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phonons in conventional and auxetic honeycomb lattices

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The modes of vibrations of conventional and auxetic honeycomb structures are studied by means of models where lattices are represented by planar networks, in which rodlike particles are linked by strings. In these structures, the translational and rotational degrees of freedom are strongly coupled. The auxetic network is obtained by modifying a model proposed by Evans et al. in 1991 [Nature (London) 353, 124 (1991)], and is used to explain the negative Poisson’s ratio of auxetic materials. Auxetics are materials with a negative Poisson elastic parameter, meaning that they have a lateral extension, instead of shrinking, when they are stretched. The phonon dispersions obtained in the case of the auxetic model are compared with those of a conventional honeycomb network, where rigid rodlike particles are inserted. The behavior of the rotational dispersions can explain some experimental observations on the properties of sound propagation in the auxetic materials.

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I. INTRODUCTION

Auxetic materials are characterized by a Poisson ratio, that is, the relative transverse strain divided by relative axial strain, which turns out to be negative. This property means that auxetic materials exhibit lateral extension, instead of shrinking, when they are stretched. Although a negative Poisson ratio is not forbidden by thermodynamics, this property is not usually acknowledged in the behavior of elastic or crystalline materials, but it is, in fact, displayed by many elemental materials and several man-made compounds, from the molecular scale up to the macroscopic scale, covering the major classes of materials, such as metals, ceramics, polymers, and composites. Foams with auxetic structures built with polymeric materials are well known and are used in the production of seals, gaskets, energy absorption components, and sound-proofing materials. Filter and drug-release materials will soon be produced, inserting auxetic fibers in technical textiles. Natural auxetic materials and structures are occurring in biological systems, in the skin and bone tissues, and in crystalline membranes, as Bowick et al. showed recently. Let us remember just one example of natural crystalline membrane, the cytoskeleton of the red blood cells, which is a fishnetlike network of triangular plaquettes formed by proteins.

A two-dimensional model for an auxetic mechanical system was proposed in Ref. 1 and is shown in Fig. 1. In this figure, the auxetic honeycomb structure is on the right, in comparison with the conventional honeycomb lattice on the left. This auxetic model was introduced to explain in an easy way the behavior of a material with a negative Poisson ratio. The structure is a reentrant honeycomb network, where the links L’ are rigid rods: we can immediately observe that when the network is stretched parallel to L’, the structure expands instead of shrinking in the transverse direction.

We can imagine an auxetic behavior in models where rigid parts are included, preventing the collapse of the structure in the direction perpendicular to the direction of stretch. To study the vibrations of such structures, the interactions among rigid extended masses, for instance, rodlike particles, can be represented by elastic fibers or strings. An auxetic two-dimensional membrane will then be a network of fibers linking rodlike particles, where the junctions between fibers and particles are the sites of a two-dimensional lattice. We will discuss both conventional and auxetic honeycomb lattices with rodlike particles. These structures are very important in understanding the behavior of translational and rotational modes, which are equivalent in such lattices to the acoustic and optical modes of crystalline materials.

Moreover, experiments show that auxetic structures absorb noise and vibrations more efficiently than nonauxetic equivalents; an explanation for this behavior can be found in the presence of rigid and massive units, with low energy rotational modes, the optical modes in such lattices. The existence of complete band gaps in the vibration spectra, that is, of intervals of frequencies where no propagating phonons exist, can be supposed too. In crystalline lattices, for instance, optical branches stand separate from acoustic branches in all the directions of phonon propagation. Three-dimensional elastic media can show band gaps too, and for this reason, they are called “phononic crystals,” as the photonic crystals display band gaps for light waves.

The approach we follow in calculations was recently proposed by Martinsson and Movchan, these authors studied

FIG. 1. The conventional and auxetic honeycomb structures.
FIG. 2. The chain with rigid particles in the upper part (L is the length of rods and strings). (a) The dynamic forces acting on the rigid particle and (b) the axial tension of ropes.

the phonon dispersions for membranelike lattices with several structures but pointlike particles, finding phononic band gaps.

