

## Chaotic scaling trajectories and hierarchical lattice models of disordered binary harmonic chains

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It is shown that the simple position-space rescaling method developed by Gonçalves da Silva and Koiller to compute the local density of states (DOS) in disordered harmonic chains is exact on certain hierarchical lattices and in the limit of zero impurity concentration. It is demonstrated that their method can be improved even though convergence to the true DOS cannot be achieved simply. Partial information on eigenvectors can be extracted from the scaling trajectories. For an ordered chain, delocalized states can in general be identified with chaotic behavior. Analogies with critical phenomena may be found from a functional-integral formulation of the problem. The relationship to transfer-matrix approaches is also mentioned.

### I. INTRODUCTION

Disordered systems must in general be studied by approximate methods. One-dimensional systems seem particularly well suited to test such methods because of the existence of quite a few theorems and exact results against which to test one's ideas. Many of these theorems have been developed in the context of the Anderson localization problem,<sup>1-3</sup> others in the context of disordered harmonic chains.<sup>4,5</sup> It is well known that these problems are in fact related.

One characteristic feature of the binary chain is that the spectrum of its eigenfrequencies [or density of states (DOS)] most often exhibits many gaps and sharp features whose existence is quite well understood on a theoretical basis.<sup>4,6,7</sup> Nevertheless, all standard approximation schemes<sup>5</sup> yield a smooth DOS which does not exhibit such features. Recently though, it has been pointed out by Gonçalves da Silva and Koiller<sup>8</sup> (GK) that DOS which closely resemble computer simulation results<sup>4</sup> may be obtained from a very simple position-space rescaling scheme (or renormalization group if one is not too strict on nomenclature). Similar, but more careful and elaborate procedures have also been used in studies of localization.<sup>9</sup>

The purpose of this paper is to point out limitations of the GK rescaling scheme and to indicate how, as suggested by GK, it may be improved while conserving its original simplicity. More importantly we believe, we show that the GK approximation and its generalizations are exact on certain hierarchical lattices. This not only proves useful to understand the results, it also provides an example of how an ordered but highly inhomogeneous system may mimic an homogeneously disordered system. That such a possibility existed was already pointed out by Kaufman and Griffiths<sup>10</sup> in their study of hierarchical lattices in the context of phase transitions. In that context, Berker and Ostlund<sup>11</sup> had proved earlier that some well-known position-space renormalization-group schemes, such as the Migdal-Kadanoff approximation, were exact on these lattices.

Hierarchical lattices have also found their way into the study of disordered systems such as spin-glasses<sup>12</sup> but there one is looking at a problem where the difficulties of both phase transitions and disorder are intermixed. Even though our problem has some of the features of critical phenomena, as is shown in Appendix A, we believe that we are mostly concentrating on disorder. While hierarchical lattices in critical phenomena are used as approximations of higher-dimensional Bravais lattices as well as approximations of disordered systems, here both the original disordered system and, in some sense, its hierarchical lattice models are one dimensional.

Note that since the hierarchical lattices for which the GK recursion relations are exact can be physically realized, this proves that the approximation scheme satisfies some essential physical requirements such as having a positive DOS. It is easy to devise other rescaling schemes which do not satisfy this property.

We also show in this paper that the scaling trajectories contain some information on eigenvectors. In particular, delocalized states in general lead to chaotic trajectories<sup>13</sup> while trajectories for localized states are attracted to fixed points. A different kind of fixed point characterizes regions where the DOS vanishes. From what has been said earlier on the structure of the DOS, it is clear that in any rescaling scheme for the disordered binary chain the attracting sets in parameter space are bound to have a very complicated structure. This is the case in the GK approximation.

In Secs. II and III, we discuss various GK-type rescalings and study their convergence to the true DOS. Section IV introduces the hierarchical lattices. Section V discusses eigenvectors and scaling trajectories. There it is also shown that the GK scheme gives the exact DOS on a single light impurity in an infinite chain. We conclude in Sec. VI with a general assessment of the method. Analogies with phase transitions are pointed out in Appendix A, while contact with transfer-matrix approaches is made in Appendix B.

## II. POSITION-SPACE RESCALING AND RENORMALIZATION GROUP

For the sake of completeness, we review in this section a few known results. Consider a harmonic chain of atoms of mass  $M_i$  at position  $i$ . Let us assume that the force constants between sites  $i$  and  $i+1$  are  $K_{i,i+1}$  and that the displacements of the atoms about their equilibrium positions are given by  $u_i$ . Then the eigenvalue equation for the angular frequency  $\omega$  is given by

$$\sum_j (A_{ij} - M_i \omega^2 \delta_{ij}) u_j = 0, \quad (2.1)$$

where

$$A_{ij} = (K_{i,i+1} + K_{i,i-1}) \delta_{ij} - K_{i,i+1} \delta_{i+1,j} - K_{i,i-1} \delta_{i-1,j} \quad (2.2)$$

is a tridiagonal symmetric matrix and  $\delta$  is a Kronecker delta function.

Let us define the Green's function  $G$  by

$$\sum_j [A_{ij} - M_i (\omega^2 + i\epsilon) \delta_{ij}] G_{jk} = M_i \delta_{ik}, \quad (2.3)$$

where  $i\epsilon$  is an infinitesimal imaginary number. Let  $\underline{I}$  be the identity matrix and  $M_{ij} \equiv M_i \delta_{ij}$  a diagonal matrix. Then, in matrix notation,

$$\underline{G} = \underline{M}^{-1/2} [\underline{M}^{-1/2} \underline{A} \underline{M}^{-1/2} - (\omega^2 + i\epsilon) \underline{I}]^{-1} \underline{M}^{1/2}. \quad (2.4)$$

Using the cyclic invariance of the trace and the fact that  $[\underline{M}^{-1/2} \underline{A} \underline{M}^{-1/2} - (\omega^2 + i\epsilon) \underline{I}]$  may be diagonalized by an orthogonal transformation, it is easy to show that

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \text{Im}[\text{Tr} \underline{G}] &= \lim_{\epsilon \rightarrow 0} \text{Tr}[\text{Im} \underline{G}] \\ &= \pi \sum_i \delta(\omega_i^2 - \omega^2) \end{aligned} \quad (2.5)$$

where  $\omega_i^2$  are real eigenvalues of  $(\underline{M}^{-1/2} \underline{A} \underline{M}^{-1/2} - \omega^2 \underline{I}) = 0$  or equivalently of Eq. (2.1). We conclude that with  $N$  the number of atoms in the chain,

$$\rho(\omega^2) = \frac{1}{\pi} \text{Im} \left[ \frac{1}{N} \sum_i G_{ii} \right] \quad (2.6)$$

is the density of states.

Consider the case of a uniform chain, i.e.,  $M_i = M$  and  $K_{i,i+1} = K$  for all values of  $i$ . Let us restrict our attention to the equations for  $G_{i0}$ . The first step (so-called decimation) of the rescaling procedure consists in eliminating all lines for which  $i$  is odd. We obtain

$$[2K^{(1)} - M(\omega^2 + i\epsilon)] G_{i0} = M \delta_{i0} + L^{(1)} (G_{i+2,0} + G_{i-2,0}) \quad (2.7)$$

where

$$L^{(1)} = \frac{L^{(0)2}}{2K^{(0)} - M(\omega^2 + i\epsilon)} \quad (2.8a)$$

$$K^{(1)} = K^{(0)} - L^{(1)}, \quad (2.8b)$$

$$K^{(0)} = L^{(0)} \equiv K. \quad (2.9)$$

In the second and last step, the scale of distances is

changed by a factor of 2 in Eq. (2.7). It is easy to see that this equation then has the same structure as the original one. Hence the above steps may easily be repeated to eliminate more and more degrees of freedom. This is conveniently done on a computer by iterating Eqs. (2.8a) and (2.8b).

When this is done,  $L^{(n)} \rightarrow 0$  after a number of iterations which depends on the value of  $i\epsilon$ . In general then,

$$G_{00} = \lim_{n \rightarrow \infty} \frac{M}{2K^{(n)} - M(\omega^2 + i\epsilon)}. \quad (2.10)$$

Using translational invariance, we have, for an infinite chain,

$$\rho(\omega^2) = \frac{1}{\pi} \text{Im} G_{00}. \quad (2.11)$$

The effect of a finite  $\epsilon$  is to insure convergence. The price paid is that the convergence is to a density of states where each of the delta functions in Eq. (2.5) is replaced by a Lorentzian.

There are clearly many ways the scaling transformation could have been performed. Instead of eliminating  $N/2$  degrees of freedom and changing the scale by a factor 2 at each iteration as we just did, one could have eliminated  $(b-1)N/b$  degrees of freedom and correspondingly changed the scale by a factor  $b$  (see Appendix B). One could also have blocked the degrees of freedom by groups of two and then eliminated blocks, etc. All these methods give the exact result in the case of the uniform chain. In fact, what we have defined here is a renormalization group since two successive rescaling transformations, one of length scale  $r$  and the other of length scale  $s$ , give the same result as a rescaling transformation of length scale  $rs$ . For a disordered system, as we shall shortly see, approximations are involved and different rescaling transformations give different results. For an arbitrary scaling transformation, a general expression may be found for the recursion formulae using, for example, projection operator techniques.<sup>14</sup>

## III. GENERALIZATION TO DISORDERED SYSTEMS

### A. The Gonçalves da Silva–Koiller (GK) approximation

Consider a harmonic chain with uniform restoring forces ( $K_{i,i+1} = K$ ) and masses  $M_A$  and  $M_B$  distributed at random. This is a model for one-dimensional binary alloys. If one eliminates degrees of freedom as in Eq. (2.7) one finds

$$2K_i^{(1)} = 2K^{(0)} - \frac{L^{(0)2}}{2K^{(0)} - M_{i+1}(\omega^2 + i\epsilon)} - \frac{L^{(0)2}}{2K^{(0)} - M_{i-1}(\omega^2 + i\epsilon)}, \quad (3.1a)$$

$$L_{i,i+1}^{(1)} = \frac{L^{(0)2}}{2K^{(0)} - M_{i+1}(\omega^2 + i\epsilon)}. \quad (3.1b)$$

Clearly, the "force constants" in the rescaled system are now random variables because the masses are randomly distributed. The GK approximation consists in replacing Eqs. (3.1a) and (3.1b) by their average. (Similar approxi-

mations have been made in the past in the theory of localization.<sup>9</sup> In general a complete probability distribution for the rescaled variables must be kept.) When we assume that the masses are independently distributed on each site with a probability equal to their relative concentrations  $c_A$  and  $c_B$ , Eqs. (3.1a) and (3.1b) become, in the GK approximation,

$$L^{(1)} = L^{(0)} \left[ \frac{c_A L^{(0)}}{2K^{(0)} - M_A(\omega^2 + i\epsilon)} + \frac{c_B L^{(0)}}{2K^{(0)} - M_B(\omega^2 + i\epsilon)} \right], \quad (3.2a)$$

$$K^{(1)} = K^{(0)} - L^{(1)}. \quad (3.2b)$$

In other words, all moments of the probability distribution for  $K$  and  $L$ , except the first one, are set equal to zero. This approximation is discussed further below.

