

Homework 2 Solutions

1. Maxwell-Boltzman distribution

(a) By definition $\langle v \rangle =$

$$\int_{\mathbf{v}} v P(\mathbf{v}) d\mathbf{v} = \int_{\mathbf{v}} v P(\mathbf{v}) d\mathbf{v} = (m/2\pi k_B T)^{3/2} \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} v \exp(-mv^2/2k_B T) v^2 \sin\theta dv d\theta d\phi$$

$$= 4\pi (m/2\pi k_B T)^{3/2} \int_0^{\infty} v \exp(-mv^2/2k_B T) v^2 dv$$

From tables of Gaussian integrals (or using your favorite symbolic math tool such as Maple

or Mathematica), we find $= \int_0^{\infty} v^3 \exp(-mv^2/2k_B T) dv = 2(k_B T/m)^2$

So the final result is $\langle v \rangle = [(8k_B T)/(m\pi)]^{1/2} \approx 1.6 (k_B T/m)^{1/2}$

(b) The “most likely” velocity is where the pdf has a maximum value with respect to all the independent variables. To see this we convert to scalar form $P(\mathbf{v})d\mathbf{v} = (m/2\pi k_B T)^{3/2} \exp(-mv^2/2k_B T)d\mathbf{v} = (m/2\pi k_B T)^{3/2} \exp(-mv^2/2k_B T) v^2 \sin\theta dv d\theta d\phi$. The most likely velocity is where $\partial P/\partial v = 0 = (m/2\pi k_B T)^{3/2} \{ \exp(-mv^2/2k_B T) 2v + v^2 \exp(-mv^2/2k_B T) (-mv/k_B T) \}$. The solution clearly is $v = (2k_B T/m)^{1/2} \approx 1.4 (k_B T/m)^{1/2}$

(c) The variance follows from the definition $(\Delta v)^2 \equiv \langle (\mathbf{v} - \langle \mathbf{v} \rangle)^2 \rangle = \langle \mathbf{v}^2 - 2\mathbf{v}\langle \mathbf{v} \rangle + \langle \mathbf{v} \rangle^2 \rangle = \langle \mathbf{v}^2 \rangle - \langle v \rangle^2$. By definition $\langle v^2 \rangle = 4\pi (m/2\pi k_B T)^{3/2} \int_0^{\infty} v^4 \exp(-mv^2/2k_B T) dv$. But from Gaussian

integral tables (or your favorite symbolic math tool), we find $= \int_0^{\infty} v^4 \exp(-mv^2/2k_B T) dv =$

$(3/8)(\pi)^{1/2} (2k_B T/m)^{5/2}$. So after some fortuitous cancellations, $\langle v^2 \rangle = (3k_B T/m)$. And thus $\langle v^2 \rangle - \langle v \rangle^2 = (k_B T/m)(3 - 8/\pi)$, and $v_{rms} = [\langle v^2 \rangle - \langle v \rangle^2]^{1/2} \approx 0.67 (k_B T/m)^{1/2}$

(d) $M(v)dv = \int_0^{\pi} \int_0^{2\pi} P(v) dv d\theta d\phi = (m/2\pi k_B T)^{3/2} \int_0^{2\pi} \int_0^{\pi} \exp(-mv^2/2k_B T) v^2 \sin\theta dv d\theta d\phi =$

$4\pi (m/2\pi k_B T)^{3/2} \exp(-mv^2/2k_B T) v^2 dv$. Thus $dM/dv = 4\pi (m/2\pi k_B T)^{3/2} \exp(-mv^2/2k_B T) v^2$ which is evaluated on the attached Excel spreadsheet and plotted below. Here we clearly see the most likely velocity value as the peak of the curve. And the average value is slightly above the peak, consistent with the fact that the averaging process is skewed by the long Gaussian “tail”. We also see that the rms deviation (often called the “standard” deviation) represents the range above and below the average value over which the $M(v)dv$ is large. The fact that it is relatively tight allows one to deal with the entire distribution simply by dealing with the most likely or average values exclusively – an approximation behind the kinetic theory that is so useful in the most basic form of transport theory, known as kinetic theory.

