Speed of Sound in a Solid with Lagrangian Mechanics

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Introduction

In this problem we derive an expression for the longitudinal speed of sound in a homogeneous isotropic elastic solid by modelling the solid as a three-dimensional cubic lattice. We first determine the speed of sound in terms of microscopic parameters of the material; subsequently we shall express the speed of sound in macroscopic material properties. For simplicity, we consider the case of a rectangular prism.

Part I

Consider a solid rectangular prism of dimensions $a \times b \times c$ at rest. We tie our inertial reference frame to a corner of the prism with axes along those of the prism as shown in **Figure 1** (so more precisely, we require this corner to be at rest). We may model this solid

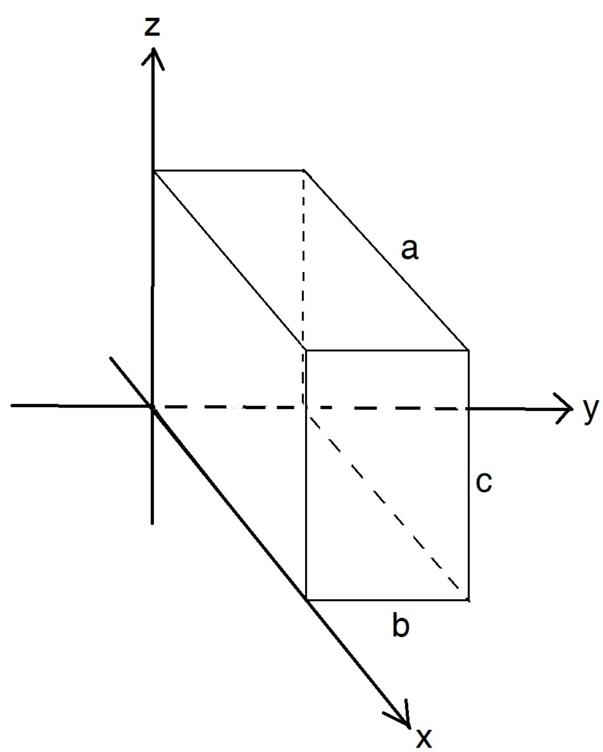
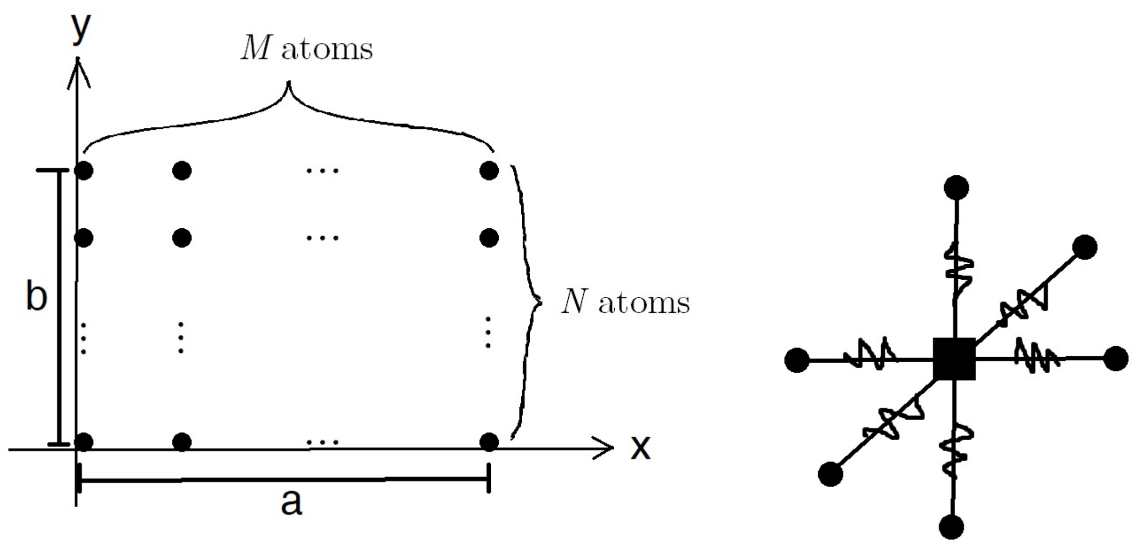


