# 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. Note that the oscillations of atoms about equilibrium will be small compared to the bond length (this is not a small oscillations problem, however).

## 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 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 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 $j$, $P(j)$. As a second bonus, relax the assumption of isotropy. That is, $l_0$ and $K$ need not be equal for springs along different coordinate axes.**

To get started, how many degrees of freedom in this system? What set of generalized coordinates could you use to describe this system?
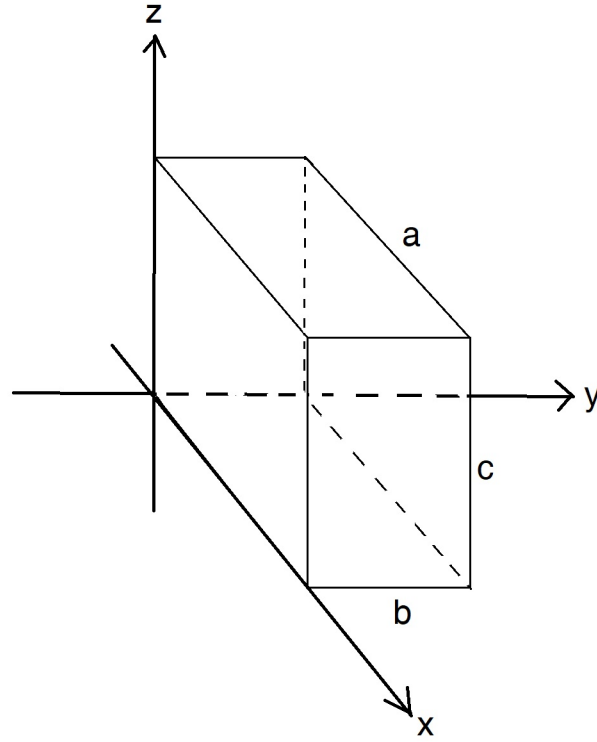
Figure 1: Sketch of the solid prism and our inertial reference frame for **Part I**. The solid is of side lengths $a$, $b$, and $c$ along the $x$-, $y$-, and $z$-axes, respectively.

## 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 $i = 0$, $j = 0$, and $k = 0$. Then our indices range over $0 \leq i \leq M - 1$, $0 \leq j \leq N - 1$, and $0 \leq k \leq P - 1$. The atom adjacent in the $x$-direction to the origin corner atom, for example, would have indices $(i, j, k) = (1, 0, 0)$. Two atoms above this atom in the $z$-direction would have indices $(i, j, k) = (1, 0, 2)$, 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? Are there any conserved quantities? Find them. Neglect gravitational effects.
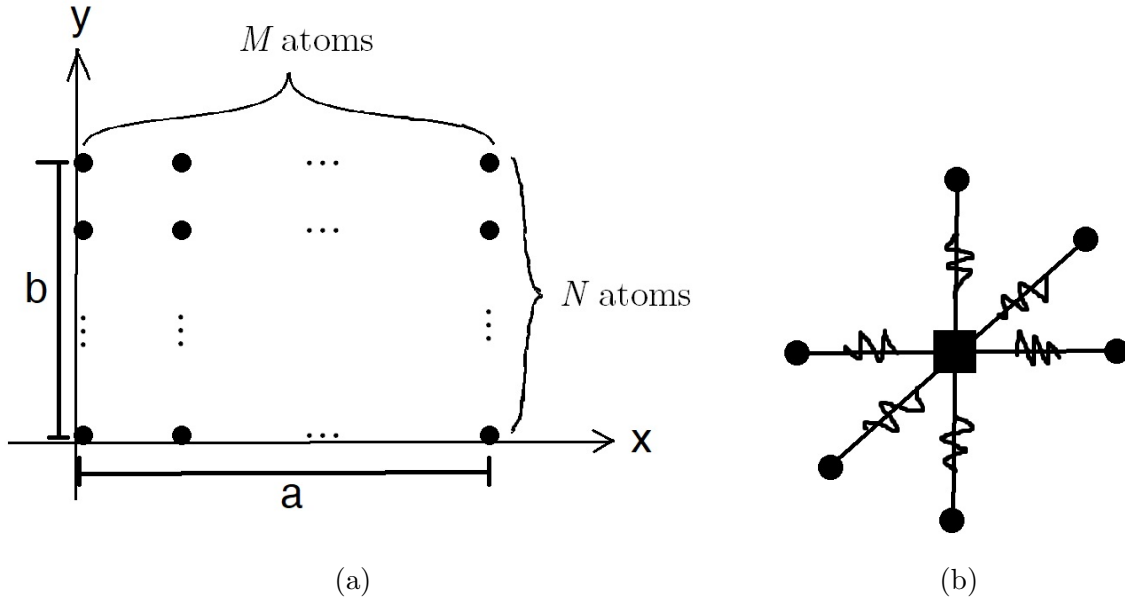
Figure 2: (a) Sketch of the crystal lattice projected on the $xy$-plane. The black dots represent atoms; each atom in the lattice is spaced out by a distance $l_0$ at equilibrium. In total there are $M$, $N$, and $P$ atoms along the $x$-, $y$-, and $z$-axes, respectively. Although this is not depicted, 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).