2. Single particle level as Boltzman subsystem.

(a) Starting with the Boltzman pdf, derive the mean number of particles $\langle n_i \rangle$ in the single state of total energy (kinetic + potential) u_i .

(b) Now derive the variance or mean-square fluctuations, $\langle (\Delta n_i)^2 \rangle$. [clue: start with the Boltzman distribution and utilize the general result for random variables, $\langle (\Delta n_i)^2 \rangle = \langle (n - \langle n_i \rangle)^2 \rangle = \langle n_i^2 \rangle - \langle n_i \rangle^2$].

(a) Since each Boltzmann subsystem is now a single state but with arbitrary population, the mean number

of particles in this state is $\langle n_i \rangle = \frac{\sum_{n_i=0}^{\infty} n_i \exp[-n_i \cdot u_i / k_B T]}{\sum_{n_i=0}^{\infty} \exp[-n_i \cdot u_i / k_B T]}$ (note the summation over n_i , not i ; this reflects

the fact that the state itself is the subsystem – the various populations of that state constitute the different terms of the statistical ensemble). The denominator (inverse normalization constant) can be evaluated

using elementary calculus as a convergent geometric series: $\sum_{n_i=0}^{\infty} \exp[-n_i \cdot u_i / k_B T] = \frac{1}{1 - \exp(-u_i / k_B T)}$.

The numerator can be evaluated using the same type of trick as described in lecture: this time take advantage of the fact that

$$\sum_{n_i=0}^{\infty} n_i \exp[-n_i \cdot u_i / k_B T] = \sum_{n_i=0}^{\infty} -k_B T \cdot \frac{d}{du_i} \exp[-n_i \cdot u_i / k_B T] = -k_B T \frac{d}{du_i} \sum_{n_i=0}^{\infty} \exp[-n_i \cdot u_i / k_B T]$$

where the last step follows by interchanging the order of summation and differentiation (allowable for well behaved functions). So by summing the geometric series, we get for the next step

$$-k_B T \cdot \frac{d}{du_i} \left\{ \frac{1}{1 - \exp(-u_i / k_B T)} \right\} = \frac{\exp(-u_i / k_B T)}{[1 - \exp(-u_i / k_B T)]^2}$$

So by taking the ratio of numerator to denominator, we get simply $\langle n_i \rangle = \frac{\exp(-u_i / k_B T)}{1 - \exp(-u_i / k_B T)} = \frac{1}{\exp(u_i / k_B T) - 1}$, the famous Planck function when $u_i = h\nu$

(b) To get the variance, we start with a fundamental result that follows from the statistical nature,

$$\langle (\Delta n_i)^2 \rangle \equiv \langle (n_i - \langle n_i \rangle)^2 \rangle = \langle n_i^2 \rangle - 2\langle n_i \rangle \langle n_i \rangle + \langle n_i \rangle^2 = \langle n_i^2 \rangle - 2\langle n_i \rangle^2 + \langle n_i \rangle^2 = \langle n_i^2 \rangle - \langle n_i \rangle^2$$

where $\langle n_i \rangle$ was derived in (a) and $\langle n_i^2 \rangle = \frac{\sum_{n_i=0}^{\infty} n_i^2 \exp[-n_i \cdot u_i / k_B T]}{\sum_{n_i=0}^{\infty} \exp[-n_i \cdot u_i / k_B T]}$. The latter can be evaluated by the same

type of trick as in (a) using the fact that

$$\sum_{n_i=0}^{\infty} n_i^2 \exp[-n_i \cdot u_i / k_B T] = \sum_{n_i=0}^{\infty} \left(\frac{k_B T}{u_i} \right)^2 \cdot \frac{d^2}{du_i^2} \exp[-n_i \cdot u_i / k_B T] = \left(\frac{k_B T}{u_i} \right)^2 \cdot \frac{d^2}{du_i^2} \sum_{n_i=0}^{\infty} \exp[-n_i \cdot u_i / k_B T]$$

