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# The absence of localization in one-dimensional disordered harmonic chains

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**Abstract.** We study one-dimensional harmonic chains in which clusters of two or three defect atoms are embedded randomly. The disorder in the systems appears in the masses of the atoms. Reflectionless modes are obtained by studying different kinds of correlation among the masses. The localization behaviour of the modes around these special frequencies is examined analytically as well as numerically. To discern the nature of the modes at and around those frequencies, density of states, bandwidth scaling and site Green functions are studied. If the special frequencies lie within the common band of the constituent atoms and at zero the modes are extended at and around them. However, the modes are critical when the special frequency appears at the upper band edge of the host system. The number of non-scattered modes is estimated for all cases. It is  $\sim \sqrt{N}$  for the dimer problem. For the trimer problem with degenerate resonances appearing inside the constituent band it is  $\sim N^{3/4}$ . If the degenerate resonances of the trimer appear at zero frequency the number of non-scattered modes is  $\sim N^{5/6}$ .

## 1. Introduction

In one-dimensional disordered electronic systems almost all states are exponentially localized [1–3]. Therefore, in this context the study of one-dimensional correlated disordered systems [4–22] is of immense interest from both the theoretical and the experimental point of view [23]. In the tight-binding representation if the site energies [5–11] or off diagonal interactions [14, 17] or both [4, 12, 13, 15] are correlated in binary disordered chains, it can be shown that the systems sustain a set of non-scattered states. The number of such non-scattered states in this set is  $\sim \sqrt{N}$ , where  $N$  is the length of the chain. The basic requirement for obtaining such non-scattered states is the vanishing of the reflection coefficient at a particular energy. This is called the resonance energy or special energy. The position of this energy depends on the nature of the correlation. For example in the random dimer model (RDM) [5, 6, 9] the dimer energy is the special energy. Furthermore, this resonance energy must belong to the common band of the constituent atoms. Due to the presence of such states the mean square displacement (MSD) of an initially localized particle grows as  $\sim t^{3/2}$  (i.e. superdiffusive in nature) [4–6, 14, 15]. This is true only when the resonance energy appears inside the common band of constituent atoms. But when the resonance is at the host band edges the motion appears to be diffusive. The non-scattered states are also observed in one-dimensional disordered systems with random periods [24, 25]. Since the disordered systems with special energy show anomalous transport behaviour, the recent trend is to increase the number of such non-scattered states [18–22]. This can be achieved by increasing the correlation length. Instead of taking two sites of equal strength, if we consider  $n$  sites with equal strength we obtain  $(n - 1)$  resonance energies where the reflection coefficient vanishes [18, 19]. Since each resonance energy contains a set of

$\sim \sqrt{N}$  non-scattered states [18], the number of such states increases the prefactor of the number of states. Consequently, the exponents of the MSD will not change. In our recent work [20, 21] we have shown a way to increase the number of such states at the exponent level. In RTMDR [20–22], where two resonance energies merge at a particular energy inside the constituent band the number of non-scattered states is  $\sim N^{3/4}$ . Furthermore, the MSD is found to grow as  $\sim t^{1.75}$  [21].

The one-dimensional harmonic chain can be mapped to a tight-binding model (TBM) of an electronic system. Hence, almost all normal modes are localized in the one-dimensional disordered harmonic chain. This was originally shown by Dean [26]. However, there is one important difference between the disordered one-dimensional harmonic chain and that of the electronic system in the TBM. It can be shown by using the transfer matrix method that the one-dimensional disordered harmonic chain behaves like a perfect system at the frequency  $\omega = 0$  [27, 28]. Matsuda and Ishii [27] analytically showed that in such systems  $\sim \sqrt{N}$  low-frequency modes are not localized. They also showed the behaviour of thermal conductivity due to the presence of such low-frequency modes for different boundary conditions. Recently, a model of a one-dimensional correlated disordered harmonic chain has been studied [29]. All masses in this system have been considered to be equal. The spring constants are assumed to take two values. Furthermore, one of them appears in a pair while the other one appears randomly. The presence of delocalized modes of vibration in this particular model is shown by means of multifractal analysis. However, the number of such modes is not shown clearly. The purpose of this paper is to show the non-scattered modes in various one-dimensional correlated disordered harmonic chains. In all systems we have taken the disorder in the masses of atoms. Moreover, different kinds of correlation among masses are considered. As the basic criterion for obtaining the non-scattered states in one-dimensional correlated disordered electronic systems is the vanishing of the reflection coefficient, we study here the reflection property of the harmonic chains after transforming the systems to the equivalent tight-binding models. In each case we show the existence of a reflectionless mode at frequency  $\omega_0$ . We also show that even in the correlated disordered one-dimensional harmonic chains degenerate resonances can be obtained.

The organization of this paper is as follows. In section 2 we study the reflection properties for different systems. The localization behaviour around the frequency  $\omega_0$  is also studied here analytically as well as numerically. In section 3 we study the density of states, bandwidth scaling and Green function analysis to characterize the nature of modes around  $\omega_0$ . The number of non-scattered modes around  $\omega_0$  for different cases is estimated in section 4. We end this article by summarizing our main results.