To compute the single-site density of states, one notices that  $L^{(n)} \rightarrow 0$  as  $n \rightarrow \infty$  and hence, by analogy with Eqs. (2.10) and (2.11)

$$\rho_{A(B)}(\omega^2) = \frac{1}{\pi} \lim_{n \rightarrow \infty} \left[ \text{Im} \left[ \frac{M_{A(B)}}{2K^{(n)} - M_{A(B)}(\omega^2 + i\epsilon)} \right] \right] \quad (3.3)$$

while the total density of states is given by

$$\rho(\omega^2) = c_A \rho_A(\omega^2) + c_B \rho_B(\omega^2). \quad (3.4)$$

The latter result comes from the fact that once  $n \rightarrow \infty$ , the averaging over all sites but one (either  $A$  or  $B$ ) has been performed. It is then reasonable to assume that the trace over  $G_{ii}$  reduces to (3.4).

It is well known<sup>4</sup> that the exact one-dimensional density of states of a binary chain exhibits, for large enough mass ratio, a complicated system of peaks and valleys which may be understood from the existence of isolated clusters of light atoms on all length scales. GK have pointed out that since in their approximation the averaging is not performed at the first step but only gradually,  $N/2$  sites at a time, clusters of all sizes are taken into account. Hence, apart from exact results, their method is the only one which predicts sharp features analogous to those of the real density of states. Single-site methods like the coherent potential approximation produce smooth results.<sup>4,5</sup>

As mentioned above however, the GK approximation is in a sense rather crude since at each step the probability distribution for the parameters<sup>15</sup>  $K$  and  $L$  is replaced by single values for  $K$  and for  $L$ . In general, the full probability distribution must be kept.<sup>9</sup> From that perspective, one can test the validity of the GK scheme by computing the ratio of the standard deviation to the average of  $K$  and  $L$  after each iteration. If that ratio is small, then one is justified in keeping only the average of the probability distribution and neglect its width. By actual computations, one finds that after one iteration, there are certain values of  $\omega^2$  for which the ratio of width to average is infinity. Decimating twice before averaging does not improve matters greatly. In fact, there are then more values of  $\omega^2$  for which the fluctuations are larger than the average. Nevertheless, it is conceivable that after many iterations there are well-defined average values of  $K$  and  $L$  with

small fluctuations. Hence, even though the GK scheme may be bad for the first few iterations, it may well improve afterwards and give acceptable results for the complete problem. The best way to verify this is to actually compare “exact” spectra with the results of GK. In Sec. II B we consider how to improve the GK scheme.

In Fig. 1(a), we reproduce the spectrum of GK for  $M_A=1$ ,  $M_B=3$ ,  $K=1$ ,  $c_A=0.5$ , and  $\epsilon=0.02$ . For that value of  $\epsilon$ , the spectrum converges to better than one part in  $10^{15}$  in less than 11 iterations for any  $\omega^2$ . As  $\epsilon \rightarrow 0$ , the number of iterations increases and the spectrum converges towards a set of  $\delta$  functions. For comparison, we show the “exact” spectrum obtained from computer simulations by Payton and Visscher<sup>16</sup> on a chain of 100 000 atoms. Clearly, the details of the two spectra are different, even if a few of their moments, which we discuss below, are in rather good agreement.

To clearly illustrate some of the details of the GK spectrum which are incorrect, we note that the density of states does not vanish at all the forbidden frequencies predicted by the “special frequency theorem” of Matsuda.<sup>6</sup> For any mass ratio larger than two, the theorem predicts special frequencies at  $\nu^2 \equiv 4\omega^2/\omega_{\max}^2 = 2.0, 3.0, 3.41, 3.62, \dots$ . As GK pointed out, for a mass ratio of three, there is a gap in their spectrum at  $\nu^2=2.0$ . We find that this gap is present at all concentrations, but it does not disappear when the mass ratio becomes lower than two, contrary to what exact results<sup>6</sup> and numerical calculations<sup>4</sup> suggest. At the other forbidden frequencies, there is always a concentration for which the density of states does not vanish. As the concentration of light atoms is increased, high-frequency structure ( $\nu^2 > 2$ ) slowly shifts to higher frequencies and hence the gaps do not stay at fixed energy.

Exact results of Borland<sup>7</sup> also give the integrated DOS at the above “special frequencies.” Given the remarks we just made, one cannot expect the GK approximation to exactly reproduce those results but nevertheless, the deviations are not necessarily large. For a concentration  $c_A = \frac{1}{2}$  and a mass ratio of three for example, the integrated DOS of GK does not deviate by more than 7% from Borland’s results.

## B. Generalizations of the GK scheme

From comments in Sec. II A it is clear that the GK scheme may be improved by keeping a model probability distribution for  $K$  and  $L$  which has more nonzero cumulants than just the first one. This is the standard approach. We choose a different route. As suggested by GK, we generalize their scheme in a way that preserves the very simple probability distribution at the expense of having either more complicated recursion relations (when a larger fraction of atoms is eliminated before averaging over disorder) or a larger parameter space (when blocks of atoms are kept as the basic unit of the scheme instead of single atoms). The motivation for this approach is that one wants to keep the essential simplicity of the scheme as well as its hierarchical lattice interpretation and verify to what extent it can be made into a realistic model of disordered systems. We also demonstrate below that, contrary to what one may have thought, averaging variables other than  $K$  and  $L$  (such as  $K/L$  and  $1/L$ , for example) does

not improve the GK scheme. It is meaningless.

Let us consider the first suggested improvement, i.e., eliminating a larger fraction of atoms before averaging over disorder. It seems that this procedure should lead one, in the limit, to the true spectrum. It is easy to show that this is not so. Suppose one has eliminated all  $G_{i0}$  except  $G_{00}$ . Then  $L^{(\infty)} \rightarrow 0$  and

$$G_{00} = \frac{M_0}{2K^{(\infty)} - M_0(\omega^2 + i\epsilon)}. \quad (3.5)$$

The exact average density of states on a site of mass  $M_0$  may be obtained by calculating Eq. (3.5) for all possible

chain configurations with a mass  $M_0$  at site 0 and averaging. One obtains

$$G_{00} = \left\langle \frac{M_0}{2K^{(\infty)} - M_0(\omega^2 + i\epsilon)} \right\rangle. \quad (3.6)$$

The GK approximation would give

$$G_{00} = \frac{M_0}{\langle 2K^{(\infty)} \rangle - M_0(\omega^2 + i\epsilon)}. \quad (3.7)$$

In view of Eq. (3.6), it is tempting to write the set of equations for the disordered system's Green's function in the form

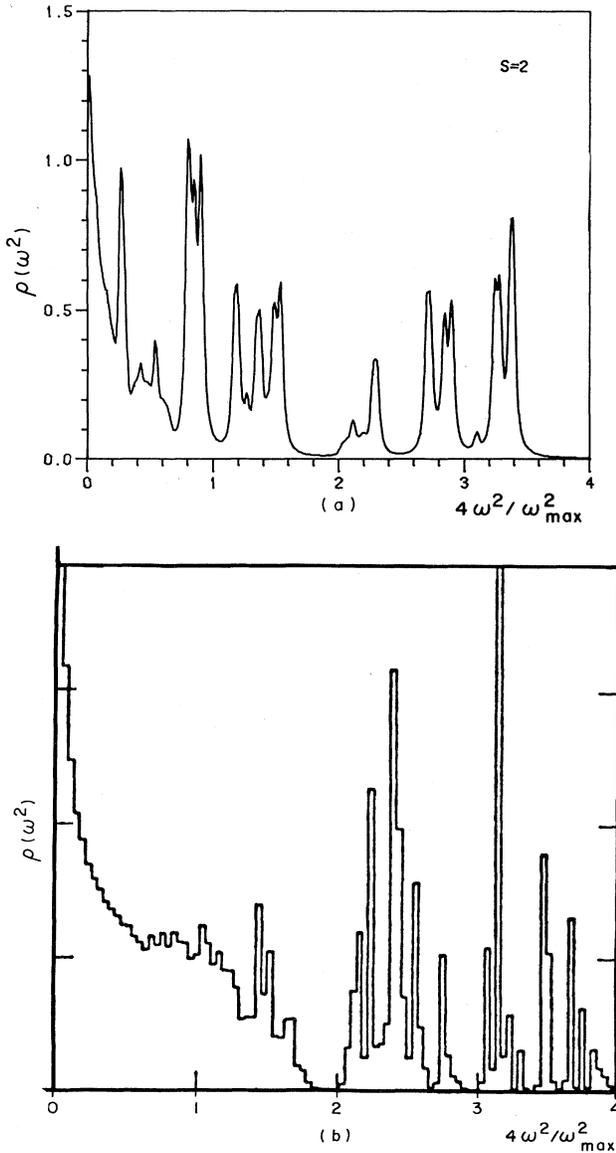


FIG. 1. (a) Density of states  $\rho(\omega^2)$  in the GK approximation for  $M_B/M_A=3$ ,  $c_A=0.5$ , and  $\epsilon=0.02$ .  $\nu^2=4\omega^2/\omega_{\max}^2$ . The length rescaling factor is  $S=2$ . (b)  $\rho(\omega^2)$  in arbitrary units, as obtained by Payton and Visscher (Ref. 16) from computer simulations on 100 000 atoms.  $M_B/M_A=3$ ,  $c_A=0.5$ ,  $\nu^2=4\omega^2/\omega_{\max}^2$ .

