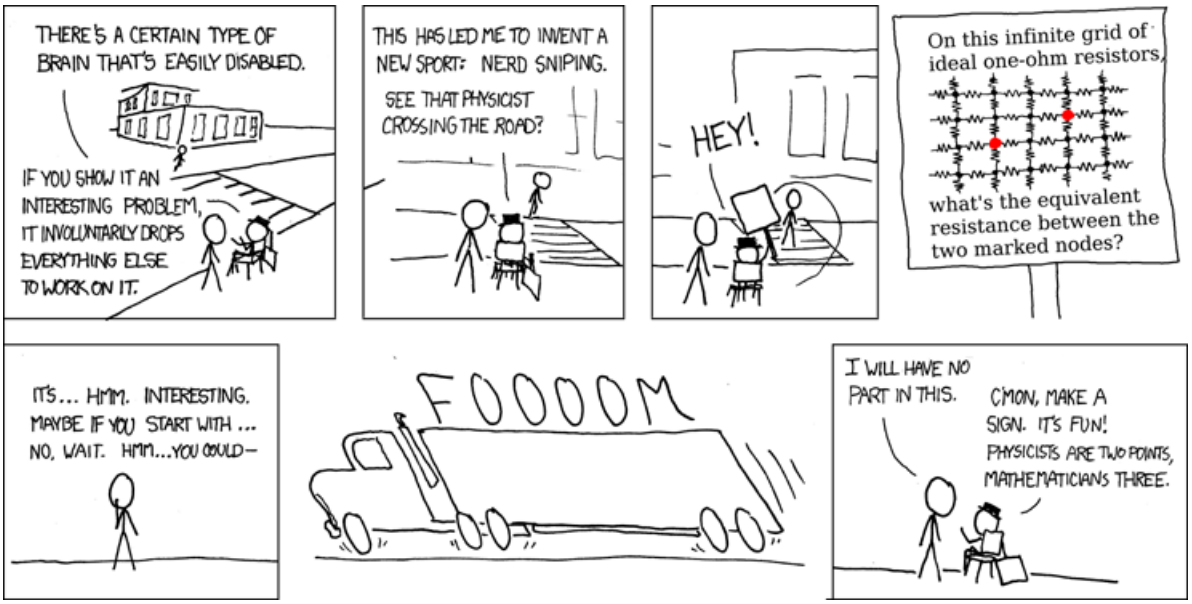
Speed of Sound in a Solid with Lagrangian Mechanics

James Wu, 92277235

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.

My inspiration for this problem came while I was reading the following xkcd comic:



I was likely thinking about PHYS 350 while reading this, because the infinite resistor grid looked like a grid of springs to me. Falling for the bait like the physicist in the comic, I thought about the mechanics of a three-dimensional lattice of springs and wrote down the Lagrangian and Euler-Lagrange equations. Playing around with the equations led me to obtain the speed of sound in a solid, which is now the focus of my project.

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

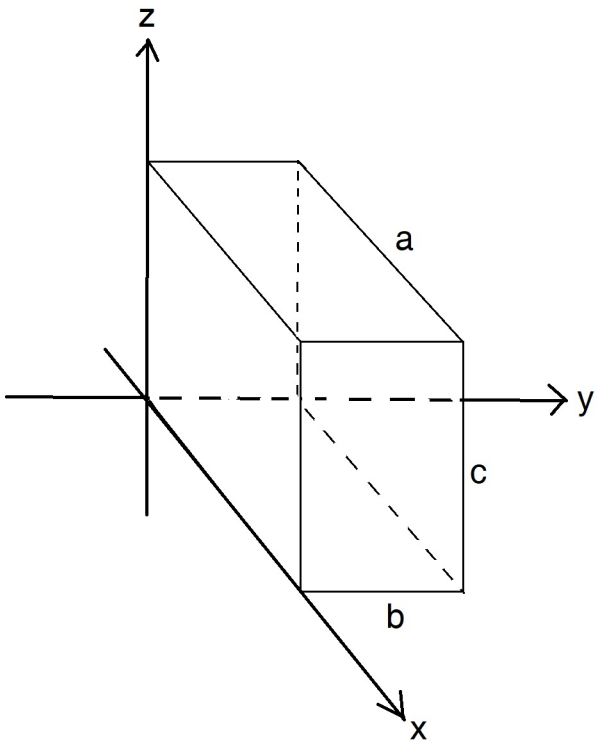
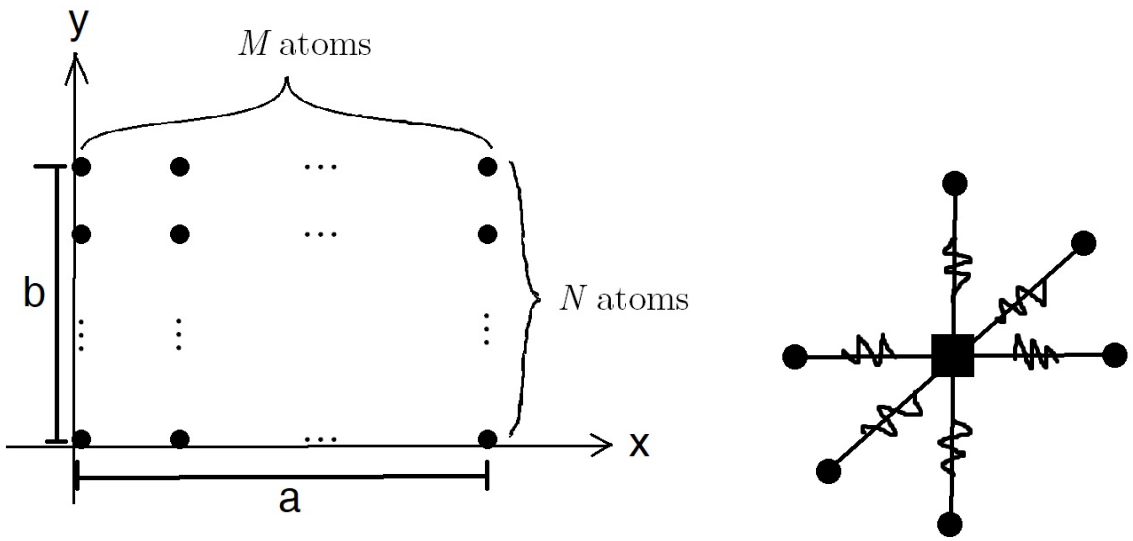


Figure 1: Sketch of the solid prism and our inertial reference frame for **Part I**. The solid is of side lengths a, b, and c along the x-, y-, and z-axes, respectively.

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 (this would also account for gravity).

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



(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).

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.

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

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

for a given mesh size of Δx. We (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 Δx 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 δ. In terms of generalized coordinates, we now constrain $x_{Mjk} = a + \delta$ for all
$0 \leq j \leq N-1, 0 \leq k \leq P-1$ 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 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. 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

$$\left.\frac{\partial \tilde{X}}{\partial x}\right|_{x=a} = q$$

or the Robin boundary condition

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

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.