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Energy transport in one-dimensional harmonic chains

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We study the spatial evaluation of a localized energy pulse in one-dimensional perfect as well as mass-disordered (uncorrelated and correlated) harmonic chains. In the classical case the behavior of the second moment $M_2(t)$ of energy distribution strongly depends on the initial excitations, especially in disordered systems. Two types of initial excitations are considered here, namely (a) impulse excitation and (b) displacement excitation. The excitation is applied at a particular mass of the chain. We have shown that $M_2(t)$ can be expressed in terms of the velocity-velocity correlation function in the case of impulse excitation. On the other hand, it is the energy-current–energy-current correlation function for the displacement excitation. The origin of these results has been shown to appear due to the different kinds of initial occupation probability of the modes of the system. For a perfect harmonic chain the difference is seen at the amplitude of $M_2(t)$. On the other hand, the effect is observed in the time exponent of $M_2(t)$ in disordered systems. The effect of mass correlation on the energy transport is investigated. Our numerical calculations support the analytical results. The possible implications of these results are also mentioned.

I. INTRODUCTION

Several unusual features have been recently observed[1,2] in amorphous systems. For example, thermal conductivity shows quadratic temperature dependence at low temperatures, plateau at intermediate temperatures[1] and further increase at higher temperature.[2] The behavior of the thermal conductivity from the plateau to the high-temperature region appears to be determined by disorder and anharmonicity.[3] It is, therefore, essential to study thoroughly the effect of disorder and anharmonicity in the transport of energy. As a prelude, we, therefore, study here the transport of energy in different kinds of uncorrelated and correlated disordered harmonic chains to understand the role of residual nonscattered modes. It has been shown previously[4,5] that uncorrelated mass-disordered systems contain a set of nonscattered modes around the zero frequency. We[6] further showed that the correlations in masses produce extra nonscattered modes in the system. We investigated transmission coefficient, individual bandwidth scaling[7] and density of states to prove the presence of extra nonscattered modes. The number of such modes has also been estimated. Nonscattered modes have also been found in classical one-dimensional harmonic chains with dimeric correlation in spring constants.[8] Generalized moments, the second moment of which is inverse participation ratio, have been analyzed to show that such systems indeed sustain a set of nonscattered modes.

Recently, the spatial evaluation of a localized energy pulse and the second moment of energy distribution have been studied[9–12] to gain a better understanding of the energy transport in amorphous systems. It should be noted that the second moment is related to the thermal conductivity by the Kubo formula. One advantage to study the second moment is that the quantity does not depend upon the boundary conditions of the system. Consequently, the results obtained from this study is very reliable. The most conspicuous feature, however, is that it exhibits different behavior for different kinds of initial excitations, especially in disordered system. Two types of initial conditions are considered here, namely, (a) impulse excitation and (b) displacement excitation. They are given at a particular mass of the system. In earlier works[10,12] the origin of this feature, however, has not been traced. The dependence of the second moment on the nature of initial excitations requires a thorough understanding. This is a further motivation behind this work. Another important point to note is that our work is completely done in Fourier space. This type of calculation is invariably done in real space.[9–12] To the best of our knowledge we show here for the first time that such a calculation can be done in the Fourier space without using directly the properties of Bessel functions. As the results of perfect harmonic chain is known[9] we first study this system. Inasmuch as we show that the second moment of energy distribution is nothing but the velocity-velocity correlation function, we clearly established that the second moment discussed in the text has a status similar to the mean-square displacement of an electron in electronic systems. Although the second moment appears to be energy-current–energy-current correlation function in the case of displacement excitation, we further show that the difference appears due to the different kinds of initial occupation probability given to the modes of the system. This work also gives us further opportunity to check the formula of Dunlap, Kundu and Phillips[13] (DKP) which is used to predict the time exponent of the mean-square displacement of an electron in correlated disordered systems.

II. FORMALISM

We consider here a one-dimensional perfect and infinite harmonic chain, called Hamiltonian chain, consist-

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ing of masses M and springs with spring constant f. The Hamiltonian $\widetilde{H}$ for this system is

$$\widetilde{H} = \sum_m \tilde{h}_m(t) \tag{1}$$

and

$$\tilde{h}_m(t) = \frac{\widetilde{P}_m^2}{2M} + \frac{f}{4}\left[(\widetilde{Q}_{m+1} - \widetilde{Q}_m)^2 + (\widetilde{Q}_m - \widetilde{Q}_{m-1})^2\right]. \tag{2}$$

Here $\widetilde{P}_m$ and $\widetilde{Q}_m$ define the momentum and the displacement of the mass at the mth site. We now define

$$\begin{aligned} \omega^2 &= f/M, \\ P_m &= \widetilde{P}_m/M\omega, \\ Q_m &= \widetilde{Q_m} \\ \tau &= \omega t, \\ h_m(t) &= \tilde{h}_m(t)/M\omega^2. \end{aligned} \tag{3}$$

Then the transformed Hamiltonian can be written as

$$H = \sum_m h_m(\tau) = \frac{\widetilde{H}}{M\omega^2} \tag{4}$$

and

$$h_m(\tau) = \frac{P_m^2}{2} + \frac{1}{4}\left[(Q_{m+1} - Q_m)^2 + (Q_m - Q_{m-1})^2\right]. \tag{5}$$

