Midterm Exam

Born–von Karman boundary condition. Lattice Fourier transform

Introduce Born–von Karman boundary condition and prove that for any quantity $Q_{\mathbf{n}}$ satisfying this condition there takes place the Fourier transform

$$Q_{\mathbf{n}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{m}}^{BZ} \mathrm{e}^{i\mathbf{q_m}\cdot\mathbf{T_n}} F_{\mathbf{m}} , \tag{1}$$

$$F_{\mathbf{m}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{n}}^{\text{(system)}} \mathrm{e}^{-i\mathbf{q_m}\cdot\mathbf{T_n}} Q_{\mathbf{n}} , \tag{2}$$

where $\mathbf{T_n}$ are translation vectors and

$$\mathbf{q_m} = \frac{m_1\mathbf{b}_1}{N_1} + \frac{m_2\mathbf{b}_2}{N_2} + \frac{m_3\mathbf{b}_3}{N_3} . \tag{3}$$

Summation in the wavevector space

Show that for a macroscopic crystal the summation over the wavevector $\mathbf{q} \equiv \mathbf{q_m}$ can be replaced with integration by the following rule:

$$\sum_{\mathbf{q}} (\ldots) \;\to\; \frac{V}{(2\pi)^3} \int_{BZ} d^3q\,(\ldots) . \tag{4}$$

Also show that one can write the Fourier transform in terms of the dimensionless wavevector

$$\mathbf{g_m} = 2\pi \left(\frac{m_1}{N_1}, \frac{m_2}{N_2}, \frac{m_3}{N_3} \right) , \tag{5}$$

and that in this case

$$\sum_{\mathbf{g}} (\ldots) \;\to\; \frac{N}{(2\pi)^3} \int_{BZ} d^3g\,(\ldots) . \tag{6}$$

Quantum theory of phonons

Derive the theory of quantum harmonic modes starting from the Hamiltonian ($\hbar = 1$)

$$H = \sum_\alpha \frac{p_\alpha^2}{2m_\alpha} + \frac{1}{2}\sum_{\alpha,\beta} A_{\alpha\beta}\, u_\alpha u_\beta \,, \tag{7}$$

where $\{u_\alpha\}$ is the set of scalar coordinates (displacements); $p_\alpha = -i\partial/\partial u_\alpha$ is the momentum operator, m_α is the mass, and the matrix $A_{\alpha\beta}$ is real and symmetric. Apply this theory to phonons by using $\alpha = (i, j, \mathbf{n})$. In particular, derive the relation

$$\langle\, (u_{\mathbf{n}j}^i)^2 \rangle = \frac{1}{m_j} \sum_\nu \int_{BZ} \frac{d^d g}{(2\pi)^d}\, |v_{j\nu}^i(\mathbf{g})|^2\, \frac{\bar{n}_{\nu\mathbf{g}} + 1/2}{\omega_\nu(\mathbf{g})} \,. \tag{8}$$

P715 Midterm Exam

I) Born-Von Karman boundary condition. Lattice Fourier transform

- Born-von Karman boundary conditions are also known as periodic boundary conditions.
- Let $\vec{a}_1$ $\vec{a}_2$ $\vec{a}_3$ denote the basis for lattice translations in a 3D crystal.
- Define the lattice translation vector:

$$\vec{T}_{\vec{n}} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

- The vector $\vec{n}$ is an "integer vector". It is a dimensionless list of three integers. $\vec{n}$ is unique for each "primitive cell" of the crystal.
- The whole crystal can be thought of as a repetition of identical primitive cells, onto a Bravais lattice.
- The set of all translations translations belong to the group $\mathcal{G}_T$.
- Define the "reciporical" (or momentum space) lattice vectors $\vec{b}_1$ $\vec{b}_2$ $\vec{b}_3$ such that

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij},$$

which are the basis for translations in reciporical space.

- Define the reciporical lattice translation vector:

$$\vec{G}_{\vec{m}} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

- Vector $\vec{m}$ is another integer vector (dimensionless), or $\vec{m} = (m_1, m_2, m_3)$.
- The set of all translations in reciporical space belong to the group $\mathcal{G}_G$.
- Vectors $\vec{T}_{\vec{n}}$ and $\vec{G}_{\vec{m}}$ relate by:

$$\vec{G} \cdot \vec{T} = 2\pi \cdot \text{integer}$$

- The volume of a primitive cell is:

$$V_c = \left| \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \right|$$

- The volume of a corresponding primitive cell in reciporical space is:

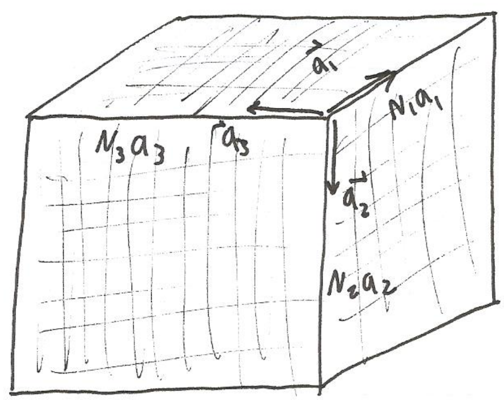
$$V_c^{(R)} = \left| \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) \right|$$

- The volumes are related: $V_c^{(R)} \cdot V_c = (2\pi)^d$

(d is the # of dimensions)

- Choose three macroscopically-large integers N_1 N_2 N_3 that define the sizes of the system in the directions $\vec{a}_1$ $\vec{a}_2$ $\vec{a}_3$.

