

Disordered binary harmonic chains with site-dependent force constants

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A hierarchical lattice model for a disordered two-component one-dimensional harmonic chain with three force constants, corresponding to the three possible pairs of nearest neighbors, is studied. Differences of as little as 20% between the various force constants can appreciably modify the density of states. These changes in the spectrum allow one to roughly characterize which type of interaction and which atoms are involved in the eigenmodes contained in certain frequency ranges.

The disordered harmonic chain problem has been a recurring theme in the study of random one-dimensional systems.¹⁻³ Well-known analogies^{2,4} between that problem and other one-dimensional problems, such as electronic or random walk problems, certainly contribute to the continued popularity of that subject. Perhaps the most striking property of the random harmonic chain is the very irregular shape of its local density of states as was revealed first by computer simulations.³ None of the standard mean-field-like analytic methods (such as coherent potential approximation) have been able to reproduce such complicated spectra even though the existence of a large number of gaps in the density of states has been understood from exact calculations.¹

Not too long ago, Gonçalves da Silva and Koiller⁵ (GK) proposed a very simple but approximate position-space rescaling scheme which accounts for clusters of atoms on all length scales and thus reproduces at least the qualitative features of the computer simulations. Even though quantitative details of the local density of states may be wrong, the first few moments agree rather well with exact results. As shown in Ref. 6 the GK scheme may be improved and it also has the virtue of being exact on certain hierarchical lattices. To obtain physical results, the latter property is a very useful guide since partial averaging schemes of the GK type may easily produce negative densities of states when the wrong quantity is averaged.

In this paper, we wish to investigate an explicit example of extension of the GK scheme to the case where disorder is present in the force constants as well as in the masses.⁷ More specifically, we consider the case where atoms of type 1 and 2 are distributed at random and interact through force constants K_{11} between atoms of type 1, $K_{12}=K_{21}$ between atoms of two different types, and K_{22} between atoms of type 2. Even though this kind of model appears much more physical than the standard model with uniform force constants, it has, to our knowledge, not been the subject of much attention. A different type of problem which is equivalent to force constants which are random but do not depend on site occupation have, however, been considered earlier.⁴

We use the simplest GK scheme where half of the sites are eliminated to give renormalized parameters which are then averaged over the distribution of eliminated degrees of freedom. That scheme may be improved by working with groups of atoms instead of single atoms as our basic unit or by eliminating more atoms before averaging⁶ but in all cases this type of approximation basically forces the probability distribution back to its original form after each iteration while an exact treatment would let this distribution evolve under renormalization.⁸

The basic "miniaturization"⁹ step which allows us to construct the hierarchical lattice corresponding to our problem is illustrated in Fig. 1. The variables i, j, k can take the value 1 or 2. Note that the left (right) label for the force constants is the same as that of the site to its left (right) end. It is important to realize that under renormalization one must introduce new parameters to be able to work in a closed parameter space. Consider, for example, Fig. 1(a) and assume that it now represents the effective sites and force constants after n iterations on a hierarchical lattice of length 2^{n+1} . Then the equation of motion for the displacement u_j of the atom at site j is,

$$({}^L K_{ij}^{(n)} + {}^R K_{jk}^{(n)} - M_j \omega^2) u_j = L_{ij}^{(n)} u_i + L_{jk}^{(n)} u_k \quad (1a)$$

while for the atom at site k we have,

$$({}^L K_{jk}^{(n)} - M_k \omega^2) u_k = L_{jk}^{(n)} u_j. \quad (1b)$$

Note in particular that a K "bond" (for example, $K_{jk}^{(n)}$) can take a different value when considered from a site to its left or to its right: Hence the extra superscripts R or L . However, when the recursion relations for ${}^L K_{ij}$ and ${}^R K_{ij}$ are written down explicitly, one notices that the relation ${}^L K_{ij} = {}^R K_{ji}$ is preserved under iteration so that one may keep, for example, only ${}^R K_{ij}$ and dispose of the extra label R .

