Total and surface density of states on the Bethe lattice

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We present a new method for calculating the average integrated total density of states $\langle N(E)\rangle$ of a disordered system on a Bethe lattice terminating on a closed surface. We first give a rigorous proof of a "negative eigenvalue" theorem and subsequently derive exact expressions for $\langle N(E)\rangle$. The node-counting property for the Bethe lattice is then straightforwardly deduced. We apply our method to obtain $\langle N(E)\rangle$ for the cases of Lorentzian and Gaussian disorder. The behavior of $\langle N(E)\rangle$ is dominated by the surface states due to the special topology of the system. Thus, we finally discuss the relevance of our results to the densities of surface states in real lattices in connection to relevant material from the literature.

I. INTRODUCTION

The node-counting method that relates the number of zeros (nodes) of an eigenstate of energy E to the integrated density of states of the system up to that energy, first introduced by Schmidt[1] in the studies of one-dimensional (1D) random systems, has been extensively used in calculating energy spectra of such systems. The usefulness of the method relies in the fact that it is rather straightforward to calculate the expectation value of the number of nodes of eigenstates around an energy E in a given ensemble of random 1D systems. The restriction to 1D systems on the other hand limits the usefulness of the method and the spectra of random systems in two or three dimensional lattices are derived by other generally approximate methods like the coherent-potential approximation[2] (CPA) for example.

The simple tridiagonal form of the Hamiltonian of a 1D random system with nearest-neighbor interactions (simple linear chain) is a central feature that simplifies the formalism and makes the method tractable. A block-tridiagonal form of the Hamiltonian is again a central feature in the "negative eigenvalue" method proposed by Dean and Martin[3] and reviewed by Hori.[4] The integrated density of states in that method is related to the number of negative eigenvalues of appropriate block matrices appearing in the secular equation of the system. Higher-dimensional lattices can have such block-tridiagonal Hamiltonians and their spectra have been calculated this way.[4]

In another approach to problems involving general Hamiltonian matrices, Mattis[5] has proposed a systematic method of reducing the problem to the study of tridiagonal matrices which are isomorphic to the simple linear chain and for which node counting can be properly utilized.

In this paper we study the spectral properties of a tight-binding Hamiltonian on a Bethe lattice, by showing that it can be written in a proper block-tridiagonal form. A rigorous proof of a properly restated "negative eigenvalue" theorem is given and exact expressions for the integrated density of states are derived. The node-counting property for the Bethe lattice is a direct consequence of this analysis.

The case of a Bethe lattice is special in the sense that locally it can be made to resemble the structure of various two- or three-dimensional lattices, while it possesses a special topological structure that is drastically different from the structure of those lattices. The above properties of the Bethe lattice have two very important consequences. First, the average total density of states can be calculated with the method presented here. Second, its topological structure emphasizes the surface of the lattice where most of the sites lie. (For large Bethe lattices $N_{\rm tot}/N_{\rm surf}\rightarrow 1$ for $Z\gg 2$, where the N's are the number of sites, total and surface, respectively, Z is the lattice coordination.) Therefore in such a system the total density of states is dominated by its surface part.

In what follows we present in Sec. II the steps leading to the proof of the node counting property for the Bethe lattice. We then develop an exact method for calculating the average total density of states of a tight-binding, disordered Bethe system terminating on a closed surface. The method has been outlined in a previous paper.[6]

In Sec. III we present the behavior of the total density of states for the cases of Lorentzian (Sec. III A) and Gaussian (Sec. III B) randomness. The form of the bulk density of states is well known since the Bethe lattice has been used extensively[7] for such calculations. The total density of states in our system differs drastically from such forms in the case of weak disorder due to the domination of the surface states. In the limit of strong disorder the form of both bulk and surface densities of states is dominated by the form of the randomness. Thus in Sec. III C we conclude this work by discussing the relevance of the above results to the surface density of states of disordered real lattices.

II. NODE COUNTING ON THE BETHE LATTICE

A. The model

We consider a Bethe lattice of coordination number Z branching out of a central lattice site, in n homocentric layers of sites (Fig. 1). The lattice terminates in an external boundary layer labeled 0. Moving inwards we label $1,2,\ldots,n$ the successive layers of the lattice up to the central "layer" n which contains only one site labeled c. Each layer $k<n$ contains $N_k=Z(Z-1)^{n-k-1}$ lattice sites, each labeled (k,l), where $l=1,2,\ldots,N_k$ is an intralayer site label and the central site c is thus alternatively labeled $(n,1)$. Consequently the lattice as a whole (excluding the boundary 0 layer) contains a total $N=[Z(Z-1)^{n-1}-2]/(Z-2)$ sites and every site (k,l) has $Z-1$ nearest neighbor (NN) sites

$$(k-1,l';k-1,l'+1;\ldots;k-1,l'+Z-2)$$

on layer $k-1$ and one NN is the $(k+1,l'')$ on layer $k+1$ (see Fig. 1).

We consider the layer 1, adjacent to the boundary layer 0, as the surface of our system which then contains $N_s=Z(Z-1)^{n-2}$ sites. Note that $N_s/N\to(Z-2)/(Z-1)$ as $n\to\infty$ i.e., the surface contains a finite fraction of all sites even at the limit of the infinitely large system.

We assume a one-electron tight-binding Hamiltonian for particles on the above lattice, of the form

$$H=\sum_{k=1}^{n}\sum_{l=1}^{N_k}|k,l\rangle\varepsilon_{k,l}\langle k,l|-V\sum_{(k,l)(i,j)}{}'|k,l\rangle\langle i,j| \ . \tag{2.1}$$

The $|k,l\rangle$ are Wannier-like vectors forming the basis. The $\varepsilon_{k,l}$ are the diagonal matrix elements of H, V is the energy transfer integral, and the primed summation is over NN sites only. We adopt the boundary condition $\varepsilon_{0,l}=+\infty$ for every site $(0,l)$ on the external layer 0.

