

Damping of Long-Wavelength Acoustic Phonons in a Disordered Anomalous Solid with Parabolic Phonon Dispersion

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(Received April 11, 2010)

We propose a new anomalous soft solid with parabolic acoustic phonon dispersion relation, which yields a strong damping of long-wavelength acoustic phonons (sonic or super-sonic wave) under an induced weak disorder. The proposal is confirmed by calculating the damping rate of the acoustic phonons numerically.

The damping rate (Lyapunov exponent) corresponding to the inverse of localization length has a remarkable peak at very low frequency. Both the peak value and corresponding characteristic frequency are power-law increasing functions of the strength of disorder. When we derive the peak value of the Lyapunov exponent as a function of the characteristic frequency, the peak value numerically appears proportional to the root of the characteristic frequency in our one- and two-dimensional cases. The numerical result is enough for us to confirm a strong localization of the acoustic phonons in the frequency region of sound wave of the order of 10^3 Hz in one and two dimensions.

PACS numbers: 43.55.Ti, 62.65.+k, 63., 63.20.-e, 63.20.D-, 63.20.Pw, 63.50.Gh

I. INTRODUCTION

It is widely known that acoustic lattice vibration of solids of long-wavelength limit is understood as the vibration of a corresponding continuous elastic homogeneous media, and it is described by a normal wave equation, which is characterized only by wave velocities [1, 2]. That is, the eigenfrequency ω of acoustic phonons depends linearly on the wave number k in the long-wavelength (that is low-frequency) region. Exceptional case has been known in the bending modes of plate and twisting modes of rod (which are called as flexural modes) with parabolic acoustic-phonon dispersion relations [1–3]. We had believed that we do not have parabolic dispersion in bulk phonons. However, the parabolic dispersion seems to be observed in graphite [4–10]. In addition, it is expected to be observed in a soft mode of acoustic phonons at the Γ point in a solid near a ferro-elastic transition point [11–15].

Recently, we have proposed that we can construct the parabolic dispersion for bulk acoustic phonons within the framework of harmonic approximation [16–18]. We can find the parabolic dispersion when we have a solid in which some negative force constants of the

harmonic lattice keep a good balance with other positive force-constants. In this case, the linear term with respect to wave number disappears in acoustic-phonon dispersion, and the parabolic term appears. When a very small linear term survives with the parabolic term, we can find a very small cut-off frequency ω_c , which divides a “normal” frequency region on the lower side and an “anomalous” frequency region on the higher side.

The bulk phonons with pure parabolic dispersion exhibit a “mechanical instability” and a “thermal instability,” as in the flexural modes [17, 18]. The mechanical instability is the one by which the solid is unstable under a uniform deformation such as uniform expansion or uniform shear. The special unstable modes are characteristic to the solids with free boundary condition and do not appear in those with periodic boundary condition. The thermal instability comes from a high density of state ρ , that is, a low spectral dimension, of the acoustic phonons in the low-frequency region. The spectral dimension d^* is $d/2$, that is, $\rho(\omega) \propto \omega^{(d/2-1)}$, where d is the space dimension. The low dimensionality of the acoustic phonons leads us to the divergence of the mean square displacement of atoms at finite temperature. The divergence is an ultra-red divergence coming from the high density of state near $\omega = 0$. The instabilities can be suppressed by an unharmonicity or by inducing a cut-off frequency ω_c (cut-off wave-number), which recovers the normal character of solids in the long-wavelength limit [17, 18].

In the anomalous solid, low-energy phonons are like massive Bosons and the group velocity vanishes in the long-wavelength limit. This suggests a strong localization of long-wavelength acoustic phonons in the disordered system, which has been dramatically observed in the systems with flat dispersion relation [19–22].

We firstly made a numerical computer simulation of the dynamics of an injected wave packet in the disordered anomalous solid of one and two dimensions in a very low frequency region of the acoustic phonons around the cut-off frequency ω_c [16]. We found a remarkable strong damping of the wave packets in the transmission of low-frequency acoustic phonons.