So the numerator above becomes (with some good algebra)

$$\left(\frac{k_B T}{u_i} \right)^2 \left(\frac{d^2}{du_i^2} \right) \left[\frac{1}{1 - \exp(-u_i / k_B T)} \right] = \frac{\exp(-u_i / k_B T) [1 + \exp(-u_i / k_B T)]}{[1 - \exp(-u_i / k_B T)]^3}$$

Thus, we have $\langle n_i^2 \rangle = \frac{\exp(-u_i / k_B T) [1 + \exp(-u_i / k_B T)]}{[1 - \exp(-u_i / k_B T)]^3} = \frac{\exp(u_i / k_B T) + 1}{[\exp(u_i / k_B T) - 1]^2}$

$$\text{so } \langle n_i^2 \rangle - \langle n_i \rangle^2 = \frac{\exp(u_i / k_B T) + 1}{[\exp(u_i / k_B T) - 1]^2} - \frac{1}{[\exp(u_i / k_B T) - 1]^2} = \frac{\exp(u_i / k_B T)}{[\exp(u_i / k_B T) - 1]^2} = \langle n_i \rangle (\langle n_i \rangle + 1)$$

This is a remarkable result of discrete statistics: the greater the population of a state, the greater its variance.

3. Independent of its location, the electron in an singly-ionized hydrogen molecule creates an attractive force on both protons governed by Coulomb's law:

$$\vec{F}_{12} = \frac{e^2}{4\pi\epsilon_0} \frac{\hat{r}_{12}}{r_{12}^2} \quad \text{and} \quad \vec{F}_{13} = \frac{e^2}{4\pi\epsilon_0} \frac{\hat{r}_{13}}{r_{13}^2}$$

\hat{r}_{12} is the unit vector pointing from the left proton [labeled 2 in Fig. 1(a)] to the electron, \hat{r}_{13} is the unit vector pointing from the right proton [labeled 3 in Fig. 1(a)] to the electron, and r_{12} and r_{13} are the distanced between each pair. These forces can be defined in Cartesian coordinates as shown in Fig. 1(a). A necessary, but by no means sufficient, condition for a stable bond is that the x component of the net force between the protons and electron be attractive with respect to the protons. In other words, the effect of the electron should be to draw the protons closer together, not further apart. This is a necessary condition because the Coulomb force between the protons alone is always repulsive. So unless the electron induces an attractive effect, there is no chance for a stable bond. It is not a sufficient condition because, in principle, the induced attractive force must exceed the repulsive force between the protons if the bond is to be absolutely stable. This sufficient condition can also be analyzed mathematically, as done below.

Ignoring for the moment the proton-proton repulsion, the net electrostatic force induced by the electron on the two protons will be attractive along the x direction when

$$F_{12,x} - F_{13,x} > 0$$

Assuming the origin in Fig. 1(a) lies at the midpoint between the protons and the electron is located at (x,y), we have

$$r_{12}^2 = (x+a)^2 + y^2 \quad \text{and} \quad r_{13}^2 = (x-a)^2 + y^2$$

$$\hat{r}_{12,x} = \frac{(x+a) \cdot \hat{x}}{[(x+a)^2 + y^2]^{1/2}} \quad \text{and} \quad \hat{r}_{13,x} = \frac{(x-a) \cdot \hat{x}}{[(x-a)^2 + y^2]^{1/2}}$$

So the net-attractive condition becomes (after multiplying by $4\pi\epsilon_0/e^2$)

$$\frac{x+a}{[(x+a)^2 + y^2]^{3/2}} - \frac{x-a}{[(x-a)^2 + y^2]^{3/2}} > 0 \tag{1}$$