The Hamilton's equations obtained from (4) and (5) are

$$\begin{aligned} \dot{P}_m(\tau) = \frac{\partial H}{\partial Q_m} &= -\{(Q_{m+1} - Q_m) - (Q_m - Q_{m-1})\} \\ &= -(J_{m+1} - J_m) \end{aligned} \tag{6}$$

and

$$\dot{Q}_m(\tau) = -\frac{\partial H}{\partial P_m} = -P_m(\tau). \tag{7}$$

By $\dot{P}_m(\tau)$ and $\dot{Q}_m(\tau)$ we imply $dP_m/d\tau$ and $dQ_m/d\tau$, respectively. From (6) and (7) we finally obtain

$$\ddot{J}_m(\tau) = J_{m+1} + J_{m-1} - 2J_m \tag{8}$$

and

$$\ddot{P}_m(\tau) = P_{m+1} + P_{m-1} - 2P_m. \tag{9}$$

Since the perfect system is translationally invariant, if we introduce excitation at a mass, called origin, then the following conditions must hold good:
(a) $P_m = P_{-m}$,
(b) $Q_m = Q_{-m}$.
Condition (b) further implies that
(c) $J_m = J_{-(m-1)}$.
Because of condition (c) it can be shown that if q is an odd integer

$$\sum_{m=-\infty}^{\infty} m^q J_m^2 = \sum_{m=0}^{\infty}\sum_{p=1}^{q-1}\binom{q}{p}(-m)^p J_m^2 + \frac{1}{2}\sum_{m=-\infty}^{\infty} J_m^2.$$

Then for $q = 1$, we obtain

$$\sum_m mJ_m^2 = \frac{1}{2}\sum_m J_m^2. \tag{10}$$

The explicit solution for $J_m(\tau)$ and $P_m(\tau)$ can be obtained from the lattice Fourier transform of these quantities. We define

$$F_k(\tau) = \sum_m e^{ikm} f_m(\tau), \tag{11}$$

where $f_m(\tau)$ is either $J_m(\tau)$ or $P_m(\tau)$. Then from (8) as well as (9) we obtain

$$\ddot{F}_k(\tau) + \Omega_k^2 F_k(\tau) = 0, \tag{12}$$

where

$$\Omega_k^2 = 4\sin^2(k/2). \tag{13}$$

The solution of (12) is

$$F_k(\tau) = F_k(0)\cos(\Omega_k\tau) + \frac{\dot{F}_k(0)}{\Omega_k}\sin(\Omega_k\tau), \tag{14}$$

where $F_k(0)$ and $\dot{F}_k(0)$ are obtained from the initial conditions. Before passing to the next section we would like to note that for any integer, q

$$\sum_m m^{2q} f_m^2(\tau) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left|\frac{\partial^q F_k(\tau)}{\partial k^q}\right|^2 dk. \tag{15}$$

Although this is a trivial result, to the best of our knowledge, this is the first paper where this result will find its applicability.

III. MOMENTS OF HAMILTONIAN CHAIN

We note that $h_m(\tau)$ being a sum of positive quantities, satisfies $h_m(\tau) \geq 0$. Furthermore, H is a constant of motion and $0 \leq h_m(\tau)/H \leq 1$. The quantity $h_m(\tau)/H$ gives the fraction of energy that resides at the mth site at time τ. Consequently, it can be interpreted as the probability measure of a localized energy packet of unit strength to be found at the site m at time τ. With this interpretation of $h_m(\tau)/H$ the qth moment of the energy distribution, M_{qn} is defined as

$$M_{qn}(\tau) = \sum_m (m-n)^q h_{m,n}(\tau)/H, \tag{16}$$

where the initial excitation is introduced at the nth mass. For a translationally invariant system, M_{qn} is independent of n. Furthermore, the corresponding first moment $M_1(\tau)$ and second moment $M_2(\tau)$ attain a status similar to the average displacement and the mean-square displacement, respectively, of an electron in a crystal. It is a trivial matter to show that $M_1(\tau)$ is identically zero for a perfect harmonic chain. So, the diffusion coefficient, D of an energy packet through the harmonic chain is

$$D = \frac{1}{2} \lim_{\tau \to \infty} \frac{dM_2(\tau)}{d\tau} \tag{17}$$

while by defination $M_0(\tau) = 1$. $M_2(\tau)$ in Eq. (16) is given by

$$M_2(\tau) = \frac{1}{2H} \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \left[\left| \frac{\partial P_k}{\partial k} \right|^2 + \left| \frac{\partial J_k}{\partial k} \right|^2 \right] \right\} \tag{18}$$

and

$$H = \sum_m h_m(\tau) = \frac{1}{4\pi} \int_{-\pi}^{\pi} dk \left[|P_k|^2 + |J_k|^2 \right]. \tag{19}$$

Equation (18) is obtained by using Eqs. (10) and (15). Equation (19) follows from Eqs. (5) and (15). Higher moments can also be calculated by this procedure. We discuss below the analytical calculation of $M_2(\tau)$ for two different types of initial conditions, namely, (a) impulse excitation and (b) displacement excitation.