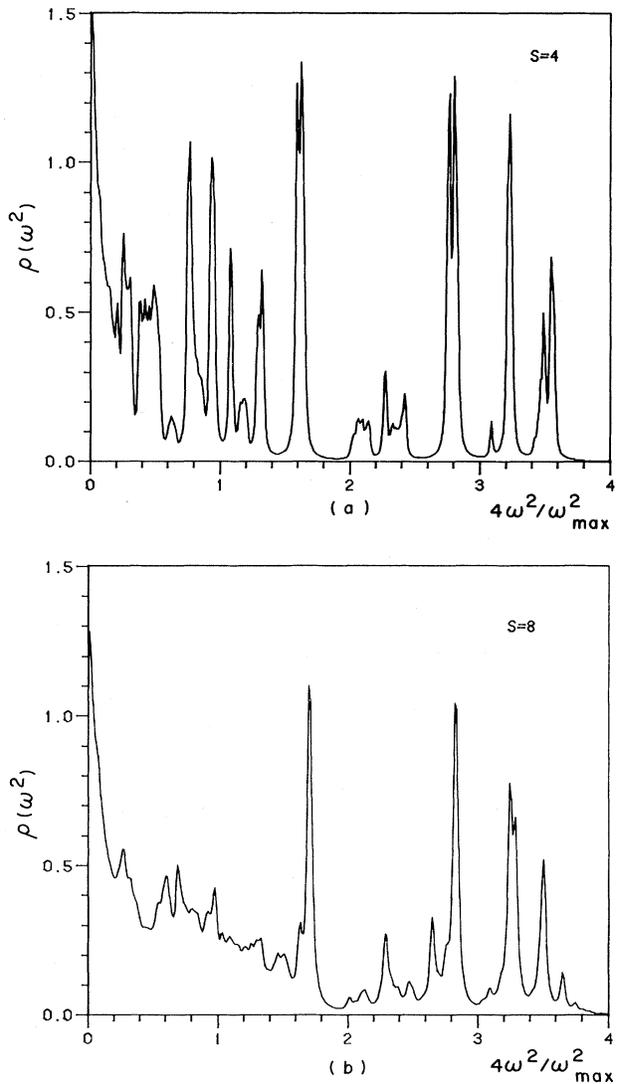


FIG. 2. (a) Density of states  $\rho(\omega^2)$  obtained for the same parameters as in Fig. 1 but this time  $\frac{3}{4}$  of the atoms are eliminated before they are averaged over. Hence  $S=4$ . The density of states at  $\nu^2=0$  is 1.59 for the value of  $\epsilon$  chosen (0.02). The vertical scale stops at 1.5 for uniformity in display. (b)  $\frac{7}{8}$  of the atoms are eliminated before averaging.  $S=8$ .

$$G_{i0} = \frac{M_i \delta_{i0}}{2K^{(0)} - M_i(\omega^2 + i\epsilon)} + \frac{L^{(0)}(G_{i+1,0} + G_{i-1,0})}{2K^{(0)} - M_i(\omega^2 + i\epsilon)} \quad (3.8)$$

and to perform the GK approximation on the variables

$$\alpha_{A(B)}^{(0)} \equiv \frac{M_{A(B)}}{2K^{(0)} - M_{A(B)}(\omega^2 + i\epsilon)} \quad (3.9a)$$

and

$$x_{A(B)}^{(0)} \equiv \frac{L^{(0)}}{2K^{(0)} - M_{A(B)}(\omega^2 + i\epsilon)} \quad (3.9b)$$

instead of on  $K$  and  $L$  as in Eqs. (3.2a) and (3.2b). It turns out that this procedure gives negative densities of states. The possible reason for this state of affairs and various other comments on the convergence of the GK approximation are touched upon in Appendix A. The next section will also demonstrate that the density of states obtained from the GK approximation has to be positive since it is an exact result for hierarchical lattices which can in principle be physically realized. In Sec. V we also show that the GK approximation is exact in the single impurity limit.

Despite the above remarks, performing more decimations before averaging can improve the spectrum in certain frequency ranges. In Figs. 2(a) and 2(b), we show spectra for  $M_B = 3M_A$  and  $c_A = 0.5$ , computed by eliminating  $3N/4$  and  $7N/8$  degrees of freedom before averaging. This corresponds to scale changes of 4 and 8. These results can be directly compared with the GK spectrum and the “exact” spectrum of Figs. 1(a) and 1(b). Eliminating more degrees of freedom apparently improves the DOS. The ameliorations are mostly in the lower ( $\nu^2 < 2$ ) and higher ( $\nu^2 > 3$ ) frequency regions. The central zone of the spectrum ( $1.5 < \nu^2 < 3$ ) remains in poor agreement with the “exact” DOS. This feature becomes more dramatic when the mass ratio is increased to a very large value.

Figures 3(a)–3(c) show the DOS obtained with the “exact” method and with the GK approximation for a rescaling of 2 and 8. The mass ratio is  $10^4$  and the two mass concentrations are equal. Once again, it is clear that increasing the scale change improves the DOS. But it also seems impossible to obtain appreciable intensity for the central peak, whose frequency corresponds to the localized mode of a single light atom oscillating between two heavy

atoms. The reason for the absence of this frequency is that the GK approximation is equivalent to calculating the DOS of an atom moving against parallel groups of atoms which have masses proportional to  $M_A$  and  $M_B$  (more details will be given in the next section). So, even if  $M_B$  is infinitely large, there are still light atoms against which the central atom is vibrating.

The simplest way to obtain this peak is to perform decimations on blocks of three atoms instead of a single atom as done before. The result of this calculation is shown in Fig. 3(d). This demonstrates that using blocks of atoms keeps more information on the short-range order.<sup>17</sup> This blocking procedure is the second way, mentioned above, which can improve the GK scheme. This method converges to the exact result in the limit of very large blocks ( $10^5$  atoms, for example). In their paper, Goncalves da Silva and Koiller use the exact moments of order one to five to justify their method. (See *Note added in proof.*)

We conclude that since, at sufficiently high mass ratio, the highest and lowest frequencies of a given spectrum correspond to the largest clusters of either light or heavy atoms, decimating a larger number of atoms before averaging improves these portions of the spectrum. The central part of the spectrum, on the other hand, depends more on the local environment of light atoms and hence it is preferable to treat exactly blocks of three or more atoms to obtain this portion of the DOS correctly. When larger and larger blocks are kept as the basic element of the GK scheme and more and more of the blocks are decimated before averaging, one expects the results to improve.

#### IV. HIERARCHICAL LATTICES

To understand some of the results discussed in the preceding section, it is useful to keep in mind that the GK recursion relations are exact for certain hierarchical lattices. Not only does that fact prove that the GK scheme and its generalizations give positive densities of states, it also helps to understand certain spectral features of the DOS. We now demonstrate the exactness of the GK recursion relations for certain hierarchical lattices, which, incidentally, are not translationally invariant.

Consider the GK recursion relations Eqs. (3.2a) and (3.2b). After one decimation, one can write the equations of motion for the remaining degrees of freedom (say the even sites for definiteness) in the following form:

$$\left[ 2K^{(0)}(c_A + c_B) - 2c_A L^{(0)} \left[ \frac{L^{(0)}}{2K^{(0)} - M_A(\omega^2 + i\epsilon)} \right] - 2c_B L^{(0)} \left[ \frac{L^{(0)}}{2K^{(0)} - M_B(\omega^2 + i\epsilon)} \right] - M_i(\omega^2 + i\epsilon) \right] G_{i0} \\ = M_i \delta_{i0} + (G_{i+2,0} + G_{i-2,0}) \left[ c_A L^{(0)} \left[ \frac{L^{(0)}}{2K^{(0)} - M_A(\omega^2 + i\epsilon)} \right] + c_B L^{(0)} \left[ \frac{L^{(0)}}{2K^{(0)} - M_B(\omega^2 + i\epsilon)} \right] \right]. \quad (4.1)$$

This expression came from eliminating odd sites and averaging but instead, one may interpret it as coming from the elimination of two sites of mass  $c_A M_A$  and  $c_B M_B$  on each odd site, attached to their neighboring even sites with respective intersite force constants  $c_A K^{(0)}$ ,  $c_A L^{(0)}$  and  $c_B K^{(0)}$ ,  $c_B L^{(0)}$ . Indeed, considering the lattice of Fig. 4(a), one can see that the equation of motion for the site

marked  $i + 1$ , for example, is (with  $i$  even)

$$c_A [(2K^{(0)} - M_A(\omega^2 + i\epsilon)) G_{i+1,0}^A = c_A [L^{(0)}(G_{i+2,0} + G_{i,0})]. \quad (4.2)$$

Canceling  $c_A$  and substituting analogous equations for the other odd sites in the equations of motion for the unde-

cimated atoms, it is easy to see that Eq. (4.1) follows.