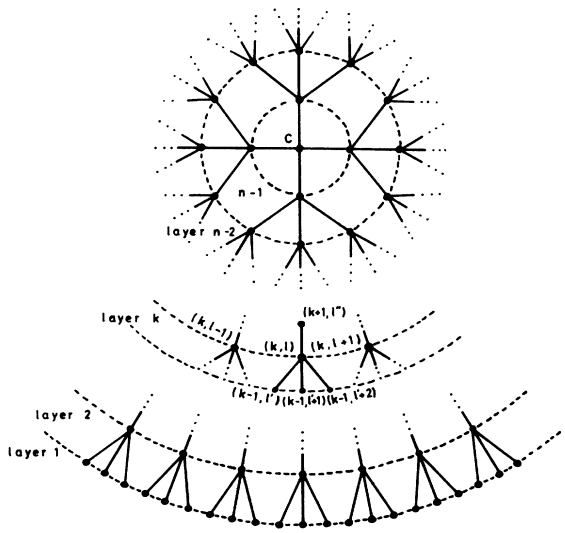

FIG. 1. Bethe lattice of coordination $Z=4$ in n homocentric layers. Layer 1 is the surface layer and C is the central lattice site. The sites in layer k are labeled (k,l), l being an intralayer label.

We observe that the matrix representing our Hamiltonian (Eq. 2.1) in the Wannier-like basis has the block-tridiagonal form:

$$H=\begin{bmatrix} A_1 & B_1 & 0 & & & & \\ B_1^T & A_2 & B_2 & & 0 & & \\ 0 & & & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & & & & 0 & \\ & 0 & & B_{n-2}^T & A_{n-1} & B_{n-1} & \\ & & & 0 & B_{n-1}^T & A_n & \end{bmatrix} . \tag{2.2}$$

The diagonal elements A_k, $k<n$, are $N_k\times N_k$ diagonal matrices, k being a layer level, with $(A_k)_{ij}=\varepsilon_{k,i}\delta_{ij}$, $A_n=\varepsilon_c$ and the off-diagonal elements B_k are $N_k\times N_{k+1}$ matrices (B_k^T denoting the transpose) which can be written in block-diagonal form as $(B_k)_{ij}=\bar{V}\delta_{ij}$, for $k=1,2,\ldots,n-1$, where $\bar{V}=(-V,-V,\ldots,-V)^T$ (column vector), containing $Z-1$ elements. The last off-diagonal elements B_{n-1} adjacent to the central site n are $(-V,-V,\ldots,-V)^T$ (column vector), containing Z elements.

The eigenvalues $\{E_i\}$ of H are the zeros of the characteristic equation

$$\Delta(E)\equiv\det(H-EI_N)=0 \tag{2.3}$$

where I_N is the $N\times N$ unit matrix. Then

$$\Delta(E)\equiv\prod_{i=1}^{N'}(E_i-E)^{\lambda_i} , \tag{2.4}$$

where λ_i the degeneracy of the zero E_i with $\sum_{i=1}^{N'}\lambda_i=N$. The expression

$$N_n(E)\equiv\frac{1}{N}\sum_{i=1}^{N'}\lambda_i\Theta(E-E_i) , \tag{2.5}$$

where Θ is the Heaviside unit-step function gives apparently the percentage of eigenvalues that are smaller than E. Thus $N_n(E)$ is the total integrated density of states per site (TIDOS) of our system.

B. Negative factor counting

When H has a block tridiagonal form, Dean and Martin[3] have shown that

$$\det(H-EI_N)=\prod_{k=1}^{n}\det U_k(E) , \tag{2.6}$$

where the $U_k(E)$ are real symmetric matrices given by the recurrence relation:

$$U_k(E)=A_k-EI_{N_k}-B_{k-1}^T U_{k-1}^{-1}(E)B_{k-1}$$

$$\text{with } U_1(E)=A_1-EI_{N_1} . \tag{2.7}$$

In our case of the Bethe lattice, all the $U_k(E)$ are diagonal matrices as can be easily verified by induction from

(2.7), because of the special form of our A_k and B_k [see (2.2)]. Then

$$\det U_k(E)=\prod_{l=1}^{N_k} X_{k,l}(E) , \tag{2.8}$$

where $X_{k,l}(E)$ are the N_k eigenvalues of $U_k(E)$ and from (2.7) we see that the $X_{k,l}(E)$ obey recurrence relations,

$$X_{k,l}(E)=\varepsilon_{k,l}-E-V^2\sum_{m=l'}^{l'+Z-2} X_{k-1,m}^{-1}(E) \tag{2.9}$$

with

$$X_{1,l}(E)=\varepsilon_{1,l}-E \tag{2.9a}$$

on the first layer and

$$X_c(E)=\varepsilon_c-E-V^2\sum_{l=1}^{Z} X_{n-1,l}^{-1}(E) \tag{2.9b}$$

at the central "layer" n (i.e., the site c). Furthermore we obtain using (2.3), (2.6), and (2.8)

$$\Delta(E)=\prod_{k=1}^{n}\prod_{l=1}^{N_k} X_{k,l}(E) . \tag{2.10}$$

Dean and Martin[3] have given a rather general proof that the number of negative eigenvalues of the matrices $\{U_k(E)\}$ at some energy E equals the number of eigenvalues E_i of H with $E_i<E$. They called this statement "the Negative Eigenvalue Theorem." In stage (1) of their proof (see Ref. 3, pp. 410 and 411) they assume that $\Delta(E)$ have no zeros in common with $\prod_{k=1}^{n-1}\det U_k(E)$. Thus, they claim, the zeros of $\Delta(E)$ coincide with those of $\det U_n(E)$ [see (2.6)]. We verified that in our case of the Bethe lattice the above assumption is not generally true, even when all eigenvalues are distinct, as Dean and Martin require, and that there may be such common zeros. A modified statement of their theorem is nevertheless true for our case as we show in the Appendix, where we present a rigorous proof of our negative eigenvalue theorem for the Bethe lattice.

According to the theorem the TIDOS of the system (see the Appendix) is given as

$$N_n(E)=\frac{1}{N}\sum_{k=1}^{n}\sum_{l=1}^{N_k}\Theta(-X_{k,l}^{\mathrm{LT}}(E)) . \tag{2.11}$$

where Θ is again the Heaviside unit-step function and the $X_{k,l}^{\mathrm{LT}}(E)$ are defined in the Appendix.

