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Absence of localization in one dimensional disordered harmonic chains

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32

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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 appear in the masses of the atoms. Reflectionless modes are obtained by studying different kinds of correlations among the masses. The localization behavior 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, bandwidths 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 it. However, the modes are critical when it appears at the upper band edge of the host system. The number of nonscattered modes is estimated for all cases. It is $\sim \sqrt{N}$ for dimer problem. For trimer problem with degenerate resonances appearing inside the constituent band it is $\sim N^{3/4}$. If the degenerate resonances of trimer appear at zero frequency the number of nonscattered 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 both from the theoretical as well as 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 nonscattered states. The number of such nonscattered states in this set is $\sim \sqrt{N}$, where N is the length of the chain. The basic requirement for obtaining such nonscattered states is the vanishing of reflection coefficient at a particular energy. This is called resonance energy or special energy. The position of this energy depends on the nature of correlation. For example in the random dimer model (RDM) [5, 6, 9] the dimer energy is the special energy. Furthermore, this resonance enrgy must belongs to the common band of the constituent atoms. Due to the presence of such states the mean square displacement (msd) of a initially localized particle grows like $\sim t^{3/2}$ (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 nonscattered states are also observed in one dimensional disordered systems with random periods [24, 25]. Since the disordered systems with special energy show anamolous transport behavior, the recent trend is, therefore, to increase the number of such nonscattered 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 $(n-1)$ number of resonance energies where reflection coefficient vanishes [18, 19]. Since each resonance energy contains a set of $\sim \sqrt{N}$ number of nonscattered states, [18] the number of such states, therefore, increases the prefactor of the number of states. Consequently, the exponents of 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 nonscattered states is $\sim N^{3/4}$. Furthermore, the msd is found to grow as $\sim t^{1.75}$ [21].

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 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 electronic system in 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]. Mutsuda and Ishii [27] analytically showed that in such systems $\sim \sqrt{N}$ number of low frequency modes are not localized. They also showed the behavior of thermal conductivity due to presence of such low frequency modes for different boundary conditions. Recently, a model of 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 pair while the other one appears randomly. The presence of delocalized modes of vibration in this particular model are shown by means of multifractal analysis. However, the number of such modes are not shown clearly. The purpose of this paper is to show the nonscattered 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 correlations among masses are considered. As the basic criteria for obtaining the nonscattered states in one dimensional correlated disordered electronic systems is the vanishing of reflection coefficient, we study here the relection 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 ω_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 behavior around the frequency ω_0 is also studied here analytically as well as numerically. In section 3 we study the density of states, bandwidths scaling and Green function analysis to characterize the nature of modes around ω_0. The number of nonscattered modes around ω_0 for different cases is estimated in section 4. We end this article by summerizing of our main results.

2 Special frequencies and localization behavior

2.1 Reflection coefficient

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

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

Here β_i is the spring constant of the ith spring that couples the two masses m_i and m_{i+1}. ω is the frequency of the harmonic chain and u_i is the Fourier transform of the amplitude of vibration of the ith mass, m_i. We consider the case where all β_i's 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

$$\begin{pmatrix} u_{i+1} \\ u_i \end{pmatrix} = T_i \begin{pmatrix} u_i \\ u_{i-1} \end{pmatrix} \tag{2}$$

where the transfer matrix

$$T_i = \begin{pmatrix} 2 - m_i\omega^2 & -1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

Note also that T_i is a unimodular matrix. The problem of lattice vibration is, however, mathematically equivalent to the TBM of electron. The equivalence between the two systems can be obtained through the following mapping,

$$\begin{aligned} 2 - m_p\omega^2 &\rightarrow E \\ (m_i - m_p)\omega^2 &\rightarrow \epsilon_i \\ \beta &\rightarrow V. \end{aligned} \tag{4}$$

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 ϵ_i respectively. The nearest neighbor 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 monoatomic harmonic chain which contains a pair of defect atoms with mass m_a. For the host monoatomic 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 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 monoatomic lattice lies between 0 and 4 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 neighbor coupling between atoms appears in pair but otherwise it 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 nth Chebysev polynomial of second kind. The argument of the polynomial is the half of the trace of the constituent transfer matrix [31].

In the hierarchy the next system of interest is a symmetric cluster of 3 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 TBM. If the site energies of the trimer can be denoted as ϵ_s, ϵ_0 and ϵ_s and all nearest neighbor interactions are unity, the transformations (4) can be written as

$$\begin{aligned} 2-\omega^2 &\rightarrow E \\ (m_0-1)\omega^2 &\rightarrow \epsilon_0 \\ (m_s-1)\omega^2 &\rightarrow \epsilon_s. \end{aligned} \tag{5}$$

Since m_p is the reference mass, the site energies of the host lattice in the transformed TBM is zero. To obtain the reflectionless modes of vibration or the special frequencies we set the numerator of the reflection coefficient $|R|^2$ for 3 sites correlation in TBM to zero. Consequently, we obtain [20]

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

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

$$\begin{aligned} \omega_0^2 &= 0 \\ \omega_0^2 &= \left(\frac{1}{m_0}+\frac{1}{m_s}\right)\pm\sqrt{\frac{1}{m_0^2}+\frac{1}{m_s^2}-\frac{1}{m_0m_s}\left(\frac{1-m_0}{1-m_s}\right)}. \end{aligned} \tag{7}$$

The criteria to obtain these reflectionless modes are that the frequency, ω_0 should be real, positive and inside the common band of the constituent atoms.

