -V & E & -(Z-1)V & 0 & \cdots & 0 \\ 0 & -V & E & -(Z-1)V & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & -V & E \end{pmatrix}}\ , \tag{11}$$

and for $E=ZV$,

$$g_{0,N}(E)=\frac{\det\begin{pmatrix} -V & ZV & -(Z-1)V & \cdots & 0 \\ 0 & -V & ZV & \cdots & 0 \\ 0 & 0 & -V & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & -V \end{pmatrix}}{\det\begin{pmatrix} ZV & 0 & 0 & \cdots & 0 \\ -V & (Z-1)V & 0 & \cdots & 0 \\ 0 & -V & (Z-1)V & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & -V & (Z-1)V \end{pmatrix}}=\frac{V^N}{Z(Z-1)^NV^{N+1}}=\frac{1}{ZV(Z-1)^N}\ . \tag{12}$$

(ii) If the surface is ignored (i.e., $g_{0N}=0$) we recover Eq. (7b).

(iii) The sum Σ_N is entirely dominated by the correlation between the central atom and the surface ones for $Z > 2$, because of the very large factor $(Z-1)^N$.

(iv) The limit of Σ_N when $N\to\infty$ is *not* Σ_∞. This can be seen by writing the surface term in terms of the Chebyshev polynomials of the second kind (u_n). In this way we get

$$ZV(Z-1)^N g_{0,N}=\frac{(Z-1)^{(N+1)/2}}{u_N(x/2)}\left[\frac{(Z-1)x}{2}-(Z-1)^{-1/2}\frac{x}{u_N(x/2)u_{N-2}(x/2)}+\frac{u_{N-3}(x/2)}{u_{N-2}(x/2)}\right]^{-1}, \tag{13}$$

where

$$x=\frac{E}{(Z-1)^{1/2}V} . \tag{14}$$

The imaginary part of (13) will consist of a divergent collection of $(N+1)$ δ functions, alternating in sign, whose weight increases like $Z(Z-1)^{(N+1)/2}$.

We expected the inconsistency between Eqs. (7) and (10) because the presence of the surface prevents the existence of the uniform mode. A way of illustrating this is to suppress the surface in a finite Bethe lattice. Realizing that the only difference between surface sites and bulk sites is the coordination, one could always close the surface by joining in pairs the surface dangling orbitals which is the natural way (i.e., periodic boundary conditions) for $Z=2$. Therefore Eq. (2) now reads

$$Eg_{0,N}=Vg_{0,N-1}+(Z-1)Vg_{0,N} . \tag{2'}$$

In this case it is clear that

$$\Sigma'_N=\frac{1}{E-ZV} \tag{15}$$

for all N. This equation gives a δ function as in (7). Of course, this way of getting rid of the surface is not equivalent to neglecting it, because the original topology of the Bethe lattice is destroyed. We expect the uniform mode to exist in any fully coordinated finite system with energy $E=ZV$ and weight 1 in agreement with (15). However, in any *finite* system with a free surface there is no uniform mode and we cannot strictly regard (7) as the limit of (10) when $N\to\infty$. In fact, there is not a simple way to deal with the surface in the infinite network because of the large number of distant sites.

We conclude that attempts to give any physical significance to results arising from long-range correlations in a Bethe lattice are not correct. This has been pointed out in connection with phase transitions of the Ising model in the Bethe lattice.[7,8]

In practice, when calculating physical properties of this sort one can avoid the surface by arguing, on physical grounds, that there must be a decay in the correlations and that only near-atom correlations are important in determining the responses. This has been done when dealing with the Raman spectrum of a-Si (Ref. 9) or the infrared spectrum of a-Si:H (Ref. 10) and SiO_2 (Ref. 11), all giving reasonably satisfactory results.

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