## Part IV

Find the Euler-Lagrange equations of the system (note that the equations for boundary atoms will be different in pattern to those for interior atoms).

## Part V

Now let us consider longitudinal acoustic wave (sound) propagation along the $x$-axis. We do so by taking $y_{ijk}(0) = \tilde{y}_{ijk}$, $z_{ijk}(0) = \tilde{z}_{ijk}$, and $\dot{y}_{ijk}(0) = \dot{z}_{ijk}(0) = 0$ in our initial conditions. Furthermore, we consider the case where the acoustic waves are symmetrical across the cross-section (to the $x$-axis). We do so by requiring $x_{ijk}$ to be invariant across $j$ and $k$ in the initial conditions (when we add boundary conditions later, those too will be symmetrical). $y_{ijk}$ and $z_{ijk}$ will remain constant as a result. Furthermore, $x_{ijk}$ will remain invariant across $j$ and $k$. The longitudinal wave propagation is therefore described by the longitudinal displacement (from equilibrium) $X_i$ of point $(i, j, k)$: $X_i = x_i - \tilde{x}_i$. We only need the $i$ index given that $x_{ijk}$ only depends on $i$. As for $\tilde{x}_{ijk}$, you may verify that your expression in **Part II** is independent of $j$ and $k$.

Show that $\ddot{y}_{ijk}$ and $\ddot{z}_{ijk}$ are initially zero from their EL equations under our assumptions for the initial condition. Since $\dot{y}_{ijk}$ and $\dot{z}_{ijk}$ are initially zero, $y_{ijk}$ and $z_{ijk}$ will consequently remain at their equilibrium values. Simplify the EL equations for $x$, applying this fact. Verify that $\ddot{x}_{ijk}$ is independent of $j$ and $k$ at $t = 0$. Since $x_{ijk}$ and $\dot{x}_{ijk}$ are invariant with respect to $j$ and $k$ at $t = 0$, we have that $x_{ijk}$ will forever be independent of $j$ and $k$ (notice that the EL equations are time invariant). With all this in mind, we may reduce the $3(MNP - 1)$ equations to $M - 1$ equations ($x_0$ is fixed). Rewrite these equations in terms of $X_i$.

## 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

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

for a given mesh size of $\Delta x$. We (you) 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, the equations appear to be finite difference equations, however $X_{ijk}$ this is not a function of $x$, $y$, and $z$. However, $X_{ijk}(t)$ is a discretization of some twice differentiable function $\tilde{X}(x, y, z, t)$, where the EL equations serve as the difference equations. We may interpret $X_{ijk}$ to be $\tilde{X}$ evaluated at the point where the $(i, j, k)$ atom's equilibrium location is. Because there are a very large number of atoms along each dimension in a macroscopic solid, the finite difference discretization is very accurate; that is, the values of $X_{ijk}$ will be approximately equal the actual values of $\tilde{X}$ (which is governed by the corresponding differential equation) evaluated at those points.

Express the equations for the interior points obtained in **Part V** as a set of finite difference equations for $\tilde{X}$. What should the mesh spacing $\Delta x$ be?

## 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 some continuous (in fact continuously twice differentiable) field $\tilde{X}$; at lattice points, this field is simply the longitudinal displacement of the corresponding atom. Now 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 $\delta$. In terms of generalized coordinates, we now constrain $x_{Mjk} = a + \delta$ for all $0 \le j \le N - 1, 0 \le k \le P - 1$ under the deformation. If initially the system was at rest with no deformation applied (i.e. 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 $E$* ($E_x$ if you are not assuming isotropy) 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 $\rho$ 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. To finish off, as a bonus exercise let us consider the boundary conditions of the prism. The boundary condition for $\tilde{X}$ at $x = 0$ is already constrained to be

$$\tilde{X}(x = 0, y, z, t) = 0$$

as we require the corner to be fixed at rest. Symmetry in $y$ and $z$ requires this to be the case for the entire $yz$ face. At the other end's $yz$ face, however, we are free to specify any boundary condition provided that it is symmetric in $y$ and $z$. For example, we may specify

the Dirichlet boundary condition

$$\tilde{X}(x = a, y, z, t) = p$$

the mixed boundary condition

$$\frac{\partial \tilde{X}}{\partial x}\bigg|_{x=a} = q$$

or the Robin boundary condition

$$\alpha \tilde{X}(x = a, y, z, t) + \beta \frac{\partial \tilde{X}}{\partial x}\bigg|_{x=a} = \gamma$$

for $\alpha, \beta \neq 0$.

Physically speaking, what is happening to the $x = a$ face for the Dirichlet, mixed, and Robin boundary conditions, respectively? How do the constants $p, q, \alpha, \beta, \gamma$ relate to what is being applied to the $x = a$ face for each boundary condition? It may help to create "ghost" points $X_{M,j,k}$ and use the right finite difference introduced in **Part VI** for the first derivative.