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

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

Since m_0 is a real and positive quantity, m_s cannot be less than 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 $m_s=3/4$, the special frequency ω_0 is obtained at the upper band edge of the host as shown in figure 1(b). This type of behavior is also obtained in RTMDR [20, 21]. The number of nonscattered 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 nonscattered modes we should expect the same behavior in this case. In this vibrational system we find that the degenerate frequency moves towards $\omega=0$ with increasing the value of 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,

$$m_0=3-2m_s \tag{9}$$

is obeyed (see figure 1(c)). Inasmuch as m_0 is a real and positive quantity we must have $0<m_s<3/2$. These are the major results in this paper. It should be noted that in all constraints for 3 atoms 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 behavior

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 chains 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 $\omega_o = \sqrt{2/m_a}$. For trimer problem with degenerate special frequency it can be shown that the transfer matrix commutes with the perfect site transfer matrix. Due to the vanishing of the reflection coefficient at the special frequencies a neighborhood characterized by vanishingly small reflection is obtained. Hence, the inverse localization length or Lyapunov exponent (γ) of the modes in this neighborhood can be approximately written as [5, 9, 32]

$$\gamma \sim |R|^2. \tag{10}$$

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

We now study the localization behavior 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 (γ^{-1}) shows $(\omega - \omega_0)^{-2}$ and $(\omega - \omega_0)^{-1}$ type singular behavior depending on whether ω_0 is less than or equal to 2. The similar procedure can be used to obtain the localization behavior of the modes for trimer problem with degenerate special frequencies. The reflection coefficient of this case in the neighborhood of ω_0 behaves like $\sim (\omega-\omega_0)^4$, $(\omega-\omega_0)^3$ and $(\omega-\omega_0)^6$ when ω_0 is inside the common band of constituent atoms, 2 and 0 respectively. Consequently, the localization length shows the singular behavior like $(\omega-\omega_0)^{-4}$, $(\omega-\omega_0)^{-3}$ and $(\omega-\omega_0)^{-6}$ for the cases discussed above. This type of behavior of $|R|^2$ hence of γ, can be analyzed 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 ω^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 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 ω^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, first and second derivative of $|R|^2$ with respect to ω^2 along with the function vanishes. Furthermore, ω_0^2 is inside the common band of constituent atoms. Consequently, $|R|^2$ should be symmetric around ω_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 behavior numerically to substantiate our analytical result.

The displacement of Nth atom with frequency ω, $u_N(\omega)$ 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]

$$\begin{pmatrix} u_{N+1} \\ u_N \end{pmatrix} = T_N T_{N-1} \cdots T_2 T_1 \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}. \tag{11}$$

The Lyapunov exponent, γ is [16]

$$\gamma = \lim_{N \to \infty} \frac{1}{N} \mathrm{Re}\, K_N(\omega^2), \tag{12}$$

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

$$Q_N(\omega^2) = \prod_{i=1}^{N} T_i(\omega^2). \tag{13}$$

In figure 3 we have plotted the average localization length around the special frequency as a function of $|\omega - \omega_0|$ for dimer system and trimer with degenerate frequencies. For dimer we consider the case where ω_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 behavior 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 behavior of the density of states (DOS). The fluctuations in DOS corresponds to the localized modes and the smoothness of it around a frequency indicates the possible presence of nonscattered 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 ω^2 is the number of negative values of $h_i (i = 1, 2, \cdots, N)$ where h_i is determined by

$$h_{i+1} = A_i - \omega^2 - B_i^2/h_i; \quad i = 1, 2, \cdots, N-1 \tag{14}$$

and

$$h_1 = A_1 - \omega^2. \tag{15}$$

Here,

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

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 ω^2. The DOS as a function of ω^2 for different cases are shown in figure (4). When ω_0 is inside the band of constituent atoms the DOS shows the smooth behavior around it. But when ω_0 is at the spectral boundaries the DOS shows the divergence behavior like a perfect system. So, the study of density of states suggest the possible presence of delocalized modes around the special frequencies in correlated disordered harmonic chains. We study next the scaling behavior 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 neighborhood of special frequencies. Since $Q_N(\omega^2)$ is a unimodular matrix the bands in ω^2-space are characterized

by $|\mathrm{Tr}Q_N(\omega^2)| \leq 2$. If Δ_i defines the width of the ith 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 β_i is a constant. In the neighborhood 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 this can be used as the reference band (numbered as 0) to analyze the scaling behavior 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 other side the bands are numbered as 1L, 2L, 3L etc. Here, we show the scaling behavior 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 behavior of the bands 0, 5R and 5L are presented in figure 5(a). The bandwidth with index i, Δ_i for large value of N is found to obey

$$\ln \Delta_i = \ln c_i - \alpha_i \ln N \tag{17}$$

where c_i is the index dependent constant. The values of c and α are presented in table 1 for different region of N. The bands do not partition in a systematic way due to disorder for small value of N. Hence, equation (17) is not strictly obeyed in that region. But for large values of N they show good scaling behavior 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 behavior increases with the band index i. This further implies that the number of extended modes increases with increasing the system size N. As the system is a disordered vibrational chain it is obvious that all bands do not show $\alpha \sim 1$ for finite value of N. This can be explained by invoking the concept of 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 systemetic way.