A. Impulse excitation

The initial excitation is given at the mass at site $n = 0$, i.e., $P_n(0) = \frac{\delta_{n,0}}{M\omega}$ and $Q_n(0) = 0$ for all n. This yields $H = \frac{1}{2M^2\omega^2}$ and

$$M_2(\tau) = \frac{\tau^2}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial \Omega_k}{\partial k} \right)^2 dk + \frac{1}{2\pi} \int_{-\pi}^{\pi} \sin^2(\Omega_k \tau)\, dk, \tag{20}$$

which finally yields

$$M_2(\tau) = \tau^2/2 + [1 - J_0(4\tau)]/8. \tag{21}$$

Since the last term of the above equation is bounded we obtain, therefore,

$$\lim_{\tau \to \infty} M_2(\tau) = \tau^2/2. \tag{22}$$

B. Displacement excitation

In this case the initial excitation is $P_n(0) = 0$ and $Q_n(0) = \delta_{n,0}$. This, in turn, gives $H = 1$ and

$$M_2(\tau) = \frac{1}{4\pi} \left[\tau^2 \int_{-\pi}^{\pi} \left(\Omega_k \frac{\partial \Omega_k}{\partial k} \right)^2 dk + \int_{-\pi}^{\pi} \left(\frac{\partial \Omega_k}{\partial k} \right)^2 dk + \frac{1}{4} \int_{-\pi}^{\pi} \Omega_k^2 \cos^2(\Omega_k \tau)\, dk \right]. \tag{23}$$

From Eq. (23) we ultimately obtain

$$M_2(\tau) = \frac{\tau^2}{4} + \frac{1}{4} + \frac{1}{8} \left[1 + J_0(4\tau) - J_2(4\tau) \right]. \tag{24}$$

Furthermore due to the boundedness of the last term in Eq. (24) we obtain

$$\lim_{\tau \to \infty} M_2(\tau) = \tau^2/4. \tag{25}$$

These results have already been obtained in Ref. 9. Predictably our results agree with the published results. However, this calculation has a few distinctive features which require special mention. First of all, this type of calculations is invariably done in the real space. To the best of our knowledge we show for the first time that a calculation of this type can be done in the reciprocal space with the help of Eq. (15). Furthermore, this method is quite simple because it does not directly deal with Bessel functions. Instead it exploits the property of their generating function. We would also like to emphasize that the explicit expressions for the leading-order term of $M_2(\tau)$ for both the impulse excitation and displacement excitation are now obtained. This clearly shows the power of this method.

Inasmuch as the definition of $M_2(\tau)$ employed here gives it a status of the mean-square displacement of say, an electron in a perfect crystal, it is worthwhile to discuss the significance of the leading term of Eqs. (20) and (23). We write

$$\widetilde{M}_{2P}(\tau) = \frac{\tau^2}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial \Omega_k}{\partial k} \right)^2 dk \tag{26}$$

and

$$\begin{aligned} \widetilde{M}_{2Q}(\tau) &= \frac{\tau^2}{4\pi} \int_{-\pi}^{\pi} \left(\Omega_k \frac{\partial \Omega_k}{\partial k} \right)^2 dk \\ &= \frac{\tau^2}{2\pi} \int_{-\pi}^{\pi} \left(\frac{\partial E(k)}{\partial k} \right)^2 dk \end{aligned} \tag{27}$$

with

$$E(k) = \frac{1 - \cos k}{\sqrt{2}}. \tag{28}$$

P and Q stand for impulse and displacement excitation, respectively. The significance of Eq. (26) can be understood if we use the phonon language. We take a phonon with wave vector k and mix with it adjoining phonon to form a wave packet with a spread of a few lattice sites. The group velocity of this phonon wave packet $v_k = \partial \Omega_k / \partial k$. Hence, $\widetilde{M}_{2P}(\tau)$ is simply the phonon-velocity–phonon-velocity correlation function. Consequently, the propagation of an energy packet through a harmonic chain can be thought of as diffusion of phonons through the chain. In the case of position excitation, we obtain the electron-velocity–electron-velocity correlation function of an electron in a perfect tight binding crystal with $E(k)$ given by Eq. (28). Hence, the propagation of an energy packet in this case may be interpreted, albeit misleadingly, as the diffusion of an electron in a perfect crystal. Since we are considering a phonon system not an electronic system it is, therefore, prudent to interpret Eq. (27) as the energy-current–energy-current correlation function. The apparent disimilarity of these two expressions can be understood from the standard definition of the velocity-velocity autocorrelation function, as we show below.

The Hamiltonian of the system can be written as

$$H = \sum_k h_k(\tau) = \frac{N}{2\pi}\int_{-\pi}^{\pi} h_k(\tau)\, dk. \qquad (29)$$

Due to the initially given impulse excitation the initial occupation probability of the modes $p_k(0)$, is $h_k(0)/H = 1/N$. The expression of $h_k(0)$ can be obtained by comparing Eqs. (29) and (19). As the second moment $M_2(\tau)$ is equivalent to the mean-square displacement in an electronic system, it should be expressed in terms of velocity-velocity correlation function. So, the second moment can be written as

$$M_2(\tau) = \tau^2 \sum_k v_k^2\, p_k(0) = \frac{\tau^2}{2\pi}\int_{-\pi}^{\pi} v_k^2\, dk.$$

This is exactly obtained in Eq. (26). In the case of initially applied displacement excitation the initial occupation probability of the modes is $p_k(0) = \Omega_k^2/2N$. Using the same formula for the second moment we obtain

$$M_2(\tau) = \frac{\tau^2}{4\pi}\int_{-\pi}^{\pi} (\Omega_k v_k)^2\, dk,$$

which is nothing but Eq. (27). So, the difference arises because of the different kinds of initial occupation probability of the modes of the system. For the case of impulse excitation the initial occupation probability of all the modes are equal and it is $1/N$. On the other hand, displacement excitation makes the initial occupation probability of the modes to depend on k through $\Omega_k^2/2N$. The relevance of this discussion will be transparent in the subsequent sections where we discuss the behavior of $M_2(\tau)$ in the totally disordered and correlated disordered systems.