## 2. Special frequencies and localization behaviour

### 2.1. Reflection coefficient

The equation of motion for a one-dimensional array of masses  $\{m_i\}$  coupled by harmonic springs is

$$(\beta_{i-1} + \beta_i - \omega^2 m_i)u_i = \beta_{i-1}u_{i-1} + \beta_i u_{i+1}. \quad (1)$$

Here  $\beta_i$  is the spring constant of the  $i$ th spring that couples the two masses  $m_i$  and  $m_{i+1}$ .  $\omega$  is the frequency of the harmonic chain and  $u_i$  is the Fourier transform of the amplitude of vibration of the  $i$ th mass,  $m_i$ . We consider the case where all constants  $\beta_i$  have the same value and without any loss of generality this value can be taken to be unity. So, the

disorder in the harmonic chain arises due to the randomly placed atoms of different masses. The transfer matrix equation is

$$\begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} = \mathbf{T}_i \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix} \quad (2)$$

where the transfer matrix

$$\mathbf{T}_i = \begin{pmatrix} 2 - m_i \omega^2 & -1 \\ 1 & 0 \end{pmatrix}. \quad (3)$$

Note also that  $\mathbf{T}_i$  is a unimodular matrix. The problem of the lattice vibration is, however, mathematically equivalent to the TBM of the electron. The equivalence between the two systems can be obtained through the following mapping:

$$2 - m_p \omega^2 \rightarrow E \quad (m_i - m_p) \omega^2 \rightarrow \epsilon_i \quad \beta \rightarrow V. \quad (4)$$

Since our motivation in this present paper is to study the resonance properties of disordered binary systems,  $m_p$  and  $m_i$  here denote the mass of the host and impurity atoms respectively. In the transformed tight-binding model  $E$  is the electronic energy and the site energies of the host and impurity sites are 0 and  $\epsilon_i$  respectively. The nearest-neighbour interactions are  $V$  which is considered to be unity.

To study the resonance property of the correlated disordered systems, it is essential to examine the resonance property of a perfect system with a single correlated impurity unit [9, 30]. So, we consider first a one-dimensional monatomic harmonic chain which contains a pair of defect atoms with mass  $m_a$ . For the host monatomic chain, we assume that the mass of each atom  $m_p$  is unity. Inasmuch as this system is equivalent to a single dimer in a perfect host system in the TBM [5], in the lattice vibration model we call this pair of defect atoms a 'dimer'. By using the mapping (4) it can be shown that the mode of frequency  $\omega_0 = \sqrt{2/m_a}$  is reflectionless, provided this special frequency belongs to the common band of the constituent atoms. Note that the band of the monatomic lattice lies between zero and four while for the other constituent atom of mass  $m_a$  we have  $0 \leq \omega^2 \leq 4/m_a$ . Hence, the restriction on the defect mass for obtaining the reflectionless mode is that  $m_a \geq 0.5$ . This feature is also obtained in the lattice vibration where the nearest-neighbour coupling between atoms appears in pairs but otherwise is random [29]. Instead of taking a cluster of two equal masses one can also consider a cluster of  $n$  atoms of equal mass. By equating the transfer matrix of the cluster to the unit matrix, it can be shown that the system has  $(n - 1)$  reflectionless modes. The frequency of these modes can be obtained from the zeros of the  $n$ th Chebysev polynomial of the second kind. The argument of the polynomial is half of the trace of the constituent transfer matrix [31].

In the hierarchy the next system of interest is a symmetric cluster of three defect atoms embedded in a perfect chain. The mass of the atoms in the host lattice,  $m_p$ , is again assumed to be unity. The mass of the central atom in the cluster is  $m_0$  while the other mass is  $m_s$ . Again all spring constants are considered to be unity. The system is equivalent to a trimer [20] in a perfect chain in the TBM. If the site energies of the trimer can be denoted as  $\epsilon_s$ ,  $\epsilon_0$  and  $\epsilon_s$  and all nearest-neighbour interactions are unity, the transformations (4) can be written as

$$2 - \omega^2 \rightarrow E \quad (m_0 - 1) \omega^2 \rightarrow \epsilon_0 \quad (m_s - 1) \omega^2 \rightarrow \epsilon_s. \quad (5)$$

Since  $m_p$  is the reference mass, the site energies of the host lattice in the transformed TBM are zero. To obtain the reflectionless modes of vibration of the special frequencies we set the numerator of the reflection coefficient  $|R|^2$  for the three-site correlation in the TBM to zero. Consequently, we obtain [20]

$$[E^2 - (\epsilon_0 + \epsilon_s)E + \epsilon_0\epsilon_s - 2]\epsilon_s + \epsilon_0 = 0. \quad (6)$$

Using the transformations (5) in (6) we obtain a third-order algebraic equation in  $\omega^2$ . The solutions of this equation are

$$\omega_0^2 = 0 \quad \omega_0^2 = \left(\frac{1}{m_0} + \frac{1}{m_s}\right) \pm \sqrt{\frac{1}{m_0^2} + \frac{1}{m_s^2} - \frac{1}{m_0 m_s} \left(\frac{1 - m_0}{1 - m_s}\right)}. \quad (7)$$

The criteria to obtain these reflectionless modes are that the frequency,  $\omega_0$ , should be real, positive and inside the common band of the constituent atoms.