Secondly, we conducted an IPR (Inverse Participation Ratio) analysis for the eigenstates of the disordered anomalous solids in one and two dimensions [17]. We found a remarkable peak of a trend of localization again around the cut-off frequency ω_c of the acoustic phonons. That is, the both strong localization phenomena appeared around the characteristic frequency ω_c .

However, the abovementioned studies are qualitative ones. We have not made a quantitative argument of the localization of acoustic phonons in the disordered anomalous solid. This is the principal motive of us for pursuing the present study. We show in this paper some numerical results of the damping rate (Lyapunov exponent of the wave function, abbreviated as L-exponent throughout this paper) of the low-frequency acoustic phonons as a function of eigenfrequency and strength of disorder. The localization length of the eigenfunction is understood as the inverse of the L-exponent.

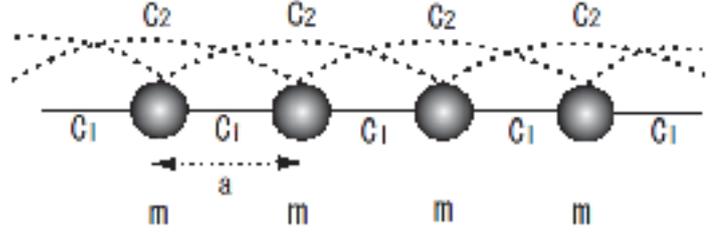


FIG. 1: Conceptual figure of a simple one-dimensional anomalous harmonic solid with a mass m , the nearest-neighbor interaction of force constant c_1 , the second-neighbor interaction of c_2 , and the lattice constant a .

II. DAMPING RATE OF LOW-FREQUENCY ACOUSTIC PHONONS IN ONE- AND TWO-DIMENSIONAL DISORDERED ANOMALOUS SOLIDS

The damping rate of the wave function is numerically obtained by calculating the L-exponent of wave function for a sufficiently long system of length N of the order of $10^5 \sim 10^6$ unit cells. In two dimensions, we impose cyclic boundary condition in the direction of the “width” of the “strip,” and we change the width S from 6 to 20 unit cells and estimate the $S \rightarrow \infty$ limit of L-exponent by using “width scaling.” The calculation is performed by adopting QR decomposition for the product of transfer matrices transferring the amplitudes of the wave function along the linear chain (in one dimension) or along the quasi-one-dimensional system (in two dimensions).

II-1. One-dimensional case

We start by describing the simplest mono-atomic anomalous linear chain with mass m , the nearest-neighbor force constant c_1 , the second-neighbor force constant c_2 , and the lattice constant a , as shown in Fig.1 for the case of periodic system.

The Newton’s dynamical equation of motion of the displacement u of the n -th atom from the equilibrium position at time t is written, assuming the harmonic solution $u(n,t) = u(n)\exp\{-i\omega t\}$ as

$$\begin{aligned}
 -m\omega^2 u(n) &= c_1(n+1, n)(u(n+1) - u(n)) - c_1(n, n-1)(u(n) - u(n-1)) \\
 &\quad + c_2(n+2, n)(u(n+2) - u(n)) - c_2(n, n-2)(u(n) - u(n-2)), \\
 (n &= 1 \sim N),
 \end{aligned} \tag{1}$$

where ω is the eigenfrequency. The eigenvalue equation is solved for periodic system by