IV. THE BEHAVIOR OF $M_2(\tau)$ IN UNCORRELATED AND CORRELATED DISORDERED HARMONIC CHAINS

There is one-to-one correspondence between the eigenstates of site disordered tight binding Hamiltonian (TBH) and the normal modes of a mass-disordered harmonic chain.[6] It is a well established result that all eigenstates of a site disordered TBH are exponentially localized.[14] Hence, by corollary all normal modes of a harmonic chain are exponentially localized with exception of modes around $\Omega_0 = 0$.[15] Since disorder in a mass-disordered harmonic chain vanishes at $\Omega_0 = 0$, it has been shown that the system sustains $\sim \sqrt{N}$ nonscattered modes in the neighborhood of the zero-frequency mode.[5] N defines the size of the sample. Reflectionless modes at frequencies other than zero can be obtained in disordered harmonic chains by introducing correlation among the masses.[6] For example, consider a disordered binary system composed of masses m_p with say, $m_p = 1$ and m_a. The spring constant is considered to be unity. If m_a is constrained to appear in pair, we obtain a random dimer chain. This chain has another reflectionless mode at $\Omega_{k_0} = \sqrt{2/m_a}$ provided Ω_{k_0} lies inside the common band of the mass-spring system. Similarly if m_a is constrained to appear as n-mer, we obtain random n-mer chain. This chain can sustain $(n-1)$ reflectionless modes along with the mode at $\Omega_0 = 0$. Another interesting example is a disordered binary chain composed of unit masses and a symmetric trimeric mass system. The central mass of this trimer is m_0 and other two masses are m_s. When $m_0 = m_s(1 \pm \sqrt{4m_s - 3})$ and $m_s > \frac{3}{4}$ two reflectionless modes of this disordered binary system coalesce at $\Omega_{k_0} = \sqrt{1/m_s + 1/m_0}$. Similarly, if $m_0 = 3 - 2m_s$ and $0 < m_s < \frac{3}{2}$, a doubly degenerate reflectionless mode is obtained at $\Omega_0 = 0$. The nature of the modes around the reflectionless mode in these systems has been thoroughly investigated in our previous work.[6]

Although the exact calculation of $M_2(\tau)$ for the uncorrelated and correlated disordered systems is desired, the calculation by the present method or by the real-space method will be quite arduous. However, the asymptotic behavior of $M_2(\tau)$ in time, τ can be discerned by simple physical consideration. If $\tau_{\rm loc}$ is the time taken by the phonon wave packet to traverse the most probable localization length $\tilde{l}_{\rm loc}$ of the normal modes, for $\tau >> \tau_{\rm loc}$, $M_2(\tau)$ can at best grow subdiffusively due to contribution from localized modes. So, if $M_2(\tau)$ grows diffusively or superdiffusively in the asymptotic limit, the propagation of phonons through the nonscattered modes must be responsible for it. DKP formula[13] used this concept and predicts the asymptotic time exponent of the mean-square displacement of an electron in correlated disordered systems. So, we employ here the DKP formula to calculate the asymptotic behavior of $M_2(\tau)$ in τ for the two different initial conditions.

A. Impulse excitation

Suppose the system has l sets of nonscattered modes and the width of the ith set in the reciprocal space, $\Delta k_i \sim N^{-\beta_i}$ and $\beta_i > 0$. We further assume that group velocity of phonon, i.e., $d\Omega_k/dk$ does not vanish in the sets under consideration. Then according to DKP,

$$M_2(\tau) \sim \frac{\tau^2}{2\pi}\sum_{i=1}^{l}\int_{k_{i(\min)}}^{k_{i(\max)}} \left(\frac{\partial\Omega_k}{\partial k}\right)^2 dk$$

$$\sim \frac{\tau^2}{2\pi}\sum_{i=1}^{l}\cos^2(k_{0(i)}/2)/N^{\beta_i}. \qquad (30)$$

$k_{0(i)}$ in the above equation determines the reflectionless mode of a single cluster of impurity atoms in the perfect chain for the ith set. Furthermore, if v is the average group velocity of the phonons which is constant for the systems discussed here then we can write $N = v\tau$. Consequently equation (30) yields

$$M_2(\tau) \sim \frac{1}{2\pi}\sum_{i=1}^{l}\frac{\tau^{2-\beta_i}}{v^{\beta_i}}(1-\Omega^2_{k_{0(i)}}/4). \tag{31}$$

Note that if all β_i's are the same, we obtain from the above equation

$$M_2(\tau) \sim \frac{\tau^{2-\beta}}{2\pi v^{\beta}}\left[l-\sum_{i=1}^{l}\Omega^2_{k_{0(i)}}/4\right]. \tag{32}$$

So, the amplitude of $M_2(\tau)$ will increase. This is actually observed in the case of random dimer chain (discussed later). We now consider various cases.

1. Uncorrelated random chain

Here we have a set of nonscattered modes around $\Omega_0 = 0$. Furthermore, $\Delta k \sim N^{-1/2}$ and $v \sim 1$. So, the second moment for the system is

$$M_2(\tau) \sim \tau^{3/2}/2\pi.$$

2. Random dimer chain

Here we have two sets of nonscattered modes. One set is around $\Omega_0 = 0$ and the other one is around $\Omega_{k_0} = \sqrt{2/m_a}$ with Δk_1 and $\Delta k_2 \sim 1/\sqrt{N}$. So, from formula (32) we obtain

$$M_2(\tau) \sim \frac{\tau^{3/2}}{2\pi\sqrt{v}}(2-\Omega^2_{k_0}/4).$$

So, the presence of an extra set of nonscattered modes with the same nature of width only alters the amplitude of $M_2(\tau)$.