This is because of scattering effect. But with increasing the value of N the band enters inside the SSZ and the scattering effect becomes negligibly small. Then the band shows good scaling behavior. In figure 5(b) we have shown the scaling behavior of the bands 0, 5R and 10R for the case where 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 Van-hove singularity in DOS of this system at $\omega = 0$. All bands show nice scaling behavior 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 behavior 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 neighborhood of $\omega_0 = 2$ are not truly extended. This is done by analyzing the pole behavior of site Green function [36]. The scaling behavior 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.

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. 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 mode is localized. On the other hand the reflection coefficient vanishes at $\omega_0 = 2$ and 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 neighborhood of $\omega_0 = 2$ are algebraically localized. Similar behavior 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 one dimensional harmonic chain. Note that in electronic systems the site Green function shows the same behavior at both the spectral boundaries. The origin of this difference is due to the fact that localization for disordered harmonic chain starts from the upper band edge. The localization from the lower band edge is strictly forbidden due to the positiveness of ω^2. On the other hand the localization starts from both the band edges in electronic systems.

4 Number of nonscattered modes of vibration

If the nonscattered modes are defined as the modes whose localization length (γ^{-1}) is superior to the sample size (N) then $\sim \sqrt{N}$ number of 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 nonscattered modes than in completely disordered systems. In the previous section we have shown the presence of a set of nonscattered modes of vibration around the special frequencies in correlated disordered chains. The number of such modes can be estimated from the scaling behavior of the total bandwidth [10]. We, however, estimate the number such modes using the result of localization behavior and the bandwidth scaling analysis. We define the frequency width around ω_0 where these nonscattered modes are observed by $\Delta\omega$. Then the width of the nonscattered modes decays like $\Delta\omega \sim N^{-p}$. This is obtained from the localization behavior of the modes around ω_0. Again from the bandwidth scaling method we find that the modes decay like $\sim 1/N$ around ω_0. If we assume that the nonscattered modes whose localization length

is of the order of sample length follow $\sim 1/N$ type scaling behavior in bandwidth analysis then the number of nonscattered modes Δn within the region $\Delta\omega$ is

$$\Delta n \sim N^{1-p}. \tag{18}$$

The above expression is true only when ω_0 inside the constituent band. Since, for random dimer vibrational system $p = 1/2$, the number of nonscattered modes around ω_0 is $\sim \sqrt{N}$. For random trimer vibrational systems with degenerate special frequency (except $\omega_0 = 0$ and 2) $p = 1/4$, and the number of nonscattered modes is $\sim N^{3/4}$. Although for $\omega_0 = 0$ the bandwidths decay as $\sim 1/N^2$ around ω_0 the modes can be shown to decay like $\sim 1/N$ in ω-space. So, the number of nonscattered 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 nonscattered modes. However, all the results discussed above are true only when ω_0 is inside the common band of the constitute 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 (ω_0) mode where reflection coefficient vanishes if ω_0 belongs to the band of constituent atoms. This special property of the system gives rise to the presence of a set of nonscattered 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 behavior of the systems around ω_0 is discussed analytically as well as numerically. The study of density of states suggests the possible presence of delocalized modes around ω_0. The bandwidth scaling analysis together with the Green function analysis confirms the extended nature of the modes around ω_0 for ω_0 is either inside the constituent

band or at zero. But when ω_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 behavior in bandwidth analysis then the random dimer harmonic chain contains $\sim \sqrt{N}$ number of nonscattered modes. Here, N is the length of the chain. The same behavior is also obtained around $\omega = 0$ in disordered harmonic chain. So, due to presence of pair correlation in disordered chain the number of nonscattered modes increases in amplitude. In random trimer chain we obtain $\sim N^{3/4}$ number of nonscattered modes when the doubly degenerate special frequency appears inside the constituent band. When the doubly degenerate frequency appears at $\omega = 0$, $\sim N^{5/6}$ number of nonscattered modes are obtained. The concentration and mass dependence of defect atoms on the number of nonscattered modes are not discussed here. However, the increase in the number of nonscattered modes in the exponent level for the case of degenerate special frequency in random trimer chain should be reflected in the low temperature thermal conductivity. This work is in progress.