C. The TIDOS of the disordered Bethe lattice

We consider hereafter an ensemble of systems with H given by (2.1) in which the probability of every configuration $\{\varepsilon_{k,l}\}$ for the diagonal elements of H is given as

$$P\{\varepsilon_{k,l}\}=\prod_{k=1}^{n}\prod_{l=1}^{N_k} P_0(\varepsilon_{k,l}) , \tag{2.12}$$

i.e., the $\varepsilon_{k,l}$ are statistically uncorrelated random variables having a common probability distribution $P_0(\varepsilon_{k,l})$. We are interested in the ensemble average value $\langle N_n(E)\rangle$ of the $N_n(E)$ and from (2.11) we see that

$$\langle N_n(E)\rangle=\frac{1}{N}\sum_{k=1}^{n}\sum_{l=1}^{N_k}\langle\Theta(-X_{k,l}^{\mathrm{LT}}(E))\rangle . \tag{2.13}$$

Having assumed uniform boundary conditions on the surface, we have statistical homogeneity within every layer. We shall then need the probability distribution $\Phi_k(X_k,E)$ of $X_k(E)$ (we hereafter drop the intralayer index l) in terms of which we have from (2.13)

$$\langle N_n(E)\rangle=\sum_{k=1}^{n}\frac{N_k}{N}\int_{-\infty}^{0}\Phi_k(X;E)dX . \tag{2.14}$$

One can easily show that the sequence of $\langle N_n(E)\rangle$ as $n\to\infty$ (the infinitely large system) converges uniformly to

$$\langle N(E)\rangle=\lim_{n\to\infty}\langle N_n(E)\rangle=\sum_{k=1}^{\infty}\frac{Z-2}{(Z-1)^k}\int_{-\infty}^{0}\Phi_k(X;E)dX \tag{2.15}$$

For the calculation of the $\Phi_k(X_k;E)$ we use the recurrence relations (2.9) with the initial condition (2.9a). We have

$$\Phi_1(X_1;E)=\int_{-\infty}^{+\infty}\delta(X_1-(\varepsilon_1-E))P_0(\varepsilon_1)d\varepsilon_1=P_0(E+X_1) \tag{2.16}$$

Also, observing that the $\varepsilon_{k,i},\{X_{k-1,m}\}$ in (2.9) are statistically uncorrelated to each other,[8] we obtain in a fashion similar to (2.16) the integral recurrence relation

$$\Phi_k(X_k;E)=\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}P_0\left[E+X_k+V^2\sum_{i=1}^{Z-1}y_i^{-1}\right]\times\prod_{i=1}^{Z-1}\Phi_{k-1}(y_i;E)dy_i , \tag{2.17}$$

which together with (2.16) permits the calculation of all $\Phi_k(X_k;E)$.

Since the X_k obey "continued-fraction" type of recurrence relations like (2.9), the $\Phi_k(X;E)$ converge as $k\to\infty$ to $\Phi_\infty(X;E)$ provided the $P_0(\varepsilon)$ is well behaved,[9] where $\Phi_\infty(X;E)$ is the solution of the integral equation obtained from (2.17) by putting $\Phi_k(X;E)=\Phi_{k-1}(X;E)=\Phi_\infty(X;E)$. In the case where $P_0(\varepsilon)$ is a Lorentzian [see (3.1)], Eggarter[10] has given an elegant proof of the above statement. Due to the convergence property of $\Phi_k(X;E)$ we calculate $\langle N(E)\rangle$ by considering a convergence range of k_s layers for Φ_k and expressing $\langle N(E)\rangle$ from (2.15) in the form

$$\langle N(E)\rangle=\sum_{k=1}^{k_s}\frac{Z-2}{(Z-1)^k}\int_{-\infty}^{0}\Phi_k(X;E)dX+(Z-1)^{-k_s}\times\int_{-\infty}^{0}\Phi_\infty(X;E)dx , \tag{2.18}$$

where k_s depends on the degree of randomness in the system.

The node counting property is a direct consequence of the above analysis through the following reasoning.

Starting from the eigenvalue equation $H|\Psi,E\rangle = E|\Psi;E\rangle$ in a matrix form, where H is given by (2.1) and $|\Psi;E\rangle$ is a column vector $|\{a_{k,l}\}\rangle$ [$a_{k,l}$ being the amplitude of $|\Psi;E\rangle$ at site (k,l)], we introduce the quotients $\Pi_{k,l}(E)\equiv Va_{k+1,l'}/a_{k,l}$. From the eigenvalue equation one can see that the $\Pi_{k,l}(E)$ obey the same recurrence relations (2.9) as the $X_{k,l}(E)$ and therefore their probability distributions $P_k(\Pi_k;E)$ coincide with the $\Phi_k(X_k;E)$ as given by the same integral recurrence relations (2.17). Thus the percentage of negative $X_{k,l}(E)$ appearing in the right-hand side of the expression (2.18) for $\langle N(E)\rangle$ coincides with the percentage of negative $\Pi_{k,l}(E)$. The negative $\Pi_{k,l}(E)$ are associated with the zeros of the eigenstates around E since they simply register the local changes of sign of the amplitudes of $|\Psi;E\rangle$ and the node counting property is likewise established.

We conclude this section by giving below the Fourier transform (FT) version of Eq. (2.17)

$$\hat{\Phi}_k(-\omega;E)=(\sqrt{2\pi})^{Z-1}e^{-i\omega E}\hat{P}_0(-\omega)[\hat{f}_{k-1}(\omega;E)]^{z-1} \tag{2.19}$$

where $\hat{}$ indicates the FT of Φ, f and

$$f_k(X;E)\equiv\frac{V^2}{X^2}\Phi_k(V^2/X;E)\ , \tag{2.20}$$

which we shall need in the next section for obtaining results in the Lorentzian and Gaussian randomness case.