In order to perform the next decimation, Eq. (4.1) is first rewritten with the help of Eqs. (3.2a) and (3.2b),

$$(2K^{(1)} - M_i \omega^2) G_{i0} = M_i \delta_{i0} + L^{(1)} (G_{i+2,0} + G_{i-2,0}). \quad (4.3)$$

We are thus back to the original problem. Decimating and using the same point of view as above, one finds that after the second decimation the GK approximation is exact for the lattice of Fig. 4(b). Repeating this process, a whole lattice is generated.

From an alternate point of view, the basic building block of the hierarchical lattice is Fig. 5(a). To generate the lattice, each bond of force constant  $K$  is replaced by four springs and two masses as indicated in Fig. 5(b). To construct the hierarchical lattice which is the exact solution of the GK recursion relations iterated  $n$  times, one simply repeats the operations leading from Fig. 5(a) to 5(b)  $n$  times. The final lattice contains  $2 \times 4^n$  springs and  $(4^{n+1} - 1)/3$  masses. It can sustain at most as many modes as there are masses. If the central mass is  $M_A$  or  $M_B$  then, correspondingly,  $\rho_A(\omega^2)$  or  $\rho_B(\omega^2)$  is the exact density of states for this atom in the lattice.<sup>18</sup> Depending on the value of the small imaginary part  $\epsilon$ , the peaks corresponding to each eigenfrequency will be more or less broad.

Note that the different generalizations of the GK scheme mentioned in the preceding section correspond to obvious generalizations of the hierarchical lattice just discussed. Note also that one may interpret the hierarchical lattice as being built, starting from Fig. 5(a), by replacing each spring  $K$  by  $c_A$  parallel units of type, say  $A$ , and  $c_B$  parallel units of type  $B$ . Units of type  $A$  would consist of a mass  $M_A$  attached to two springs of constant  $K$  and units  $B$  would instead have a mass  $M_B$  and two springs of constant  $K$ . This procedure would lead to the same recursion relations and is identical to that used in critical phenomena.<sup>12</sup> However, since  $c_A$  and  $c_B$  here are fractional numbers, we find it preferable to think in terms of realizable lattices of the type described earlier. We also think much insight into the significance of the results in critical phenomena<sup>12</sup> could be obtained by similarly working with fractional numbers of bonds and trying to interpret the recursion relations obtained there as originating from some type of average over randomness.

Finally, we should point out the figures we used here are just pictorial representations of the lattice. They should be interpreted as one dimensional. Figure 6 illustrates how one would physically realize the lattice of Fig. 5(b).

## V. EIGENVECTORS AND SCALING TRAJECTORIES

Information on the eigenvectors is contained in the scaling trajectories. We first show this explicitly in the case of a pure chain<sup>19</sup> and in the single impurity limit where the GK recursion relations are exact. The relation between eigenvectors on the hierarchical lattice and those of the lattice it is supposed to model is discussed afterwards.

The following relation will be useful shortly:

$$G_{ij} = \sum_{\alpha} \frac{u_{i,\alpha} u_{j,\alpha} M_j}{\omega_{\alpha}^2 - (\omega^2 + i\epsilon)}. \quad (5.1)$$

In this expression,  $\alpha$  numbers the eigenvalues  $\omega_{\alpha}^2$  and the corresponding eigenvectors with amplitudes  $u_{j,\alpha}$  on sites  $j$ . These eigenvectors are normalized as follows:

$$\sum_{\alpha} u_{i,\alpha} u_{j,\alpha} M_j = \delta_{ij}, \quad \sum_i u_{i,\alpha} u_{i,\beta} M_i = \delta_{\alpha\beta}. \quad (5.2)$$

### A. Pure chain and single impurity limit

When the recursion relations (2.8a) and (2.8b) are iterated  $n$  times and Eqs. (2.10) and (2.11) are used, one obtains the exact DOS on the central atom of a chain containing  $2^{n+1} - 1$  atoms with the boundary condition that the last atoms are attached to a rigid wall by a spring of constant  $K$ . Alternatively, this procedure gives the DOS for a chain of  $2^{n+1}$  atoms with antiperiodic boundary conditions.

At frequencies for which the DOS is different from zero, Eq. (5.1) shows that the central atom must be moving and, by symmetry, displacements to the left and to the right must be equal. Hence, starting from

$$(2K - M\omega_{\alpha}^2)u_{0,\alpha} = K(u_{1,\alpha} + u_{-1,\alpha}), \quad (5.3)$$

one sees that after  $m$  iterations

$$\frac{u_{2^m,\alpha}}{u_{0,\alpha}} = \frac{(2K^{(m)} - M\omega_{\alpha}^2)}{2L^{(m)}} \equiv y^{(m)}. \quad (5.4)$$

Defining

$$\omega_{\alpha}^2 = \frac{2K}{M} (1 - \cos k_{\alpha} a) \quad (5.5)$$

one can show from the recursion relations and from Eq. (5.4) that

$$\frac{u_{2^m,\alpha}}{u_{0,\alpha}} = \cos(2^m k_{\alpha} a). \quad (5.6)$$

Given the above boundary conditions, Eq. (5.5) will be an eigenvalue only if

$$\cos(2^n k_{\alpha} a) = 0. \quad (5.7)$$

One concludes that from the right-hand side of Eq. (5.4), which may be computed directly from the recursion relations with real  $\omega^2$ , one obtains information about the eigenvectors. In particular, a delocalized eigenvector such as Eq. (5.6) will lead to a value of  $y^{(m)}$  which strictly speaking iterates to zero but which in practice follows a rather chaotic trajectory.

Indeed the eigenvalues are found from the DOS calculated with a small imaginary part and hence they are not quite exact, i.e., the relation (5.7) is only approximately satisfied. In fact, for the uniform chain one finds for  $n$  large enough that any  $\omega^2$  satisfying Eq. (5.5) with  $k$  real is an eigenvalue. In general, this leads to chaotic trajectories since the recursion relations (2.8a) and (2.8b) when written in terms of the variable

$$w^{(m)} = \frac{1}{2} (1 - y^{(m)}) \quad (5.8)$$

are of the form

$$w^{(m+1)} = \lambda w^{(m)} (1 - w^{(m)}) \quad (5.9)$$

with  $\lambda = 4$ . This is easily recognized as the logistic map.<sup>19,20</sup> The value  $\lambda = 4$  is the last accumulation point of

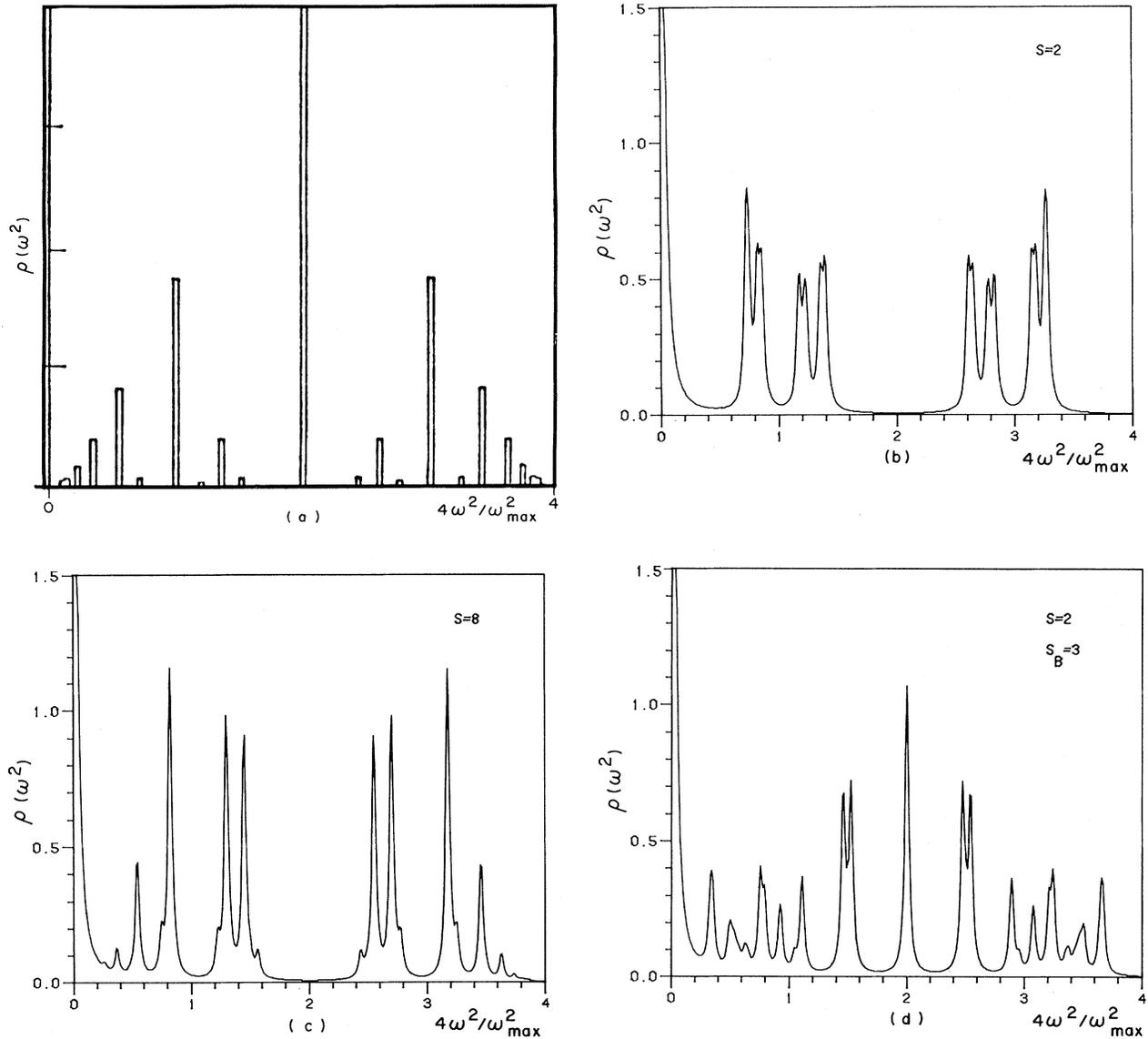


FIG. 3. (a) Density of states  $\rho(\omega^2)$  in arbitrary units for  $M_B/M_A=10000$ ,  $c_A=0.5$  obtained by Payton and Visscher (Ref. 16) from simulations on a chain of 8000 atoms. (b) Density of states in the GK approximation ( $S=2$ ).  $M_B/M_A=10000$ ,  $c_A=0.5$ ,  $\epsilon=0.02$ .  $\rho(0)=7.96$  but the vertical axis is truncated at  $\rho(\omega^2)=1.5$  for uniformity in display. (c) Same parameters as for (b) but  $\frac{7}{8}$  of the atoms are eliminated before averaging.  $S=8$ ,  $\rho(0)=7.96$ . (d) This time,  $\frac{1}{2}$  of the atoms are eliminated ( $S=2$ ) but by blocks of three ( $S_B=3$ ). The remaining blocks of three form a new chain identical to the initial one.  $\rho(0)=7.96$ .