Two special frequencies will coincide at  $\omega_0 = \sqrt{1/m_s + 1/m_0}$  (see figure 1(a)) provided

$$m_0 = m_s \left(1 \pm \sqrt{4m_s - 3}\right)/2. \quad (8)$$

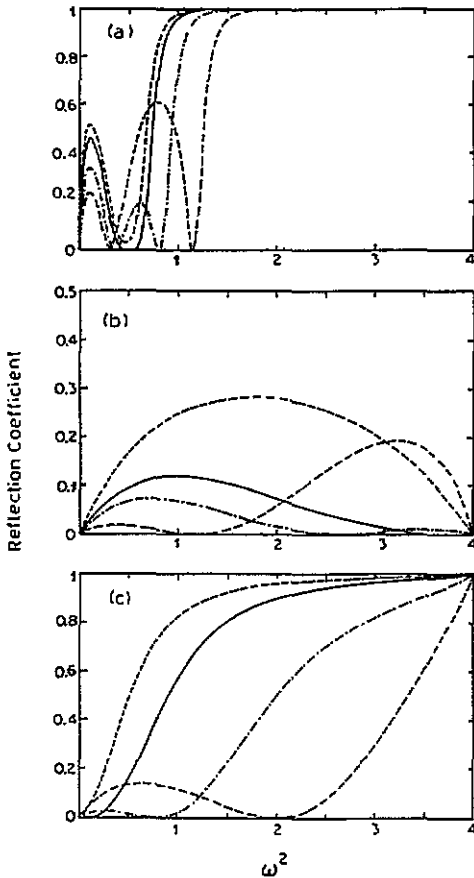
Since  $m_0$  is a real and positive quantity,  $m_s$  cannot be less than  $\frac{3}{4}$ . This is the lower bound of  $m_s$ . Furthermore to ensure that  $m_0$  is real for all values of  $m_s$ , we should choose the positive sign in (8). When  $m_s = \frac{3}{4}$ , the special frequency  $\omega_0$  is obtained at the upper band edge of the host as shown in figure 1(b). This type of behaviour is also obtained in the RTMDR [20, 21]. The number of non-scattered states in the RTMDR has been shown to increase as  $\sim N^{3/4}$ , where  $N$  is the length of the sample. So, in relation to the non-scattered modes we should expect the same behaviour in this case. In this vibrational system we find that the degenerate frequency moves towards  $\omega = 0$  with increasing  $m_s$  as well as  $m_0$ . But the degenerate solution does not superimpose on  $\omega = 0$  for any finite value of  $m_s$ . However,  $\omega = 0$  will be a second solution of equation (6) if the relation

$$m_0 = 3 - 2m_s \quad (9)$$

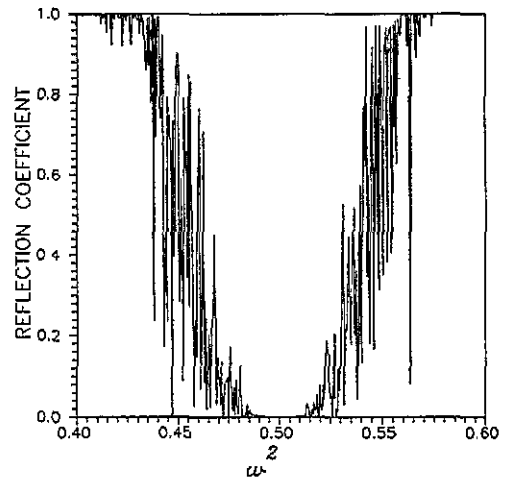
is obeyed (see figure 1(c)). Inasmuch as  $m_0$  is a real and positive quantity we must have  $0 < m_s < \frac{3}{2}$ . These are the major results of this paper. It should be noted that in all constraints for three-atom correlated systems the mass of the host lattice is also connected with  $m_0$  and  $m_s$ . So, arbitrary host systems cannot be taken to observe the merging of the solutions of equation (6).

## 2.2. Localization behaviour

So far we have considered systems with a single cluster of defect atoms. Now we consider a disordered harmonic chain where dimers or trimers are randomly distributed in an otherwise perfect chain of mass  $m_p$ . The reflection coefficient of this type of correlated disordered chain also vanishes at the special frequencies. The case of the trimer with degenerate resonances is shown in figure 2 as an example. The vanishing of the reflection coefficient at the special frequencies happens due to the commutation of the cluster transfer matrix with the perfect site transfer matrix at that frequency [15, 20]. For example, in the dimer case, the dimer transfer matrix reduces to the unit matrix at  $\omega_0 = \sqrt{2/m_a}$ . For the trimer problem with degenerate special frequency it can be shown that the transfer matrix commutes



**Figure 1.** Plot of reflection coefficient as a function of  $\omega^2$  for a single trimer in the perfect harmonic chain. (a) Here  $m_s = 3$  for all cases. The long-dashed curve corresponds to  $m_0 = 2.5$ ; the dot-dashed curve to  $m_0 = 4$ ; the solid curve corresponds to  $m_0 = 6$ , where two resonances merge. The short-dashed curve is for  $m_0 = 7$ . (b) Same as (a) but  $m_s = 0.75$ ,  $m_0 = 0.8, 0.5, 0.375$  (in this case two resonances merge) and  $0.1$  respectively. (c) Same as (a) but  $m_s = 0.5$ ,  $m_0 = 0.5, 1, 2$  (in this case two resonances merge) and  $3$  respectively.



**Figure 2.** Plot of reflection coefficient as a function of  $\omega^2$  for a random segment of length of  $N = 10^4$  where trimer clusters with concentration  $\rho = 0.25$  are distributed randomly. Here  $m_s = 3$  and  $m_0 = 6$ .

with the perfect site transfer matrix. Due to the vanishing of the reflection coefficient at the special frequencies a neighbourhood characterized by vanishingly small reflection is obtained. Hence, the inverse localization length or Lyapunov exponent ( $\gamma$ ) of the modes in this neighbourhood can be approximately written as [5, 9, 32]

$$\gamma \sim |R|^2. \quad (10)$$

$|R|^2$  in (10) is the reflection coefficient of a host system containing only one dimer or trimer. Since  $|R|^2$  contains in it information about the scattering of an incident wave by impurities, this is a reasonable approximation of  $\gamma$ .