II. FLEXIBLE AND RIGID PARTS IN THE MESH

To understand the behavior of a mechanical two-dimensional mesh including rigid extended particles, let us start from a one-dimensional chain, a composed of rigid rodlike particles and string linking the particles, where \( L' \) is the length of the rigid masses \( M \), and \( L \) the length of the strings between masses (see Fig. 2). \( l \) will be the moment of inertia. The chain vibrations that we are considering are those perpendicular to the chain. In fact, there are two possible directions perpendicular to the chain, but we consider only one direction because they are degenerate. The unit cells of the lattice have positions given by means of the primitive lattice vector \((L+L')\). For simplicity, \( L=L' \). In the chain, the two points within the basis are denoted by 0 and \( B \).

Let us investigate the harmonic vibrations of the chain supposed to be infinite with displacements of lines and nodes 0, \( B \) in the transversal direction. Let us indicate with \( a \) the two possible determinations 0 and \( B \). \( u_{i,B} \) is the displacement from the equilibrium position of one of the two nodes in the basis at the lattice reticular position \( i \). With \( w_{ji,0} \), it is called the displacement of a string connecting a node \( i \) in the lattice with the nearest neighbor node \( j \). A linear coordinate \( \zeta \) ranges from zero to the length \( L_{ji,0} \) of the string. For strings, the equation in the case of transverse vibrations is the usual wave equation, with a phase velocity \( v = \sqrt{T_o/\rho} \). Solving the equation of motion for the strings, we have

\[
w_{ji,0}(\zeta) = u_{i,B} \cos(\kappa \zeta) + \frac{u_{i,0} - u_{i,B} \cos(\kappa L)}{\sin(\kappa L)} \sin(\kappa \zeta)
\]

and, in the case of a time-harmonic oscillation of frequency \( \omega \), \( \kappa = \omega / v \). The dynamic force that the string exerts at node 0 is equal to

\[f = -T_o \frac{d^2w_{ji,0}}{d\zeta^2} \bigg|_{\zeta=0} = T_o \frac{\omega u_{i,B} \cos(\kappa L) - u_{i,0}}{\sin(\kappa L)}. \]

Assuming the rodlike particles in the chain as rigid masses, we write the equations for the motion of the center of mass and for rotation around it in a plane perpendicular to the chain. In the case of small displacements, equations are the following:

\[
d^2(u_{i,0} + u_{i,0}) = \frac{T_o}{M} \left( \frac{dw_{ji,0}}{d\zeta} + \frac{dw_{ji,0}'}{d\zeta} \right),
\]

\[
d^2(u_{i,B} - u_{i,0}) = \frac{L^2 T_o}{2L} \left( \frac{dw_{ji,0}}{d\zeta} - \frac{dw_{ji,0}}{d\zeta} \right) - \frac{LT_o}{2L} (u_{i,B} - u_{i,0}),
\]

where index \( j \) denotes the lattice point connected with site \( i \) on the right, and index \( j' \) the site connected with \( i \) on the left of the rigid particle. Let us remember that \( dw_{ji,0}/d\zeta, dw_{ji,0}/d\zeta \) are proportional to the force components perpendicular to the chain, as from Eq. (2), and then pulling the rigid body. The force component parallel to the chain is considered equal to \( T_o \). In Eq. (4), the first contribution on the right-hand side (rhs) represents the torque of the dynamic forces \( f \) on the rigid mass; the second contribution represents the torque of axial tension \( T_o \) on the rodlike particle. In Fig. 2, a diagram shows forces on the rodlike particle. Figure 2(b) illustrates how the axial forces produce a torque on the rodlike mass when the mass is not in equilibrium position.