III. BEHAVIOR AND SIGNIFICANCE OF $\langle N(E)\rangle$

In the present section we study the behavior of $\langle N(E)\rangle$ [Eq. (2.15)] in the case of (A) Lorentzian and (B) Gaussian diagonal disorder of the Bethe lattice and in (C) we discuss the applicability for our results for studying the surface DOS of disordered real lattices.

A. The Lorentzian disorder case

We consider here the Lorentzian (or Cauchy) distribution $\mathcal{L}(X;\alpha,\gamma)$ centered at α and of width γ

$$\mathcal{L}(X;\alpha,\gamma)\equiv\frac{1}{\pi}\frac{\gamma}{(X-\alpha)^3+\gamma^2} \tag{3.1}$$

having the following properties:

$$\text{(a)}\quad \hat{\mathcal{L}}(\omega;\alpha,\gamma)=\frac{1}{\sqrt{2\pi}}\exp(-\gamma|\omega|-i\alpha\omega)\ , \tag{3.2}$$

where $\hat{\mathcal{L}}(\omega;\alpha,\gamma)$ is the *FT* of $\mathcal{L}(X;\alpha,\gamma)$.

(b) The function

$$l(X;A,\Gamma)\equiv\frac{1}{X^2}\mathcal{L}(1/X;\alpha,\gamma)$$

is again a Lorentzian with

$$A=\frac{\alpha}{a^2+\gamma^2},\quad \Gamma=\frac{\gamma}{\alpha^2+\gamma^2}\ , \tag{3.3}$$

and

$$\text{(c)}\quad \int_{-\infty}^{0}\mathcal{L}(X;\alpha,\gamma)dX=\frac{1}{2}-\frac{1}{\pi}\arctan(\alpha/\gamma) \tag{3.4}$$

We assume a Lorentzian disorder for the common probability distribution $P_0(\varepsilon)$ of the diagonal elements $\varepsilon_{k,l}$ of our Hamiltonian (2.1). Thus, expressing the energies in units of V [i.e., taking $V=1$, Eq. (2.1)],

$$P_0(\varepsilon)\equiv\mathcal{L}(\varepsilon;0,\gamma_0)\ , \tag{3.5}$$

where $\mathcal{L}(\varepsilon;0,\gamma_0)$ (see 3.1) is centered at $\varepsilon=0$ and is of width γ_0. Next we observe from (2.16) that $\Phi_1(X;E)$ is a Lorentzian with $a_1=-E$, $\gamma_1=\gamma_0$, and so is $f_1(X;E)$ [see (2.20), (3.3)], with (A_1,Γ_1) given in terms of (α_1,γ_1) as in (3.3). Using the FT of f_1 we see that all subsequent Φ_k, $k=2,3,4,\ldots$ produced by iterating relation (2.19) are also Lorentzians with (α_k,γ_k) obeying the following algebraic recurrence relations:

$$\begin{aligned}\alpha_k&=-E-(Z-1)\frac{\alpha_{k-1}}{\alpha_{k-1}^2+\gamma_{k-1}^2}\ ,\\ \gamma_k&=\gamma_0+(Z-1)\frac{\gamma_{k-1}}{\alpha_{k-1}^2+\gamma_{k-1}^2}\ ,\end{aligned} \tag{3.6}$$

since now only FT's of the Lorentzian appear in relation (2.19), and then (2.19) is satisfied when the exponents appearing in both sides of it [see (3.2)] obey relations (3.6).

As mentioned in Sec. II, Eggarter[10] has shown that the iteration of (3.6) makes the values of α_k,γ_k converge exponentially fast to $\alpha(E),\gamma(E)$, where $(\alpha(E),\gamma(E))$ is obtained as the solution of the algebraic system derived from (3.6) when setting $\alpha_k=\alpha_{k-1}=\alpha(E)$ and $\gamma_k=\gamma_{k-1}=\gamma(E)$, that obeys $\alpha^2(E)+\gamma^2(E)>Z-1$. We find

$$\begin{aligned}\alpha(E)&=-\tfrac{1}{2}E(1+q)\ ,\\ \gamma(E)&=\tfrac{1}{2}\gamma_0(1+1/q)\ ,\end{aligned} \tag{3.7}$$

where

$$q\equiv|E|^{-1}(\tfrac{1}{2}[E^2-\gamma_0^2-4(Z-1)]+\{\tfrac{1}{4}[E^2-\gamma_0^2-4(Z-1)]^2+\gamma_0^2E^2\}^{1/2})^{1/2}\ .$$

Thus, the Φ_k as $k\to\infty$ converge to Φ_∞ given by $(\alpha(E),\gamma(E))$ [see (3.1)].

The average TIDOS (2.15) is expressed using (3.4) and (3.6) as

$$\langle N(E)\rangle=\frac{1}{2}-\frac{Z-2}{\pi}\sum_{k=1}^{\infty}(Z-1)^{-1}\arctan(\alpha_k/\gamma_k)\ , \tag{3.8}$$

having the limiting behavior

$$\langle N(E)\rangle\to\frac{1\pm1}{2}-\frac{\gamma_0}{\pi E}\ \text{as}\ E\to\pm\infty\ .$$

Dancz and Edwards,[11] using the Green's-function techniques, have also derived an integral expression for the averaged-total density of states of the Cayley tree, in the

case of an infinitely large system with Lorentzian disorder.

Figure 2 shows the behavior of the total average DOS

$$\rho(E)=\frac{d}{dE}\langle N(E)\rangle$$

for the cases $\gamma_0=0.1V$ (low disorder) and $\gamma_0=0.5V$ (intermediate disorder) of a Bethe lattice with $Z=4$.

