Localized vibrations in graded lattices: Gradons

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Abstract. We have studied localized vibrational modes in graded elastic lattices in which vibrating masses or nearest-coupling force constants vary linearly in a uniaxial direction. We found localized modes, called gradons, whose characteristics are peculiar to graded systems and are qualitatively different from localized states due to diffusive scattering in disordered media and confined excitations trapped by impurity potentials. The spectral properties and features of mode profiles of gradons are presented in a simple one-dimensional graded chain. In addition, it is shown that a variety of gradons can be excited in graded diatomic chains. We also demonstrate that a band overlapping picture is efficient to understand the variety of gradon modes and their transitions to extended phonon modes.

1. Introduction

Great advancement of recent nanofabrication technology enables us to manufacture various types of inhomogeneous systems. Vibrational properties of normal modes in inhomogeneous materials have also attracted much interest. In particular, the localization problem of vibrations in disordered lattices has been extensively studied because spatial extents of normal modes are deeply related to thermal and electronic properties of materials \cite{1, 2}. Most of previous works regarding vibrational localization in harmonic systems can be classified into two types. One is a consequence of interference of coherent vibrational waves due to diffusive scattering, which includes the Anderson localization of classical waves \cite{3} and fractons in fractal systems \cite{4}. The other type of localization is caused by confinement by impurities such as defect modes or surface phonons \cite{5}. In the former, localization occurs whenever the elastic mean free path becomes comparable to the wave length. The significant nature of this type of localization is the existence of universality near the localization-delocalization transition. The delocalization transition occurs in a continuous band without any spectral singularity at the transition frequency $\omega_c$, and the localization length $\xi$ diverges according to a power law of $|\omega - \omega_c|$. On the contrary, localized impurity modes are rather trapped by local potentials. Such a mode constructs a point-like spectrum, and the corresponding frequency lies outside the band isolatedly. Therefore, there is no delocalization transition in a continuous single band by impurities. Since it is not easy to control localization lengths and positions of localization centers in both cases, the availability of these localized modes for actual functional materials is limited.
In this work, we study theoretically vibrational normal modes in graded elastic systems modelled by graded spring-mass networks. Although graded lattices are one of the simplest inhomogeneous systems, they possess great potential in the materials science and a novel technology of functional materials. By combining analytical arguments and numerical calculations, we show a new type of localized vibrational states, named gradons, and their transition to extended modes. Due to a lack of universality near the transition, there exist various kinds of gradons depending on dimensions, lattice types, and so on. Since spectral properties and mode profiles of gradons are well described analytically, which is a rare example in inhomogeneous systems, graded lattices studied here provide a good candidate as functional graded materials.

2. Gradons in graded monatomic chains

As mentioned in the previous section, properties of vibrational excitations in graded lattices strongly depend on details of systems. Thus, one can expect various characteristics of normal modes peculiar to specific graded lattices. Nevertheless, fundamental features of localized modes in graded systems can be understood by demonstrating vibrations with scalar displacements in a one-dimensional graded chain with linearly graded masses or graded force constants [6]. The motion of each atom in the graded chain with $N$ atoms is described by

$$M_n \ddot{u}_n = K_{n-1}(u_{n-1} - u_n) + K_n(u_{n+1} - u_n),$$  \hspace{1cm} (1)

where $u_n$ is the scalar displacement of the $n$th atom with mass $M_n$, and $K_n$ denotes the force constant of the linear spring connecting the $n$th atom to the $(n+1)$th atom. In the graded mass model, we choose

$$M_n = m_0 - C_M \frac{n-1}{N-1},$$  \hspace{1cm} (2)

and a fixed $K_n(=k_0)$, while in the graded force constant model these are defined as $K_n = k_0 + C_K(n-1)/(N-1)$, and a fixed $M_n(=m_0)$. Due to the duality between force constants and masses, the graded force constant model is essentially the same with the graded mass model.