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Figures

Figure 1. Plot of reflection coefficient as a function of ω^2 for a single trimer in the perfect harmonic chain. (a) Here $m_s = 3$ for all cases. The big dashed curve corresponds to $m_0 = 2.5$; the dot-dashed curve for $m_0 = 4$; the solid curve corresponds to $m_0 = 6$, where two resonances merge. The small dashed curve 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 ω^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 $m_0 = 6$.

Figure 3. Log - Log plot of localization length (γ^{-1}) with $|\omega - \omega_0|$ for different cases. (a) The dimer clusters of mass $m_s = 2$ 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 ω^2 for different cases. The length of the segment here is 10^5 for all cases. (a) The dimer clusters of mass $m_s = 2$ are distributed randomly with concentration $\rho = 0.33$ in an otherwise perfect chain. The smooth behavior 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 $\omega^2 = 4$.

Figure 5. Log - Log plot of bandwidth (Δ_i) with N for different cases. In all cases the trimer clusters are randomly distributed with concentration $\rho = 0.25$ in an otherwise perfect chain. constant factor Σ is added to the ordinate for clarity. (a) Here $m_s = 3$ and $m_0 = 6$. The scaling behavior is shown in two regions of N. The scaling exponents for different regions are given in table 1. The values of Σ are taken from 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 Σ takes the value zero here. (c) Same as (b) but $m_s = 0.75$ and $m_0 = 0.375$.

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 neighbor of m_0 as a function of ω^2. The thin solid line corresponds to $G = \frac{1}{(m_s-1)\omega^2}$. (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 $\omega^2 = 0$.

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

Range of N	$10^2 - 10^3$		$10^3 - 10^4$	
Band index (i)	c	α	c	α
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

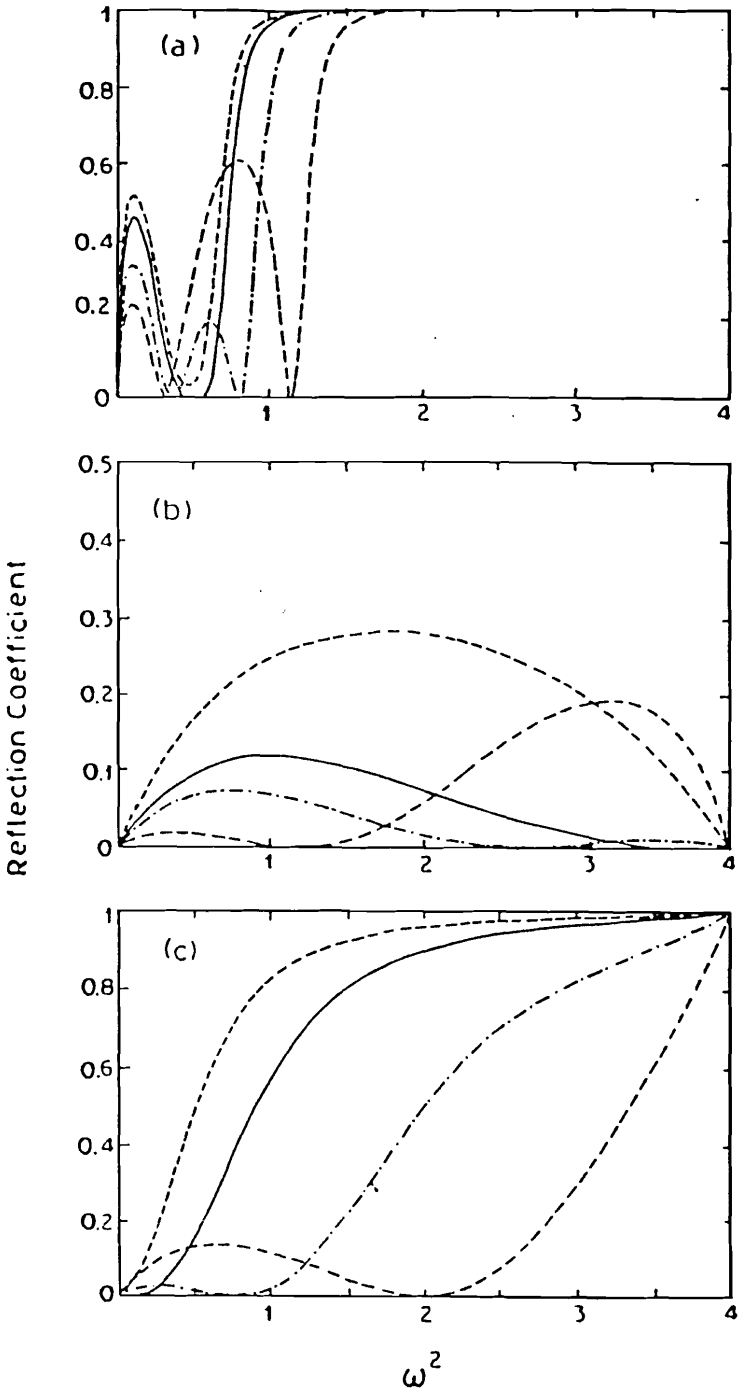
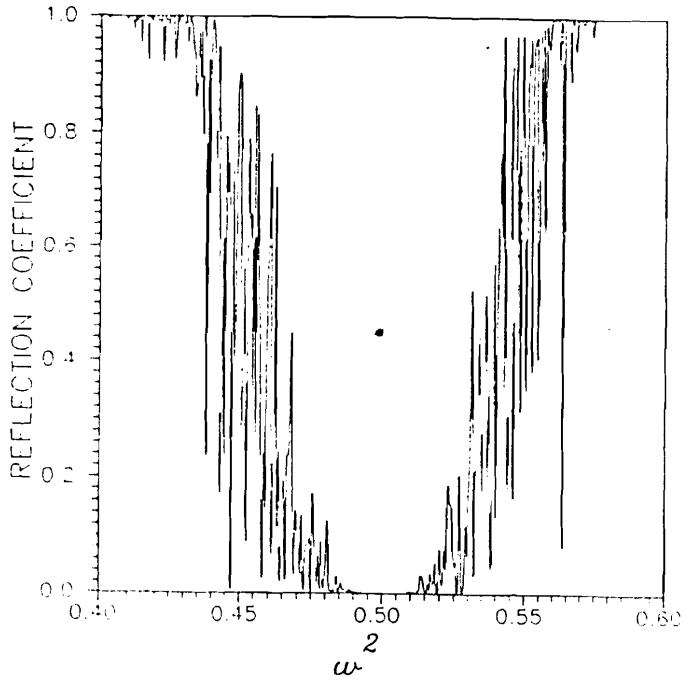