B. The Gaussian disorder case

We consider here the Gaussian distribution $G(X;\sigma)$, centered at $X=0$ and of width σ

$$G(X;\sigma)=\frac{1}{\sqrt{2\pi}\sigma}\exp(-X^2/2\sigma^2) \tag{3.9}$$

having a FT

$$\hat{G}(\omega,\sigma)=\frac{1}{\sqrt{2\pi}}\exp(-\sigma^2\omega^2/2)\ . \tag{3.10}$$

We assume a Gaussian disorder of width σ for the common probability distribution $P_0(\varepsilon)$ of the diagonal elements $\varepsilon_{k,l}$ of our Hamiltonian (2.1). Thus expressing the energies in units of V as in Sec. III A, we have

$$P_0(\varepsilon)\equiv G(\varepsilon;\sigma)\ . \tag{3.11}$$

In the present case we proceed to obtain numerically the Φ_k needed for the calculation of the TIDOS $\langle N(E)\rangle$ [see (2.15)]. Starting at the surface of the system with [see (2.16)]

$$\Phi_1(X;E)=G(E+X;\sigma)\ , \tag{3.12}$$

we use again the FT version (2.19) of the recurrence scheme for the subsequent Φ_k. In this scheme it is most convenient to use an expansion of Φ_k,f_k in terms of orthonormalized Hermite function[12]

$$\Psi_m(X;\alpha)=C_m e^{-\alpha X^2/2}H_m(X;\alpha)\ , \tag{3.13}$$

where H_m, $m=1,2,\ldots$, are Hermite polynomials obeying

$$H_m=2\alpha X H_{m-1}-2\alpha(m-2)H_{m-2}\ ,$$

$$H_1(X;\alpha)=1,\quad H_2(X;\alpha)=2aX\ ,$$

$$C_m=\left[\left(\frac{\pi}{2}\right)^{1/2}[(m-1)!](2\alpha)^{m-1}\right]^{-1/2}\ ,$$

and α is a positive definite parameter.

This expansion is always possible since the Φ_k,f_k are square integrable functions.[13] The FT of Ψ_m is given as

$$\hat{\Psi}_m(\omega,\alpha)=(-i)^{m-1}\Psi_m(\omega;1/\alpha) \tag{3.14}$$

and then the FT of Φ_k,f_k is directly given from the expansion of Φ_k,f_k in the X space; if

$$f(X)=\sum_{m=1}^{\infty}A_m(\alpha)\Psi_m(X;\alpha)\Longrightarrow\hat{f}(\omega)$$

$$=\sum_{m=1}^{\infty}A_m(\alpha)\hat{\Psi}_m(\omega;\alpha)\ ,$$

where

$$A_m(\alpha)=\int_{-\infty}^{+\infty}f(X)\Psi_m(X;\alpha)dX\ . \tag{3.15}$$

Using (3.12), (2.20), (3.15), and (3.14) we introduce in (2.19) $\hat{f}_1(\omega)$ properly expanded in terms of $\hat{\Psi}_m(\omega;\alpha)$ and we obtain $\hat{\Phi}_2(\omega)$. Purseval's theorem[14] permits us to express the $B_m^{(2)}(\alpha)$ entering the expression $\Phi_2(X)=\sum_{m=1}^{\infty}B_m^{(2)}(\alpha)\Psi_m(X;\alpha)$, in terms of $\hat{\Phi}_2(\omega)$ as

$$B_m^{(2)}(\alpha)=\int_{-\infty}^{+\infty}\hat{\Phi}_2(-\omega)\hat{\Psi}_m(\omega;\alpha)d\omega\ .$$

Having obtained thus $\Phi_2(x)$, we use (2.20) to obtain $\hat{f}_2(\omega)$ properly expanded in terms of $\hat{\Psi}_m(\omega;\alpha)$ using again (3.15) and (3.14), and the iteration proceeds likewise to obtain all subsequent $\Phi_k(X)$.

In performing the calculation we used the first fifty-two Hermite functions and the overall accuracy in the calculation of the Φ_k is estimated to be 3–5 %. We found that the $\Phi_k(X;E)$ converge to a function $\Phi_\infty(X;E)$ in a number k_s of iterations (corresponding to k_s surface layers) that, as expected, depended on E and decreased rapidly with increasing disorder σ. The average TIDOS $\langle N(E)\rangle$ is calculated using (2.15) and Fig. 3 shows the behavior of the total average DOS

$$\rho(E)=\frac{d}{dE}\langle N(E)\rangle$$

for the cases (a) $\sigma=0.5$ and (b) $\sigma=1$ and $2\sqrt{3}$ (all σ in

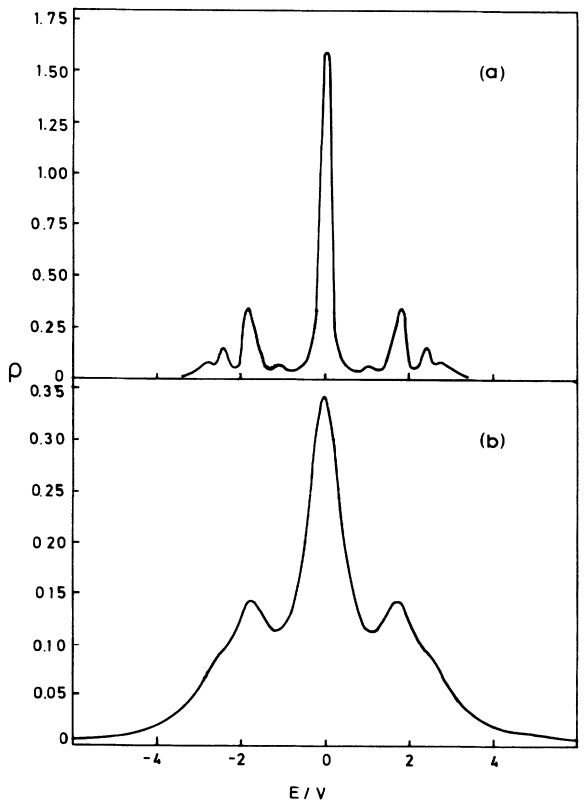

FIG. 2. Total density of states per site ρ vs E/V of a system with $Z=4$ and Lorentzian diagonal disorder of width (a) $\gamma_0=0,1V$ and (b) $\gamma_0=0.5\ V$.