If we are looking for Bloch waves with wave vector \( k \), it is possible to write for each lattice site:

\[u_{i,0} = u_0 \exp(i\omega t - 2ikL), \quad u_{i,B} = u_B \exp(i\omega t - 2ikL)\]

and then the dispersion relations for the frequency \( \omega \) can be obtained from the dynamic equations (3) and (4) of the rods. To study translational and rotational modes, a very useful approach is the use of the Bogoliubov transformation. The Bogoliubov rotation of \( u_0, u_B \) is the following:

\[u_0 = \eta + i\theta, \quad u_B = \eta - i\theta\]

and then we have the translation and rotation degrees of freedom explicitly coupled in a system of two equations:

\[-M \omega^2 \eta = \frac{T_o}{v^S} \left\{ \eta_0 [\cos(\kappa L) - C] + \theta_0 \sin(\kappa L) \right\},\]

\[-2L^2 \omega^2 \theta = \frac{T_o}{v^S} \left\{ -\theta_0 [\cos(\kappa L) + C] - S \theta + \eta_0 \sin(\kappa L) \right\},\]

where \( C = \cos(\kappa L) \) and \( S = \sin(\kappa L) \). For \( \sin(\kappa L) = 0 \), for any \( \kappa \) standing wave, modes exist corresponding to the internal vibration of the strings with no associated nodal displacements. Let us consider the reduced frequency \( \Omega = \omega / \omega_o \), where \( \omega_o = T_o / M L^2 \). The reduced dispersion relations of the chain as functions of the wave number \( k \) are shown in Fig. 3 for different values of ratio \( I / ML^2 \). This ratio can be hardly greater than 1, but, to understand the behavior of dispersion.
and ropes with length \( L \) between sites, substituting all the bonds parallel to one of the lattice directions. The lattice has one rod per unit cell, and the structure is centered orthorhombic with space group \( C2mm \).

It is straightforward to investigate the harmonic vibrations of this two-dimensional honeycomb mesh if the mesh is supposed to be infinite with displacements of lines and nodes in the direction perpendicular to its plane. As in the case of the one-dimensional lattice, \( u_{i,j} \) is the displacement of one of the nodes in the lattice basis from the equilibrium position. The same is true for \( w_{j,b} \), which is the displacement of a string linking a node in the lattice cell with the nearest neighbor node. If we are looking for Bloch waves with wave vector \( \mathbf{k} \), it is possible to write the displacements as

\[
u_{i,0} = u_0 \exp(i\omega t - i \mathbf{k} \cdot \mathbf{L}_i), \quad u_{i,B} = u_B \exp(i\omega t - i \mathbf{k} \cdot \mathbf{L}_i)
\]

If the basis has two sites, the dispersion relations for the frequency \( \omega \) are obtained solving the following equations of rod dynamics:

\[
-o^2(u_{i,B} + u_{i,0}) = \frac{T}{M} \sum_{j,j'} \left( \frac{dw_{i,j,0}}{d\xi} + \frac{dw_{i,j',0}}{d\xi} \right),
\]

\[
-o^2(u_{i,B} - u_{i,0}) = \frac{L^2T_o}{2I} \sum_{j,j'} \left( \frac{dw_{i,j,0}}{d\xi} - \frac{dw_{i,j',0}}{d\xi} \right)
\]

\[
-\frac{L}{2I} \sum_{j,j'} T_{o,j} (u_{i,B} - u_{i,0}),
\]

where \( j, j' \) are the indices of nearest neighbor sites, as in the one-dimensional chain. The second term on the rhs of the second equation contains the component \( T_{o,j} \) of forces, parallel to the axial direction of the rod in its equilibrium configuration. For the honeycomb cell, \( T_{o,\parallel} = T_o \cos(\pi/3) \).

In the case of the honeycomb lattice, there are two forces applied to each end of the rod, 0 or \( B \): the contribution of the components of these two forces is positive, giving a resulting torque which stabilizes the rodlike oscillators. Equation (9) becomes

\[
-o^2(u_{i,B} + u_{i,0}) = \frac{T}{M} \sum_{j,j'} \left( \frac{dw_{i,j,0}}{d\xi} + \frac{dw_{i,j',0}}{d\xi} \right),
\]

\[
-o^2(u_{i,B} - u_{i,0}) = \frac{L^2T_o}{2I} \sum_{j,j'} \left( \frac{dw_{i,j,0}}{d\xi} - \frac{dw_{i,j',0}}{d\xi} \right)
\]

\[
-\frac{L}{2I} T_o (u_{i,B} - u_{i,0}).
\]

The dispersion relations for the frequency \( \omega \) can be easily obtained by solving system (10) or the following equations, rewritten after the Bogoliubov rotation:

\[
-M \omega^2 \eta = \frac{T_o}{\sqrt{3}} \left[ \eta_0 \left[ \cos(\mathbf{k} \cdot \mathbf{L}_1) + \cos(\mathbf{k} \cdot \mathbf{L}_2) - C \right] 
+ \theta \omega \left[ \sin(\mathbf{k} \cdot \mathbf{L}_1) + \sin(\mathbf{k} \cdot \mathbf{L}_2) \right] \right].
\]
ascertain the proportion of the lattice parameters characteristic of the structure.