bifurcation points of this map and except on a set of measure zero, it leads to chaotic trajectories. The values of  $y$  corresponding to (5.7) are on this set of measure zero.<sup>21</sup>

We thus conclude that for the uniform chain, the ratio (5.4) remains of order unity and may change sign upon successive rescalings, whatever the chain length. In practice, the scaling trajectories are chaotic. This should characterize delocalized modes even in disordered systems.

For localized modes, the ratio (5.4) should decrease exponentially with distance measured from the proper origin. This can be checked explicitly in the single impurity

limit. In that limit, the GK approximation is exact for the DOS on a light impurity atom of mass  $M_A$  located at the center of a pure chain of atoms of mass  $M_B$ . In that case, the recursion relations for  $K$  and  $L$  are exactly given by Eqs. (3.2a) and (3.2b) with  $c_A=0$ . The local density of states  $\rho_A(\omega^2)$  on atom  $A$  is calculated from Eq. (3.3) with  $M=M_A$ . For an infinite chain with an infinitesimal concentration of  $A$  atoms, the DOS is given to linear order in the concentration by the GK equation (3.4). This neglects corrections to the DOS on the  $B$  atoms which may also occur but do not give rise to gap modes.

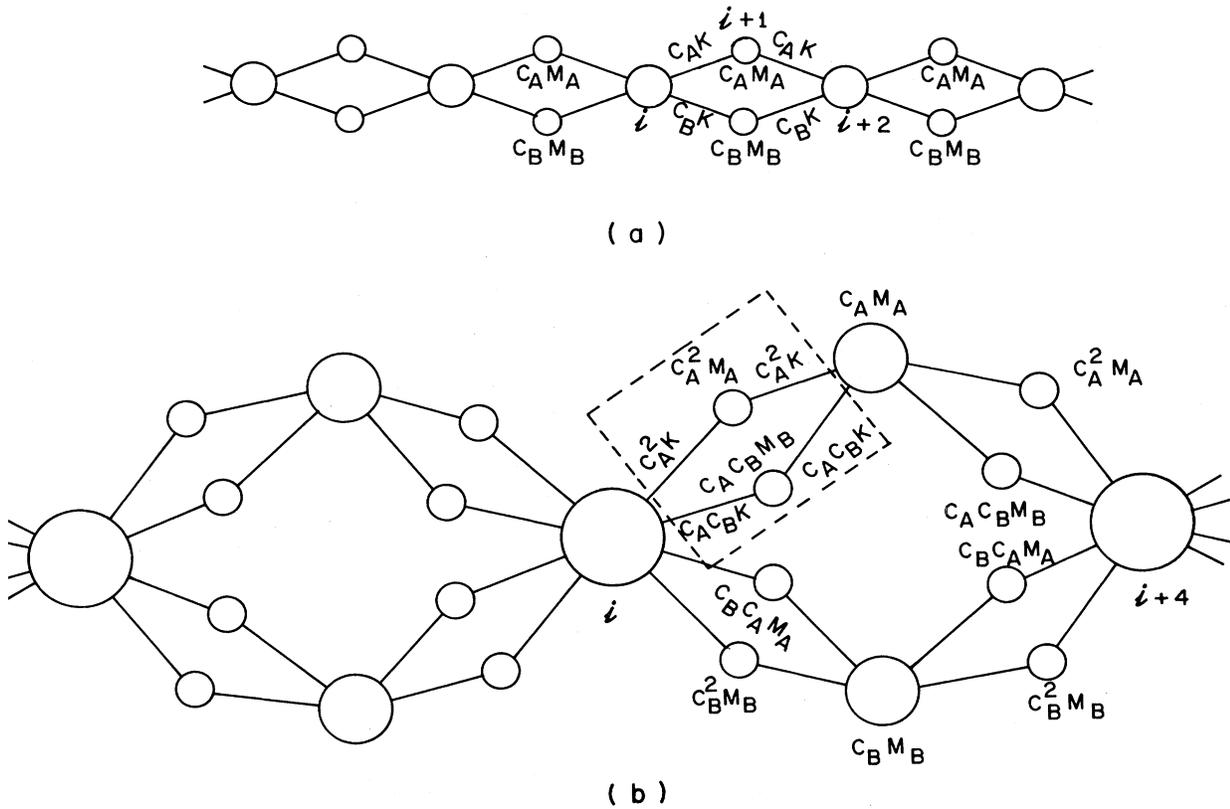


FIG. 4. (a) Lattice which leads to the GK expressions for  $K^{(1)}$  and  $L^{(1)}$  when all pairs of sites  $c_A M_A, c_B M_B$  are eliminated. Note that the masses on sites  $i, i+2$ , etc. need not be specified. The force between sites  $i$  and  $i+1$  with mass  $M_A$  is  $c_A K^{(0)}(u_{i+1}-u_i)$  but it is easier to see how it generalizes to further recursions when written in the form  $c_A(K^{(0)}u_{i+1}-L^{(0)}u_i)$ . (b) Lattice which would reproduce the GK expressions for  $K^{(2)}$  and  $L^{(2)}$ . Notice that pairs of masses and springs on the smallest length scale (dotted square) are analogous to those which, when eliminated, yielded  $L^{(1)}$  in (a). The difference here is that all elements in the dotted square (level zero) are multiplied by  $c_A$ . Hence, when eliminated, this dotted square gives  $c_A L^{(1)}$  and  $c_A K^{(1)}$  as may be checked from Eqs. (3.2a) and (3.2b).

Iterating the recursion relations (3.2a) and (3.2b) one finds that there is a finite density of states on the impurity atom outside the band for the pure chain at

$$\omega_\alpha^2 = \frac{4K}{M_B} \frac{1}{1-\delta^2}, \quad (5.10)$$

where  $\delta = 1 - (M_A/M_B)$ . This is in agreement with the exact result. Taking the displacements to be even around the A atom by symmetry, one finds that

$$\frac{u_{2^m, \alpha}^B}{u_{0, \alpha}^A} = \frac{(2K^{(m)} - M_A \omega_\alpha^2)}{2L^{(m)}} = (-e^{-\kappa a})^{2^m}, \quad (5.11)$$

where the inverse localization length is given by<sup>22</sup>

$$\kappa = \frac{1}{a} \ln \left[ \frac{1+\delta}{1-\delta} \right]. \quad (5.12)$$

Note that in regions where the DOS vanishes, ratios such as (5.11) grow under iteration.<sup>1,2</sup> In the case of the pure chain, the chaotic and growth regimes of iteration are separated by fixed points<sup>21</sup> which give some information on the singularities of the DOS at the band edges.<sup>13</sup> The scaling function which allows this information to be extracted is discussed in Appendix A.

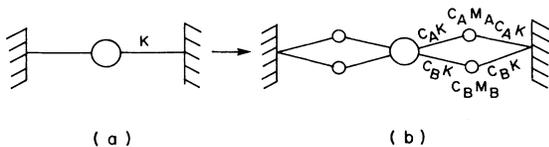


FIG. 5. Hierarchical lattice may be built by considering the spring  $K$  in (a) as being a unit formed of four springs and two masses as indicated in (b), and then considering each of the springs in that figure as another such unit and so on.

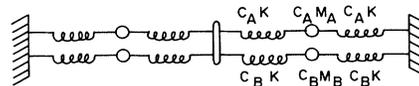


FIG. 6. Physical realization of the lattice of Fig. 5(b). Notice that the central object may move sideways but not rotate.

### B. Hierarchical lattice and disordered chain

In the completely disordered case, one may first ask for the character of eigenvectors on the hierarchical lattice and then try to compare it to eigenvectors on a truly disordered chain. Given an eigenfrequency, it is possible to find the relative displacements of atoms on the hierarchical lattice. An eigenfrequency for a finite chain (i.e., for a fixed number of iterations) may rapidly be found numerically, to thirteen significant figures for example, by identifying a maximum in the DOS using a rather large value of  $\epsilon$ , then looking at a smaller energy range around that maximum with a smaller value of  $\epsilon$ , and repeating the process until  $\epsilon=10^{-13}$ . Each time, the DOS is computed for intervals of  $\omega^2$  equal to  $\epsilon$ .