At first, we consider the spectral density of vibrational states of an infinite one-dimensional graded mass chain ($N \to \infty$). Let us divide the infinite system into small subchains. Each of subchains is so small comparing to the whole chain that the mass gradient can be neglected inside the subchain, but still infinite. Since we treat the nearest-neighbor couplings, the number of degrees of freedom related to the inter-subchain coupling is much smaller than that related to the intra-subchain coupling, and one can neglect them. Therefore, the density of states (DOS) $D(\omega)$ of the infinite graded chain is just the average of the DOS $D_{\text{sub}}(\omega, M)$ of the subchain with the uniform mass $M$, namely,

$$D(\omega) = \frac{1}{C_M} \int_{m_0-C_M}^{m_0} D_{\text{sub}}(\omega, M)dM.$$

We call the above treatment the band overlapping picture, because the DOS of the whole graded chain is regarded as the spectral superposition over subchains. Since the subchain is infinite and has a constant mass, the DOS $D_{\text{sub}}(\omega, M)$ is given by $2\theta[\omega_D(M) - \omega]/\pi \sqrt{\omega_D^2(M) - \omega^2}$, where $\theta(x)$ is the step function and $\omega_D(M) = 2\sqrt{k_0/M}$. Substituting this expression of $D_{\text{sub}}(\omega, M)$ into equation (3), we have
heavier region. The boundary between these two regions is determined by the mode pattern has finite amplitudes only in the lighter region, while no amplitude in the modes with \( \omega < \omega_c \) because masses in this region are too heavy to vibrate with the frequency \( \omega \). A mode with a frequency \( \omega > \omega_m \) shows the profile of the analytically calculated DOS for the graded mass model with \( N = 1000 \). Therefore, the site position of the gradon front (the site with the largest amplitude) coincides with numerical results indicates the validity of our interpretation of gradon localization.

The localization nature of gradons is qualitatively different from that of usual localized modes, such as the Anderson localization and localized impurity modes. For example, (i) even impurity modes provide a localization-delocalization transition within a continuous band, (ii) the

\[
D(\omega) = \begin{cases} 
\frac{2}{2 \pi C_M \omega^2} (m_0 - C_M) \sqrt{\omega_m^2 - \omega^2} & (0 < \omega \leq \omega_c) \\
\frac{2}{2 \pi C_M \omega^2} (m_0 - C_M) \sqrt{\omega_m^2 - \omega^2} + \frac{4k_0}{\pi C_M \omega^2} \tan^{-1} \left( \frac{\omega_m^2 - \omega^2}{2 \omega \sqrt{\omega_m^2 - \omega^2}} \right) + \frac{\pi}{2} & (\omega_c < \omega \leq \omega_m) 
\end{cases}
\]

and \( D(\omega) = 0 \) for \( \omega > \omega_m \), where \( \omega_c = 2\sqrt{k_0/m_0} \) and \( \omega_m = 2\sqrt{k_0/(m_0 - C_M)} \). A similar expression can be obtained for the DOS for a graded force constant model. Solid line in figure 1 shows the profile of the analytically calculated DOS for the graded mass model with \( k_0 = 1, m_0 = 1, \) and \( C_M = 0.5 \). Open circles represent the DOS for a finite graded mass model with \( N = 1000 \) obtained by a numerical diagonalization of the dynamical matrix describing equation (1), which agrees well with the analytical expression equation (4).

The DOS clearly exhibits a singularity at \( \omega = \omega_c (= 2.0) \). From this behavior, we expect that modes with \( \omega > \omega_c \) are qualitatively different from modes with \( \omega < \omega_c \). In order to clarify this point, we plot in figure 2 numerically calculated eigenvectors \( e(\lambda) \) of the dynamical matrix, where three typical modes with \( \omega = 2.399 (> \omega_c), 1.999 (\approx \omega_c), \) and \( 0.399 (< \omega_c) \) are presented. These mode patterns show that modes with \( \omega > \omega_c \) are localized within lighter regions, whereas modes with \( \omega < \omega_c \) are extended. We call localized modes with \( \omega > \omega_c \) gradons. Gradons also appear in the graded force constant model in which gradons are localized in harder regions. The mechanism of gradon localization is basically the same with that of localized impurity modes. A mode with a frequency \( \omega \) larger than \( \omega_c \) cannot have amplitudes in a heavier region because masses in this region are too heavy to vibrate with the frequency \( \omega \). As a consequence, the mode pattern has finite amplitudes only in the lighter region, while no amplitude in the heavier region. The boundary between these two regions is determined by \( \omega = 2\sqrt{K_n/M_n} \). Therefore, the site position of the gradon front (the site with the largest amplitude) \( n_c \) is given by \( n_c = (Nm_0/C_M)(1 - \omega_c^2/\omega^2) \) for the graded mass model and \( n_c = (Nk_0/C_K)(\omega^2/\omega_c^2 - 1) \) for the graded force constant model. The fact that the gradon front predicted by these relation coincides with numerical results indicates the validity of our interpretation of gradon localization.

