Physics 489 S 04 Lecture 9
Lattice Vibrations II (Ashcroft and Merminchapter 21, 22)

1. Generalization to D = 2 and 3 dimensions.
   Normal modes described by wavevector $\mathbf{k}$ in one primitive cell of reciprocal lattice
   Convenient choice: Brillouin Zone

2. Counting of modes
   Number of allowed k values = number of unit cells in crystal
   Density of allowed values of $\mathbf{k}$ is $(L/2\pi)^D$
   Thus $(1/V)\sum_{\mathbf{k}} \to (1/2\pi)^D \int_{BZ} d^D k$, exactly the same as for electrons described in Lecture 2

3. Types of motion
   Motions in D = 2 or 3 directions: Longitudinal, transverse motions
   For S atoms per cell: D × S dispersion curves; D acoustic; D(S-1) optic

4. D = 1,2, or 3 dimensions - one atom per cell
   Define displacements $u_\mu(\mathbf{R}_i^0)$, where $\mathbf{R}_i^0$ is the position of the atom in cell i and $\mu =$ vector direction ($\mu = 1, 2, 3$ if D=3)
   $E_{tot} = E_0 + 1/2 \sum u_\mu(\mathbf{R}_i^0) D_{\mu,\nu}(\mathbf{R}_i^0 - \mathbf{R}_j^0) u_\nu(\mathbf{R}_j^0)$, where $D_{\mu,\nu}(\mathbf{R}_i^0 - \mathbf{R}_j^0) = d^2 E_{tot}/du_\mu(\mathbf{R}_i^0) du_\nu(\mathbf{R}_j^0)$
   Note: $D_{\mu,\nu}(\mathbf{R}_i^0 - \mathbf{R}_j^0) = D_{\mu,\nu}(\mathbf{R}_j^0 - \mathbf{R}_i^0)$
   and $\sum_i D_{\mu,\nu}(\mathbf{R}_i^0) = 0$ ("translation invariance")

5. Equation of motion for 1 atom per cell in 3 dimensions.
   $u_\mu(\mathbf{R}_i^0) = e_\mu exp(i\mathbf{k} \cdot \mathbf{R}_i^0 - i\omega t)$, general form of solution.
   $M\omega^2 e_\mu = D_{\mu,\nu}(\mathbf{k}) e_\nu$ is the eigenvalue equation.
   $D_{\mu,\nu}(\mathbf{k}) = \sum_i D_{\mu,\nu}(\mathbf{R}_i^0) exp(i\mathbf{k} \cdot \mathbf{R}_i^0)$ is Fourier transform.
   Using symmetry and $\sum_i D_{\mu,\nu}(\mathbf{R}_i^0) = 0$, it follows that
   $D_{\mu,\nu}(\mathbf{k}) = -2\sum_i D_{\mu,\nu}(\mathbf{R}_i^0) sin^2(\mathbf{k} \cdot \mathbf{R}_i^0/2)$
   Real symmetric matrix has 3 real eigenvalues, $\lambda_s(\mathbf{k})$, and eigenvectors, $e_s(\mathbf{k})$.
   Eigenvalues give dispersion relation: $\omega_s = (\lambda_s(\mathbf{k})/M)^{1/2}$
   Eigenvectors give polarization of mode, longitudinal or transverse.

6. Example: Dispersion curves for Pb. See A&M page 441.
   Modes of a 2D triangular lattice.

7. Speed of sound derived from matrix of force constants.
   When $k << \pi/a$ can approximate $sin(kR/2) \to kR/2$
   Leads to $\omega = v_{sound} k$ for one longitudinal and D-1 transverse sound waves.

8. Relation to elasticity theory
   $\mathbf{u}(\mathbf{R}_j) = \mathbf{u}(\mathbf{R}_i) + (\mathbf{R}_j - \mathbf{R}_i) \cdot \frac{\partial \mathbf{u}}{\partial \mathbf{R}}$, where $\frac{\partial \mathbf{u}}{\partial \mathbf{R}}$ is the strain tensor
   $E_{\sigma\mu\tau\nu} = -1/2 \sum_{\mathbf{R}} \mathbf{R}_\sigma D_{\mu,\nu}(\mathbf{R}) \mathbf{R}_\tau$, 4th rank elasticity tensor.
   Rewrite as $C_{\sigma\mu\tau\nu}$ for conventional elasticity tensor.
   $\{\sigma\mu\} = \{xx, yy, zz, xy, yz, zx\} \to \{1, 2, 3, 4, 5, 6\}$
   General crystal has 21 independent elements of tensor
   Cubic crystal has 3 independent elements: C_{11}, C_{12}, C_{44}