To find the relative displacements of atoms, let us consider Fig. 4(b). If the atoms to the extreme left and right are replaced by walls, then that figure represents the atoms which are eliminated (except for the central atom) by the last two decimations. Using the equation of motion for the atom of mass  $c_A M_A$ , it is easy to see that in an eigenmode  $\alpha$ , if  $n$  iterations eliminate all atoms but the central one, then

$$\frac{u_{2^{n-1},\alpha}^A}{u_{0,\alpha}} = \frac{1}{2y_A^{(n-1)}} \quad (5.13)$$

where

$$y_A^{(n-1)} = \frac{(2K^{(n-1)} - M_A \omega_\alpha^2)}{2L^{(n-1)}}. \quad (5.14)$$

Similarly, from the equation of motion for the atom of mass  $c_A^2 M_A$  to the extreme right, one finds

$$\frac{u_{2^{n-2n-2},\alpha}^A}{u_{2^{n-1},\alpha}^A} = \frac{1}{2y_A^{(n-2)}}, \quad (5.15)$$

or, from Eq. (5.13),

$$\frac{u_{2^{n-2n-2},\alpha}^A}{u_{0,\alpha}} = \frac{1}{2y_A^{(n-2)} 2y_A^{(n-1)}}. \quad (5.16)$$

These relations may easily be generalized (see below). From these, the displacements of atoms at any distance from the central atom may also be found but the expressions are not so simple.

Clearly then, the character of a mode may not be inferred from the behavior of recursion relations as simply as in the case of the pure chain, both because the displacements of atoms do not follow trivially from the recursion relations and because, on a hierarchical lattice, the displacements of the many atoms at a given distance from the central site are in general different from each other.

Another clue on the general character of an eigenmode may be obtained from the behavior of the energy of a given mode as the size of the lattice is increased. Consider, for example, a single impurity in a pure finite chain of length  $2l=2^{n+1}a$ . Perturbation theory gives the eigenfrequency  $\omega^2$  of the localized mode as,

$$\omega^2 - \omega_\infty^2 = -\omega_\infty^2 (2\delta e^{-2l\kappa a} \sinh \kappa a), \quad (5.17)$$

where  $\delta$  and  $\kappa$  are defined, respectively, below Eq. (5.10) and in Eq. (5.12) and  $\omega_\infty^2$  is given by Eq. (5.10). For a

delocalized mode on a finite pure chain on the other hand, the eigenfrequency for symmetric modes is given by Eq. (5.5) with

$$k_\alpha = (m + \frac{1}{2})\pi/l, \quad (5.18)$$

where  $m=0,1,2,\dots$  and  $l=2^n a$ . Hence, when the chain is doubled in size, there are twice as many eigenvalues and the splitting between these is

$$\Delta\omega^2 = \left[ \frac{2K}{M} \sin k_\alpha^0 a \right] \left[ \frac{\pi}{2l} \right] a. \quad (5.19)$$

As one keeps increasing the size of the chain, the splitting of the new eigenvalues which appear close to the original one are clearly proportional, when  $k_\alpha^0 a \gg 1$ , to the inverse chain length.

In the case of a single impurity, where the GK recursion relations are exact ( $c_A=0$ ), one may verify numerically that the result (5.17) holds. For the more general case, we find that for each eigenenergy on a central atom, for example,  $A$ , two new eigenfrequencies appear when the chain length is doubled. This behavior is illustrated, for small chains, by the tree diagram of Fig. 7. The splitting between eigenfrequencies does not however follow the inverse length dependence discussed above. Instead, the splitting between the two lowest frequencies of the tree have the following dependence on chain length:

$$\Delta\omega^2(l) = C/l^\mu \quad (5.20)$$

with  $C$  a constant and  $\mu=2.39$  for the special case in Fig. 7. A law of this form is also found for the splittings of the two highest frequencies corresponding to each chain length on the tree of Fig. 7. However, for a chain of a

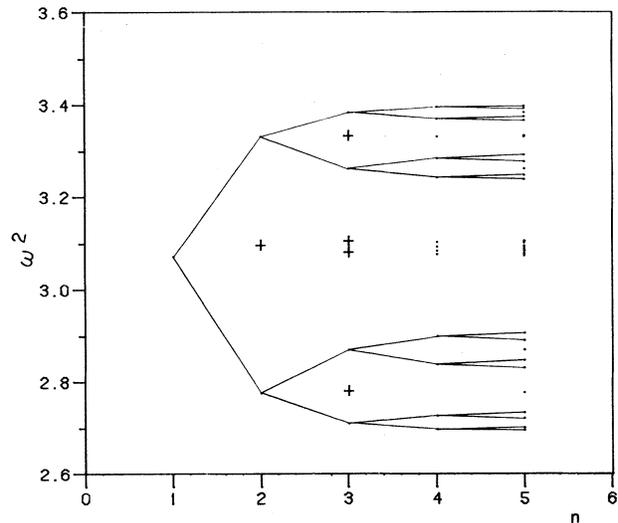


FIG. 7. Eigenfrequencies around  $\omega^2=3$  as a function of  $n=\log_2(l)$ , where  $2l$  is the hierarchical lattice length. For an  $A$  central atom, the eigenfrequencies are represented by points. Some of them have been joined by straight lines to illustrate the bifurcation structure. The crosses are for a  $B$  central atom. For clarity, the crosses have not been marked for  $n \geq 4$ .  $c_A=0.5$ ,  $M_B=3M_A$ .

given length, the many splittings do not compare very easily with one another. By analogy with Eq. (5.17), one also finds that for a chain of length  $l$ , the lowest frequency  $\omega^2(l)$  in Fig. 7 for that chain follows the law

$$\omega^2(l) - \omega_\infty^2 = C'/l^\mu \quad (5.21)$$

with  $\mu$  the same as in Eq. (5.20) and where  $\omega_\infty$  is the lowest frequency on the continuation of the tree of Fig. 7.

We should also point out that an eigenfrequency for an  $A$ -type central atom, in general finds itself barely shifted for a  $B$  central atom on a chain twice the size, and vice versa. A few of the eigenfrequencies for  $B$ -type central atoms are marked with crosses on Fig. 7. In general though, these frequencies correspond to a small density of states compared with that on the  $A$ -type atom in Fig. 7, and hence one may surmise that for these frequencies, the average displacement is larger away from the central atom, a fact one may confirm by looking at eigenvectors.

The type of behavior we have just described in Fig. 7 has also been observed for atoms of mass  $M_A$  or  $M_B$ , for small or intermediate concentrations and for energies ei-

ther above or below the band edge of the pure chain of heavy atoms. It is interesting to point out though that in the latter case, when the DOS is calculated for a heavy central atom, the power-law behavior of the splittings sets in for longer chains only suggesting that the eigenvector has more structure or a longer "localization length" in the sense that its asymptotic large distance decay comes in at a larger distance from the central atom.

These results on energy splittings suggest some sort of "algebraic localization" of the modes. This may be checked by looking in detail at the eigenvectors although, as we discussed at the beginning of this section, it is a much more difficult task. We must first compute some sort of average over the displacements of atoms at a given distance from the central atom. We tried arithmetic averages over the displacements or their absolute values, but it seems that the geometric mean has a more regular behavior. More specifically, using the results (5.13) and (5.16), and their generalizations, we calculate the average displacements of atoms at a distance (in units where  $a = 1$ )  $2^n - 2^{n-m}$  from the central atom of a chain of length  $2 \times 2^n$  as follows:

$$\ln(\bar{u}_{2^n - 2^{n-m}, \alpha} / u_{0, \alpha}) \equiv \sum_{i_1=1}^2 \sum_{i_2=1}^2 \cdots \sum_{i_m=1}^2 c_{i_1} c_{i_2} \cdots c_{i_m} \ln |x_{i_1}^{(n-1)} x_{i_2}^{(n-2)} \cdots x_{i_m}^{(n-m)}|, \quad (5.22)$$

where  $1 \leq m \leq n$  and,

$$x_i^{(n)} = \begin{cases} 1/(2y_A^{(n)}), & i=1 \\ 1/(2y_B^{(n)}), & i=2. \end{cases}$$

To check the validity and understand the meaning of this formula, we first consider the eigenvector corresponding to the lowest frequency on a hierarchical lattice with either an  $A$  or  $B$  central atom. In that limit ( $\omega \rightarrow 0$ ), the GK approximation should be exact since the mass disappears from the problem [Eqs. (2.1) and (2.2)] and hence there is no more disorder.<sup>23</sup> One finds that Eq. (5.21) is satisfied with  $\mu=2$ , i.e.,  $\omega$  goes to zero as  $1/l$  in agreement with the fact that this lowest-frequency mode should be delocalized. Furthermore, since  $\cos(\pi x/2l)$  is the eigenvector corresponding to the lowest-frequency mode of a uniform chain, we can check whether calculations from Eq. (5.22) fit the function

$$\ln \cos \left[ \frac{\pi}{2} \left( 1 - \frac{1}{2^m} \right) \right]. \quad (5.23)$$

We find this to be the case to about 8% accuracy for chains of length  $2 \times 2^3$  and to about 0.03% for chains of length  $2 \times 2^{11}$ . Note in passing that for sufficiently large values of  $m$ , Eq. (5.23) reduces to

$$-m \ln 2 + \ln(\pi/2) \quad (5.24)$$

which is independent of  $n$  and should be contrasted with the result (5.25) below.

For a more general case, the results of calculations with Eq. (5.22) are illustrated in Fig. 8. The various straight lines are for different chain lengths. For each of these chains, the energy is chosen as the lowest on the tree of

Fig. 7. The points are all averages over atoms closer to the boundaries than to the central atom where the DOS is calculated and hence they represent the long-distance behavior of the eigenvectors. The curves on Fig. 8 may all be fitted by the following:

$$\ln(\bar{u}_{2^n - 2^{n-m}, \alpha} / u_{0, \alpha}) = m(\beta m - \gamma n). \quad (5.25)$$

This result indicates a behavior that is more complicated than Eq. (5.20) but that does however have the nice feature

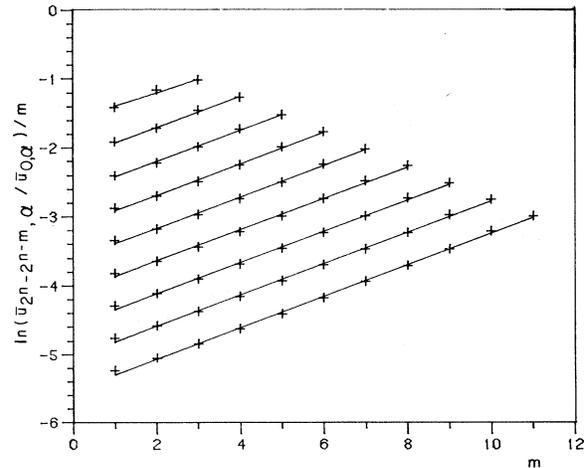


FIG. 8.  $\ln(\bar{u}_{2^n - 2^{n-m}, \alpha} / u_{0, \alpha})$  is defined in Eq. (5.22). The fact that we have straight lines on this figure shows that the relation (5.25) is correct. The crosses are the results of calculations and the straight lines are least-square fits.

