Anomalous sound propagation in a solid with a special acoustic phonon dispersion relation

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Abstract. We investigate a new type of solids which has a special acoustic phonon dispersion relation of \(\omega = ak^2\) type. This has been partially observed in graphite. This type of solids usually has a mechanical instability under a homogeneous expansion or a homogeneous deformation and also has a thermal instability. These instabilities can be eliminated by introducing a small cut-off wave number or a suitable unharmonic inter-atomic interaction. We remove the former one by introducing the periodic boundary condition. Some general features of the peculiar “solid” are investigated theoretically and numerically. Especially we investigate the anomalous wave propagation of the dispersive acoustic phonons numerically. The computer simulation of the wave–packet dynamics shows us a stronger localisation character than that in a normal solid in the case of 1-dimensional disordered systems.

1. Introduction

The long-wave acoustic phonons in homogeneous solids have the frequency (\(\omega\)) – wavenumber (\(k\)) dispersion relation of \(\omega = ck\) type. Elastic properties of the normal materials are well described by the linear dispersion relation and the long-wavelength limit of them are described by the well known wave equation. However, \(\omega = ck^2\) type dispersion relation has partially been found in graphite and been confirmed theoretically by using force constants model [1,2]. We thus try in this paper to investigate the general theoretical background of finding the peculiar dispersion relations in crystals and to consider numerically the physical significance of them, within the framework of the force-constants model.

We first show the condition of finding the peculiar solids, and clarify that it reads to an instability against a homogeneous expansion or a homogeneous deformation. We will show some examples in 1-, 2- and 3-dimensions. The solids have \(k = 0\) soft modes inducing phase transitions. But when the instabilities are stabilized by a boundary condition, a very small cut off wave number or an anharmonicity, we can expect to find a peculiar world. It has the spectral dimension \(d^* = d/2\), where \(d\) is the spatial dimension, and the elastic motion is governed by a special wave equation.
We next show the peculiar wave propagation of the acoustic waves. The important points are its dispersion and the anomalously slow sound velocity in the long-wave region. The slow sound velocity recalls the flat-band localization in the electronic case which reads us to a strong insulator when we introduce a weak disorder into it [3].

2. Condition of finding the anomalous solids

Let us describe the process of finding the anomalous solid by examining the simplest case of one-dimensional periodic linear chain of equally spaced $N$ atoms (with lattice constant $a$) with nearest-neighbour and second nearest-neighbour harmonic interactions (of force constants $\alpha_1$, $\alpha_2$) under the cyclic boundary condition. Then we have the Bloch solution $u(n,t) = \exp\{i(k,na - \omega(k)t)\}$ for the displacement of atom at site $n$ at time $t$, and have the frequency ($\omega$)-wavenumber ($k$) dispersion relation

$$\omega^2(k_i) = \frac{2\alpha_1}{m}(1-\cos k_i a) + \frac{2\alpha_2}{m}(1-\cos k_i 2a)$$

$$= \frac{1}{m}(\alpha_1 + 4\alpha_2)a^2 k_i^2 + \frac{1}{12m}(-\alpha_1 - 16\alpha_2)a^4 k_i^4 + O(a^6 k_i^6) \tag{1}$$

where $\omega(k_i)$ is the eigenfrequency of the eigenmode specified by the wave number $k_i = (2\pi / Na)i a$, ($i = \{-N/2 \ldots -1,0,1,{-N/2}\}$). In the normal case where the coefficient $(\alpha_1 + 4\alpha_2)$ does not vanish, we obviously have the normal linear dispersion relation. But if we consider the special case where the relation $(\alpha_1 + 4\alpha_2) = 0$ is kept between the force constants, then we have the positive coefficient $(-\alpha_1 - 16\alpha_2)$ and have the anomalous dispersion relation of $\omega = ck_i^2$ type. One may wonder about accepting a negative force constant $\alpha_2 = -\alpha_1 / 4$ assuming $\alpha_1$ is positive. However, the negative force constant only works together with the stronger positive one and does not make any pure imaginary or complex eigenfrequency. The only exception is the eigenfrequency 0 for the wave number 0, which corresponds to the well-known unstable mode of the parallel shift (or the rotation in the case of 2 and 3 dimensions) of the entire crystal. We usually kill these kinds of instability by fixing the centre of inertia of the crystal at some specific point and also by fixing the angular variables of the entire crystal in the case of 2 and 3 dimensions.