We now study the localization behaviour of modes around  $\omega_0 = \sqrt{2/m_a}$  for the dimer problem. The leading-order term in the Taylor series expansion of  $|R|^2$  is  $\sim (\omega - \omega_0)^2$  when  $\omega_0 < 2$  and  $\sim (\omega - \omega_0)$  for  $\omega_0 = 2$ . So, the localization length ( $\gamma^{-1}$ ) shows  $(\omega - \omega_0)^{-2}$  and  $(\omega - \omega_0)^{-1}$  type singular behaviour depending on whether  $\omega_0$  is less than or equal to two. A similar procedure can be used to obtain the localization behaviour of the modes for the trimer problem with degenerate special frequencies. The reflection coefficient in this case in the neighbourhood of  $\omega_0$  behaves as  $\sim (\omega - \omega_0)^4$ ,  $(\omega - \omega_0)^3$  and  $(\omega - \omega_0)^6$  when  $\omega_0$  is inside the common band of constituent atoms, two and zero respectively. Consequently, the localization length shows singular behaviour as  $(\omega - \omega_0)^{-4}$ ,  $(\omega - \omega_0)^{-3}$  and  $(\omega - \omega_0)^{-6}$  for the cases discussed above. This type of behaviour of  $|R|^2$ , and hence of  $\gamma$ , can be analysed very easily. Since  $|R|^2$  is a positive semidefinite function, the curve will show a minimum at  $\omega_0^2 = 2/m_a$  for the dimer problem. Inasmuch as the minimum value of  $|R|^2$  is zero, the first derivative of it with respect to  $\omega^2$  vanishes at the special frequency. This, of course, requires the special frequency to be inside the constituent band. Therefore, the series starts with  $(\omega^2 - \omega_0^2)^2$ . Hence, the quoted result follows. In the case of the special frequency appearing at any one of the band edges,  $|R|^2 = 0$  is no longer the minimum of the curve of  $|R|^2$ . This can be shown by analytical continuation of  $|R|^2$ . Hence, the leading-order term in the Taylor series expansion of  $|R|^2$  will be  $(\omega^2 - \omega_0^2)$ . Since, at the lower band edge,  $\omega_0 = 0$ , the series starts with  $\omega^2$ . For  $\omega_0^2 = 4$ , the leading-order term is first order in  $(\omega - \omega_0)$ . In the trimer problem with doubly degenerate special frequency one maximum and two minima merge at the special frequency. So, the first and second derivatives of  $|R|^2$  with respect to  $\omega^2$  along with the function vanish. Furthermore,  $\omega_0^2$  is inside the common band of constituent atoms. Consequently,  $|R|^2$  should be symmetric around  $\omega_0$ . Hence, the third derivative also vanishes. Thus the series starts with  $(\omega^2 - \omega_0^2)^4$ . However, at the spectral boundaries, previous arguments also hold good here. Hence, the series expansion of  $|R|^2$  starts with  $(\omega^2 - \omega_0^2)^3$  around  $\omega_0^2 = 0$  and  $\omega_0^2 = 4$ . We then obtain  $\gamma(\omega) \sim \omega^6$  around  $\omega_0 = 0$  and  $\gamma \sim (2 - \omega)^3$  around  $\omega_0 = 2$ . We will study next the localization behaviour numerically to substantiate our analytical result.

The displacement of the  $N$ th atom with frequency  $\omega$ ,  $u_N(\omega)$  in the vibrational system can be calculated by using the transfer matrix method. For given values of  $u_1$  and  $u_0$ , ( $u_1^2 + u_0^2 \neq 0$ ) it is given by [27]

$$\begin{pmatrix} u_{N+1} \\ u_N \end{pmatrix} = \mathbf{T}_N \mathbf{T}_{N-1} \dots \mathbf{T}_2 \mathbf{T}_1 \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}. \quad (11)$$

The Lyapunov exponent,  $\gamma$ , is [16]

$$\gamma = \lim_{N \rightarrow \infty} \frac{1}{N} \operatorname{Re} K_N(\omega^2) \quad (12)$$

where  $K_N(\omega^2)$  is the logarithm of the eigenvalue of  $\mathbf{Q}_N(\omega^2)$  whose modulus is greater than unity. Here,  $\mathbf{Q}_N(\omega^2)$  is defined as

$$\mathbf{Q}_N(\omega^2) = \prod_{i=1}^N \mathbf{T}_i(\omega^2). \quad (13)$$

In figure 3 we have plotted the average localization length around the special frequency as a function of  $|\omega - \omega_0|$  for the dimer system and the trimer with degenerate frequencies. For the dimer we consider the case where  $\omega_0$  is inside the common band of constituent atoms. For the trimer we consider the cases where the degenerate frequency appears inside the constituent band as well as at  $\omega_0 = 0$ . The observed scaling behaviour is given in the corresponding figures (see figure 3). The average is taken over twenty different realizations of the systems. The maximum length of the system considered is  $10^7$ . Our numerical results show a good agreement with the analytical results obtained above.