TABLE I. Results obtained from various trees of the type illustrated in Fig. 7.  $\omega_1^2$  is the eigenfrequency square (for a chain of length 4) from which the tree branches.  $c_A$  is the concentration of  $A$ -type atoms ( $M_B = 3M_A$ ). In the next column, is the maximum number of iterations necessary to study the longest chain (of length  $2l$ ) for that tree. For the first two lines of the table, longer chains were beyond the precision of the computer. The central atom is that on which the DOS is computed,  $\mu$  is defined in Eqs. (5.20) and (5.21), while  $\beta$  and  $\gamma$  appear in Eq. (5.25). Note that the result marked with an asterisk applies only to the longest chains and is the most uncertain.

$\omega_1^2$	$c_A$	$\log_2 l$	Central atom	$\mu$	$\beta$	$\gamma$
2.391 284 000 256 7	0.001	8	$A$	6.52	1.86	3.86
1.980 909 373 849 6	0.005	7	$A$	5.35	1.53	2.95
3.071 697 493 336 6	0.5	11	$A$	2.39	0.228	0.475
0.882 686 932 815 51	0.5	11	$B$	2.3*	0.213	0.480

that it extrapolates to  $\bar{u}_{2^n-2^{n-m},\alpha} = u_{0,\alpha}$  when  $m=0$ . Also, once again, a law of the form (5.25) sets in only for longer chains when we look at a low energy mode on a heavy atom where we expect less ‘‘localization.’’

The results for the cases we studied in detail are summarized in Table I. The exponent  $\beta$  is obtained from the slopes of lines like in Fig. 8 and  $\gamma$  from the slope of the graph of the intercept of these lines as a function of  $n$ . Since  $\beta$  is not constant, but seems to reach a limit as the chain length increases, we quote our estimate of this limiting value. The same is true for  $\gamma$ . Error estimates from least-square fits give an uncertainty of not more than 5 on the third digit. Within a more conservative error bound of 1 on the second digit, note that  $\gamma=2\beta$ . Assuming that this equality holds and using Eqs. (5.22) and (5.25) one finds

$$\ln \left[ \frac{\bar{u}_{2^n-2^{n-m},\alpha}}{\bar{u}_{2^n-2^{n-(m-1)},\alpha}} \right] = \sum_{i=1}^2 c_i \ln |x_i^{(n-m)}|$$

$$= \gamma(m-n) - \frac{\gamma}{2}. \quad (5.26)$$

This relates more directly the behavior of recursion relations with eigenvectors.

Even though we have looked only at a small number of cases, it is tempting to suggest that the above behavior of energy splittings [Eq. (5.20)] and of average displacements [Eq. (5.25)], is typical for that kind of model. Note also that given the complicated topology of the hierarchical lattice and the somewhat artificial meaning of the average displacements defined by Eq. (5.22), it is not really surprising to find that the behavior of energy splittings and average displacements are not simply related.

To compare the eigenmodes on the hierarchical lattice with those of a real one-dimensional chain it is supposed to model, one should recall that there, disorder induces exponential localization.<sup>2</sup> This is clearly not observed for the hierarchical lattice. It may be tempting to compute an average localization length using the Herbert-Jones-Thouless<sup>24,25</sup> formula and the real part of the average Green’s function, which may be computed from the GK scheme. That is not really justified, however, unless there is exponential localization.

The lack of exponential localization on our lattice is not all that surprising given that the hierarchical lattice is not

really a one-dimensional structure. Remarking that each time the length scale is changed by a factor of 2 the number of springs is changed by a factor of 4, the hierarchical lattice looks, from that point of view, two dimensional. In fact the connectivity is different from atom to atom<sup>10,11</sup> and the structure is neither one nor two dimensional. Hence it is not all that surprising to find that the behavior is somewhere between exponential localization, like for one-dimensional systems, and logarithmic localization, like a two-dimensional system.

## VI. CONCLUSION

We have demonstrated that the particular type of rescaling and of averaging over quenched disorder proposed<sup>8</sup> by GK is exact for the single-site DOS of the central atom of a hierarchical lattice. This lattice is self-similar but not translationally invariant. This connection suggests perhaps that self-similar lattices may be a useful vehicle for the study of disordered systems.<sup>26</sup> It also helps to understand the positivity, as well as some of the details of the GK spectrum. The GK scheme is also exact in the single impurity limit and, for arbitrary concentrations, in the limit of equal masses.

We have also shown that, even though the GK approximation is the simplest one to give sharp features analogous to those of the true DOS, these features do not necessarily compare in detail with those of the true DOS. Nevertheless, it is possible to generalize the scheme to obtain better DOS while retaining the essential simplicity of the original method as well as the hierarchical lattice interpretation. Eliminating more atoms before averaging seems to improve the part of the spectrum which involves longer-range properties, while taking a larger number of atoms as the basic units improves the results for modes which depend more on short-range properties. This latter type of approximation is in a sense a generalization of cluster Bethe-lattice methods<sup>27</sup> where a Bethe lattice is attached to various clusters of atoms. Here, a hierarchical lattice of clusters is attached to the central cluster being studied. The exact result must be obtained when a large enough block is taken as the basic unit. In standard rescaling approaches, the exact result is reached by taking a larger and larger parameter space to describe the probability law. Our point of view is different but equally valid.

Some qualitative information on the localization of the modes can evidently be obtained from their sensitivity to the particular approximation scheme used, but it is also

possible to be more quantitative by looking at the dependence of the energy splittings on chain length or even by studying directly the eigenvectors. That kind of analysis is tedious and not totally straightforward, but it tends to show some kind of ‘‘algebraic’’ localization of the modes. In energy ranges where the modes are expected to have a more extended character, the asymptotic algebraic behavior tends to set in only for rather long chains.

Finally, in Appendix A we show to what kind of quenched disorder averaging the GK scheme leads in the generating functional. The analogies between the generating functional and critical phenomena suggest that similar considerations applied to statistical mechanics might help to understand the connection between hierarchical lattices used, for example, for the spin-glass problem<sup>12</sup> and the real disordered systems they are supposed to represent.

*Note added in proof.* After this paper was submitted for publication we received a manuscript from M. O. Robbins and B. Koiller where it is shown analytically that in the simple GK approximation the first five moments of the exact spectrum are preserved. These authors also discuss how many of the exact moments are reproduced when one uses more elaborate schemes such as the ones considered here.

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#### APPENDIX A: GENERATING FUNCTIONAL AND ANALOGY WITH CRITICAL PHENOMENA

The generating functional presented in this appendix allows one to draw analogies with renormalization-group approaches in critical phenomena. This functional was implicitly used in an earlier paper<sup>13</sup> to extract exponents for the band-edge singularities from the behavior of recursion relations near fixed points. The generating functional also allows us to give yet another argument for the positivity of the DOS in the GK approximation or generalizations thereof.

Let us define<sup>28</sup>

$$\mathcal{F}(\omega^2, K, \{M_i\}, \{\phi_i\}) = \ln \left[ \int \mathcal{D}u \exp[iS_\omega^{(0)}(\{u_i\}, \omega^2, K, \{M_i\}, \{\phi_i\})] \right], \quad (\text{A1})$$

where

$$\int \mathcal{D}u \equiv \int_{-\infty}^{\infty} \prod_{j=1}^N du_j \quad (\text{A2})$$

and

$$S_\omega^{(0)} = \sum_{j=1}^N \left[ \frac{1}{2} M_j (\omega^2 + i\epsilon) u_j^2 - \frac{1}{2} K (u_{j+1} - u_j)^2 - \phi_j u_j \right]. \quad (\text{A3})$$

The classical action is equal to the Fourier sum of  $S_\omega$  over frequencies. Units may be chosen such that  $S_\omega$  is dimensionless. Notice that the term proportional to  $\epsilon$  makes the integral convergent. Integrating by parts<sup>29</sup> one obtains

$$\int \mathcal{D}u \left[ \frac{\delta}{\delta u_l} e^{iS_\omega^{(0)}} \right] u_k M_k = -M_k \delta_{kl}. \quad (\text{A4})$$

One can easily show that this leads directly to the equations of motion (2.3) if the following definition of the Green’s function is used:

$$G_{lk} = \frac{i \int \mathcal{D}u (u_l u_k M_k) e^{iS_\omega^{(0)}}}{\int \mathcal{D}u e^{iS_\omega^{(0)}}}. \quad (\text{A5})$$

This definition closely parallels the result (5.1). The quantity  $\mathcal{F}$  in Eq. (A1) is thus a generating functional since the Green’s function Eq. (A5) may be obtained from it by taking functional derivatives with respect to  $\phi_j$  or other parameters such as  $M$  or  $\omega^2$ .

The generating functional is analogous to the free energy in phase transitions except that here it can be complex. The recursion relations (2.8a) and (2.8b) may be obtained from that functional by performing the Gaussian integrals over half of the sites and regrouping the coefficients of the remaining variables (say even sites) to write  $S_\omega$  in the form

$$S_\omega^{(1)} = \sum_{j=1}^{N/2} \left\{ \frac{1}{2} [M_j (\omega^2 + i\epsilon) - 2K^{(1)}] u_{2j}^2 + L^{(1)} u_{2j} u_{2(j+1)} \right\}. \quad (\text{A6})$$

$\phi_j$  can be set equal to zero for this purpose since to find the DOS on a single site, it suffices to eliminate all sites but this one.