Because of the inequality, this expression defines a region in space which can be defined very

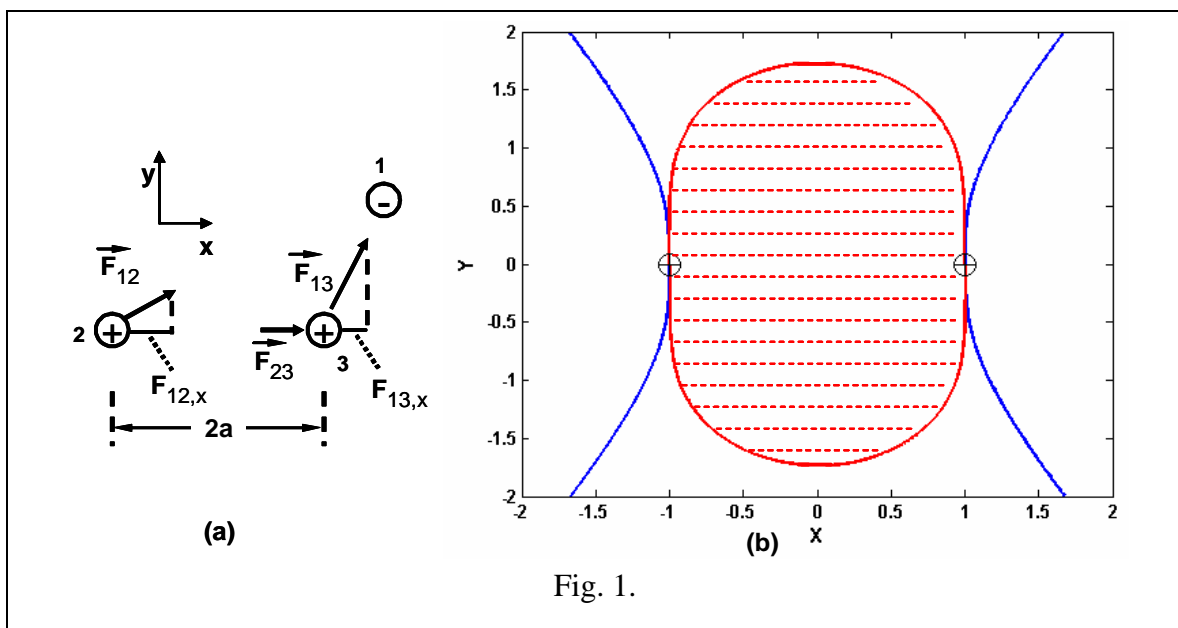


Fig. 1.

simply along the x axis (i.e., $y = 0$). Under this condition, we have

$$\frac{x+a}{[(x+a)^2]^{3/2}} - \frac{x-a}{[(x-a)^2]^{3/2}} > 0$$

where the exponentiation is maintained in the denominator to remind us that the denominators should always be positive, regardless of x . By inspection, the inequality is satisfied only for $-a < x < a$. This makes sense physically since when the electron is located between the two protons, the induced net attraction will always be larger than the proton-to-proton repulsion. An analytic solution to Eqn (1) is tedious, but a numerical solution is easy by a number of different methods. Shown in Fig. 1(b) (solid blue lines) is the solution for equality in Fig. (1) obtained with a simple MATLAB function (hydrogen.m on course Website) assuming $a = 1$. Each solution locus is a hyperbola that intersects the two protons represented by plus signs. Clearly, the inequality is satisfied at all (x,y) values between these two loci.