The essential points are the same even when we proceed to the more complex cases, two-dimensional square lattice shown in Fig.1 and honeycomb lattice shown in Fig.2, and three-dimensional square lattice. The obtained transverse acoustic- and optical- phonon dispersions of honeycomb lattice (graphene) in Fig.2 is quite similar to the corresponding ones experimentally observed in graphite [4].

![Figure 1. Anomalous in-plane phonon dispersion of a square lattice. The frequency $\omega$ is written in an arbitrary unit](image)
3. Mechanical and thermal instabilities
In all the cases we are concerned, the anomalous solids have special additional unstable modes of zero frequency. They are homogeneous expansion in the case of longitudinal phonon and homogeneous deformation in the case of transverse phonon. We can give a general proof of the instabilities in a simple class of systems. When we expand $\omega^2$ by even power of $k$, the coefficient of $k^2$ just corresponds to the energy gain for the homogeneous expansion or deformation. These homogeneous unstable modes can disappear when we introduce fixed or periodic boundary condition, or we have a small cut-off wave number which comes from a characteristic length recovering the normal character of the solid. Another way of eliminating the unstable modes is to expect a suitable unharmonicity which recover the unharmonic restoration force when the displacement of atom $u(n,t)$ becomes large.

Another instability comes from the divergence of the mean square displacement $<(u)^2>$, because the spectral dimension is $d^* = d/2$, where $d$ is the one for the normal solid or the spatial dimension. The divergence comes from the density of states $D(\omega) \propto \omega^{d^*-1}$ at $\omega = 0$. The instability also disappears when we have a small cut-off wave number (small cut-off frequency) or the unharmonicity mentioned above.

4. Anomalous wave propagation and localization of acoustic phonons
Let us return to the case of one-dimension. Because of the dispersive dispersion relation, a wave packet cannot keep the wave shape, which is exemplified in Fig.3.

Figure 3. Snap shots of a wave packet (central wave number $k_0 = (20/1000)(\pi/a)$) initially injected (written at the left end of (a)) from the left through a normal solid toward the anomalous “solid”. (a) Soon after it reached the internal boundary (the horizontal dash). (b) More time elapsed after then. The unit of the time step is 0.01, and $t = 0$ when the packet reached the internal boundary.

We next simulate the wave-packet dynamics for the case where the anomalous “solid” on the right hand side contains disorder. A striking feature we find in the disordered anomalous “solid” is a remarkably localized character in the long-wave acoustic phonons, which is in strong contrast with
that in the ordinary normal disordered solids. This characteristic comes from the vanishing of the
group velocity in the long-wave limit.

Figure 4. Snap shots of a wave packet (central wave number \( k_0 = (20/1000)(\pi/a) \)) initially
injected (written at the left end of (a)) from the left through a normal solid toward a dis-ordered
anomalous “solid”, (a) Soon after it reached the internal boundary (the horizontal dash), (b) More time
elapsed after then. The unit of the time step is 0.01, and \( t = 0 \) when the packet reached the internal
boundary. The mass in the disordered phase has been uniformly distributed from 0.75 to 1.25.

We are studying the system-size dependence of the inverse participation ratio (IPR) of the
eigenmodes of the low-frequency acoustic phonons in disordered systems. We have not completed the
analysis but have a partial information insisting the stronger localization in the disordered anomalous
solid. The expectation of the strong localization of acoustic phonons comes from the observation that
the anomalous solid has the same type of dispersion relation as the normal electronic system has.
When we introduce disorder into the electronic system, we usually find a strong localization on both
band edges because the group velocity vanishes in the regular system.

5. Concluding remarks
To summarize, we presented a new aspect of anomalous elastic properties of a new class of crystalline
solids. The solids are expandable or deformable but can be controlled and be stabilized by some
suitable boundary conditions, a cut-off wave number or a suitable unharmonicity. The expected elastic
properties are an extremely soft mechanical response accompanied by an extremely slow sound
velocity, and a characteristic dispersion of the sound wave. When this material is fabricated, we can
expect various interesting peculiar phenomena. The obtained results in this paper are quite new, and
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