Figure 1: Sketch of the solid prism and our inertial reference frame for **Part I**. The solid is of side lengths a, b, and c along the x-, y-, and z-axes, respectively.

prism as a $M \times N \times P$ cubic lattice of point masses, each with mass m. These point masses represent the solid's atoms. This is illustrated in **Figure 2a**. The bond potential energy



(a) (b)

Figure 2: (a) Sketch of the crystal lattice projected on the xy-plane. The black dots represent atoms; each atom in the lattice is spaced out by a distance l_0 at equilibrium. In total there are M, N, and P atoms along the x-, y-, and z-axes, respectively. Although this is not depicted, this lattice repeats similarly along the z-axis. (b) Sketch of the interaction between an interior atom (square) and its six neighbours (circles). This interaction is modelled as a spring of equilibrium length l_0 and spring constant K. It follows that these springs lie along the x-, y-, and z-axes (two on each).

between two adjacent atoms experiences a local minimum at an equilibrium length l_0. Applying the small oscillations approximation to this stable equilibrium, we model the interaction between two adjacent atoms as a harmonic oscillator (i.e. spring) of equilibrium displacement l_0 and spring constant K. Furthermore, we take the interaction between non-adjacent atoms to be negligible. For interior (i.e. not on the solid's boundary) atoms, this is depicted in **Figure 2b** (as we shall see, the boundary atoms and their interactions with the external environment determine the boundary conditions). Finally, we neglect gravity throughout this problem.

As a bonus challenge, complete all parts of this problem for an arbitrary prismatic solid. That is, take P to be a function of j, $P(j)$.

To get started, how many degrees of freedom in this system? What set of generalized coordinates could you use to describe this system?

Part II

We may label each atom in the lattice with indices i, j, and k. We shall label the corner atom at the origin with $i = 1$, $j = 1$, and $k = 1$. Then our indices range over $1 \le i \le M$, $1 \le j \le N$, and $1 \le k \le P$. The atom adjacent in the x-direction to the origin corner atom, for example, would have indices $(i, j, k) = (2, 1, 1)$. Two atoms above this atom in the z-direction would have indices $(i, j, k) = (2, 1, 3)$, etc. We may denote the (global i.e. when every atom is at equilibrium) equilibrium x, y, and z positions of the (i, j, k) atom as $\tilde{x}_{ijk}$, $\tilde{y}_{ijk}$, and $\tilde{z}_{ijk}$, respectively.

Determine $\tilde{x}_{ijk}$, $\tilde{y}_{ijk}$, and $\tilde{z}_{ijk}$ in terms of i, j, k, and l_0. What are the dimensions a, b, and c of the prism in terms of M, N, P, and l_0?

Part III

We similarly may denote the (current) x, y, and z positions of the (i, j, k) particle as x_{ijk}, y_{ijk}, and z_{ijk}, respectively. In terms of these coordinates, find the total kinetic and potential energies of the system. What is the Lagrangian?

Part IV

Find the Euler-Lagrange equations for the (i, j, k) interior atom ($2 \le i \le M - 1$, $2 \le j \le N - 1$, $2 \le k \le P - 1$). For simplicity, find the EL equations only for x_{ijk} (the equations for y_{ijk} and z_{ijk} are then determined by symmetry). We will consider the boundary atoms later.

Part V

Now let us consider longitudinal acoustic wave (sound) propagation along the x-axis. That is, we consider wave propagation where y_{ijk} and z_{ijk} are not displaced from their equilibrium values. For example, we could have a hammer uniformly striking the yz face of the prism opposite to the origin. The longitudinal wave propagation is therefore described by the longitudinal displacement (from equilibrium) X_{ijk} of point (i, j, k): $X_{ijk} = x_{ijk} - \tilde{x}_{ijk}$. We are focusing on the case where external acoustic stimuli are applied uniformly along j and k so that X_{ijk} is constant in j and k.

