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

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

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 approximate

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

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

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

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

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

Our Lagrangian is thus

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

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.

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

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

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

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 $(i, j, k) \neq (0, 0, 0)$ (the corner atom does not have any degrees of freedom),

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

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

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

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 $(i,j,k) \neq (0,0,0)$)

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

Part V

At $t = 0$, we have $y_{ijk} = jl_0$ and $z_{ijk} = kl_0$. Consequently, y_{ijk} is invariant in i and k, while z_{ijk} is invariant in i and j. This means that for $m > n$

$$\begin{aligned}
\sqrt{(x_{mjk} - x_{njk})^2 + (y_{mjk} - y_{njk})^2 + (z_{mjk} - z_{njk})^2} &= |x_{mjk} - x_{njk}| = x_{mjk} - x_{njk}\\
\sqrt{(x_{imk} - x_{ink})^2 + (y_{imk} - y_{ink})^2 + (z_{imk} - z_{ink})^2} &= |y_{imk} - y_{ink}| = y_{imk} - y_{ink} = (m-n)l_0\\
\sqrt{(x_{ijm} - x_{ijn})^2 + (y_{ijm} - y_{ijn})^2 + (z_{ijm} - z_{ijn})^2} &= |z_{ijm} - z_{ijn}| = z_{ijm} - z_{ijn} = (m-n)l_0
\end{aligned}$$

The absolute values resolve given that the oscillations about equilibrium points are assumed to be small; the spatial order of the atoms will therefore be preserved. Then

$$(y_{i+1,j,k} - y_{ijk}) - \lambda^y_{i:i+1,i} l_0 = 0 - 0 = 0$$

$$(y_{i,j+1,k} - y_{ijk}) - \lambda^y_{j:j+1,j} l_0 = l_0 - \frac{l_0}{l_0} l_0 = 0$$

Similar calculations to the first equation can be done for the k index to yield zero (for $i : i, i-1$ we simply shift the index). Adding terms together, this gives $m\ddot{y}_{ijk} = 0$ and so $\ddot{y}_{ijk} = 0$ at $t = 0$. By symmetry, we must have $\ddot{z}_{ijk} = 0$ initially. □

We can also perform similar calculations for the terms replacing the j and k indices in the x_{ijk} equation as we did for the term in the y_{ijk} equation with $i : i+1, i$ to obtain zero. Meanwhile,

$$\lambda^x_{i:i+1,i} = \frac{x_{i+1,j,k} - x_{ijk}}{\sqrt{(x_{i+1,j,k} - x_{ijk})^2}} = 1$$

noting that the absolute value resolves. Shifting indices to apply this to $i : i, i-1$, we now attain

$$m\ddot{x}_{ijk} = K\left((x_{i+1,j,k} - x_{ijk}) - l_0\right)\delta'_{i,M-1} - K\left((x_{ijk} - x_{i-1,j,k}) - l_0\right)\delta'_{i,0}$$

At initial conditions, we reduce $x_{ijk} \mapsto x_i$ seeing that the x_{ijk} is independent of j and k. Then

$$m\ddot{x}_{ijk} = K\left((x_{i+1} - x_i) - l_0\right)\delta'_{i,M-1} - K\left((x_i - x_{i-1}) - l_0\right)\delta'_{i,0}$$

Seeing that the right-hand side is independent of j and k (and so is m), we have demonstrated that $\ddot{x}_{ijk}$ is independent of j and k (at initial conditions). □

Indexing with i, we know have

$$m\ddot{x}_i = K\left((x_{i+1} - x_i) - l_0\right)\delta'_{i,M-1} - K\left((x_i - x_{i-1}) - l_0\right)\delta'_{i,0}$$

For $1 \le i \le M-2$ this simplifies to

$$m\ddot{x}_i = K\left((x_{i+1} - x_i) - l_0\right) - K\left((x_i - x_{i-1}) - l_0\right) = K\left(x_{i+1} + x_{i-1} - 2x_i\right)$$

$$\boxed{m\ddot{x}_i = K\left(x_{i+1} + x_{i-1} - 2x_i\right),\ 1 \le i \le M-2}$$

As for $i = M-1$,

$$\boxed{m\ddot{x}_{M-1} = -K\left((x_{M-1} - x_{M-2}) - l_0\right)}$$

Note that x_0 is no longer a degree of freedom.