### 3. Nature of normal modes at and around the special frequencies

#### 3.1. Density of states

The nature of states in the systems can be anticipated from the behaviour of the density of states (DOS). The fluctuations in the DOS correspond to the localized modes and its smoothness around a frequency indicates the possible presence of non-scattered modes there [17]. We study the DOS numerically using Dean's method [33], which is based on the negative eigenvalue theorem. The negative eigenvalue theorem states that the number of eigenstates with eigenvalues less than or equal to  $\omega^2$  is the number of negative values of  $h_i$  ( $i = 1, 2, \dots, N$ ) where  $h_i$  is determined by

$$h_{i+1} = A_i - \omega^2 - B_i^2/h_i \quad i = 1, 2, \dots, N - 1 \quad (14)$$

and

$$h_1 = A_1 - \omega^2. \quad (15)$$

Here,

$$A_i = 2/m_i \quad B_i = 1/\sqrt{m_{i-1}m_i} \quad (16)$$

and

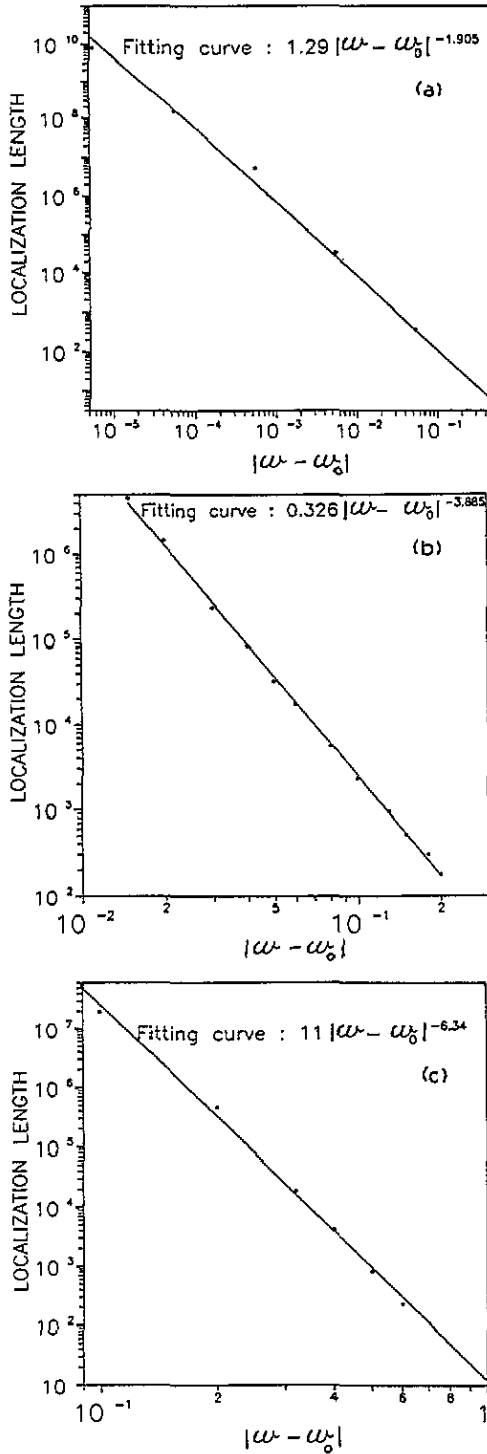
$$h_i = \frac{u_i}{m_{i-1}u_{i-1}}.$$

The definition of  $h_1$  by equation (15) implies that the mass of the atom at  $i = 0$  is infinite. Hence,  $u_0$  is zero. The negative eigenvalue theorem gives the integrated density of states (IDOS). So, the DOS can be obtained by differentiating the IDOS with respect to  $\omega^2$ . The DOS as a function of  $\omega^2$  for different cases is shown in figure 4. When  $\omega_0$  is inside the band of constituent atoms the DOS shows smooth behaviour around it, but when  $\omega_0$  is at the spectral boundaries the DOS shows divergence behaviour like a perfect system. So, the study of density of states suggests the possible presence of delocalized modes around the special frequencies in correlated disordered harmonic chains. We study next the scaling behaviour of bandwidths for further characterization of the modes around the special frequency.