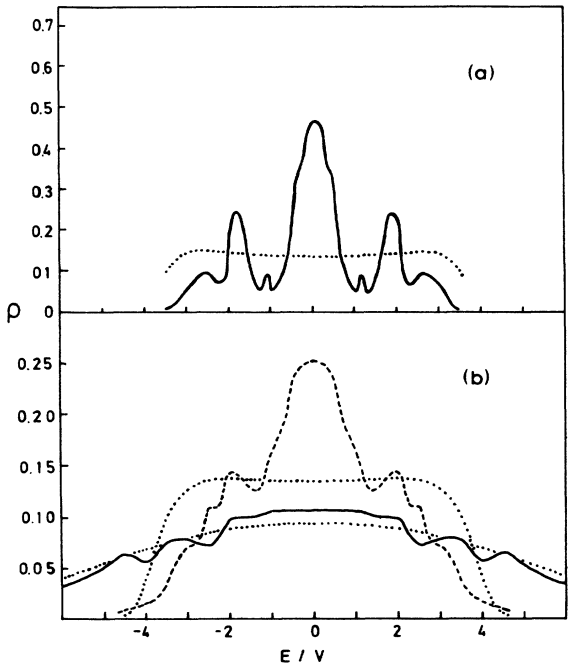

FIG. 3. Total density of states per site ρ vs E/V of a system with $Z=4$ and Gaussian diagonal disorder of width (a) $\sigma=0.5V$ and (b) $\sigma=1.0V$ (dashed line) and $\sigma=2\sqrt{3}V$ (solid line). The bulk density of states in all three cases is also shown by dotted lines. Note that V introduces energy scale proportional to the unperturbed bandwidth $B_0=4\sqrt{Z-1}V$.

units of V). The bulk DOS $\rho_b(E)$ given[8,13] by

$$\rho_b(E)=\int_{-\infty}^{+\infty}\Phi_\infty(X;E)\Phi_\infty(1/X;E)dX\ ,$$

is also shown on the same figure by dotted lines.

C. DOS in the surface region of disordered real lattices

The local DOS in the surface region of real systems has been studied by many authors using tight-binding methods[15–20] and more recently by *ab initio* procedures.[21–24] Though it is quite clear that these *ab initio* methods have shown the importance of deriving the electron charge distribution at the surface self-consistently in order to obtain correctly the surface DOS, a task which is not envisioned here, these methods are incapable of handling large amounts of disorder and often require large amounts of computer work. With this in mind it is interesting to examine the extent to which qualitative features from our calculated DOS agree with those from relevant *ab initio* and tight-binding calculations, as an intermediate check, prior to studying the behavior of the local DOS in the surface region in the case of systems with intermediate and strong disorder, where such checks do not exist. As we discuss below our results should become dramatically more realistic as the disorder of the system is increased. Therefore the discovery of some qualitative resemblances of the weak disorder behavior of our model to the existing results for ordered systems, should provide reasonable evidence for the pertinence of our results to real systems when intermediate or strong disorder is present.

The centrosymmetric Bethe-lattice construction used in our model (see Fig. 1), apart from the obvious advantage stemming from the simplicity of the formalism, which makes the solution tractable for any amount of disorder present in the system, has at first sight an advantage as well as a disadvantage over other possible constructions using Bethe or real lattices. The advantage lies in the capability of the construction to imitate locally a real lattice topology in every neighborhood of the whole surface layer and not only in the vicinity of an appropriate cluster of sites, as in the usual Bethe lattice applications.[7] The disadvantage of the construction is its dramatic failure to imitate the topology of successive real lattice layers, because the number of lattice sites in our layers decreases geometrically fast inward from the surface. This fact would also make unjustifiable the use of anything beyond the tight-binding Hamiltonian.

A more careful examination reveals though, that the advantage becomes truly significant only if a large amount of disorder is present. Because then, the eigenstates are localized rather strongly and their DOS depends mainly on the local lattice topology explained above.

A more careful examination reveals also that the disadvantage is a minor one in the overall scheme, if one is interested in the electronic structure of the first few layers of the surface region, in the presence of large amounts of disorder, for the following reasons: As discussed in the Introduction, most of the lattice sites in our construction lie in those first few layers (for example 96% of the sites lie in the first three layers for $Z=4$). Then, if due to disorder the states are well localized at every part of the system, the total DOS we calculate has a rather small contribution from the states localized in the rest of the system. In the above example the rest of the system contains less than 4% of the total number of sites. In other words, our total DOS is then dominated by the states localized in the first few layers.

We come now to compare our results in the case of weak disorder with relevant ones for ordered systems, from the extensive literature associated with surface electronic structure. We note first that electron charge redistribution affects almost exclusively the first surface layer (see for example Fig. 10 of Ref. 23) and therefore the local density of states in subsequent layers (second from the surface, etc.) should show little influence from charge redistribution. Therefore, when a calculation of local DOS in the surface region includes self-consistently the charge redistribution, its results should differ substantially from ours only in the first surface layer. With that in mind, we compared our results to a variety of local DOS's obtained by various Hamiltonians and interestingly enough we found them to have common basic features, in the layers adjacent to the first surface layer.

We first mention Ref. 16 (Fig. 1 therein) and Ref. 20 (Fig. 21 therein) where in a non-self-consistent tight-binding scheme they obtain the same basic three-peak structure of the surface DOS, although the structure is shifted with respect to the band center in Ref. 20 due to

the second-neighbor overlap integrals that shift the band but do not change the bandwidth. A similar behavior has the non-self-consistently calculated surface DOS presented in Fig. 2 (dashed line) of Ref. 17.

We then examine a number of papers where the calculations of surface DOS contain various degrees of self-consistency in charge redistribution. Comparison of our results with the local DOS of the first surface layer contained in these references shows substantial discrepancies due to charge redistribution as discussed above, and such discrepancies are more dramatically obvious in the work of Kerker *et al.* (see Fig. 3 of Ref. 22). On the other hand, the behavior of the DOS in the second layer from the surface exhibits again the basic three-peak structure in all cases examined, and we mention Fig. 1 and Fig. 2 of Ref. 18, Fig. 1 of Ref. 19, Fig. 12 of Ref. 23 and Fig. 16(c) of Ref. 24. In Figure 4 we show two of the cases referred to above, namely the self-consistent calculation for the second from the surface layer presented in Fig. 12 of Ref. 23 (solid line) and the non-self-consistent calculation for the surface layer presented in Fig. 2 of Ref. 17 (dashed line), for comparison with our calculated surface DOS presented in Fig. 3(a) above (dash-dotted line). One should notice the good qualitative agreement consisting of a coincidence in the positions (unlike their magnitudes), of most of our peaks, to the corresponding ones of the other two curves, especially the solid curve.