Finally, note that $x_i = X_i + il_0$ and $\ddot{X}_i = \ddot{x}_i$. Then for $1 \le i \le M-2$,

$$m\ddot{X}_i = K\left(X_{i+1} + (i+1)l_0 + X_{i-1} + (i-1)l_0 - 2\left(X_i + il_0\right)\right) = K\left(X_{i+1} + X_{i-1} - 2X_i\right)$$

$$\boxed{m\ddot{X}_i = K\left(X_{i+1} + X_{i-1} - 2X_i\right),\ 1 \le i \le M-2}$$

And for $i = M-1$

$$m\ddot{X}_{M-1} = -K\left((X_{M-1} + (M-1)l_0 - X_{M-2} - (M-2)l_0) - l_0\right)$$

$$\boxed{m\ddot{X}_{M-1} = -K\left(X_{M-1} - X_{M-2}\right)}$$

Part VI

For the interior points, we rearrange the X_i equation to get

$$\ddot{X}_i = \frac{K}{m}\left(X_{i+1} + X_{i-1} - 2X_i\right)$$

This equation looks similar to the second derivative difference equation. The mesh points are indexed at $i-1$, i, and $i+1$. Since X_i describes the deviation from equilibrium at $\tilde{x}_i$, the mesh spacing must be the spacing in $\tilde{x}_i$. This is simply l_0. Thus,

$$\boxed{\Delta x = l_0}$$

Hence

$$\boxed{\ddot{X}_i = \frac{Kl_0^2}{m}\frac{X_{i+1} + X_{i-1} - 2X_i}{l_0^2}}$$

Part VII

The discrete equation corresponds to the differential equation

$$\frac{\partial^2 \tilde{X}}{\partial t^2} = \frac{Kl_0^2}{m}\frac{\partial^2 \tilde{X}}{\partial x^2}$$

Seeing that X is constant in j and k, we have $\tilde{X}$ be constant in y and z. Then $\frac{\partial^2 \tilde{X}}{\partial y^2} = \frac{\partial^2 \tilde{X}}{\partial z^2} = 0$. This means that $\nabla^2 \tilde{X} = \frac{\partial^2 \tilde{X}}{\partial t^2}$. Hence

$$\boxed{\frac{\partial^2 \tilde{X}}{\partial t^2} = \frac{Kl_0^2}{m}\nabla^2 \tilde{X}}$$

This gives $c^2 = \frac{Kl_0^2}{m}$. Thus

$$\boxed{c = l_0\sqrt{\frac{K}{m}}}$$

In numerical applications, time must be discretized as well. However, in our equations, time is a continuum. Therefore the discrete equations serve as a better approximation to the wave differential equation than a full discretization would.

Part VIII

Notice that j and k symmetries are preserved when we deform x_{Mjk} by δ. Then we use the equations for X_i from **Part V**. At rest, $\ddot{X}_i = \ddot{x}_i = 0$. We then have the equations

$$X_{i+1} + X_{i-1} - 2X_i = 0$$

for $1 \le i \le M-2$. Moreover, we have the boundary conditions $X_0 = 0$ and $X_{M-1} = \delta$. We may rearrange the X_i equation to

$$X_i = \frac{X_{i+1} + X_{i-1}}{2}$$

That is, X_i is the average value of its two neighbours. We now have M linear equations in M unknowns (two equations are from the boundary conditions). The coefficient matrix is tridiagonal and therefore invertible. Hence there is a unique solution to these equations. By inspection, the solution is

$$X_i = \frac{i}{M}\delta$$

for $0 \le i \le M-1$. Notice that under j and k symmetry, the potential energy simplifies to

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

$$= \frac{NPK}{2} \sum_{i=0}^{M-2} ((X_{i+1} + (i+1)l_0 - X_i - il_0) - l_0)^2 = \frac{NPK}{2} \sum_{i=0}^{M-2} (X_{i+1} - X_i)^2$$
$$= \frac{NPK}{2} \sum_{i=0}^{M-2} \left(\frac{\delta}{M}\right)^2 = \frac{(M-1)NPK\delta^2}{2M^2} \approx \frac{NPK\delta^2}{2M}$$