Figure 1.



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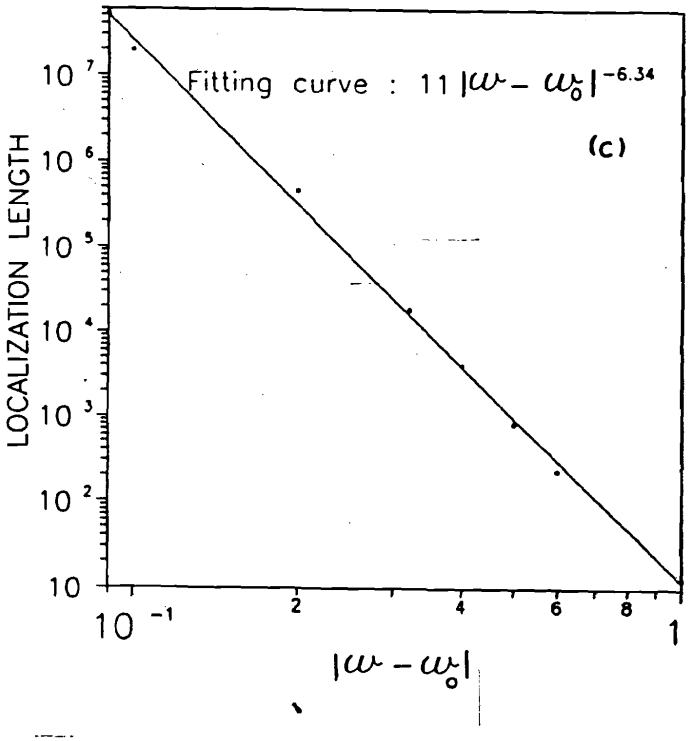

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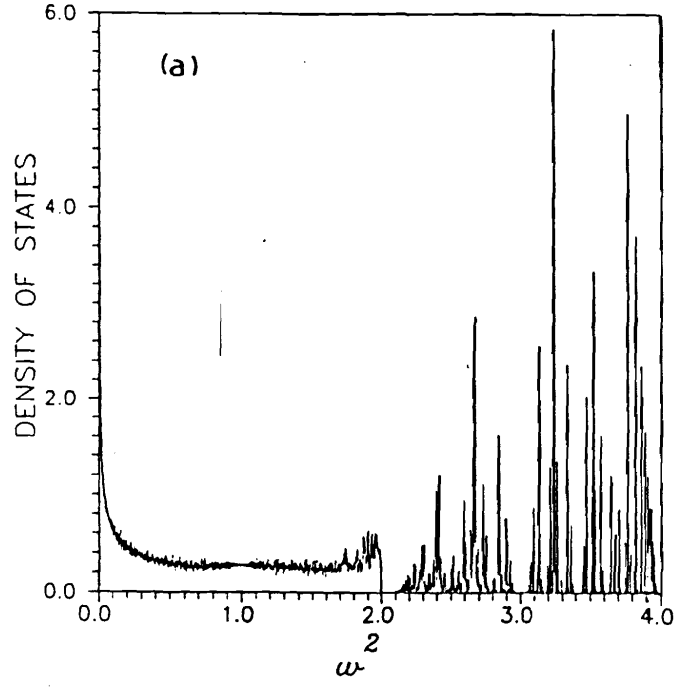