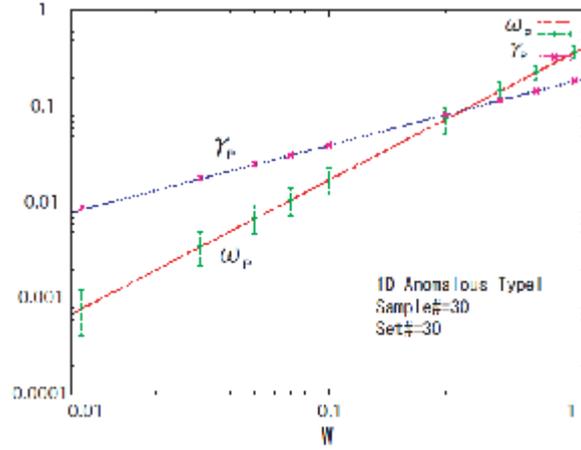


FIG. 2: Peak value of L-exponent γ_p and the corresponding frequency ω_p of the disordered anomalous solid of type I as a function of the strength of disorder W . The error bars have been calculated for 30 sets of the averaged value taken over 30 randomly generated sample systems. The straight lines are for the help to our eyes.

assuming the Bloch-type eigenfunction $u(n) = \exp\{ikna\}$ with wave number k and taking the Fourier transform of it, and we get the following dispersion relation:

$$\omega^2(k_i) = \frac{2c_1}{m}(1 - \cos k_i a) + \frac{2c_2}{m}(1 - \cos k_i 2a) \quad (2)$$

$$= \frac{1}{m}(c_1 + 4c_2)a^2 k_i^2 + \frac{1}{12m}(-c_1 - 16c_2)a^4 k_i^4 + O(a^6 k_i^6) \quad (3)$$

where $k_i = (2\pi/Na)i$ with $(i = -[N/2] \sim -1, 0, 1, \sim [N/2])$ is the i -th wave number. In the normal case where the coefficient $(c_1 + 4c_2)$ is positive and hence does not vanish, we obviously have a normal linear dispersion relation near the Γ -point. But if we consider a special case where the “vanishing condition”

$$(c_1 + 4c_2) = 0, \quad (4)$$

is kept between the force-constants, assuming $c_1 > 0$, then we have the positive coefficient $(-c_1 - 16c_2)$ and a parabolic dispersion relation. The negative force-constant $c_2 = -(1/4)c_1$ only works together with the positive one c_1 and hence yields no complex (pure-imaginary in this case) eigenfrequency except for $k=0$ at the Γ -point, which is the same as the case of normal solid with linear dispersion relation. In this study, we call the solid as “anomalous” solid for the case $c_1 = 4$ and $c_2 = -1$, and “normal” solid for the case $c_1 = 4$ and $c_2 = 1$.

We next introduce a disorder in each of the force constants c_1 and c_2 , independent of site n , with a probability distribution. We first define a fundamental uniform distribution $p(\delta)$, which takes the value of $1/W$ for the argument δ over the period of $-(1/2)W \sim$

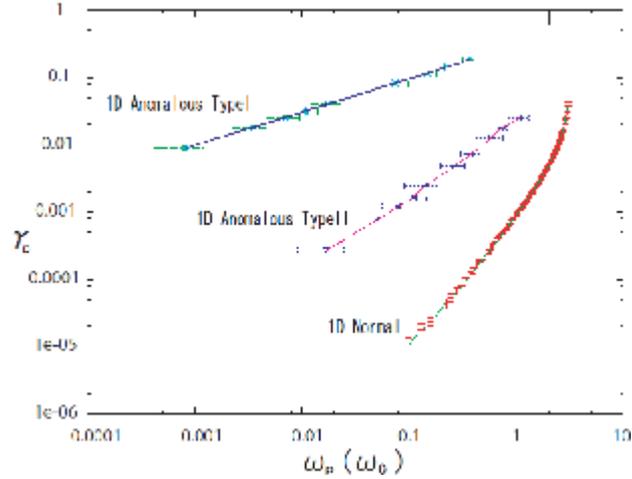


FIG. 3: Peak values of L-exponent γ_p of disordered anomalous solids of type I and type II as a function of the corresponding frequency ω_p or ω_c . The ω dependence of L-exponent γ of normal disordered systems is shown for reference. The error bars have been calculated for 30 sets of the averaged value taken over 30 randomly generated sample systems. The lines are for the help to our eyes.