The localization nature of gradons is qualitatively different from that of usual localized modes, such as the Anderson localization and localized impurity modes. For example, (i) even impurity modes provide a localization-delocalization transition within a continuous band, (ii) the
The delocalization transition is realized even in one dimension, and (iii) the delocalization transition accompanies a spectral singularity. The most striking difference is that gradons in infinite graded systems are localized in infinite spatial region, namely, gradon modes are localized only in the sense that a finite part of the whole system has vibrational amplitudes, while usual localized modes are localized within a finite region even in infinite systems. This character of localized gradons appears also in the inverse participation ratio (IPR) for a finite system. Approximating the envelope function of a gradon mode by a simple step-like function, it seems that the IPR becomes proportional to $1/N$ as in the case of extended modes. The numerical result shown in figure 3, however, exhibits that the IPR, $P^{-1}$, is proportional to $\log N/N$. This makes a remarkable contrast with $P^{-1} \propto N^{-1}$ for extended modes and $P^{-1} \sim \text{const.}$ for usual localized modes. The anomalous size dependence of the IPR enables us to distinguish gradons from usual localized states.

3. Gradons in graded diatomic chains

In order to demonstrate a variety of gradon excitations in various graded systems, we present gradons in graded diatomic chains (GDC). In a GDC, two types of atoms (type-1 and type-2) are alternatively placed along the chain. As in the case of graded monatomic chains, it is possible to construct both GDC models with graded masses and graded force constants. For simplicity, we focus on the GDC with graded masses [7]. Masses of type-1 and type-2 atoms at the $n$th cell (including a pair of these atoms), denoted respectively by $M_n^{(1)}$ and $M_n^{(2)}$, are chosen as

$$M_n^{(1)} = m_0^1 - C_M \frac{n-1}{N-1}, \quad M_n^{(2)} = m_0^2,$$

and the force constant is assumed to be constant ($k_0$). A homogeneous diatomic chain ($C_M = 0$) has two bands corresponding to acoustic and optical branches, while in the GDC there are two cases. If $M_n^{(1)}$ is always larger or smaller than $m_0^2$, we have two bands separated by a gap. Otherwise, all modes lie in a single band.

Employing the band overlapping picture as in the monatomic case, we can analytically obtain the DOS for the GDC by averaging DOS’s for segmental homogeneous diatomic subchains with various sets of $M^{(1)}$ and $M^{(2)}$ [7]. The spectrum of the GDC can be characterized by five frequencies, $\omega_1 = \sqrt{2k_0/m_0^1}$, $\omega_2 = \sqrt{2k_0/(m_0^1-C_M)}$, $\omega_3 = \sqrt{2k_0/m_0^2}$.
Figure 4. (a) Mode classification for the GDC with $\omega_1 \leq \omega_2 < \omega_3 < \omega_4 \leq \omega_5$ by the band overlapping picture. (b), (c), (d), and (e) show typical mode patterns of ALG, OLG, OHG, and OLHG, respectively.

$$\omega_4 = \sqrt{2k_0(1/m_0^4 + 1/m_5^4)}$$

and

$$\omega_5 = \sqrt{2k_0[1/(m_0^4 - C_M) + 1/m_5^4]}.$$  

Spectral properties are strongly affected by the order of these frequencies. Depending on $m_0^4$, $m_5^4$, and $C_M$, we have five possible order relationships between $\omega_1, \omega_2, \ldots, \omega_5$. We discuss in detail mode profiles in the case of $\omega_1 \leq \omega_2 < \omega_3 < \omega_4 \leq \omega_5$ as an example. In this case, $\omega_1$ and $\omega_2$ represent the upper bounds of the acoustic modes in the heaviest and lightest subchains, respectively. Therefore, acoustic dispersions of subchains lie in the gray region surrounded by $\omega_1$, $\omega_2$, and $\omega = 0$ in figure 4(a).