Eqn (1) is just a necessary condition because the Coulomb force between the protons is always repulsive. So unless the electron induces an attractive effect, there is no chance for a stable covalent bond. To be a sufficient condition, the induced attractive force must exceed the repulsive force between the protons. This can also be analyzed mathematically by adding to Eqn (1) the corresponding x component of the repulsive force.

$$\frac{x+a}{[(x+a)^2 + y^2]^{3/2}} - \frac{x-a}{[(x-a)^2 + y^2]^{3/2}} - \frac{1}{4a^2} > 0 \quad (2)$$

The numerical solution corresponding to this condition is also plotted in Fig. 1(b). The solid red line denotes equality in Eqn. 1(b), and the shaded region denotes where the inequality is satisfied. As might be expected intuitively, the additional constraint in Eqn. (2) limits the possible electron position a much smaller area (shown by the red cross hatch) than satisfies Eqn. (1). This smaller region “between the protons” is where bonding of ionized hydrogen molecule can occur.

4. Given the following form of the compliance matrix,

$$\begin{matrix} 0.7664 & -0.2130 & -0.2130 & 0 & 0 & 0 \\ -0.2130 & 0.7664 & -0.2130 & 0 & 0 & 0 \\ -0.2130 & -0.2130 & 0.7664 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.2563 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.2563 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.2563 \end{matrix}$$

we expect the inverse (stiffness) matrix to have exactly the same form; i.e., all nonzero elements in the upper-left quadrant; all zeroes in the lower left and upper right quadrants; and nonzero elements only along the diagonal of the lower-right quadrant.

(b) substitution of this matrix into Matlab and using the inv.m function (matrix inversion) leads to the result.

$$\begin{matrix} 1.6600 & 0.6390 & 0.6390 & 0 & 0 & 0 \\ 0.6390 & 1.6600 & 0.6390 & 0 & 0 & 0 \\ 0.6390 & 0.6390 & 1.6600 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.7960 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.7960 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.7960 \end{matrix}$$

Given the units of 10^{11} N/m² we have $C_{11} = 166$ GPa, $C_{12} = 63.9$ GPa, and $C_{44} = 79.6$ GPa - the three distinct coefficient for crystalline silicon !

5. (Young's modulus and Poisson's ratio). An isotropic solid is subject to tension along the x axis
i. Find the stiffness coefficients in terms of Young's modulus and Poisson's ratio

In the notes there is general form of the compliance matrix for an isotropic solid:

$$\begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{xz} \\ e_{xy} \end{bmatrix} = \begin{bmatrix} 1/Y & -\sigma/Y & -\sigma/Y & 0 & 0 & 0 \\ -\sigma/Y & 1/Y & -\sigma/Y & 0 & 0 & 0 \\ -\sigma/Y & -\sigma/Y & 1/Y & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1+\sigma)/Y & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1+\sigma)/Y & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1+\sigma)/Y \end{bmatrix} \begin{bmatrix} P_{xx} \\ P_{yy} \\ P_{zz} \\ P_{yz} \\ P_{xz} \\ P_{xy} \end{bmatrix}$$

We expect the stiffness matrix to have the form:

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{bmatrix}$$

By definition, the stiffness matrix is the inverse of the compliance matrix. Stated mathematically, this means that if X is the matrix product of the two matrices, then

$$X_{MN} = \sum_K C_{MK} S_{KN} = \delta_{M,N} \text{ where } \delta_{M,N} \text{ is the Kronecker delta function } (= 1 \text{ if } M = N; = 0 \text{ if } M$$

$\neq N$). It is easy to show $X_{11} = X_{22} = X_{33} = 1 = (C_{11} - 2C_{12}\sigma)/Y$ (*), and $X_{12} = X_{13} = X_{21} = X_{23} = X_{31} = X_{32} = 0 = [C_{12} - \sigma(C_{11} + C_{12})]/Y$ (**). Multiplying (*) by σ and adding to (**) (to eliminate dependence on C_{11}), we get $\sigma Y = -2C_{12}\sigma^2 + C_{12}(1 - \sigma)$, or

$$C_{12} = \sigma Y / (1 - \sigma - 2\sigma^2).$$

Substitution of this back into (*) yields $C_{11} = Y + 2\sigma^2 Y / (1 - \sigma - 2\sigma^2)$, or