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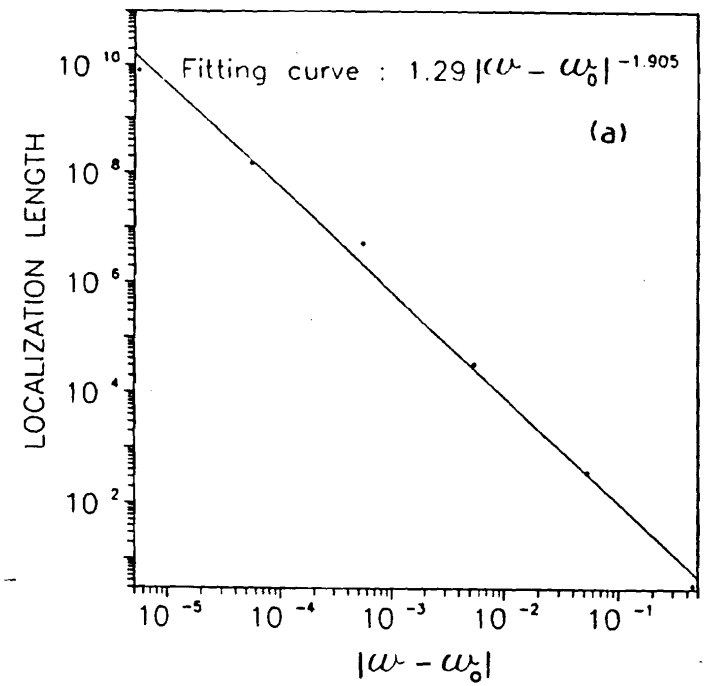

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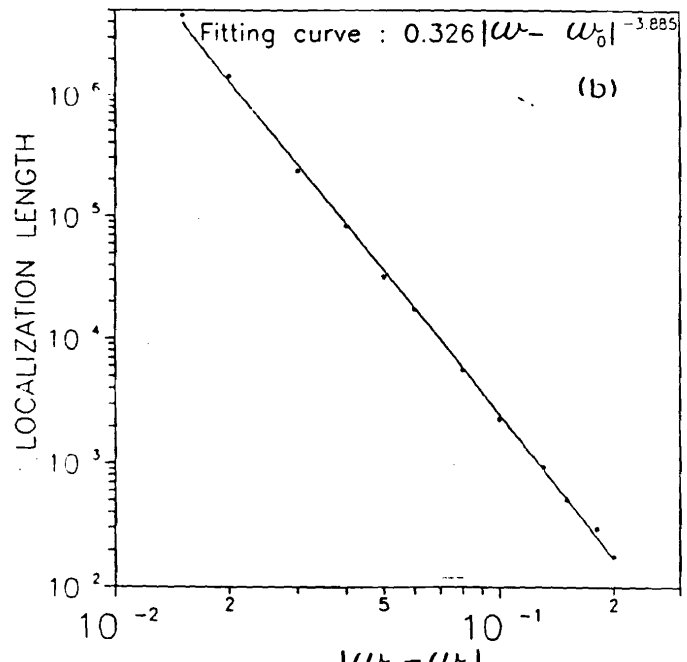

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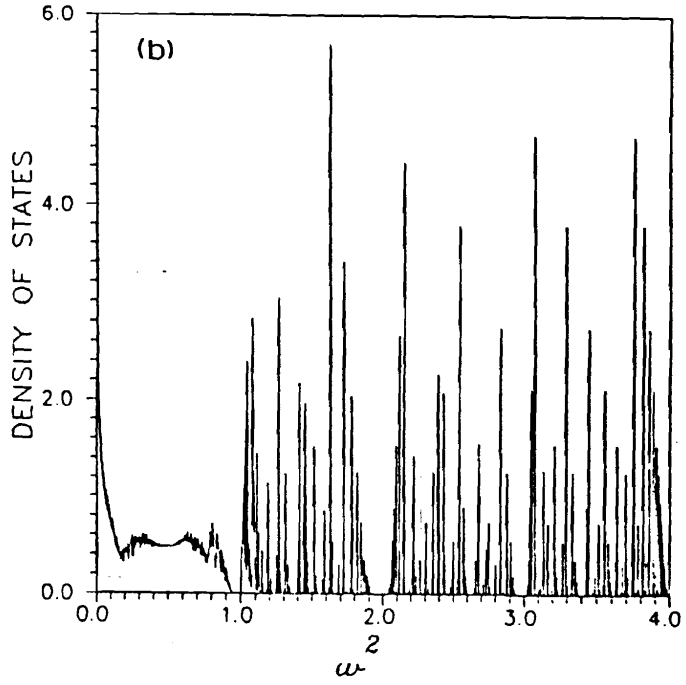