Similarly, optical dispersions of subchains lie in the gray region surrounded by $\omega_3$, $\omega_4$, and $\omega_5$. In the frequency region $[0, \omega_1]$, all acoustic dispersions of any subchains share this region, which implies that all subchains can vibrate at a common frequency and leads spatially extended vibrational excitations, acoustic phonons (AP), in the GDC. In the frequency region between $\omega_1$ and $\omega_2$, however, some of dispersion relations of segmental subchains (i.e., local dispersions in the GDC) do not occupy a part of this region. This implies that the vibrational mode of $\omega$ in the GDC has finite amplitudes only in a part with $M_n^{(1)} < 2k_0/\omega^2$, namely localized in a lighter part of the GDC. We call these modes acoustic light gradons (ALG) [figure 4(b)]. On the other hand, the frequency region between $\omega_3$ and $\omega_4$ is shared by all optical dispersions of any segmental subchains. Thus, we can expect extended optical phonons (OP) in this frequency region. On the contrary, the local dispersions only partially occupy the frequency region $[\omega_1, \omega_5]$, which implies optical modes at frequencies contained in this region (optical light gradons: OLG) are localized in lighter parts of the GDC [figure 4(c)] as in the acoustic case. From these arguments based on the band overlapping picture, we can summarize characteristics of vibrational modes in the GDC satisfying the condition $\omega_1 \leq \omega_2 < \omega_3 < \omega_4 \leq \omega_5$ as depicted in figure 4(a).

Applying the band overlapping picture to other cases of the order relations of $\omega_1, \omega_2, \ldots, \omega_5$, we have optical heavy gradons (OHG) which are localized in heavier parts of the GDC [figure 4(d)] and appear in the frequency region $\omega_2 < \omega < \omega_3$ if $\omega_1 < \omega_3 < \omega_2 \leq \omega_4 < \omega_5$. In addition, in the frequency region $\omega_4 < \omega < \omega_5$ when $\omega_1, \omega_3 < \omega_4 < \omega_2 < \omega_5$, vibrational excitations have no amplitudes both in the lighter and heavier sides as depicted by figure 4(e). We refer these modes as optical light-heavy gradons (OLHG).

Transitions between these modes are clearly displayed by the IPR profile. Figure 5(a) shows the IPR of the GDC with $m_0^4 = 1.5$, $m_5^4 = 1.0$, and $C_M = 1.1$ as a function of frequency, which indicates the transitions AP $\rightarrow$ ALG $\rightarrow$ OLG $\rightarrow$ OLHG $\rightarrow$ OLHG at $\omega_1$, $\omega_3$, $\omega_4$, and $\omega_5$, respectively. It is interesting that the IPR for OLHG’s increases with frequency though the size of the vibrating region of the OLHG is insensitive to frequency. As shown in figure 5(b), the size dependence of the IPR also distinguishes gradons from extended modes. Namely, the IPR’s $P^{-1}$ for various
kinds of gradons are proportional to $\log N/N$, while $P^{-1} \propto N^{-1}$ for AP’s. This unusual property is consistent with the similarity and difference in shapes of the humps (at $n = n_c$) of the variety of gradon modes depicted in figure 4.

4. Conclusions
The nature of gradons excited in graded lattices has been studied by demonstrating vibrational modes in one-dimensional graded chain. Although the mechanism of gradon localization is essentially the same with that of localized impurity modes, spectral properties and features of mode profiles of gradons are largely different from those of conventional localized states. In particular, the system-size dependence of the inverse participation ratio $P^{-1}$ obeys an anomalous power law, $P^{-1} \propto \log N/N$. Many of characteristics of gradons, including spectral densities of states, positions of gradon fronts, and transition frequencies between gradons and phonons, can be analytically understood by the band overlapping picture based on the superposition of dispersion relations of small segments into which the whole graded system is divided. This picture predicts the existence of several kinds of gradons in a graded diatomic chain as shown in this paper. The diversity of gradons is due to the lack of universality in gradon excitations, and we can expect various types of gradons in different kinds of graded systems [8, 9]. Predictability of the gradon nature makes a great step forward in providing theoretical insights in the wave functional behaviors of functional graded materials.

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