(1/2) W and takes the value of 0 for the others. We call W a strength of disorder. Then we can define $p_1(c_1) = p(c_1 - 4)$ and $p_2(c_2) = 4p(4(c_2 - (-1)))$ as type I, in which the statistical average of c_1 , $\langle c_1 \rangle$, is 4 and that of c_2 , $\langle c_2 \rangle$, is -1. Thus, the statistically averaged solid describing the long wavelength limit of the disordered system satisfy the vanishing condition $(\langle c_1 \rangle + 4 \langle c_2 \rangle) = 0$. We can also define $p_1(c_1) = p(c_1 - (4 + W/2))$ and $p_2(c_2) = 4p(4(c_2 + 1))$ as type II, in which $\langle c_1 \rangle = 4 + W/2$ and $\langle c_2 \rangle = -1$, and hence, $(\langle c_1 \rangle + 4 \langle c_2 \rangle) = W/2 > 0$. In type II, the characteristics of normal solid should recover in the low frequency region below ω_c . We study types I and II in this paper as well as the normal disordered system (with $p_1(c_1) = p(c_1 - 4)$ and $p_2(c_2) = 4p(4(c_2 - 1))$) as a reference system representing a normal disordered solid.

Eq.1 can be understood as a recurrence equation, which derives $u(n+2)$ from $u(n+1)$, $u(n)$, $u(n-1)$, and $u(n-2)$. We can thus define a transfer matrix t_n and the product of the transfer matrices T_N , which relate the amplitude vector $u_n = (u(n+1), u(n), u(n-1), u(n-2))^T$ for two adjacent n 's and also for two distant n 's as

$$u_{n+1} = t_n u_n, \quad u_{N+1} = T_N u_1, \quad T_N = t_N t_{N-1} \cdots t_2 t_1. \quad (5)$$

Then, we can define L-exponent γ of wave function by finding the minimum eigenvalue $\lambda_m^2(N)$ of $M_N = (T_N)^T T_N$ bigger than or equal to unity as

$$\gamma = \lim_{N \rightarrow \infty} \gamma(N), \quad \gamma(N) = \frac{1}{2N} \log \lambda_m^2(N). \quad (6)$$

The eigenvalues of T_N or M_N usually diverge and vanish exponentially with respect to N and we cannot numerically calculate T_N and M_N directly by making the product of the transfer matrices. We thus use the QR algorithm to get $\gamma(N)$ numerically.

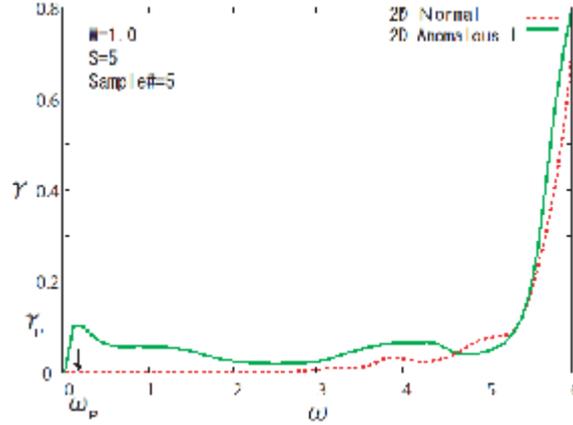


FIG. 4: Typical overall feature of the ω dependence of the L-exponent γ of disordered anomalous solid of type I, for the case of the strength of disorder $W=1.0$ and of the width of the strip $S=5$. The L-exponent has been averaged over 5 random sample systems. The corresponding L-exponent of normal disordered systems is shown for reference.