On points 0 or B of the rigid masses, three ropes and three forces are acting. A force is parallel to the rod, then $T_{o,1} = T_o$; the other two have components $T_{o,1} = T_o \cos(2 \pi / 3)$, but are negative with respect to the rod axis. If only these two forces were present in the model, the resulting torque in Eq. (9) would be destabilizing the acoustic oscillations of the membrane, in the case of oscillations with the wave vector $k$ in the $X$ direction.

Moreover, in the model in Fig. 4 on the right, the strings parallel to the rigid masses can have a different tension $T_{o} = \xi T_o$. These ropes have a sound speed $v_2 = \sqrt{\xi T_o} / \rho$ different from the sound speed $v_1 = \sqrt{T_o} / \rho$ of the other ropes. The reduced frequency we use in the calculations is $\Omega = \omega / \omega_o$, with $\omega_o = T_o / M v_1$. Equation (9) must be rewritten in the following form:

$$- \omega^2 (u_{i,B} + u_{i,0}) = \frac{T_o}{M} \sum_{j,j'} \left( \frac{dw_{ij,B0}}{d\zeta} + \frac{dw_{ij',0B}}{d\zeta} \right)$$

$$+ \frac{\xi T_o}{M} \sum_{k,k'} \left( \frac{dw_{ik,B0}}{d\zeta} + \frac{dw_{ik',0B}}{d\zeta} \right)$$

$$- \omega^2 (u_{i,B} - u_{i,0}) = \frac{L^2 T_o}{2I} \sum_{j,j'} \left( \frac{dw_{ij,B0}}{d\zeta} - \frac{dw_{ij',0B}}{d\zeta} \right) + \frac{L^2 \xi T_o}{2I} \sum_{k,k'} \left( \frac{dw_{ik,B0}}{d\zeta} - \frac{dw_{ik',0B}}{d\zeta} \right)$$

where indices $j, j'$ are used when sites are connected by ropes with tension $T_o$, and $k, k'$ when sites are connected with ropes with tension $T_{o} = \xi T_o$. Note the different signs from Eq. (10). The approach to solve system (12) with the Bogoliubov transformation can be proposed too. As a result, we have the following equations:

$$- M \frac{F}{T_o} \omega^2 \eta = \frac{\omega_o}{3} \left( c_1 + c_2 + C + \frac{F}{F'} (c_3 - C') \right)$$

$$+ \frac{\omega_o}{3} \left( s_1 + s_2 + \frac{F}{F'} s_3 \right)$$

$$- \frac{L^2 T_o}{2I} \omega^2 \theta = - \frac{F}{L^2} \frac{\omega_o}{3} \left( c_1 + c_2 + C + \frac{F}{F'} (c_3 - C') \right)$$

$$+ \frac{F}{L^2} \frac{\omega_o}{3} \left( s_1 + s_2 + \frac{F}{F'} s_3 \right)$$

where $C = \cos(\kappa_1 L)$, $S = \sin(\kappa_1 L)$, $C' = \cos(\kappa_2 L)$, $S' = \sin(\kappa_2 L)$, $F = v_1 S$, $F' = v_2 S'$, $C' = \cos(\kappa_2 L)$, $\kappa_1 = \omega / v_1$, and $\kappa_2 = \omega / v_2$. The coefficients containing the wave number are $c_1 = \cos(\mathbf{k} \cdot \mathbf{l}_1)$, $s_1 = \sin(\mathbf{k} \cdot \mathbf{l}_1)$, $c_2 = \cos(\mathbf{k} \cdot \mathbf{l}_2)$, $s_2 = \cos(\mathbf{k} \cdot \mathbf{l}_2)$, $c_3 = \cos(\mathbf{k} \cdot (\mathbf{l}_1 + \mathbf{l}_2))$, and $s_3 = \sin(\mathbf{k} \cdot (\mathbf{l}_1 + \mathbf{l}_2))$.
Figure 6 shows the reduced phonon dispersions of the auxetic honeycomb lattice for values of ratio $I/ML^2$ ranging from 0.1 to 10, and for $\xi = 1$. As we did when studying the chain, we consider also high values of $\xi$ to show the behavior of dispersions. In both models, conventional and auxetic honeycomb, the rodlike masses are viewed by the waves in the lattice $Y$ direction as pointlike ones.