3. Symmetric random trimer chain with degenerate resonances

Here also we have nonscattered modes around $\Omega_0 = 0$ and $\Omega_{k_0} = \sqrt{1/m_s + 1/m_0}$. The assumption is that $m_s > \frac{3}{4}$. Furthermore, $\Delta k_1 \sim 1/\sqrt{N}$ and $\Delta k_2 \sim 1/N^{1/4}$. Then,

$$M_2(\tau) \sim \frac{1}{2\pi}\left[\frac{\tau^{3/2}}{v^{1/2}} + \left\{1-\frac{1}{4}(1/m_s + 1/m_0)\right\}\frac{\tau^{1.75}}{v^{1/4}}\right].$$

When two resonances merge at $\Omega_0 = 0$ we have $\Delta k \sim N^{-1/6}$ and $v \sim 1$. Hence, from formula (32) we obtain

$$M_2(\tau) \sim \frac{\tau^{11/6}}{2\pi}.$$

B. Displacement Excitation

We first examine the situation where a set of nonscattered modes is obtained around $\Omega_0 = 0$. The group velocity here is considered to be unity around $\Omega_0 = 0$ and this gives $N \sim \tau$. So, we obtain

$$M_2(\tau) \sim \frac{\tau^2}{4\pi}\int_0^{k_{\max}} \sin^2 k\, dk$$
$$\sim \frac{\tau^{2-3\beta}}{12\pi}. \tag{33}$$

Since for the completely random system $\beta = \frac{1}{2}$, Eq. (33) gives

$$M_2(\tau) \sim \frac{\tau^{1/2}}{12\pi}.$$

On the other hand, for the symmetric trimer model with degenerate resonances at ($\Omega_0 = 0, \beta = \frac{1}{6}$). Consequently, for this system we obtain

$$M_2(\tau) \sim \frac{\tau^{1.5}}{12\pi}.$$

We now analyze the random dimer chain and symmetric random trimer chain with nonzero degenerate resonances. If we consider the constant value of v we obtain $N \sim \tau$. These systems contain another reflectionless mode along with the zero mode. If we consider the width of the nonscattered zone around the nonzero reflectionless mode behaves like $\Delta k \sim N^{-\beta}$, we obtain

$$M_2(\tau) \sim \frac{\tau^2}{4\pi}\int_{k_{\min}}^{k_{\max}}\left(\Omega_k\frac{\partial\Omega_k}{\partial k}\right)^2 dk$$
$$\sim \frac{1}{4\pi}\left[\Omega^2_{k_0}\left(1-\Omega^2_{k_0}/4\right)\frac{\tau^{2-\beta}}{v^{\beta}} + \frac{\cos(2k_0)}{12}\frac{\tau^{2-3\beta}}{v^{3\beta}}\right]. \tag{34}$$

For random dimer chain $\beta = \frac{1}{2}$ and including the contribution from the nonscattered modes around $\Omega_0 = 0$ we finally obtain

$$M_2(\tau) \sim \frac{\tau^{1/2}}{12\pi v^{3/2}}\left\{1+\frac{\cos(2k_0)}{4}\right\}$$
$$+\frac{\Omega^2_{k_0}(1-\Omega^2_{k_0}/4)}{4\pi v^{1/2}}\tau^{3/2}.$$

Similarly the symmetric random trimer model with degenerate resonances for which $\beta = \frac{1}{4}$ yields

$$M_2(\tau) \sim \frac{\tau^{1/2}}{12\pi v^{3/2}} + \frac{\cos(2k_0)}{48\pi v^{3/4}}\tau^{1.25}$$
$$+\frac{\Omega^2_{k_0}(1-\Omega^2_{k_0}/4)}{4\pi v^{1/4}}\tau^{1.75}.$$

Consider now the situation when $\Omega_{k_0} \to 0$. In the random dimer mass chain for the second term to dominate we need $\tau >> \tau_c$ and τ_c is determined by $\tau_c^{1/2} \sim \Omega^2_{k_0}\tau_c^{3/2}$. This in turn yields $\tau_c \sim \Omega_{k_0}^{-2}$. Since in the second model the second term always dominates the first term, τ_c is obtained by comparing the second term and the last term and this consideration yields $\tau_c = \Omega_{k_0}^{-4}$.

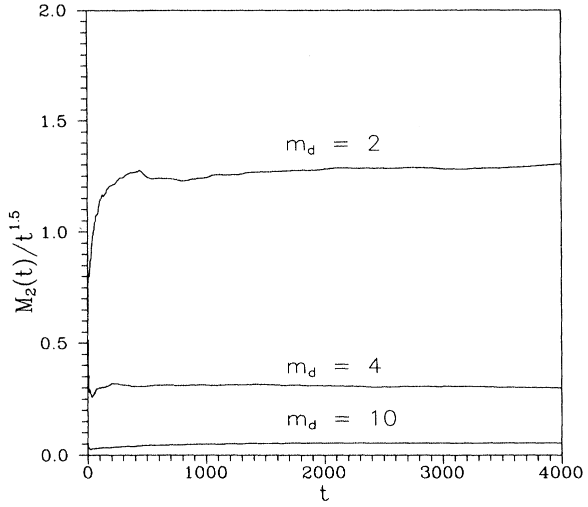

FIG. 1. Plot of $M_2(t)/t^{1.5}$ with time t for uncorrelated mass-disordered harmonic chains with the initially given impulse excitation. The concentration of the defect masses m_d, is $c = 0.5$.

V. NUMERICAL CALCULATIONS OF $M_2(T)$ AND DISCUSSION

In this section we present our numerical calculations of $M_2(t)$ for the uncorrelated and correlated mass disordered harmonic chains. We consider both the impulse excitation and displacement excitation. For a chain of N masses we have N coupled second-order differential equations of $\widetilde{P}_m(t)$ and $\widetilde{Q}_m(t)$. These differential equations are solved on expanding lattice using fourth order Runge-Kutta method. Furthermore we employed binary distribution of masses. Our results are discussed below.