We first confirmed the convergent property of $\gamma(N)$ and that of the sample fluctuation $\sigma(N)$, both with respect to N . The numerical value of $\gamma(N)$ becomes stable for N bigger than a critical value of the order of $10^3 \sim 10^4$ depending on the given frequency ω and the strength of disorder W . On the other hand, the variance σ behaves as $\sigma(N) \propto 1/\sqrt{N}$. We calculate L-exponent for sufficiently long system until we get at least the inequality $\sigma(N)/\gamma(N) < 10^{-1}$.

A striking feature of ω -dependence of the L-exponent γ for disordered anomalous solids is that it always shows a remarkable local peak at a very low frequency. That is, $\gamma(\omega)$ does not decrease with decreasing the value of ω and it has a local maximum at a small value of ω even though the phonons are acoustic ones. The characteristics are consistent with the strongly localized wave functions found in the IPR analysis made in Ref. 18. We call the characteristic frequency as peak frequency ω_p and call $\gamma(\omega_p)$ as the peak value of L-exponent γ_p . Their W -dependences are shown in Fig.2.

From $\omega_p(W)$ and $\gamma_p(W)$ we finally get γ_p as a function of ω_p , which would be our main result (Fig.3). We get a similar result also for the disordered anomalous solid of type II, replacing ω_p into ω_c .

II-2. Two-dimensional case

As the simplest two-dimensional anomalous solid, we consider a simple square lattice with mass m and with nearest-neighbor and second-neighbor interactions of force constants c_1 and c_2 , respectively, only along x and y directions. When we observe only the x -direction or y -direction, the structure is just like the one-dimensional anomalous system shown in Fig.1. The system is obviously unstable under sheer stress, but we disregard it to save the

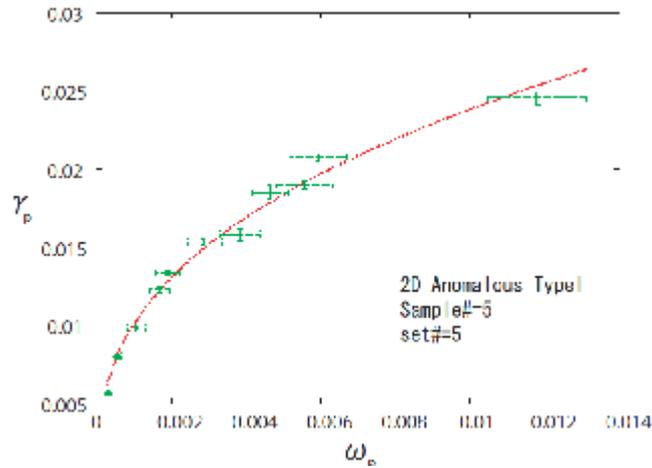


FIG. 5: Peak values of L-exponent γ_p in disordered anomalous solids of type I as a function of the corresponding frequency ω_p . The error bars have been calculated for five sets of the averaged value taken over five randomly generated sample systems. The line is for the help to our eyes.

computing time. In addition, we consider only one component of the deviation of atom, which would be perpendicular to the square lattice on the $x - y$ plane. We introduce a disorder into the system just like the case of one dimension. We introduce $p_1(c_1)$ and $p_2(c_2)$ in each of the force-constants c_1 and c_2 , respectively, independently of the lattice sites. Both type I and type II are studied.

To calculate the L-exponent of the wave function in two dimensions, we study a sufficiently long strip of length N and width S . The length N is of the order of 10^5 and the width S varies from 6 to 20. After calculating the L-exponent $\gamma(N, S)$ by the QR algorithm applied to the product of the transfer matrices suitably defined in this case, we first find the $N \rightarrow \infty$ limit $\gamma(S)$. The next step is a “width scaling” in which we plot $\gamma(S)$ as a function of $1/S$ and find the $1/S \rightarrow 0$ limit. We can thus find the L-exponent γ of a two-dimensional system for given ω and W .

