Solution: Speed of Sound in a Solid with Lagrangian Mechanics

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Part I

There are MNP atoms in this system. Each atom, being modelled as a point particle, has 3 degrees of freedom. However, we must subtract the atom at the origin, as we have constrained it to be fixed. Thus

$$\boxed{s = 3(MNP - 1)}$$

We can use the x, y, and z coordinates of each particle to describe the particle's motion. Our generalized coordinates are then

$$\boxed{\left(x_{ijk}, y_{ijk}, z_{ijk}\right),\ (0,0,0) \leq (i,j,k) \leq (M-1, N-1, P-1), (i,j,k) \neq (0,0,0)}$$

where we index the atoms with i, j, and k along the x-, y-, and z-axes, respectively.

Part II

The equilibrium position of atom (i,j,k) is

$$\boxed{(\tilde{x}_{ijk}, \tilde{y}_{ijk}, \tilde{z}_{ijk}) = (il_0, jl_0, kl_0)}$$

If we take the prism to be bounded by the point atoms, then the dimensions would be $(a,b,c) = ((M-1)l_0, (N-1)l_0, (P-1)l_0)$. Quasi-philosophically, we could, however, argue that the prism extends a bit beyond the boundary atoms; no external body can be pushed right against the boundary atoms as that would require an infinite amount of energy (the bond energy diverges to infinity as bond distance approaches zero). Regardless, this all occurs on the l_0 scale, which is small compared to the (a,b,c) scale. Hence we simply assert

$$\boxed{(a,b,c) \approx (Ml_0, Nl_0, Pl_0)}$$

Part III

The kinetic energy of particle (i,j,k) is simply

$$T_{ijk} = \frac{m}{2}\left(\dot{x}_{ijk}^2 + \dot{y}_{ijk}^2 + \dot{z}_{ijk}^2\right)$$

For the case $i = j = k = 0$, we simply have $\dot{x}_{000} = \dot{y}_{000} = \dot{z}_{000} = 0$ as a constant. This means that $T_{000} = 0$, so we may add it to the total kinetic energy of the system (despite the $(0,0,0)$ atom not being part of the system):

$$\boxed{T = \frac{m}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\dot{x}_{ijk}^2 + \dot{y}_{ijk}^2 + \dot{z}_{ijk}^2\right)}$$

In what follows, we let $x_{000} = y_{000} = z_{000} = 0$ be constants. Then for a single spring along the x-axis connecting atoms (i, j, k) and $(i+1, j, k)$, we have

$$\begin{aligned} U^x_{ijk} &= \frac{K}{2}\left(|\mathbf{r}_{i+1,jk} - \mathbf{r}_{ijk}| - l_0\right)^2 \\ &= \frac{K}{2}\left(\sqrt{(x_{i+1,j,k} - x_{ijk})^2 + (y_{i+1,j,k} - y_{ijk})^2 + (z_{i+1,j,k} - z_{ijk})^2} - l_0\right)^2 \end{aligned}$$

Then the sum of kinetic energies amongst all the x-axis springs are

$$U^x = \frac{K}{2}\sum_{i=0}^{M-2}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i+1,j,k} - x_{ijk})^2 + (y_{i+1,j,k} - y_{ijk})^2 + (z_{i+1,j,k} - z_{ijk})^2} - l_0\right)^2$$

Applying isotropic symmetry yields analogous expressions in y and z. Then the total kinetic energy $T = T^x + T^y + T^z$ (we neglect gravity in this problem) is

$$\boxed{\begin{aligned} U = &\frac{K}{2}\sum_{i=0}^{M-2}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i+1,j,k} - x_{ijk})^2 + (y_{i+1,j,k} - y_{ijk})^2 + (z_{i+1,j,k} - z_{ijk})^2} - l_0\right)^2 \\ &+ \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-2}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i,j+1,k} - x_{ijk})^2 + (y_{i,j+1,k} - y_{ijk})^2 + (z_{i,j+1,k} - z_{ijk})^2} - l_0\right)^2 \\ &+ \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-2}\left(\sqrt{(x_{i,j+1,k} - x_{ijk})^2 + (y_{i,j+1,k} - y_{ijk})^2 + (z_{i,j+1,k} - z_{ijk})^2} - l_0\right)^2 \end{aligned}}$$