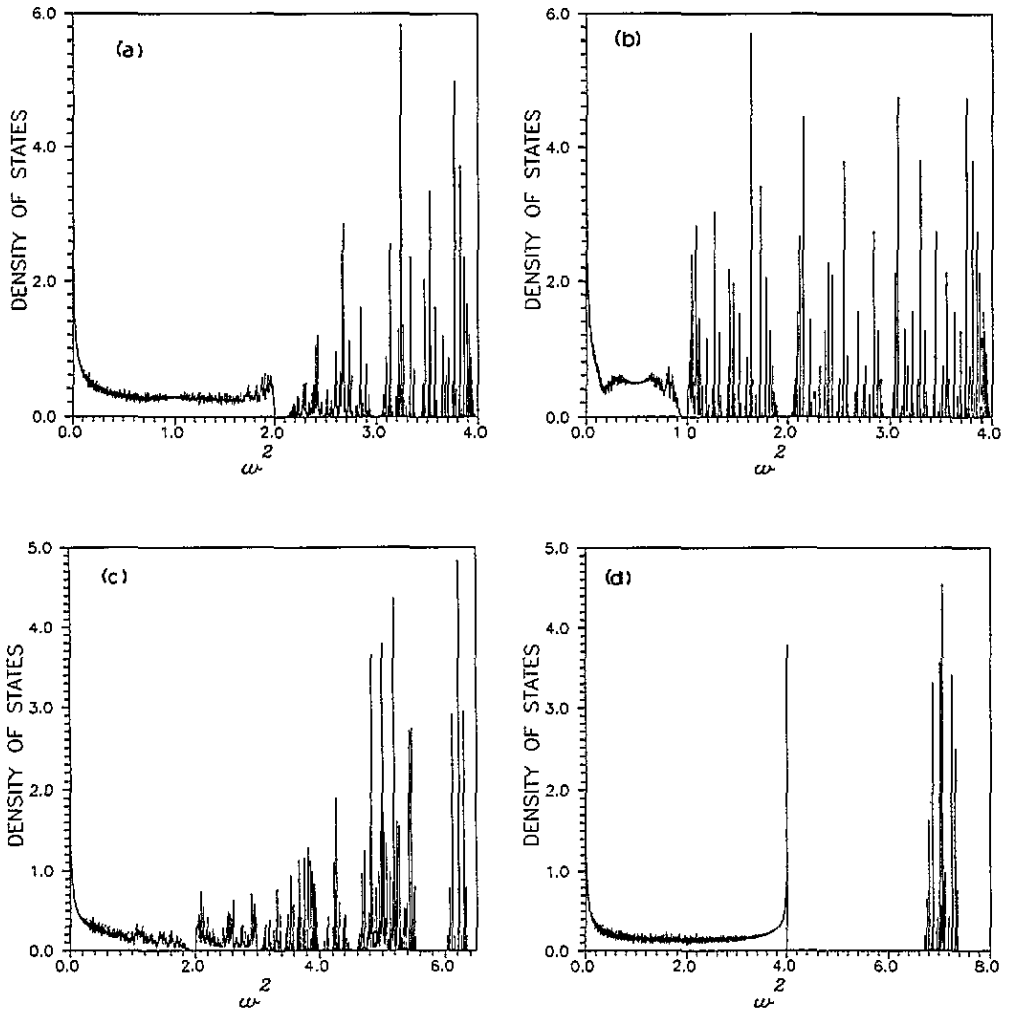
#### 3.2. Bandwidth scaling analysis

The bandwidth scaling method has been used successfully to discern the nature of states in one-dimensional quasiperiodic electronic systems [34] and deterministically aperiodic systems [35]. Recently we [10,21] applied this method with some modification to the one-dimensional correlated disordered electronic systems. This method nicely exhibits the accumulation of extended states around the resonance energies of RDM [10] and RTMDR [21]. So, we apply this method here to characterize the nature of the vibrational modes in the neighbourhood of special frequencies. Since  $\mathbf{Q}_N(\omega^2)$  is a unimodular matrix the bands in  $\omega^2$ -space are characterized by  $|\text{Tr } \mathbf{Q}_N(\omega^2)| \leq 2$ . If  $\Delta_i$  defines the width of the  $i$ th band, then the extended modes of vibration are characterized by  $\Delta_i \propto N^{-1}$ . For algebraically localized modes,  $\Delta_i \propto N^{-\alpha}$ ,  $\alpha > 1$  and for strongly localized modes,  $\Delta_i \propto \exp(-\beta_i N)$  where  $\beta_i$  is a constant. In the neighbourhood of Van Hove singularities, bands exhibit  $\Delta_i \propto N^{-2}$  [34]. The method of individual bandwidth scaling is described elaborately in [10,21]. The basic idea in this scaling analysis is that there exists a band at the special frequencies and





**Figure 3.** Log-log plot of localization length ( $\gamma^{-1}$ ) against  $|\omega - \omega_0|$  for different cases. (a) The dimer clusters of mass  $m_d = 2$  are distributed randomly with concentration  $\rho = 0.33$  in an otherwise perfect chain. (b) The trimer clusters of masses  $m_s = 3$  and  $m_0 = 6$  are distributed randomly with concentration  $\rho = 0.25$  in an otherwise perfect chain. (c) Same as (b) but here  $m_s = 0.5$  and  $m_0 = 2$ .



**Figure 4.** Plot of the density of states (DOS) as a function of  $\omega^2$  for different cases. The length of the segment here is  $10^5$  for all cases. (a) The dimer clusters of mass  $m_2 = 2$  are distributed randomly with concentration  $\rho = 0.33$  in an otherwise perfect chain. Smooth behaviour is obtained around  $\omega^2 = 1$ . (b) The trimer clusters of masses  $m_s = 3$  and  $m_0 = 6$  are distributed randomly with concentration  $\rho = 0.25$  in an otherwise perfect chain. The smoothness is observed around  $\omega^2 = 0.5$ . (c) Same as (b) but here  $m_s = 0.5$  and  $m_0 = 2$ . The DOS curve diverges like that of a perfect one-dimensional chain around  $\omega^2 = 0$ . (d) Same as (b) but  $m_s = 0.75$  and  $m_0 = 0.375$ . The DOS curve also diverges like that of a perfect chain around  $\omega^2 = 4$ .

this can be used as the reference band (numbered as zero) to analyse the scaling behaviour of various bands around it. The bands appearing to the right of the reference band will be denoted as 1R, 2R, 3R etc and similarly, for the other side, the bands are numbered as 1L, 2L, 3L etc. Here, we show the scaling behaviour of the bands for the trimer system with a doubly degenerate special frequency. First we consider the case where the degenerate frequency appears inside the common band of constituent atoms. The scaling behaviour of the bands 0, 5R and 5L is presented in figure 5(a). The bandwidth with index  $i$ ,  $\Delta_i$ , for large values of  $N$  is found to obey