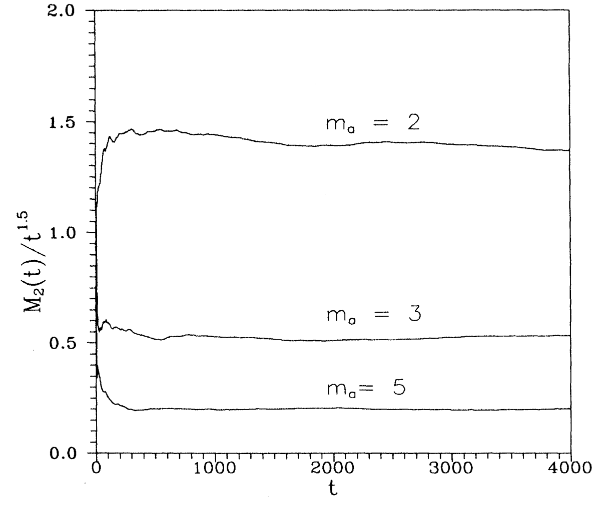

FIG. 2. Plot of $M_2(t)/t^{1.5}$ with time t for random dimer chain with initially given impulse excitation. The concentration of dimer impurity is $c = 0.33$.

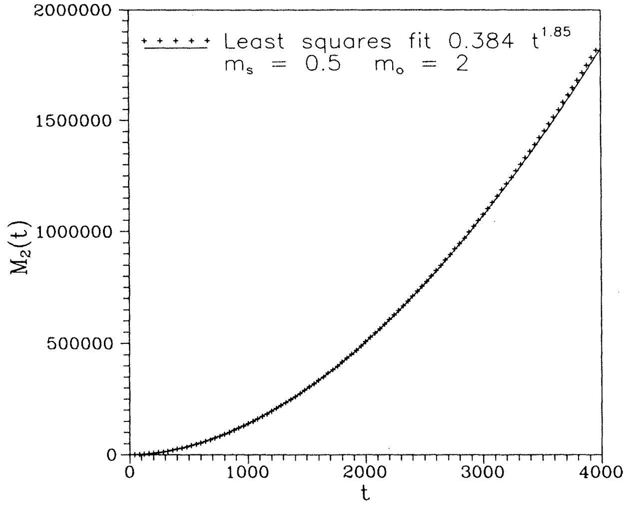

FIG. 3. Plot of $M_2(t)$ as a function of t for symmetric random trimer chain with degenerate resonances at $\Omega_0 = 0$ with the initially given impulse excitation. Here concentration of trimer is $c = 0.25$.

A. Impulse excitation

We first consider the uncorrelated disordered binary harmonic system. The system is composed of a unit mass and a second mass with mass ratio m_d. The spring constant f is considered to be unity in all the cases discussed here. $M_2(t)$ for the system is calculated for different mass ratios and in different samples. A set of prototype results is shown in Fig. 1. We find that $M_2(t) \sim At^{3/2}$. The value of the exponent is in agreement with our analytical result. $M_2(t)$ for random dimeric mass chain is also calculated. Since both sets of nonscattered modes should give

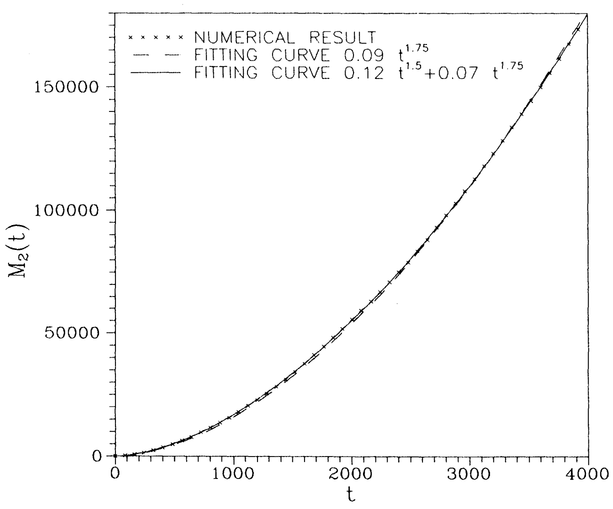

FIG. 4. Same as Fig. 3 but $\Omega_{k_0} \neq 0$. Here $m_s = 3$ and $m_0 = 6$.

~ 1.5 for the exponent, we expect that $M_2(t) \sim C t^{3/2}$ for this system. This is observed and shown in Fig. 2. $M_2(t)$ for random symmetric trimer model with doubly degenerate resonances is also studied. When $\Omega_0 = 0$ is the position of the doubly degenerate resonances, we expect that the exponent should be ~ 1.83. Our numerical result also agrees and it is shown in Fig. 3. When the doubly degenerate resonances is not at $\Omega_0 = 0$, $M_2(t)$ according to our formula is a linear combination of two terms with exponents ~ 1.5 and ~ 1.75. We indeed find that $M_2(t)$ for this model is better described by such a combination (see Fig. 4). A single exponent fitting of $M_2(t)$ with exponent of 1.75 is also included in Fig. 4. This suggests that the nonscattered modes are primarily responsible for the superdiffusive behavior in the random and this type of correlated disordered chains.