Our Lagrangian is thus

$$\boxed{\begin{aligned} \mathcal{L} = &\frac{m}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\dot{x}^2_{ijk} + \dot{y}^2_{ijk} + \dot{z}^2_{ijk}\right) \\ &- \frac{K}{2}\sum_{i=0}^{M-2}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i+1,j,k} - x_{ijk})^2 + (y_{i+1,j,k} - y_{ijk})^2 + (z_{i+1,j,k} - z_{ijk})^2} - l_0\right)^2 \\ &- \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-2}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i,j+1,k} - x_{ijk})^2 + (y_{i,j+1,k} - y_{ijk})^2 + (z_{i,j+1,k} - z_{ijk})^2} - l_0\right)^2 \\ &- \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-2}\left(\sqrt{(x_{i,j+1,k} - x_{ijk})^2 + (y_{i,j+1,k} - y_{ijk})^2 + (z_{i,j+1,k} - z_{ijk})^2} - l_0\right)^2 \end{aligned}}$$

As we will see in **Part IV**, $\frac{\partial\mathcal{L}}{\partial x_{ijk}} = m\dot{x}_{ijk}$, $\frac{\partial\mathcal{L}}{\partial y_{ijk}} = m\dot{y}_{ijk}$, and $\frac{\partial\mathcal{L}}{\partial z_{ijk}} = m\dot{z}_{ijk}$ are in general nonzero. Hence momenta are generally not conserved in this system. However, notice that the Lagrangian is time invariant: $\frac{\partial\mathcal{L}}{\partial t} = 0$. Thus energy is conserved.

$$E = \mathcal{L} - \sum_{(i,j,k)\neq(0,0,0)}\left(\dot{x}_{ijk}\frac{\partial\mathcal{L}}{\partial\dot{x}_{ijk}} + \dot{y}_{ijk}\frac{\partial\mathcal{L}}{\partial\dot{y}_{ijk}} + \dot{z}_{ijk}\frac{\partial\mathcal{L}}{\partial\dot{z}_{ijk}}\right)$$

$$
\begin{aligned}
&= \mathcal{L} - \sum_{(i,j,k)\neq(0,0,0)} \left(m\dot{x}_{ijk}^2 + m\dot{y}_{ijk}^2 + m\dot{z}_{ijk}^2\right) \\
&= \mathcal{L} - m\sum \left(\dot{x}_{ijk}^2 + \dot{y}_{ijk}^2 + \dot{z}_{ijk}^2\right)
\end{aligned}
$$

In going to the last step, we leveraged the fact that $\dot{x}_{000} = \dot{y}_{000} = \dot{z}_{000} = 0$. Hence

$$
\boxed{
\begin{aligned}
E = &\frac{m}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\dot{x}_{ijk}^2 + \dot{y}_{ijk}^2 + \dot{z}_{ijk}^2\right) \\
&+ \frac{K}{2}\sum_{i=0}^{M-2}\sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i+1,j,k}-x_{ijk})^2 + (y_{i+1,j,k}-y_{ijk})^2 + (z_{i+1,j,k}-z_{ijk})^2} - l_0\right)^2 \\
&+ \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-2}\sum_{k=0}^{P-1}\left(\sqrt{(x_{i,j+1,k}-x_{ijk})^2 + (y_{i,j+1,k}-y_{ijk})^2 + (z_{i,j+1,k}-z_{ijk})^2} - l_0\right)^2 \\
&+ \frac{K}{2}\sum_{i=0}^{M-1}\sum_{j=0}^{N-1}\sum_{k=0}^{P-2}\left(\sqrt{(x_{i,j+1,k}-x_{ijk})^2 + (y_{i,j+1,k}-y_{ijk})^2 + (z_{i,j+1,k}-z_{ijk})^2} - l_0\right)^2
\end{aligned}
}
$$