$$C_{11} = Y(1 - \sigma) / (1 - \sigma - 2\sigma^2)$$

To get C_{22} , we note $X_{44} = X_{55} = X_{66} = 1 = C_{44} 2(1+\sigma)/Y$, or

$$C_{44} = Y / [2(1 + \sigma)]$$

- ii. There is an alternate form of the stiffness matrix for an isotropic solid in terms of Lamé coefficients

$$\begin{bmatrix} P_{xx} \\ P_{yy} \\ P_{zz} \\ P_{yz} \\ P_{xz} \\ P_{xy} \end{bmatrix} = \begin{bmatrix} 2\mu_L + \lambda_L & \lambda_L & \lambda_L & 0 & 0 & 0 \\ \lambda_L & 2\mu_L + \lambda_L & \lambda_L & 0 & 0 & 0 \\ \lambda_L & \lambda_L & 2\mu_L + \lambda_L & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_L & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu_L & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu_L \end{bmatrix} \begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{xz} \\ e_{xy} \end{bmatrix}$$

These can be related directly to the Young's modulus and Poisson's ratio through the stiffness coefficients. By inspection, we have

$$\lambda_L = C_{12} = \sigma Y / (1 - \sigma - 2\sigma^2)$$

$$\mu_L = Y / [2(1 + \sigma)]$$

For self consistency we check the sum $2\mu_L + \lambda_L = Y(1 - \sigma) / (1 - \sigma - 2\sigma^2) = C_{11}$, as expected.

6. (a) For purified aluminum $Y = 73$ GPa and $\sigma = 0.33 \Rightarrow \lambda_L = 53.3$ GPa and $\mu_L = 27.4$ GPa.
For amorphous SiO_2 , $Y = 85$ GPa, and $\sigma = 0.25 \Rightarrow \lambda_L = 34.0$ GPa and $\mu_L = 34.0$ GPa (equal !)
(b) From the Lamé coefficients for aluminum, $C_{12} = \lambda_L = 53$ GPa, $C_{11} = 2\mu_L + \lambda_L = 108$ GPa
and $C_{44} = \mu_L = 27$ GPa. From the Lamé coefficients for amorphous SiO_2 ,
 $C_{12} = 34$ GPa, $C_{11} = 102$ GPa and $C_{44} = 34$ GPa

7. (Speed of Sound in an Isotropic Solid)

- i. along the \mathbf{x} , \mathbf{y} , or \mathbf{z} directions in an isotropic solid, we can use the same formulation as for a cubic solid and solve the component elastic wave equation. With a longitudinal wave $\Delta r_x = \Delta r_0 \exp[j(kx - \omega t)]$ along the x axis, for example. The solution leads to the dispersion relation $\omega = k c = k [(2\mu_L + \lambda_L)/\rho]^{1/2}$ where c is the speed of longitudinal sound in terms of the stiffness and Lamé coefficients.
- ii. For the shear wave, the solutions are $r_y = \Delta r_0 \exp[j(kx - \omega t)]$ or $r_z = \Delta r_0 \exp[j(kx - \omega t)]$ and find $\omega = k c = k (C_{44}/\rho)^{1/2}$.
- iii. Along the $\mathbf{x} + \mathbf{y} + \mathbf{z}$ axis (cube diagonal in Cartesian coordinates), we use the clue that

$u = \Delta r_x = v = \Delta r_y = z = \Delta r_z$ and the elastic wave equation becomes

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2} + C_{44} \left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + (C_{12} + C_{44}) \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 u}{\partial x \partial z} \right)$$