An overall feature of the ω -dependence of the L-exponent γ for a disordered anomalous solid of type I is exemplified in Fig.4. Again in two dimensions, $\gamma(\omega)$ does not decrease with decreasing the value of ω , and it has a local peak value γ_p at a small peak frequency ω_p , which is consistent with the result on the IPR analysis in Ref. cite18.

By calculating $\gamma_p(W)$ and $\omega_p(W)$ for various values of W , we get γ_p as a function of ω_p , which is shown in FIG. 5. We also get a similar result also for the disordered anomalous solid of type II, replacing ω_p by ω_c .

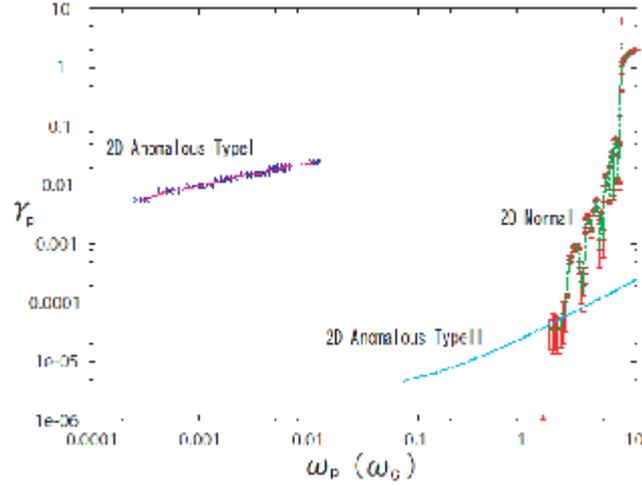


FIG. 6: Peak values of L-exponent γ_p in disordered anomalous solid of type I and type II as a function of the corresponding frequency ω_p or ω_c . The ω -dependence of L-exponent γ in normal disordered systems is shown for reference. The error bars have been calculated for five sets of the averaged value taken over five randomly generated sample systems. The lines are used for enhancing the visibility. In the case of two-dimensional anomalous solid of type II, the value of γ_p was very small and inaccurate, and we have not obtained enough results to show the data point with error bars.

III. SUMMARY AND DISCUSSIONS

We studied the damping rate (L-exponent) of wave functions for acoustic phonons of a disordered anomalous solid in one and two dimensions. We found

1. In both the dimensions, the L-exponent has a local peak γ_p at a very low peak frequency ω_p (or ω_c), which is in strong contrast with the extremely weak localization of the low-frequency acoustic phonons in normal disordered solids.
2. Both γ_p and ω_p (or ω_c) are power-law functions of the strength of disorder W .
3. The above data in 2 suggest

$$\gamma_p \propto \sqrt{\omega_p} \text{ (type I),}$$

$$\gamma_p \propto \omega_c \text{ (type II),}$$

irrespective of the dimensionality, which are in strong contrast with the corresponding relation $\gamma \propto \omega^\beta$ with $\beta = 2$ and $\beta = 4$ in one- and two-dimensional normal disordered solids, respectively.

By using the relations in (4) with some suitable values of $a \cong 1nm$, Debye frequency $\omega_D \cong 10^{13}Hz$, and by setting ω_p (or ω_c) $\cong 10^3Hz$, we get the localization length λ of the order of $10\mu m$ (one dimension) and $10^{-1}\mu m$ (two dimensions) for type I and $1m$ (one dimension) and 10^2m (two dimensions) for type II. The corresponding value of normal disordered solids is of the order of 10^6m in one dimension and $10^{18}m$ in two dimensions.

Unfortunately, we have not made the numerical calculation in three dimensions due to a tough computing time. However, we have seen that the above results do not depend on the dimensionality. Hence, they encourage us to suggest the strong localization of low-frequency acoustic phonons in disordered anomalous solid in three dimensions also. If our speculation is confirmed in near future, we will be able to expect a low-energy frequency band, within which we will have localized acoustic phonons, and below and above this, we will have the delocalized ones. This problem is open for the future study.

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