Part IV

For convenience, let us introduce the antidelta

$$\delta'_{mn} = 1 - \delta_{mn}$$

Let us first obtain the equations for x. We shall then apply symmetry to obtain the equations for y and z. Now for $(i,j,k) \neq (0,0,0)$ (this atom does not have any degrees of freedom),

$$\frac{\partial \mathcal{L}}{\partial \dot{x}_{ijk}} = m\dot{x}_{ijk} \;\therefore\; \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_{ijk}} = m\ddot{x}_{ijk}$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial x_{ijk}} = &K\left(\sqrt{(x_{i+1,j,k}-x_{ijk})^2 + (y_{i+1,j,k}-y_{ijk})^2 + (z_{i+1,j,k}-z_{ijk})^2} - l_0\right) \\
&\frac{(x_{i+1,j,k}-x_{ijk})}{\sqrt{(x_{i+1,j,k}-x_{ijk})^2 + (y_{i+1,j,k}-y_{ijk})^2 + (z_{i+1,j,k}-z_{ijk})^2}}\delta'_{i,M-1} \\
&- K\left(\sqrt{(x_{ijk}-x_{i-1,j,k})^2 + (y_{ijk}-y_{i-1,j,k})^2 + (z_{ijk}-z_{i-1,j,k})^2} - l_0\right) \\
&\frac{(x_{ijk}-x_{i-1,jk})}{\sqrt{(x_{ijk}-x_{i-1,j,k})^2 + (y_{ijk}-y_{i-1,j,k})^2 + (z_{ijk}-z_{i-1,j,k})^2}}\delta'_{i,0} \\
&+ K\left(\sqrt{(x_{i,j+1,k}-x_{ijk})^2 + (y_{i,j+1,k}-y_{ijk})^2 + (z_{i,j+1,k}-z_{ijk})^2} - l_0\right)
\end{aligned}
$$

$$
\begin{aligned}
&\frac{(x_{i,j+1,k} - x_{ijk})}{\sqrt{(x_{i,j+1,k} - x_{ijk})^2 + (y_{i,j+1,k} - y_{ijk})^2 + (z_{i,j+1,k} - z_{ijk})^2}} \delta'_{j,N-1} \\
&- K \left(\sqrt{(x_{ijk} - x_{i,j-1,k})^2 + (y_{ijk} - y_{i,j-1,k})^2 + (z_{ijk} - z_{i,j-1,k})^2} - l_0 \right) \\
&\frac{(x_{ijk} - x_{i,j-1,k})}{\sqrt{(x_{ijk} - x_{i,j-1,k})^2 + (y_{ijk} - y_{i,j-1,k})^2 + (z_{ijk} - z_{i,j-1,k})^2}} \delta'_{j,0} \\
&+ K \left(\sqrt{(x_{i,j,k+1} - x_{ijk})^2 + (y_{i,j,k+1} - y_{ijk})^2 + (z_{i,j,k+1} - z_{ijk})^2} - l_0 \right) \\
&\frac{(x_{i,j,k+1} - x_{ijk})}{\sqrt{(x_{i,j,k+1} - x_{ijk})^2 + (y_{i,j,k+1} - y_{ijk})^2 + (z_{i,j,k+1} - z_{ijk})^2}} \delta'_{k,P-1} \\
&- K \left(\sqrt{(x_{ijk} - x_{i,j,k-1})^2 + (y_{ijk} - y_{i,j,k-1})^2 + (z_{ijk} - z_{i,j,k-1})^2} - l_0 \right) \\
&\frac{(x_{ijk} - x_{i,j,k-1})}{\sqrt{(x_{ijk} - x_{i,j,k-1})^2 + (y_{ijk} - y_{i,j,k-1})^2 + (z_{ijk} - z_{i,j,k-1})^2}} \delta'_{k,0}
\end{aligned}
$$

For further brevity, let us define

$$
\lambda^x_{i:m,n} = \frac{x_{mjk} - x_{njk}}{\sqrt{(x_{mjk} - x_{njk})^2 + (y_{mjk} - y_{njk})^2 + (z_{mjk} - z_{njk})^2}}
$$

We similarly define $\lambda^x_{j:m,n}$ and $\lambda^x_{k:m,n}$ substituting the j and k indices, respectively. Also define λ^y and λ^z to use y and z coordinates in the numerator instead. Then we simplify