Taking into account the above remarks and using the hierarchical lattice or the GK procedure one obtains the following recursion relations:

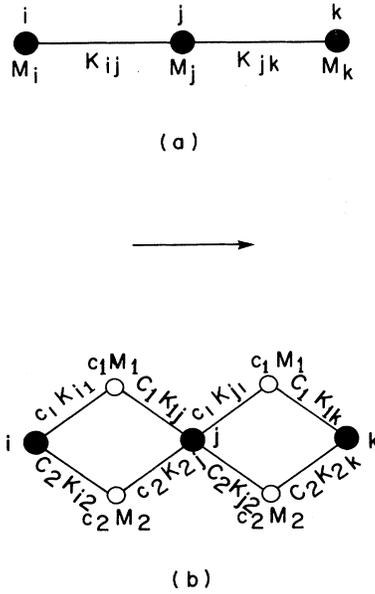


FIG. 1. Basic operation which allows one to build the hierarchical lattice which is solved exactly by the recursion relations Eq. (2).

$$K_{ij}^{(l+1)} = \sum_{s=1}^2 c_s \left[K_{is}^{(l)} - \frac{(L_{is}^{(l)})^2}{K_{si}^{(l)} + K_{sj}^{(l)} - M_s(\omega^2 + i\epsilon)} \right], \quad (2a)$$

$$L_{ij}^{(l+1)} = \sum_{s=1}^2 c_s \frac{L_{is}^{(l)} L_{sj}^{(l)}}{K_{si}^{(l)} + K_{sj}^{(l)} - M_s(\omega^2 + i\epsilon)}, \quad (2b)$$

where c_s is the concentration of atoms of type s . Note that indices in these equations refer to the type of atom, not to the site number. The small imaginary part $i\epsilon$ allows us to compute the Green's function. Indeed, $L_{ij}^{(l)}$ always iterates to zero when $\epsilon \neq 0$. The rate of convergence is faster when ϵ is larger and the peaks in the local density of states have a width⁶ proportional to ϵ . If convergence is obtained after n iterations, the Green's function at site 0 may be calculated from

$$G_{00}^s = \frac{M_s}{K_{si}^{(n)} + K_{sk}^{(n)} - M_s(\omega^2 + i\epsilon)}. \quad (3)$$

The label s in this equation refers to the type of atom at site 0. We have checked that once the $L_{ij}^{(l)}$ have converged to zero, the result of Eq. (3) is independent of whether sites i and k are of type 1 or 2. Physically, this means that for a finite value of ϵ , the chain can always be chosen long enough that the density of states is independent of the boundary conditions.

Since site 0 in Eq. (3) can be of type 1 or 2 with probability c_1 or c_2 , the average density of states is

$$\rho(\omega^2) = \pi^{-1} \text{Im}(c_1 G_{00}^1 + c_2 G_{00}^2) \equiv \sum_{s=1}^2 c_s \rho_s(\omega^2), \quad (4)$$

where $\rho_s(\omega^2)$ is a partial density of states.

The moments of the spectrum

$$\langle \omega^{2n} \rangle_s = \int d\omega^2 \omega^{2n} \rho_s(\omega^2) \quad (5)$$

were computed by numerical integration and compared with exact results which we obtained from the moment-trace theorem.³ We considered the case $c_1=0.2, 0.5$, and 0.8 with $M_1=M_2=1$, $K_{11}=1$, $K_{12}=1/\sqrt{3}$, and $K_{22}=1/3$. We used 16001 integration steps and Simpson's rule. The value of ϵ was set equal to the integration step, 2.5×10^{-4} . For the first three moments, the exact and approximate results never differ by more than 7% while the estimated numerical error is 1%. These results should be compared to the case where all force constants are equal.⁵ There, GK obtained differences of not more than 1% between the calculated first three moments and the exact ones. (See Note added in proof.)

In the rest of this paper, we discuss the case $M_1=1$, $M_2=3$, and $c_1=c_2=0.5$. The solid line in Fig. 2(a) represents $c_1 \rho_1(\omega^2)$ and the dashed line $c_2 \rho_2(\omega^2)$ in the case where all force constants are equal. Comparing with Fig. 2(b), which is the average density of states, it is easy to see that in certain regions of the spectrum, it is mainly one type of atom which is vibrating. For example, for the group of modes in the region $v^2 = 4\omega^2/\omega_{\max}^2 > 2.6$ and the one in $1 < v^2 < 2$, it is mainly atoms of type 1 which are involved. On the contrary, for $2 < v^2 < 2.4$ it is essentially atoms of type 2 which are moving.