(only dependent variable is u !). We seek the solution $u = u_0 e^{[j(k(x+y+z)/\sqrt{3}-\omega t)]}$ and

substitute to get

$$-\rho \omega^2 u_0 = -C_{11} \frac{k^2}{3} u_0 - C_{44} \left(\frac{k^2}{3} + \frac{k^2}{3} \right) u_0 - (C_{12} + C_{44}) \left(\frac{k^2}{3} + \frac{k^2}{3} \right) u_0$$

$$\rho \omega^2 = C_{11} \frac{k^2}{3} + 4C_{44} \frac{k^2}{3} + 2C_{12} \frac{k^2}{3}$$

$$\text{or } \frac{\omega}{k} = v_s = \left[\frac{1}{\rho} \left(\frac{C_{11}}{3} + \frac{2C_{12}}{3} + \frac{4C_{44}}{3} \right) \right]^{1/2} = \frac{\omega}{k} = v_s = \left[\frac{1}{\rho} \left(\frac{C_{11}}{3} + \frac{2C_{12}}{3} + \frac{4C_{44}}{3} \right) \right]^{1/2}$$

- iv. To get the velocities we first need the densities: a little searching reveals $\rho = 2700$ KG/m³ (Al) and $\rho = 2600$ KG/m³ (SiO_2), so that for compressional wave along \mathbf{x} , \mathbf{y} , or \mathbf{z} :
 $c = k(C_{11}/\rho)^{1/2} = [(2\mu_L + \lambda_L)/\rho]^{1/2} = 6325$ m/s for aluminum and 6263 m/s for SiO_2

For the shear wave along **x, y, or z**: we get $c = k(C_{44}/\rho)^{1/2} = [\mu_L/\rho]^{1/2} = 3162$ m/s for Al and 3616 m/s for SiO₂. For the compressional wave along **x + y + z** direction, we get

$$\frac{\omega}{k} = v_s = \left[\frac{1}{\rho} \left(\frac{C_{11}}{3} + \frac{2C_{12}}{3} + \frac{4C_{44}}{3} \right) \right]^{1/2} = \left[\frac{1}{\rho} \left(\frac{2\mu_L + \lambda_L}{3} + \frac{2\lambda_L + 4\mu_L}{3} \right) \right]^{1/2} = \left[\frac{2\mu_L + \lambda_L}{\rho} \right]^{1/2}$$

So the longitudinal wave is the same along the **x + y + z** as along **x, y, or z**. This can be generalized to a compressional (or shear) wave velocity independent of orientation, just what one expects in an “isotropic” solid !

8. If the solid has a cubic symmetry in an x, y, z cartesian system and is subjected to tension along the **x** axis:
 (a) Young’s modulus:

It is always true
$$\begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & \dots \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} P_{xx} \\ P_{yy} \\ P_{zz} \\ \vdots \\ \vdots \end{pmatrix},$$
 but under uniaxial stress only one P_M is

nonzero, let’s let it be P_{xx} . So we have $e_{xx} = S_{11}P_{xx}$ ($S_{11} \rightarrow$ compliance coefficient) and by definition $\nu \equiv \frac{-P_{xx}}{e_{xx}} = \frac{1}{S_{11}}$. Unfortunately, the relationship between the compliance and stiffness matrix is not as simple as for the isotropic solid. But from inversion formulae, we can solve for S_{11} by algebra in terms of elastic stiffness coefficient C.

$$S_{11} - S_{12} = \frac{1}{C_{11} - C_{12}}, S_{11} + 2S_{12} = \frac{1}{C_{11} + 2C_{12}} \Rightarrow 3S_{11} = \frac{2}{C_{11} - C_{12}} + \frac{1}{C_{11} + 2C_{12}}$$

$$\text{or } 3S_{11} = \frac{3(C_{11} + C_{12})}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \Rightarrow \nu = \frac{C_{11}^2 + C_{11}C_{12} - 2C_{12}^2}{C_{11} + C_{12}}$$

Poisson’s ratio $\sigma \equiv \frac{e_{yy}}{e_{xx}}$ or $\frac{e_{zz}}{e_{xx}}$: But $e_{yy} = S_{21}P_{xx}$, all other $P_M = 0$. So $\frac{e_{yy}}{e_{xx}} = \frac{S_{21}}{S_{11}} = \frac{S_{12}}{S_{11}}$.