Having established the kind of relevance our results bear to surface-region DOS in the case of weak disorder we proceed to some conclusions emerging from the behavior of our DOS in the case of intermediate and strong disorder. One conclusion concerns the overall shape of our DOS that is dominated there by the type of the randomness (i.e., the DOS has a Gaussian shape for Gaussian randomness as in Fig. 3). The other conclusion concerns the gradual smoothening of the structure as disorder is increased, leading to its practical disappearance in the strong disorder case. We note that such features of the DOS have been noticed in cases of bulk disorder too.[8]

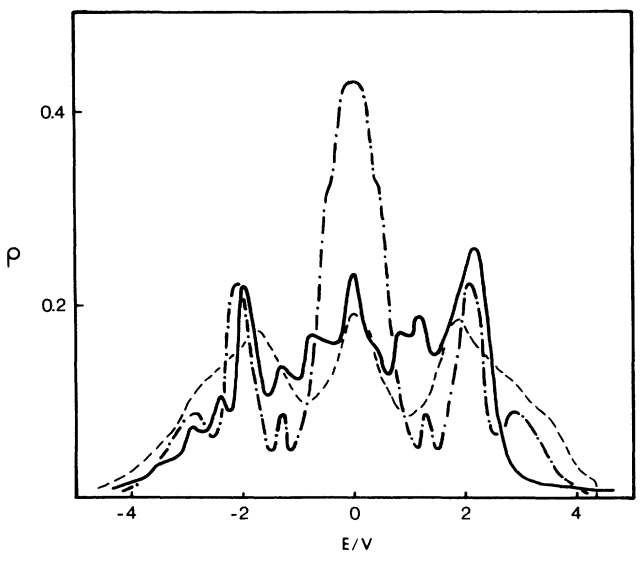

FIG. 4. Surface DOS ρ vs E/V from Fig. 12 of Ref. 23 (solid line) and from Fig. 2 of Ref. 17 (dashed line), for comparison with our Fig. 3(a) (dashed-dotted line).

In closing we should emphasize the fact that our method can be extended in a simple way to include layer-dependent randomness and can also be useful in studying interface DOS and bring about most of their qualitative features.

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APPENDIX

We consider here the functions $X_{k,l}(E)$ defined as the eigenvalues of the corresponding matrices $U_k(E)$, which obey relations (2.9). As shown by Dean and Martin, the characteristic polynomial $\Delta(E)$ is expressed as the product of all the $X_{k,l}(E)$, for all values of E that are not singular points of this product [see (2.3) and (2.10)].

In what follows, E denotes values of the variable on the real axis. We first prove the following lemma.

Lemma. The $X_{k,l}(E)$ are fractional rational functions of E with a degree of the numerator greater by 1 than the degree of the denominator. Every $X_{k,l}(E)$ is a strictly decreasing function of E, at all open intervals in which the E axis is divided by the singular points of $X_{k,l}(E)$ that lie on it. Moreover, any zeroes of a $X_{k,l}(E)$ are simple and any nonremovable singular points of it are simple poles.

Proof by perfect induction

The $X_{1,l}(E)$ obviously have all the properties stated in the lemma [see (2.9a)]. Also, differentiating (2.9) and (2.9a) with respect to E we obtain

$$\frac{d}{dE}X_{k,l}(E)=-1+V^2\sum_{m=l'}^{l'+Z-2}X_{k-1,m}^{-2}(E)\times\frac{d}{dE}X_{k-1,m}(E) \quad \text{(A1)}$$

with

$$\frac{d}{dE}X_{1,l}(E)=-1\ . \quad \text{(A1a)}$$

We now suppose that all $X_{k-1,l}(E)$ for a given k have these properties. Then it is obvious from (2.9) that all the $X_{k,l}(E)$ are rational fractions too, represented in the form of sum of a polynomial $(\varepsilon_{k,l}-E)$ of the first degree and a proper fraction. This representation being unique,[25] the degree of this polynomial represents the difference of the degree (numerator-denominator) of these new rational fractions. Also, from (A1) it is obvious that for every $X_{k,l}(E)$,

$$\frac{d}{dE}X_{k,l}(E)<0\ ,$$

for every E including the singular points E_s, in the sense that

$$\lim_{E\to E_s}\frac{d}{ds}X_{k,l}(E)<0$$

there. Then the truth of the statements about simple zeros of the $X_{k,l}(E)$ as well as their "strictly decreasing" property, follows immediately. Finally, since the $X_{k-1,m}(E)$ have simple zeros it follows from (2.9) that the poles of a $X_{k,l}(E)$, created by simple zeros of the $X_{k-1,m}(E)$ involved in (2.9), are simple. The rest of the poles of $X_{k,l}(E)$, if any, are created from removable singular points E_s of the $X_{k-1,m}(E)$ for which $\lim_{E\to E_s}X_{k-1,m}(E)=0$ and are simple too, since as shown above

$$\lim_{E\to E_s}\frac{d}{dE}X_{k-1,m}(E)<0\ .$$

Corollary: For every $X_{k,l}(E)$ we have $X_{k,l}(E)\sim -E$, $E\to\pm\infty$.

We hereafter introduce the $X^{\mathrm{LT}}_{k,l}(E)$ as being the rational fractions $X_{k,l}(E)$ in lowest terms, i.e., at all removable singular points $\{E_r\}$ of a $X_{k,l}(E)$ we define

$$X^{\mathrm{LT}}_{k,l}(E_r)=\lim_{E\to E_r}X_{k,l}(E)\ . \tag{A2}$$

Then according to the lemma, if the $X^{\mathrm{LT}}_{k,l}(E)$ have any singular points, these points are simple poles, and at all open intervals in which the axis is divided by these poles, the $X^{\mathrm{LT}}_{k,l}(E)$ are strictly decreasing functions of E. Moreover, the properties of the $X_{k,l}(E)$, namely (a) having the degree of the numerator greater by 1 than the degree of the denominator, and (b) $X_{k,l}(E)\sim -E$, $E\to\pm\infty$ shown for the $X_{k,l}(E)$ in the lemma and the corollary, are obviously shared by the $X^{\mathrm{LT}}_{k,l}(E)$ too.