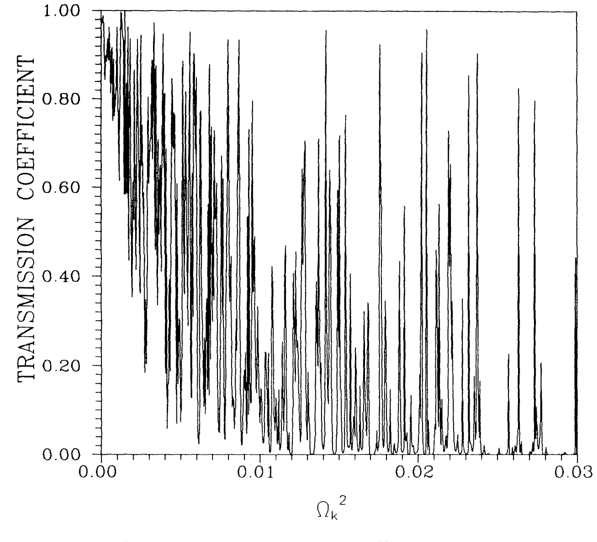

FIG. 6. Plot of transmission coefficient as a function of Ω_k^2 for uncorrelated mass-disordered harmonic chain of length $N = 5000$. Here, $m_d = 2$ and $c = 0.5$.

B. Displacement excitation

We mostly discuss here the behavior of the second moment, $M_2(t)$ in uncorrelated random system. It is pointed out in Ref. 10 that the time exponent of $M_2(t)$ with displacement excitation is significantly different from the corresponding exponent of the impulse excitation. However, neither any rigorous estimation nor any convincing explanation of this observed behavior has been provided.[10] Inasmuch as our analytical calculation predicts that the exponent of $M_2(t)$ is 0.5, some of our protype results are shown in Fig. 5. In this case we observe the oscillating behavior in $M_2(t)$ as well as the increasing tendency with time t. We fitted the plots with the exponent 0.6 of time t. The exponents, however, in this case are significantly larger than the expected value (0.5). To understand this we analyzed the transmission coefficient of this system as shown in Fig. 6. It should be noted that the spectrum contains many fringe resonances. The position of these resonances depends on the sample length as well as on the sample. Since all the nonscattered modes have equal occupation probability as $(1/N)$ in the case of momentum excitation they contribute equally to $M_2(t)$. On the other hand, for displacement excitation the occupation probability of the nonscattered modes is given by $\Omega_k^2/2N$. Therefore, the contribution of these modes to $M_2(t)$ is weighted by Ω_k. So, the contribution of the fringe resonances to $M_2(t)$ is not significantly suppressed. The fluctuation occurs because fringe resonances appear randomly. To prove

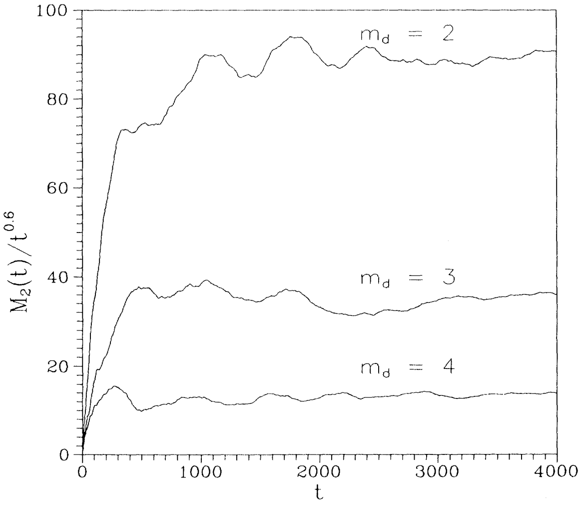

FIG. 5. Plot of $M_2(t)/t^{0.6}$ against t for uncorrelated mass-disordered harmonic chains with the initially given displacement excitation. Here $c = 0.5$.

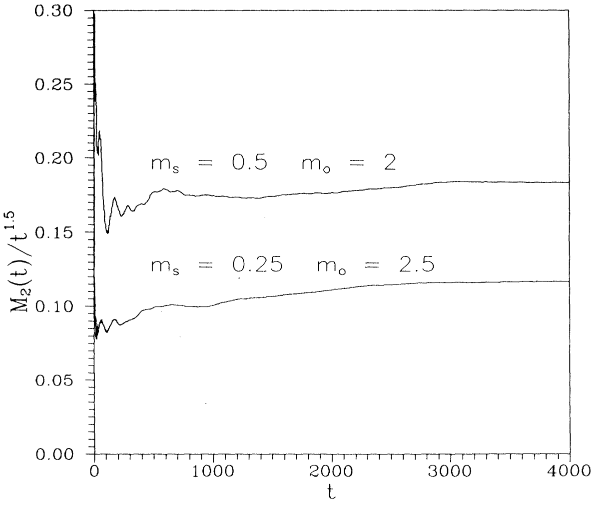

FIG. 7. Plot of $M_2(t)/t^{1.5}$ as a function t for symmetric trimer chain with degenerate resonances at $\Omega_0 = 0$ with the initially given displacement excitation. Here $c = 0.25$.

this we studied $M_2(t)$ with the displacement excitation of the symmetric random trimer model with degenerate resonances at $\Omega_0 = 0$. The expected value of the exponent is 1.5. The observed value agrees well with the prediction. Furthermore, the evolution of $M_2(t)$ does not show any perceptible fluctuation (see Fig. 7). This is obtained because the width of the nonscattered modes is large compared to that in the uncorrelated disordered system. Hence, the contribution from the fringe resonances is suppressed. We also studied the behavior of $M_2(t)$ in the random dimer mass chain as well as in the symmetric random trimer model with a degenerate resonance at $\Omega_{k_0} \neq 0$. The predictable values of the exponent for these systems are ~ 1.5 and ~ 1.75, respectively. This is observed. The behavior of $M_2(t)$ in these systems is also studied by bringing the resonance frequency Ω_{k_0} towards zero. According to the analytical calculation, we should not observe the above exponents within the critical time. Qualitatively this trend is observed in both the cases. However, no quantitative estimation is done.