We can use the freedom in the choice of force constants, which our model allows, to elucidate further the origin of the various groups of modes. Figure 3 shows how the

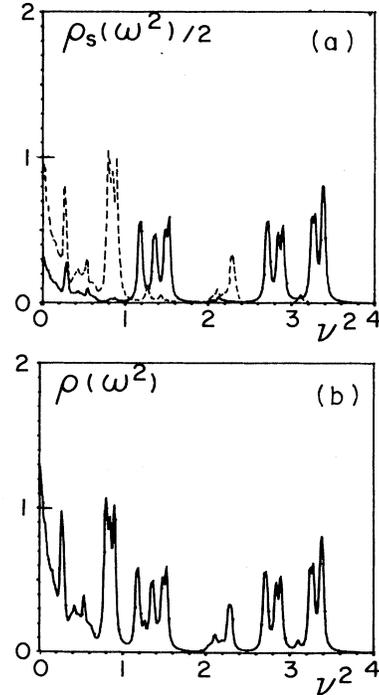


FIG. 2. (a) Partial density of states associated with type-1 atoms (solid line) or type-2 atoms (dotted line), multiplied by the respective concentration of each species, $c_1=c_2=0.5$. The other parameters are $M_1=1$, $M_2=3$, $K_{11}=K_{12}=K_{22}=1$. 401 values of $v^2 = 4\omega^2/\omega_{\max}^2$ were computed with $\epsilon=0.02$. (b) Average density of states obtained from the sum of the two curves in (a).

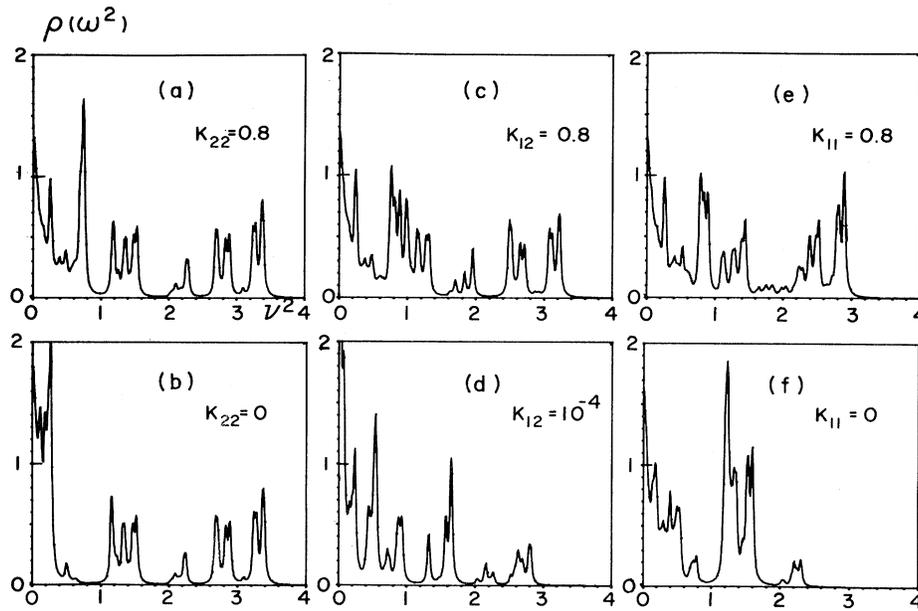


FIG. 3. Average DOS when all parameters, except the one explicitly indicated, are the same as in Fig. 2.

density of states of Fig. 2(b) evolves when the force constants are changed one at a time from 1 to 0.8 and 0. Calculations for the intermediate cases 0.5 and 0.2 reveal that the spectra change monotonously. It is important to notice, however, that we expect the hierarchical lattice results to be least representative of the real system when the force constants differ appreciably [Figs. 3(b), 3(d), and 3(f)]. Indeed these cases are analogous to the one of very large mass ratio discussed in detail in Ref. 6. In particular, it is easy to see that the hierarchical lattice solution of the problem $K_{12}=0$ [Fig. 3(d)] differs appreciably from the exact solution, which may be found from a trivial generalization of the method used by Domb *et al.*¹⁰ to solve the infinite mass ratio problem.