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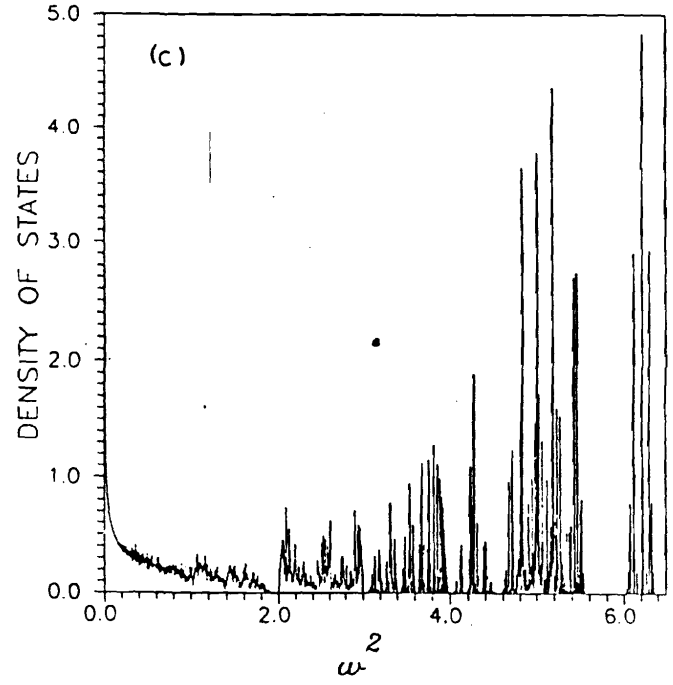

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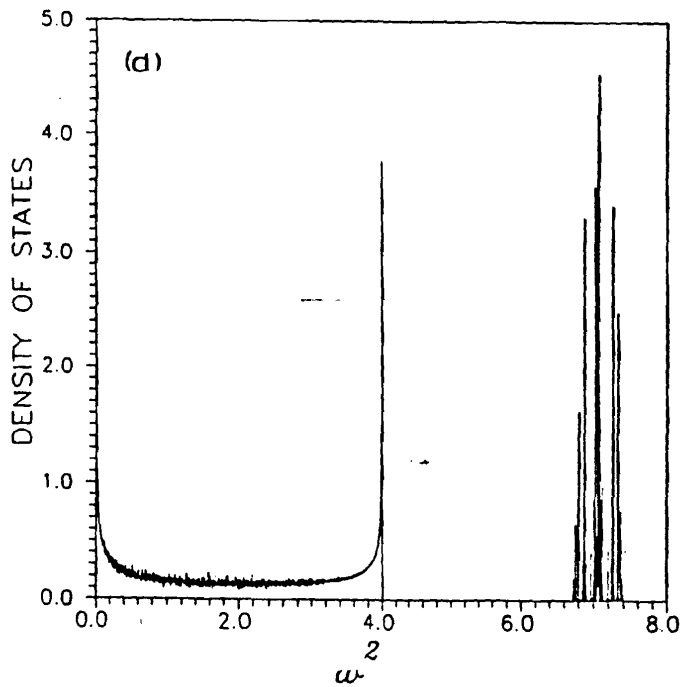

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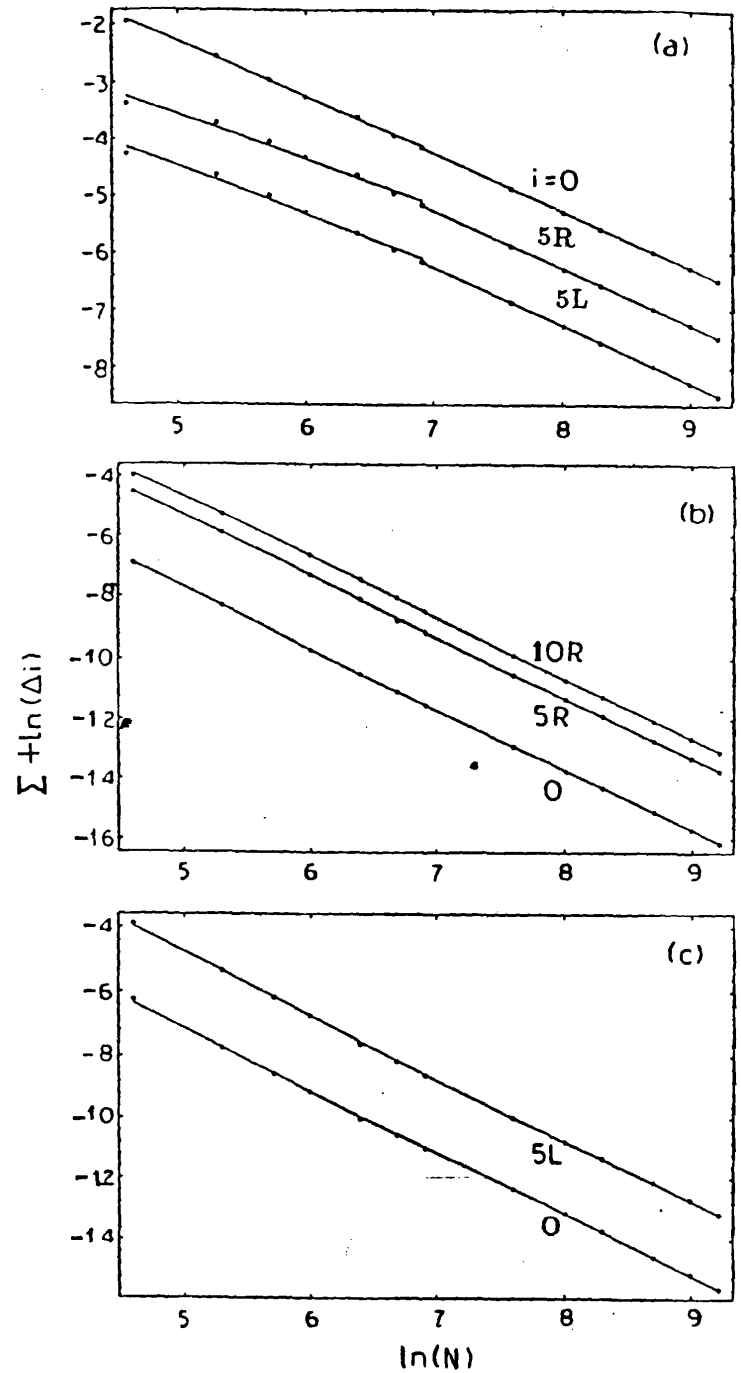