Noting that $U = 0$ when there is no deformation ($\delta = 0$), we equate

$$\frac{1}{2}E\varepsilon^2 = \frac{1}{2}E\frac{\delta^2}{a^2} = \frac{\Delta U}{V} = \frac{U}{abc} = \frac{1}{MNPl_0^3}\frac{NPK\delta^2}{2M}$$
$$E\frac{1}{a^2} = E\frac{1}{M^2 l_0^2} = \frac{1}{MNPl_0^3}\frac{NPK}{M}$$
$$E = \frac{1}{MNPl_0^3} MNPKl_0^2 = \frac{K}{l_0}$$

Meanwhile, for (average) density we have

$$\rho = \frac{m_{total}}{V} = \frac{MNPm}{MNPl_0^3} = \frac{m}{l_0^3}$$

We now have $K = El_0$ and $m = \rho l_0^3$. Then

$$c = l_0\sqrt{\frac{K}{m}} = l_0\sqrt{\frac{El_0}{\rho l_0^3}} = l_0\sqrt{\frac{E}{\rho l_0^2}}$$

$$\boxed{c = \sqrt{\frac{E}{\rho}}}$$

We have now accomplished our main objective in this problem: to determine the speed of sound in a solid in terms of its macroscopic properties. In terms of material properties, our assumption of invariance in y and z implies a material of zero Poisson's ratio.

This is indeed an accurate expression for the speed of sound in a homogeneous linear solid with zero Poisson's ratio; for example, this agrees with the expression given in *Sears and Zemansky's University Physics*. Applying these results to a few metals (aluminum, lead, and steel) gives underestimates of 15-40%. This could be due to our assumption of zero Poisson's ratio. Qualitatively, we would expect faster sound propagation under a nonzero Poisson's ratio. This is because longitudinal straining along the x-axis would induce straining along the y- and z-axes. These in turn would induce straining along the x-axis, thereby facilitating acoustic wave transport.

Part IX

<u>Dirichlet BCs</u>

Trivially, this corresponds to simply fixing the $x = a$ face at a certain x-coordinate $x = p$. Notice that $x_{M-1,j,k}$ are no longer degrees of freedom.

Mixed BCs

Let us now introduce a ghost mesh point X_M in discretizing $\tilde{X}$. Then we may rewrite

$$mX_{M-1} = -K(X_{M-1} - X_{M-2}) = K(X_M + X_{M-2} - 2X_{M-1}) - K(X_M - X_{M-1})$$

If we discretize

$$\frac{\partial \tilde{X}}{\partial x}(x = a, y, z, t) = \frac{X_M - X_{M-1}}{l_0}$$

So in the case of mixed boundary conditions

$$mX_{M-1} = K(X_M + X_{M-2} - 2X_{M-1}) - Kl_0 q$$

This means that the mixed boundary condition corresponds to a constant force F being applied uniformly on the $x = a$ face. To see why, we first see that our potential energy has an additional terms $-fx_{M-1,j,k}$ for all j and k in bounds. Then the Lagrangian would have the terms $+fx_{M-1,j,k}$. Differentiating into the EL equations gives a $+f$ term:

$$mX_{M-1} = K(X_M + X_{M-2} - 2X_{M-1}) - Kl_0 q + f$$

Here f is the force applied on each atom. Uniform application of the force maintains j and k symmetry. It follows that $F = NPf$. Applying the discretization of $\frac{\partial^2 \tilde{X}}{\partial t^2} = c^2 \frac{\partial^2 \tilde{X}}{\partial x^2}$ to the $M - 1$ mesh point, we then have

$$mX_{M-1} = K(X_M + X_{M-2} - 2X_{M-1})$$

This means that $f = Kl_0 q$. Then

$$F = NPKl_0 q = \frac{K}{l_0} NPl_0^2 q = Ebcq$$

$$\boxed{F = qEA}$$

where $A = bc$ is the cross-sectional area of the solid. In fact, under a Newtonian formalism, we have $\varepsilon = \frac{\sigma}{E} = \frac{F}{EA}$. This suggests that q is the applied strain on the solid. Geometrically, we would indeed expect $\frac{\partial \tilde{X}}{\partial x}\Big|_{x=a}$ to be the overall strain of the bar under a linear strain profile.