When parameter $\xi$ is increased, we see a complete band gap between acoustic and rotational modes, and this is shown in Fig. 7 in the case of $I/ML^2 = 1$. The threshold value is $\xi_{th} = 5$ for $I/ML^2 = 1$. Reducing the value of ratio $I/ML^2$, the threshold value is lower, $\xi = 1.7$ for $I/ML^2 = 0.1$. The increase of tension $T_X$ produces a growth of rotational frequencies, while, in the $Y$ direction, the acoustic branch remains almost unchanged. Let us note that the property of being auxetic is not, by itself, responsible for the absolute gap shown in Fig. 7. An analogous effect can be achieved by introducing stretched horizontal strings or springs between the rods in the conventional honeycomb structure. The stretched string would then exert a force, increasing the frequency of the rotational mode.

In honeycomb lattices, a complete band gap between translational (acoustic) and rotational (optical) modes can then be observed if the axial tension $T_X$ of strings aligned in the $X$ direction is increased with respect to the axial tension $T_o$ over a threshold value depending on ratio $I/ML^2$. On the contrary, it is impossible to obtain a gap in the $Y$ direction lowering the value of $I/ML^2$: acoustic and rotational branches are always crossed even if this ratio goes to zero.

The behavior of the conventional honeycomb model shown in Fig. 4 on the left is more or less the same, but the rotational frequencies are higher by about 15% if compared with those in Fig. 6 of the auxetic honeycomb model. This is in agreement with experiments showing that auxetic structures absorb vibrations more efficiently than nonauxetic equivalents, due to the presence of lower rotational energies. It would be better to estimate the Poisson ratio of the meshes, for a proper comparison of dispersions, but the estimation requires a study of in-plane strains of membranes, that is, of in-plane vibrations not discussed in this paper.

V. AUXETIC MEMBRANES

We have seen that by adjusting the lattice parameters and interactions, that is, by changing elastic properties or densities of ropes, it is possible to change deeply the phonon dispersions of the mesh. Of course, different and more complex auxetics must be proposed and studied to understand the behavior of these structures in an exhaustive way. If we consider as “auxeticlike” two-dimensional structures those structures which do not collapse when stretched along one of the in-plane directions, several membranes can be proposed, but it is necessary to insert some rigid parts in their meshes.
Let us consider, for instance, the square lattice in the upper part of Fig. 8. The thick lines represent the rodlike particles, which have different orientations in the plane of the lattice. In this case, the lattice basis contains two rigid rods. In the lower part of the figure, the phonon dispersions are shown. If rod masses in the lattice basis are different, a complete band gap appears, in agreement with the behavior of crystalline systems and mechanical systems with pointlike masses proposed in Ref. 20.

More complex two-dimensional structures can be proposed, for instance, the structure in Ref. 21 or the membrane in Ref. 13. In this reference, the in-plane vibrations of rectangular rigid particles connected by harmonic elements are discussed. Of course, different approaches to the problem of vibrations of auxetic structures are possible: for instance, a solution based on finite elements to solve a macroscopic mechanical system.22 These studies are, in fact, very important for the development and applications of auxetics. The aim of this paper is instead the investigation of the role played by rodlike particles in the lattice vibrations and the creation of auxetic counterparts, inserting rigid particles in lattices.

8 K. L. Alderson, A. Alderson, G. Smart, V. R. Simkins, and P. J. Davies, Plast. Rubber Compos. 31, 344 (2002).