One thus concludes that the renormalization procedure leaves the generating functional invariant, as in critical phenomena, and it is using this analogy that one may find the relationship between band-edge singularities and renormalization-group eigenvalues.<sup>13</sup>

In the disordered case, the above procedure may be repeated to generate the recursion relations (3.1a) and (3.1b) for any realization of the disorder. The recursion relations (3.2a) and (3.2b) in the GK approximation may be obtained by averaging *only over the eliminated sites* (say odd sites) as follows:

$$\langle \mathcal{F} \rangle_{\text{odd}} \equiv \ln \left[ \int \mathcal{D}u \exp(i \langle S^{(1)} + C^{(1)} \rangle_{\text{odd}}) \right]. \quad (\text{A7})$$

Here,  $C^{(1)}$  is a constant term containing information only on the eliminated odd sites. This process is repeated until

only one degree of freedom is left. This degree of freedom is taken as representative of an atom in an infinite disordered chain.

Clearly, the above scheme is in a sense a poor approximation since the log should be averaged. Nevertheless, since only a partial averaging is done, this seems a better approximation than averaging  $S^{(0)}$  over *all* degrees of freedom as is often done in the simplest kind of effective medium approximation. In terms of the full Green's function (2.4), one may state in an analogous manner that while the inverse matrix on the right-hand side should be averaged, one instead eliminates half of the degrees of freedom of the matrix on the left-hand side of Eq. (2.3) and then averages this matrix, which is now half the size.

Equations (A1)–(A7) are also useful to prove that the GK approximation preserves a positive density of states. The fact that the DOS is positive comes from the sign of  $\epsilon$  in  $MG^{-1} = A - M(\omega^2 + i\epsilon)$ . Since this same  $\epsilon$  is the only term which gives to the argument of the exponential a real part with the sign appropriate to insure convergence of the integral (A1), the density of states will be positive if and only if the functional integral is formally convergent. Since the quantity  $S^{(1)} + C^{(1)}$  has, before averaging, the correct properties to insure convergence of  $\mathcal{F}$  for any realization of the disorder, its average over the eliminated sites has the same properties. Note that  $C^{(1)}$  does not contribute to the density of states on the uneliminated sites.

Recursion relations for the quantities (3.9a) and (3.9b) may be derived from the functional integral by changing variables as often as necessary to insure that the coefficient of the quadratic terms ( $u^2$ ) always be equal to the same constant. However, averaging those recursion relations does not correspond to a simple procedure in the functional integral and we have not been able to deduce what this procedure implies for the DOS. In particular, we have not been able to show that this procedure guarantees positivity.

#### APPENDIX B: RELATION WITH TRANSFER MATRIX METHODS

In the case of a uniform system, the recursion relations may be found by writing the eigenvalues of the square of the transfer matrix in the same functional form as the original eigenvalues. Using this new transfer matrix

(whose eigenvalues are the square of the original ones), the number of  $T$  matrices to multiply to obtain the same generating functional is then half as much.<sup>30</sup>

The GK approximation for the disordered case does not correspond to such a simple procedure. Nevertheless, the transfer matrix may be used to express the scaling transformation for arbitrary scale change in a compact way. Starting from the equations (2.1) and (2.2) for  $u_i$ , the idea, as usual, is to eliminate  $u_{i\pm 1}$  in terms of  $u_i$  and  $u_{i\pm b}$ , where  $b$  is the scaling factor. Equations (2.1) and (2.2) may be written in the form

$$\begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} = \underline{T}_i \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix}, \quad (\text{B1})$$

where

$$\underline{T}_i = \begin{pmatrix} (2K - M_i\omega^2)/K_{i,i+1} & -K_{i,i-1}/K_{i,i+1} \\ 1 & 0 \end{pmatrix}. \quad (\text{B2})$$

Using this result, we have that

$$\begin{pmatrix} u_{i+b} \\ u_{i+b-1} \end{pmatrix} = \underline{T}_{i+b-1} \cdots \underline{T}_{i+2} \underline{T}_{i+1} \begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} \\ \equiv \tilde{\underline{T}}_{b-1,1}^i \begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} \quad (\text{B3})$$

which may be used to write  $u_{i\pm 1}$  in terms of  $u_i$  and  $u_{i\pm b}$ ,

$$u_{i\pm 1} = \frac{1}{(\tilde{\underline{T}}_{\pm b\mp 1, \pm 1}^i)_{11}} u_{i\pm b} - \frac{(\tilde{\underline{T}}_{\pm b\mp 1, \pm 1}^i)_{12}}{(\tilde{\underline{T}}_{\pm b\mp 1, \pm 1}^i)_{11}} u_i. \quad (\text{B4})$$

Substituting in Eqs. (2.1) and (2.2) we find the renormalized parameters

$$2K_i^{(1)} = 2K_i + K_{i,i+1} \frac{(\tilde{\underline{T}}_{b-1,1}^i)_{12}}{(\tilde{\underline{T}}_{b-1,1}^i)_{11}} + K_{i,i-1} \frac{(\tilde{\underline{T}}_{-b+1,-1}^i)_{12}}{(\tilde{\underline{T}}_{-b+1,-1}^i)_{11}}, \quad (\text{B5})$$

$$K_{i,i\pm 1}^{(1)} = \frac{K_{i,i\pm 1}}{(\tilde{\underline{T}}_{\pm b\mp 1, \pm 1}^i)_{11}}. \quad (\text{B6})$$

The equations may then be averaged as was done in going from Eqs. (3.1) to (3.2). When  $b=2$  the GK result is recovered.

<sup>1</sup>For reviews on localization in one dimension, see this and the next three references: K. Ishii, *Progr. Theor. Phys. Suppl.* **53**, 77 (1973).

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<sup>3</sup>D. J. Thouless, in *Ill Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, Amsterdam, 1979).

<sup>4</sup>For a review, see this and the next reference: P. Dean, *Rev. Mod. Phys.* **44**, 127 (1972).

<sup>5</sup>R. J. Elliott, J. A. Krumhansl, P. L. Leath, *Rev. Mod. Phys.* **46**, 465 (1974); E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966).

<sup>6</sup>H. Matsuda, *Progr. Theor. Phys.* **19**, 161 (1964); J. Hori, *ibid.*

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<sup>8</sup>C. E. T. Gonçalves da Silva and Belita Koiller, *Solid State Commun.* **40**, 215 (1981).

<sup>9</sup>The work of H. Aoki, *J. Phys. C* **13**, 3369 (1980) is most closely related to that of Ref. 8. Also related are calculations by S. Sarker and E. Domany, *Phys. Rev. B* **23**, 6018 (1981) and F. J. Wegner, *Z. Phys. B* **25**, 327 (1976).

<sup>10</sup>M. Kaufman and R. B. Griffiths, *Phys. Rev. B* **24**, 496 (1981); R. B. Griffiths and M. Kaufman, *ibid.* **26**, 5022 (1982).

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<sup>12</sup>S. R. McKay, A. N. Berker, and S. Kirkpatrick, *Phys. Rev. Lett.* **48**, 767 (1982); B. Derrida, J. P. Eckmann, and A. Er-

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- <sup>13</sup>This has also been noted by B. W. Southern, A. A. Kumar, P. D. Loly, and A.-M. S. Tremblay, *Phys. Rev. B* **27**, 1405 (1983). It may also happen that fixed points correspond to delocalized states. See Sec. V, and Ref. 21. See also Ref. 19.
- <sup>14</sup>D. Schmeltzer, *Phys. Rev. B* **25**, 3915 (1982). This paper extends the method discussed in Sec. II to three dimensions and to defects.
- <sup>15</sup>In general, one needs to write a joint probability distribution for  $K$  and  $L$ . These quantities are not independently distributed.
- <sup>16</sup>D. N. Payton III and W. M. Visscher, *Phys. Rev.* **154**, 802 (1967).
- <sup>17</sup>Note that decimating by blocks of  $n$  atoms allows one to take interactions with a range of  $n$  neighbors into account very easily within the GK scheme. With first-nearest-neighbor interactions only, Eqs. (3.2a) and (3.2b) are replaced by matrix equations but it turns out that most of the matrix elements need not be iterated.
- <sup>18</sup>In the GK approximation, the total DOS is  $c_A\rho_A + c_B\rho_B$  and hence one must attach two different central atoms to the hierarchical lattice and average their local DOS to model the average DOS on a disordered binary chain.
- <sup>19</sup>J. V. José, in *Proceedings of the XIX Latin American School of Physics, Cali, Columbia, 1982*, edited by A. Ruedo (World Scientific, 1983); *J. Phys. A* **16**, L205 (1983). This author also studied disordered  $d=1$  systems by a method analogous to ours.
- <sup>20</sup>R. M. May, *Nature* **261**, 459 (1976). To find the DOS, we in fact iterate the logistic map in the complex plane: see B. B. Mandelbrot, *Ann. N.Y. Acad. of Sciences* **357**, 249 (1980).
- <sup>21</sup>Some values of  $y$  which are fixed points correspond to delocalized states. For the pure chain, these states are at the band edges or if not, their position depends on the length rescaling. Indeed, from Eq. (5.6), it is clear that  $k_a a = 120^\circ$  leads to a fixed point. If the length rescaling had been 4, then  $k_a a = 72^\circ$  would have been a fixed point.
- <sup>22</sup>Since to obtain Eqs. (5.11) and (5.12) the recursion relations are iterated with real frequencies, one must be careful with numerical instabilities, which show up rather rapidly for this problem.
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- <sup>30</sup>Useful results on transfer matrices may be found, for example, in H. Matsuda, *Prog. Theor. Phys. Suppl.* **23**, 22 (1962).