$$\ln \Delta_i = \ln c_i - \alpha_i \ln N \quad (17)$$

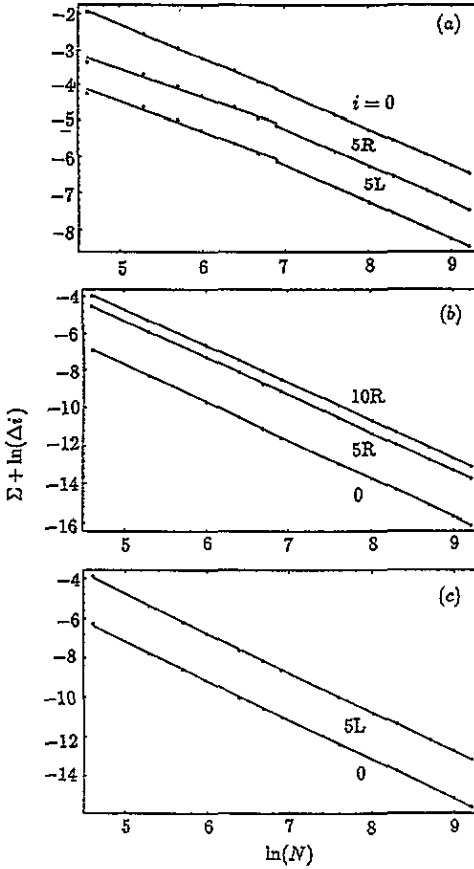
where  $c_i$  is the index-dependent constant. The values of  $c$  and  $\alpha$  are presented in table 1 for different regions of  $N$ . The bands do not partition in a systematic way due to disorder for small values of  $N$ . Hence, equation (17) is not strictly obeyed in that region. But for large values of  $N$  the bands show good scaling behaviour with the exponent,  $\alpha \sim 1$ , confirming the presence of extended modes of vibration. Of course, the value of  $N$  beyond which a band shows good scaling behaviour increases with band index  $i$ . This further implies that the number of extended modes increases with increasing system size  $N$ . As the system is a disordered vibrational chain it is obvious that not all bands show  $\alpha \sim 1$  for finite values of  $N$ . This can be explained by invoking the concept of the special spectral zone (SSZ) [10, 21]. The scattering effect due to the defect atoms is negligibly small in the SSZ. The band which is outside the SSZ is not partitioned in a systematic way. This is because of the scattering effect. But with increasing  $N$  the band enters the SSZ and the scattering effect becomes negligibly small. Then the band shows good scaling behaviour. In figure 5(b) we have shown the scaling behaviour of the bands 0, 5R and 10R for the case where the degenerate special frequency is at  $\omega_0 = 0$ . Equation (17) is also obeyed by these bands but with the scaling exponent  $\alpha \sim 2$ . This is due to the presence of the Van Hove singularity in the DOS of this system at  $\omega = 0$ . All bands show nice scaling behaviour for comparatively small values of  $N$ . This implies that the number of extended states is large compared to the previous case. The scaling exponent  $\alpha \sim 2$  is also obtained for the case where degenerate frequency  $\omega_0 = 2$ . The scaling behaviour of bands 0 and 5L is shown in figure 5(c). So, the bandwidth scaling analysis shows that the modes at and around the special frequencies are extended in nature when the special frequencies appear inside the constituent band and at zero. We next show that the modes in the neighbourhood of  $\omega_0 = 2$  are not truly extended. This is done by analysing the pole behaviour of the site Green function [36]. The scaling behaviour of the bands around special frequencies for the random dimer chain is similar to what is observed in the trimer system. This is not discussed here.

**Table 1.** The value of  $c$  and bandwidth scaling index ( $\alpha$ ) of different bands in different ranges of  $N$ . Here  $m_s = 3$ ,  $m_0 = 6$  and concentration,  $\rho = 0.25$ .

Band index ( $i$ )	Range of $N$			
	$10^2-10^3$		$10^3-10^4$	
	$c$	$\alpha$	$c$	$\alpha$
0	1.638	0.957	2.344	1.013
5R	0.556	0.794	2.241	1.008
5L	0.765	0.841	2.289	1.010

### 3.3. Green function analysis

The site Green functions are calculated for the system containing only one trimer. For this calculation transformations (5) together with the well known renormalized perturbative expansion (RPE) [36] method have been used. It is well known that the pole of the Green function at a particular energy corresponds to a localized mode at that frequency. The site Green function for the system under study shows a pole at  $\omega^2 = 4$  when the resonance frequency appears at  $\omega_0 = 2$ . This is shown in figure 6(a). This indicates that the particular



**Figure 5.** Log-log plot of bandwidth ( $\Delta_r$ ) against  $N$  for different cases. In all cases the trimer clusters are randomly distributed with concentration  $\rho = 0.25$  in an otherwise perfect chain. A constant factor  $\Sigma$  is added to the ordinate for clarity. (a) Here  $m_s = 3$  and  $m_0 = 6$ . The scaling behaviour is shown in two regions of  $N$ . The scaling exponents for different regions are given in table 1. The values of  $\Sigma$  are taken from the top as 2, 1 and 0. (b) Same as (a) but  $m_s = 0.5$  and  $m_0 = 2$ . All figures are shown here in one region of  $N$  and  $\Sigma$  takes the value zero here. (c) Same as (b) but  $m_s = 0.75$  and  $m_0 = 0.375$ .

mode is localized. On the other hand the reflection coefficient vanishes at  $\omega_0 = 2$  and the DOS diverges like that of a perfect system around that frequency. Because of this peculiarity we argue that the mode is neither truly extended nor truly localized. Hence, the modes in the neighbourhood of  $\omega_0 = 2$  are algebraically localized. Similar behaviour is also observed in the dimer system. But when  $\omega_0 = 0$  we do not observe any pole in the site Green function at that frequency as shown in figure 6(b). The Green function analysis clearly shows the difference between the two spectral boundaries in the one-dimensional harmonic chain. Note that in electronic systems the site Green function shows the same behaviour at both the spectral boundaries. The origin of this difference is the fact that localization for the disordered harmonic chain starts from the upper band edge. The localization from the lower band edge is strictly forbidden due to the positiveness of  $\omega^2$ . On the other hand the localization starts from both the band edges in electronic systems.