In Figs. 3(a) and 3(b), K_{22} decreases. For $\nu^2 > 1$ the structure of the spectra both in amplitude and frequency is literally unchanged. By contrast, for $\nu^2 < 1$ one may recognize certain spectral features of Fig. 2(b) when $K_{22}=0.8$, but this is not possible anymore for $K_{22}=0.0$ and, as one may expect, there is a shift to lower frequencies.

Figures 3(c) and 3(d) exhibit the effect of a change in K_{12} . One sees that as K_{12} varies, the high-frequency structures associated with type-1 atoms decrease in amplitude and move to the lower frequencies, which suggests that this force constant contributes to these modes. The peaks in region $2 \leq \nu^2 \leq 2.4$, which are associated with vibrations of type-2 atoms in a region where there is no eigenmode for a pure type-2 chain, are obviously very much influenced by a change in K_{12} . [This is confirmed by Figs. 3(e) and 3(f) below].

K_{11} changes in Figs. 3(e) and 3(f). As one could have expected, it is mainly the highest frequencies which are influenced. One observes a rapid shift towards low frequen-

cies, mainly for $\nu^2 > 2.6$. Comparing with Fig. 3(c), we see that in this frequency range, K_{11} is more important than K_{12} . Notice on the other hand that when $K_{11}=0.0$, the structure of Fig. 2 in the region $2 \leq \nu^2 \leq 2.4$ reappears which confirms the dominant role of the K_{12} force constant in that frequency range. (We assume that this structure was hidden in the shifted high-frequency modes when $K_{11}=0.8$). For $1 \leq \nu^2 \leq 1.6$ we know from Figs. 2, 3(a), and 3(b) that type-1 atoms are vibrating. We see that this structure persists for $K_{11}=0.8$ [Fig. 3(e)] while it disappears rapidly for $K_{12}=0.8$ [Fig. 3(c)]. We can thus surmise that it is mainly type-1 atoms and the K_{12} force constant which are involved in that frequency range.

Finally, note that a relatively small change ($\sim 20\%$) of the force constants between the lightest atoms can have a rather large effect on the shape of the spectrum at high frequencies [compare Figs. 2(b) and 3(e)]. This spectrum is thus in general sensitive to whether the force constants are equal or not.

Whether or not our results apply to the real disordered chain is obviously open to question. One could apply the improved methods suggested in Ref. 6 or perform Monte Carlo simulations.

Note added in proof. After this paper was submitted for publication, we received copies of work from M. A. Davidovich and C. E. T. Gonçalves da Silva as well as from M. O. Robbins and B. Koiller (unpublished). The former paper [which has appeared as B. Koiller, M. O. Robbins, M. A. Davidovich, and C. E. T. Gonçalves da Silva, *Solid State Commun.* **45**, 955 (1983)] considers a problem similar to the one presented here. In the latter, it is shown analytically that only the first moment of the density of states is exact for the kind of problem treated here. In the case of mass disorder only, the first five moments are ex-

act. Finally, note that numerical integrations for the moments converge much more rapidly when, using the analytic properties of the Green's function, the integration contour is deformed above the real axis (M. O. Robbins, private communication). The work of A. K. Bhattacharjee and C. E. T. Gonçalves da Silva [Solid State Commun. 45, 673 (1983)], which has just appeared in print, is also very closely related to ours.

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¹For reviews, see this and the next three references: E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension*, (Academic, New York, 1966).

²R. J. Elliott, J. A. Krumhansl, and P. L. Leath, *Rev. Mod. Phys.* 46, 465 (1974).

³P. Dean, *Rev. Mod. Phys.* 44, 127 (1972).

⁴S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, *Rev. Mod. Phys.* 53, 175 (1981).

⁵C. E. T. Gonçalves da Silva and Belita Koiller, *Solid State Commun.* 40, 215 (1981).

⁶J.-M. Langlois, A.-M. S. Tremblay, and B. W. Southern, preceding paper, *Phys. Rev. B* 28, 218 (1983).

⁷Various extensions of the GK scheme and their equivalence to hierarchical lattice models have been considered by A.-M. S. Tremblay (unpublished).

⁸H. Aoki, *J. Phys. C* 13, 3369 (1980); J. V. José (unpublished).

⁹R. B. Griffiths and M. Kaufman, *Phys. Rev. B* 26, 5022 (1982).

¹⁰C. Domb, A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Phys. Rev.* 115, 24 (1959).