Simplify the x EL equations, applying the simplification that y_{ijk} and z_{ijk} are not displaced. Rewrite these equations in terms of X. Also show that $\ddot{y}_{ijk}$ and $\ddot{z}_{ijk}$ are equal to zero in the EL equations (this ensures that if the system starts with y_{ijk} and z_{ijk} at rest for all (i, j, k), y_{ijk} and z_{ijk} will remain unperturbed).

Part VI

Turning now to the theory of finite differences, we may approximate the derivatives of a twice continuously differentiable function $f(x)$ in a mesh as

$$\left.\frac{df}{dx}\right|_{x=x_i} \approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x},\ \left.\frac{d^2 f}{dx^2}\right|_{x=x_i} \approx \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{(\Delta x)^2}$$

for a given mesh size of Δx. We will make use of the first approximation later. Of course, these finite differences have analogous formulae for partial derivatives.

Let us now concern ourselves with somehow differentiating X_{ijk}. As it stands, this is not a function of x, y, and z, which we would like it to be. But notice that in analyzing a macroscopic solid, M, N, and P are very large. Taking inspiration from fluid mechanics, however, we then define a cubic volume element to be small enough so that the prism can be decomposed into a large number of such elements, yet large enough to contain a large number of atoms. Then we can define a function $\tilde{X}(x, y, z, t)$ to be the average value of $X(t)$ for all the point masses inside the cubic volume element (whose sides run along the coordinate axes) centred at the point (x, y, z).

Observe that the EL equations for X can be massaged into a finite set of finite difference equations for $\tilde{X}(x, y, z, t)$. Perform this manipulation.

Part VII

As one of the most important equations in physics, the wave equation is

$$\frac{\partial^2 f}{\partial t^2} = c^2 \nabla^2 f$$

This represents the propagation of a quantity f through space. The constant c is known as the *wave speed*; this represents the speed at which f propagates through space. Notice that the set of equations obtained in **Part VI** is a *pseudo*-discretization of the wave equation for $\tilde{X}$.

"Undiscretize" these equations to recover the wave equation for $\tilde{X}$. Longitudinal sound wave in a solid are hence carried through $\tilde{X}$, the local average longitudinal displacement. Find the wave speed c in terms of the quantities we have encountered thus far. The equations in **Part VI** represent a *pseudo*-discretization of the wave equation; in fact, this is better than a typical finite difference discretization. Why is this the case (recall that finite difference discretizations are used to numerically compute the solutions to differential equations)?

Part VIII

Let us take a detour now to the mechanics of materials. Consider a uniaxial deformation of the prism where the yz-face opposite to the origin is displaced by an amount δ. In terms of generalized coordinates, we now constrain $x_{Mjk} = a + \delta$ for all $1 \leq j \leq N, 1 \leq k \leq P$ under the deformation. If initially the system was at rest (with no constraint on x_{Mjk}), and we take the system after the displacement to be at rest (this could be in steady state, where the oscillations of the atoms have been damped; for sound propagation we have neglected damping), then the *elastic modulus* E is defined to be the constant of proportionality such that the increase in energy per total (initial) volume is $\frac{1}{2}E\varepsilon^2$, where $\varepsilon = \frac{\delta}{a}$ is known as the *strain* of the deformation (the elastic modulus is more commonly defined in terms of forces; in the context of Lagrangian mechanics, however, we shall continue to formulate phenomena in terms of generalized coordinates and energies). Finally, the density ρ of a material is its mass per unit volume.

Express the speed of sound c in the solid in terms of its macroscopic properties.

Part IX

We have finally found the speed of longitudinal sound waves in a homogeneous isotropic elastic solid, albeit for the case of a rectangular prism. Our results, however, apply to any such prismatic solid. TODO: finish + update I2 fig