VI. CONCLUSION

We conclude the paper by mentioning primarily the salient features of this study. First of all, we show how the second moment $M_2(t)$ of the energy distribution in a Hamiltonian chain can be calculated in the Fourier space. To the best of our knowledge, this procedure has not been applied before. The power of the technique is further revealed by obtaining compact as well as revealing expressions for $M_2(t)$ for two different kinds of excitations, namely (a) impulse excitation and (b) displacement excitation. In the case of impulse excitation, the asymptotic expression of $M_2(t)$ is predictably found to be phonon velocity-velocity correlation function. On the other hand, for the displacement excitation, the expression can be interpreted as energy-current–energy-current correlation function. The apparent dissimilarity of these two expressions is shown to originate from the way modes are populated by two different kinds of excitations. In the case of impulse excitation, every normal mode is occupied with a probability $1/N$ whereas it is $\Omega_k^2/2N$ for displacement excitation. This is one of the thrust results of this paper. The importance of this understanding is best appreciated by noting that the observed growth of $M_2(t)$ in uncorrelated disordered systems with displacement excitation is subdiffusive. On the other hand, it is superdiffusive with a time exponent ~ 1.5 in the case of impulse excitation. We also predict a time exponent of ~ 0.5 for the first case. The observed discrepancy between the numerical result and the predicted exponent is also resolved by studying further $M_2(t)$ in a symmetric trimer model with degenerate resonances at $\Omega_0 = 0$. Hence, the role of fringe resonances in the energy transport is discerned. Although the subdiffusive behavior of $M_2(t)$ for displacement excitation has been observed previously, this paper rigorously established its origin. In a continuation, we also studied the effect of mass correlation on the energy transport. In the case of impulse excitation, the symmetric trimer model with doubly degenerate resonances at $\Omega_0 = 0$ yields a time exponent of 11/6. This is the largest value of the exponent in correlated disordered systems[13,16] so far obtained. Although it is theoretically possible to improve upon this value, this will most probably lead to a very complicated system. In the case of impulse excitation we have shown explicitly that the widths of the nonscattered modes with same exponent can only increase the amplitude of $M_2(t)$. We further showed that the critical time t_c beyond which the desired value of the time exponent is obtained goes as $\Omega_{k_0}^{-2}$ and $\Omega_{k_0}^{-4}$ for the dimeric and trimeric chain, respectively, as $\Omega_{k_0} \to 0$. Hence, we conclude that the time exponent of $M_2(t)$ in disordered systems depends on the correlation as well as on the initial occupation probability of the modes in the system. So, the correlation and the initial occupation probability of the modes can be used as control parameters to monitor the low-temperature thermal conductivity of amorphous materials. This study also suggests that the electrical conductivity in correlated disordered systems can be altered by selectively populating the nonscattered states. Hence, the idea of selective population may be useful in developing better electronic filters.

It should be noted that thermal conductivity of uncorrelated mass-disordered systems depends on the boundary conditions of the system. This is observed in both analytical[5] and numerical calculations.[17] Thermal conductivity diverges as $N^{1/2}$ for free end boundary condition whereas it vanishes as $N^{-1/2}$ for fixed boundary condition. We obtain the same type of behavior in diffusion coefficient for different types of initial excitations. Inasmuch as we are dealing with infinite systems, it is quite likely that the dependence of the thermal conductivity on the boundary condition in finite systems is manifested here in initial conditions. This aspect therefore, needs closer scrutiny. This work is presently in progress.

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[1] R. C. Zeller and R. O. Pohl, Phys. Rev. B **4**, 2029 (1971).

[2] D. G. Cahill and R. O. Pohl, Phys. Rev. B **35**, 4067 (1987).

[3] R. Orbach, Philos. Mag. B **65**, 289 (1992).

[4] H. Matsuda and K. Ishii, Prog. Theor. Phys. Suppl. **45**, 56 (1970).

[5] K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77 (1973).

[6] P. K. Datta and K. Kundu, J. Phys.: Condens. Matter **6**, 4465 (1994).

[7] P. K. Datta, D. Giri, and K. Kundu, Phys. Rev. B **48**, 16 347 (1993).

[8] F. Domínguez-Adame, E. Maciá, and A. Sánchez, Phys. Rev. B **48**, 6054 (1993).

[9] J. Vazquez-Marquez, M. Wagner, M. Montagna, O. Pilla, and G. Viliani, Physica B **172**, 355 (1991).

[10] M. Wagner, G. Zavt, J. Vazquez-Marquez, G. Viliani, W. Frizzera, O. Pilla, and M. Montagna, Philos. Mag. B **65**, 273 (1992).

[11] M. Wagner, A. Lütze, G. Viliani, W. Frizzera, and O. Pilla,

Physica B **190**, 285 (1993).

[12] G. S. Zavt, M. Wagner, and A. Lütze, Phys. Rev. E **47**, 4108 (1993).

[13] D. H. Dunlap, K. Kundu, and P. Phillips, Phys. Rev. B **40**, 10 999 (1989).

[14] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).

[15] P. Dean, Proc. Phys. Soc. **84**, 727 (1964).

[16] D. Giri, P. K. Datta, and K. Kundu, Physica B (to be published).

[17] W. M. Visscher, Prog. Theor. Phys. **46**, 729 (1971).