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial x_{ijk}} = {} & K \left((x_{i+1,j,k} - x_{ijk}) - \lambda^x_{i:i+1,i} l_0 \right) \delta'_{i,M-1} - K \left((x_{ijk} - x_{i-1,j,k}) - \lambda^x_{i:i,i-1} l_0 \right) \delta'_{i,0} \\
&+ K \left((x_{i,j+1,k} - x_{ijk}) - \lambda^x_{j:j+1,j} l_0 \right) \delta'_{j,N-1} - K \left((x_{ijk} - x_{i,j-1,k}) - \lambda^x_{j:j,j-1} l_0 \right) \delta'_{j,0} \\
&+ K \left((x_{i,j,k+1} - x_{ijk}) - \lambda^x_{k:k+1,k} l_0 \right) \delta'_{k,P-1} - K \left((x_{ijk} - x_{i,j,k-1}) - \lambda^x_{k:k,k-1} l_0 \right) \delta'_{k,0}
\end{aligned}
$$

Applying symmetry to obtain the y and z equations, we obtain (for $(i,j,k) \neq (0,0,0)$)

$$
\boxed{
\begin{aligned}
m\ddot{x}_{ijk} = {} & K \left((x_{i+1,j,k} - x_{ijk}) - \lambda^x_{i:i+1,i} l_0 \right) \delta'_{i,M-1} - K \left((x_{ijk} - x_{i-1,j,k}) - \lambda^x_{i:i,i-1} l_0 \right) \delta'_{i,0} \\
&+ K \left((x_{i,j+1,k} - x_{ijk}) - \lambda^x_{j:j+1,j} l_0 \right) \delta'_{j,N-1} - K \left((x_{ijk} - x_{i,j-1,k}) - \lambda^x_{j:j,j-1} l_0 \right) \delta'_{j,0} \\
&+ K \left((x_{i,j,k+1} - x_{ijk}) - \lambda^x_{k:k+1,k} l_0 \right) \delta'_{k,P-1} - K \left((x_{ijk} - x_{i,j,k-1}) - \lambda^x_{k:k,k-1} l_0 \right) \delta'_{k,0} \\
m\ddot{y}_{ijk} = {} & K \left((y_{i+1,j,k} - y_{ijk}) - \lambda^y_{i:i+1,i} l_0 \right) \delta'_{i,M-1} - K \left((y_{ijk} - y_{i-1,j,k}) - \lambda^y_{i:i,i-1} l_0 \right) \delta'_{i,0} \\
&+ K \left((y_{i,j+1,k} - y_{ijk}) - \lambda^y_{j:j+1,j} l_0 \right) \delta'_{j,N-1} - K \left((y_{ijk} - y_{i,j-1,k}) - \lambda^y_{j:j,j-1} l_0 \right) \delta'_{j,0} \\
&+ K \left((y_{i,j,k+1} - y_{ijk}) - \lambda^y_{k:k+1,k} l_0 \right) \delta'_{k,P-1} - K \left((y_{ijk} - y_{i,j,k-1}) - \lambda^y_{k:k,k-1} l_0 \right) \delta'_{k,0} \\
m\ddot{z}_{ijk} = {} & K \left((z_{i+1,j,k} - z_{ijk}) - \lambda^z_{i:i+1,i} l_0 \right) \delta'_{i,M-1} - K \left((z_{ijk} - z_{i-1,j,k}) - \lambda^z_{i:i,i-1} l_0 \right) \delta'_{i,0} \\
&+ K \left((z_{i,j+1,k} - z_{ijk}) - \lambda^z_{j:j+1,j} l_0 \right) \delta'_{j,N-1} - K \left((z_{ijk} - z_{i,j-1,k}) - \lambda^z_{j:j,j-1} l_0 \right) \delta'_{j,0} \\
&+ K \left((z_{i,j,k+1} - z_{ijk}) - \lambda^z_{k:k+1,k} l_0 \right) \delta'_{k,P-1} - K \left((z_{ijk} - z_{i,j,k-1}) - \lambda^z_{k:k,k-1} l_0 \right) \delta'_{k,0}
\end{aligned}
}
$$

Part V

TODO

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 (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 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 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. 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,α,β,γ 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.