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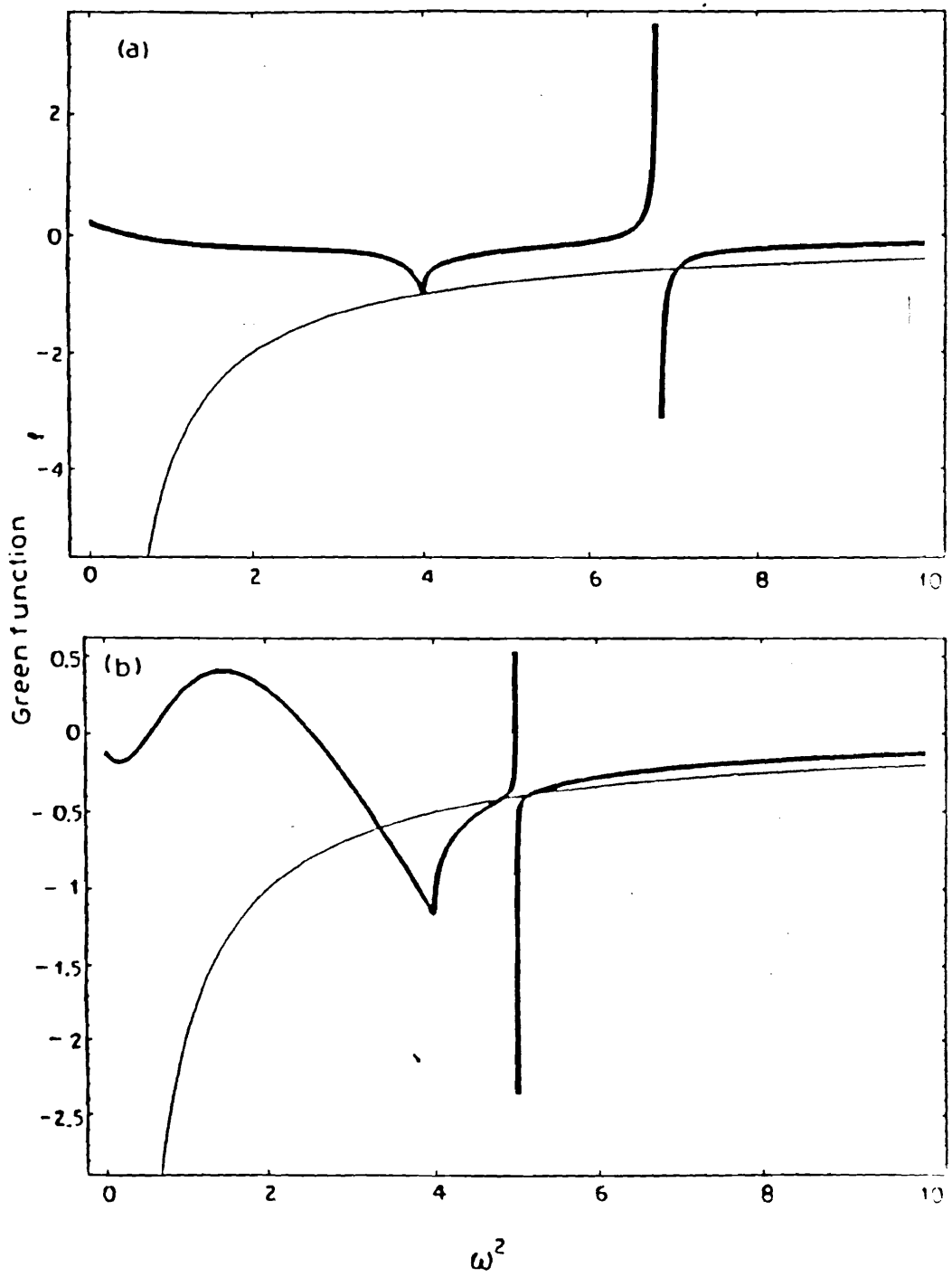

Figure 5