Finally, and most important, if a point E_i is a simple pole of a $X^{\mathrm{LT}}_{k,l}(E)$, then E_i is also a zero of at least one of the $X^{\mathrm{LT}}_{k-1,m}(E)$, where $(k-1,m)$ belongs to the "group" of corresponding lattice points [NN to (k,l)] involved in (2.9). This means that every point E_i that is a simple pole with multiplicity $\langle\mathrm{Mult}(P_i)\rangle$ given by the number of $X^{\mathrm{LT}}_{k,l}(E)$ in our system that have a simple pole at E_i, is also a zero of multiplicity $\langle\mathrm{Mult}(Z_i)\rangle$ given by the number of corresponding $X^{\mathrm{LT}}_{k',l'}(E)$ in our system that have a zero at E_i. Moreover $\langle\mathrm{Mult}(Z_i)\rangle\geq\langle\mathrm{Mult}(P_i)\rangle$. Then introducing Δm_i below, we have

$$\Delta m_i\equiv\langle\mathrm{Mult}(Z_i)\rangle-\langle\mathrm{Mult}(P_i)\geq 0\ . \tag{A3}$$

We can now proceed to show that $\Delta(E)$ defined in (2.3) can be expressed in terms of the $X^{\mathrm{LT}}_{k,l}(E)$ at every value of E. Indeed, starting from (2.10) we have

$$\Delta(E)=\prod_{k=1}^{n}\prod_{l=1}^{N_K}X^{\mathrm{LT}}_{k,l}(E)\ , \tag{A4}$$

for every E that is not a pole of any $X^{\mathrm{LT}}_{k,l}(E)$, because by expressing $\Delta(E)$ as in (A4) we eliminate all removable singular points of the $X_{k,l}(E)$, and the only singular points contained in the right-hand side (rhs) of (A4) are the simple poles of the $X^{\mathrm{LT}}_{k,l}(E)$. Therefore, since at every singular point E_i we have $\langle\mathrm{Mult}(Z_i)\rangle\geq\langle\mathrm{Mult}(P_i)$, [see (A3)], all E_i are removable singular points of the rational fraction appearing in the rhs of (A4). Then at every singular point E_i the limit $E\to E_i$ of that rhs exists and expressing that rational fraction in lowest terms we eliminate *all* these removable singular points and we are left with a polynomial. Therefore

$$\Delta(E)\equiv\left[\prod_{k=1}^{n}\prod_{l=1}^{N_k}X^{\mathrm{LT}}_{k,l}(E)\right]^{\mathrm{LT}} \tag{A5}$$

and at every point E_i for which $\langle\mathrm{Mult}(Z_i)\rangle>\langle\mathrm{Mult}(P_i)$ [i.e. $\Delta m_i\geq 1$; see (A3)] we have a zero of $\Delta(E)$ of multiplicity λ_i, where

$$\lambda_i=\Delta m_i\ , \tag{A6}$$

while the points E_i for which $\Delta m_i=0$ are the removable singular points that have been eliminated in (A5).

We can now prove the following negative eigenvalue theorem:

Theorem: The number of $X^{\mathrm{LT}}_{k,l}(E)$ that have negative values at a point E that is not a zero of $\Delta(E)$ is equal to the sum $\sum\lambda_i$ of the multiplicities λ_i of all zeros $\{E_i\}$ of $\Delta(E)$, for which $E_i<E$.

Proof: The $X^{\mathrm{LT}}_{k,l}(E)$ obey the corollary of the lemma. Therefore at $E=-\infty$ the $X^{\mathrm{LT}}_{k,l}(-\infty)$ are all positive and at $E=+\infty$ the $X^{\mathrm{LT}}_{k,l}(+\infty)$ are all negative, their total number being N [see (2.8)]. When E is crossing a point E_1 that is a $\langle\mathrm{Mult}(Z_i)\rangle$ zero and a $\langle\mathrm{Mult}(P_i)\rangle$ pole of some $X^{\mathrm{LT}}_{k,l}(E)$, then a number $\langle\mathrm{mult}(Z_i)\rangle$ of those $X^{\mathrm{LT}}_{k,l}(E)$ obviously change from positive to negative values and the rest, a number $\langle\mathrm{mult}(P_i)\rangle$ of them, obviously change from negative to positive values, the net increase of the total number of negative $X^{\mathrm{LT}}_{k,l}(E)$ being $\langle\mathrm{Mult}(Z_i)\rangle-\langle\mathrm{Mult}(P_i)\rangle$.

Starting from $E=-\infty$ where we have no negative $X^{\mathrm{LT}}_{k,l}(E)$, we increase by Δm_i their number [see (A3)] at every point E_i we encounter before a given value E. Therefore the total number $M_n(E)$ of negative $X^{\mathrm{LT}}_{k,l}(E)$ is

$$M_n(E)=\sum_{E_i\,(<E)}\Delta m_i\ ,$$

with $\sum_{E_i(<E)}\Delta m_i\sim N$, $E\to+\infty$ since at that limit all $X^{\mathrm{LT}}_{k,l}(E)$ are negative. Then, using (A6) we finally obtain

$$M_n(E)=\sum_{E_i\,(<E)}\lambda_i \tag{A7}$$

and this completes the proof.

Note: By their definitions

$$M_n(E)=\sum_{k=1}^{n}\sum_{l=1}^{N_k}\Theta(-X^{\mathrm{LT}}_{k,l}(E))$$

and

$$\sum_{E_i\,(<E)}\lambda_i\equiv\sum_{i=1}^{N'}\lambda_i\Theta(E-E_i)\ ,$$

where N' is the number of distinct energy levels and Θ is the Heaviside unit-step function. Then, relation (2.11) follows immediately from (2.5) and (A7).

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