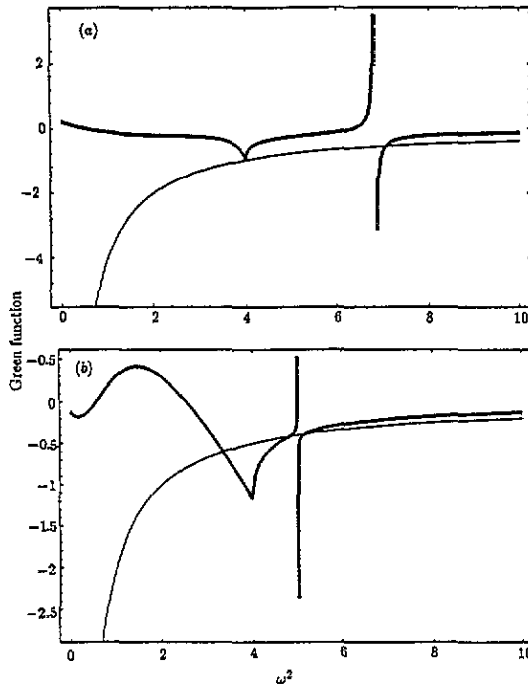


Figure 6. The thick solid line corresponds to the real part of the Green function ( $G$ ) with defect atoms of mass  $m_s$  and  $m_0$  calculated at the other nearest neighbour of  $m_0$  as a function of  $\omega^2$ . The thin solid line corresponds to  $G = 1/(m_s - 1)\omega^2$ . (a) Here  $m_s = 0.75$  and  $m_0 = 0.375$ . One of the poles is observed at  $\omega^2 = 4$ . (b) Here  $m_s = 0.5$  and  $m_0 = 2$ . No pole is observed at  $\omega^2 = 0$ .

#### 4. Number of non-scattered modes of vibration

If the non-scattered modes are defined as the modes whose localization length ( $\gamma^{-1}$ ) is superior to the sample size ( $N$ ) then  $\sim \sqrt{N}$  such states are obtained in the complete disordered vibrational systems around the zero frequency [27]. Since in the correlated disorder chain other reflectionless modes apart from the mode at zero frequency are present there will be more non-scattered modes than in completely disordered systems. In the previous section we have shown the presence of a set of non-scattered modes of vibration around the special frequencies in correlated disordered chains. The number of such modes can be estimated from the scaling behaviour of the total bandwidth [10]. We, however, estimate the number of such modes using the result of localization behaviour and the bandwidth scaling analysis. We define the frequency width around  $\omega_0$  where these non-scattered modes are observed by  $\Delta\omega$ . Then the width of the non-scattered modes decays as  $\Delta\omega \sim N^{-p}$ . This is obtained from the localization behaviour of the modes around  $\omega_0$ . Again from the bandwidth scaling method we find that the modes decay as  $\sim 1/N$  around  $\omega_0$ . If we assume that the non-scattered modes whose localization length is of the order of the sample length follow  $\sim 1/N$  type scaling behaviour in the bandwidth analysis then the number of non-scattered modes  $\Delta n$  within the region  $\Delta\omega$  is

$$\Delta n \sim N^{1-p}. \quad (18)$$

The above expression is true only when  $\omega_0$  is inside the constituent band. Since for the random dimer vibrational system  $p = \frac{1}{2}$ , the number of non-scattered modes around  $\omega_0$

is  $\sim \sqrt{N}$ . For the random trimer vibrational systems with degenerate special frequency (except  $\omega_0 = 0$  and 2)  $p = \frac{1}{4}$ , and the number of non-scattered modes is  $\sim N^{3/4}$ . Although for  $\omega_0 = 0$  the bandwidths decay as  $\sim 1/N^2$  around  $\omega_0$  the modes can be shown to decay as  $\sim 1/N$  in  $\omega$ -space. So, the number of non-scattered modes can be obtained from equation (18). Since in this case  $p = 6$ , we have  $\Delta n \sim N^{5/6}$ . Thus using the short-range correlation among the masses we have increased the number of non-scattered modes. However, all the results discussed above are true only when  $\omega_0$  is inside the common band of the constituent atoms or at zero.

## 5. Summary

We have studied one-dimensional disordered harmonic chains with different correlations among the masses. The correlation produces a special frequency ( $\omega_0$ ) mode where the reflection coefficient vanishes if  $\omega_0$  belongs to the band of constituent atoms. This special property of the system gives rise to the presence of a set of non-scattered modes around these particular frequencies. We have also shown here that by introducing appropriate correlation among the masses in the trimeric cluster two special frequencies can be overlapped. The localization behaviour of the systems around  $\omega_0$  is discussed analytically as well as numerically. The study of density of states suggests the possible presence of delocalized modes around  $\omega_0$ . The bandwidth scaling analysis together with the Green function analysis confirms the extended nature of the modes around  $\omega_0$  for  $\omega_0$  is either inside the constituent band or at zero. But when  $\omega_0$  is at the upper band edge the modes are critical like. If we consider that the modes whose localization length is larger than the sample size show  $\sim 1/N$  type scaling behaviour in bandwidth analysis then the random dimer harmonic chain contains  $\sim \sqrt{N}$  non-scattered modes. Here,  $N$  is the length of the chain. The same behaviour is also obtained around  $\omega = 0$  in the disordered harmonic chain. So, due to the presence of the pair correlation in the disordered chain the number of non-scattered modes increases in amplitude. In the random trimer chain we obtain  $\sim N^{3/4}$  non-scattered modes when the doubly degenerate special frequency appears inside the constituent band. When the doubly degenerate frequency appears at  $\omega = 0$ ,  $\sim N^{5/6}$  non-scattered modes are obtained. The concentration and mass dependence of defect atoms on the number of non-scattered modes are not discussed here. However, the increase in the number of non-scattered modes in the exponent level for the case of the degenerate special frequency in the random trimer chain should be reflected in the low-temperature thermal conductivity. This work is in progress.

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