And from Kittel, Eqn. (51): $S_{11} - S_{12} = \frac{1}{C_{11} - C_{12}}$ (i) and $S_{11} + 2S_{12} = \frac{1}{C_{11} + 2C_{12}}$ (ii)

We then divide (ii) by (i) to get

$$\frac{1 + 2S_{12}/S_{11}}{1 - S_{12}/S_{11}} = \frac{1 - 2\sigma}{1 + \sigma} = \frac{C_{11} - C_{12}}{C_{11} + 2C_{12}}. \text{ Let's call this quantity } \alpha$$

So, $1 - 2\sigma = \alpha(1+\sigma)$; $2\sigma + \alpha\sigma = 1 - \alpha \Rightarrow \sigma = (1-\alpha)/(\alpha+2)$

So we get finally,
$$\sigma = \frac{1 - \frac{C_{11}-C_{12}}{C_{11}+2C_{12}}}{\frac{C_{11}-C_{12}}{C_{11}+2C_{12}}+2} = \frac{3C_{12}}{3C_{11}+3C_{12}} = \frac{C_{12}}{C_{11}+C_{12}}$$

b) We evaluate Young's modulus for Si and NaCl (see Table 12 of Kittel). For silicon

$C_{11} = 1.66 \times 10^{11} \text{ N/m}^2$, $C_{12} = 0.639 \times 10^{11} \text{ N/m}^2$, so $Y_{Si} = \frac{C_{11}^2 + C_{11}C_{12} - 2C_{12}^2}{C_{11} + C_{12}} \cong \frac{3.000}{2.299} \times 10^{11} \text{ N/m}^2$

and $\sigma = 0.278$. For NaCl, $C_{11} = 0.487 \times 10^{11} \text{ N/m}^2$, $C_{12} = 0.124 \times 10^{11} \text{ N/m}^2$, so

$Y_{NaCl} = \frac{0.267}{0.611} \times 10^{11} \text{ N/m}^2 = 0.437 \times 10^{11} \text{ N/m}^2$ and $\sigma = 0.203$.

c) We can now evaluate the velocity of a longitudinal acoustic wave along the **x** direction and along the **x + y + z** directions for cubic Si and NaCl.

For silicon:

$C_{11} = 1.66 \times 10^{11} \text{ N/m}^2$, $C_{12} = 0.639 \times 10^{11} \text{ N/m}^2$, $C_{44} = 0.796 \times 10^{11} \text{ N/m}^2$, and

$\rho = 2.33 \times 10^3 \text{ KG/m}^3$ (from CRC handbook of Chemistry and Physics)

So, $v_s = \left[\frac{1}{2,330} 1.66 \times 10^{11} \right]^{1/2} = 8440 \text{ m/s}$ along **x, y, or z**

$v_s = \left[\frac{1}{2,330} (0.553 + 0.426 + 1.061) \times 10^{11} \right]^{1/2} = 9360 \text{ m/s}$ along **x+y+z**

So there is now anisotropy in the compressional wave speed !

For NaCl:

$C_{11} = 0.487 \times 10^{11} \text{ N/m}^2$, $C_{12} = 0.124 \times 10^{11} \text{ N/m}^2$, $C_{44} = 0.126 \times 10^{11} \text{ N/m}^2$, and

$\rho = 2.16 \times 10^3 \text{ KG/m}^3$ (from CRC handbook of Chemistry and Physics)

So, $v_s = \left[\frac{1}{2,160} 0.487 \times 10^{11} \right]^{1/2} = 4748 \text{ m/s}$ along **x, y, or z**

$v_s = \left[\frac{1}{2160} (0.162 + 0.083 + 0.168) \times 10^{11} \right]^{1/2} = 4370 \text{ m/s}$ along **x+y+z**

Again, the compressional wave is anisotropic. But in contrast to silicon, it moves a bit slower along **x + y + z** than it does along **x, y, or z**.