Robin BCs

In this case we have

$$\beta \frac{d\tilde{X}}{dx}(x = a, y, z, t) = \gamma - \alpha \tilde{X}(x = a, y, z, t)$$
$$\frac{d\tilde{X}}{dx}(x = a, y, z, t) = \frac{\gamma}{\beta} - \frac{\alpha}{\beta}\tilde{X}(x = a, y, z, t)$$

Then

$$\begin{aligned} mX_{M-1} &= K(X_M + X_{M-2} - 2X_{M-1}) - K(X_M - X_{M-1}) \\ &= K(X_M + X_{M-2} - 2X_{M-1}) - Kl_0\left(\frac{\gamma}{\beta} - \frac{\alpha}{\beta}X_{M-1}\right) \\ &= K(X_M + X_{M-2} - 2X_{M-1}) + \frac{\alpha K l_0}{\beta}\left(X_{M-1} - \frac{\gamma}{\alpha}\right) \end{aligned}$$

This corresponds to a spring of spring constant κ and equilibrium length L_0 being uniformly applied to the $x = a$ face. Let κ' be the effective spring constant on each atom. Then the potential energy gains a $+\frac{\kappa'}{2}\left(x_{M-1,j,k} - L_0\right)^2$ term. Conversely, the Lagrangian gains a $-\frac{\kappa'}{2}\left(x_{M-1,j,k} - L_0\right)^2$ term. So the EL equation for $x_{M-1} \to X_{M-1}$ gains a $-\kappa'\left(x_{M-1} - L_0\right)$ term (note the j and k symmetries being preserved):

$$mX_{M-1} = K(X_M + X_{M-2} - 2X_{M-1}) + \frac{\alpha K l_0}{\beta}\left(X_{M-1} - \frac{\gamma}{\alpha}\right) - \kappa'\left(x_{M-1} - L_0\right)$$

It follows that $\kappa' = \frac{\alpha K l_0}{\beta}$ and

$$\boxed{L_0 = \frac{\gamma}{\alpha}}$$

Of course, for the limiting case $\beta \to 0$ (in the direction of sign that agrees with α) we have a fully rigid spring holding the face fixed at $x = \frac{\gamma}{\alpha}$ (we will see shortly that κ is proportional to κ'); this agrees with our result for the Dirichlet condition that would be obtained. To relate κ' with κ, we equate the spring energies taking across the entire $x = a$ face:

$$\frac{\kappa}{2}\left(x_{M-1} - L_0\right)^2 = \sum_{j=0}^{N-1}\sum_{k=0}^{P-1}\frac{\kappa'}{2}\left(x_{M-1} - L_0\right)^2 = NP\frac{\kappa'}{2}\left(x_{M-1} - L_0\right)^2$$

This gives us $\kappa = NP\kappa'$. Thus

$$\kappa = NP\frac{\alpha K l_0}{\beta} = \frac{\alpha}{\beta}\frac{K}{l_0}NPl_0^2 = \frac{\alpha}{\beta}EA$$

We box this as

$$\boxed{\kappa = \frac{\alpha}{\beta}EA}$$

Of course, α and β must agree in sign for this spring to be stable. Then for the limiting case $\alpha \to 0$, we first rearrange the spring force to be

$$F = -\kappa\left(x_{M-1} - L_0\right) = \kappa L_0\left(1 - \frac{x_{M-1}}{L_0}\right) = \frac{\gamma}{\beta}EA\left(1 - \frac{x_{M-1}}{L_0}\right) = \frac{\gamma}{\beta}EA\left(1 - \frac{\alpha}{\gamma}x_{M-1}\right)$$

We see that as $\alpha \to 0$ we obtain $F = \frac{\gamma}{\beta}EA$, agreeing with our result for the mixed boundary condition. Interestingly, the sign of α need not agree with that of β in the limit to recover this relationship.