- The total crystal can be now regarded as a sum of these "macroscopic cells".



- Translations between these macroscopic cells are expressed by the vector

$$\vec{\mathcal{T}}_{\vec{l}} = l_1 N_1 \vec{a}_1 + l_2 N_2 \vec{a}_2 + l_3 N_3 \vec{a}_3$$

- Vector $\vec{l} = (l_1, l_2, l_3)$ is another dimensionless integer vector.

- The set of all $\vec{\mathcal{T}}_{\vec{l}}$ form the group $\mathcal{G}_{\mathcal{T}}$, a sub-group of $\mathcal{G}_T$.

- The corresponding recipocrical space has the translation vector:

$$\vec{q}_{\vec{m}} = \frac{m_1\vec{b}_1}{N_1} + \frac{m_2\vec{b}_2}{N_2} + \frac{m_3\vec{b}_3}{N_3} \qquad (3)$$

- The set of all $\vec{q}_{\vec{m}}$ belong to the group $\mathcal{G}_q$. Note $\mathcal{G}_G$ is a subgroup of $\mathcal{G}_q$.

- Now we let $Q_{\vec{n}}$ be a quantity defined in the crystal. $Q_{\vec{n}}$ exhibits PERIODIC BOUNDARY CONDITIONS:

$$Q_{\vec{n}} = Q(\vec{T}_{\vec{n}}) \equiv Q(\vec{T}_{\vec{n}} + \vec{\mathcal{J}}_{\vec{\ell}})$$

$Q_{\vec{n}}$ is invariant under translation to another macroscopic cell.

- Note: Geometric Series

$$f = 1 + x + x^2 + x^3 + \cdots + x^n$$
$$fx = x + x^2 + x^3 + \cdots + x^{n+1}$$

$$fx - f = x^{n+1} - 1 \longrightarrow f = \frac{x^{n+1} - 1}{x - 1}$$

$$1 + x + x^2 + \cdots + x^n = (x^{n+1} - 1)/(x - 1)$$

$$1 + x + x^2 + \cdots + x^{n-1} = \frac{1 - x^n}{1 - x}$$

- The periodicity and discreteness of the system allows for analysis using the FOURIER TRANSFORM. There are $N = N_1 \times N_2 \times N_3$ independent harmonics $F_{\vec{m}} = F(\vec{q}_{\vec{m}})$.

- Introduce the Fourier transform and its inverse:

$$Q_{\vec{n}} = \frac{1}{\sqrt{N}} \sum_{\vec{m}}^{B.Z.} e^{i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} F_{\vec{m}} \qquad (1)$$

$$F_{\vec{m}} = \frac{1}{\sqrt{N}} \sum_{\vec{n}}^{(system)} e^{-i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} Q_{\vec{n}} \qquad (2)$$

- B.Z. stands for the "first Brillouin zone." It is the Wigner - Seitz cell of reciporical space.

- The sum over $\vec{m}$ may be limited to a sum over the first B.Z. due to the invariance in $F_{\vec{m}}$ under translations:

$$\vec{q}_{\vec{m}_0} \longrightarrow \vec{q}_{\vec{m}_0} + \vec{G}$$

- In the above, $\sum$ means:

$$\sum_{\vec{p}} = \sum_{p_1=0}^{N_1-1} \sum_{p_2=0}^{N_2-1} \sum_{p_3=0}^{N_3-1} \qquad \left(\text{replace } p \text{ by } m, n. \right)$$

- Examine the exponential $e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}}$.

$$e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = \exp\left(\pm i \left(\frac{m_1 \vec{b}_1}{N_1} + \frac{m_2 \vec{b}_2}{N_2} + \frac{m_3 \vec{b}_3}{N_3}\right) \cdot \left(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3\right)\right)$$

$$= \exp\left(\pm i (2\pi)\left(\frac{m_1 n_1}{N_1} + \frac{m_2 n_2}{N_2} + \frac{m_3 n_3}{N_3}\right)\right)$$

$$= \left(e^{\pm i 2\pi \frac{m_1 n_1}{N_1}}\right)\left(e^{\pm i 2\pi \frac{m_2 n_2}{N_2}}\right)\left(e^{\pm i 2\pi \frac{m_3 n_3}{N_3}}\right)$$

$$= \prod_{j=1}^{3} e^{\pm i 2\pi \frac{m_j n_j}{N_j}}$$

- If m_j/N_j is integer, $\vec{q}_{\vec{m}} = \vec{G}$. The exponential becomes:

$$e^{\pm i \vec{G}_{\vec{m}} \cdot \vec{T}_n} = e^{\pm i 2\pi \cdot \tilde{n}} \quad ; \quad \tilde{n} = \text{integer}$$

- Then the sum becomes:

$$\sum_{\vec{n}}^{(\text{system})} e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = \prod_{j=1}^{3} \sum_{n_j=0}^{N_j-1} e^{i 2\pi \tilde{n}} = \prod_{j=1}^{3} N_j$$

$$= N_1 N_2 N_3 = N$$

$$\sum_{\vec{n}}^{(\text{sys.})} e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = N \qquad \text{if} \quad \vec{q}_{\vec{m}} = \vec{G}.$$

- By a similar argument,

$$\sum_{\vec{m}}^{\text{B.Z.}} e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = N \qquad \text{if} \quad \vec{T}_{\vec{n}} = \vec{J}.$$

- Now examine the sum when m_j/N_j is not an integer. (Any m_j/N_j works.)

$$\sum_{n_j=0}^{N_j-1} e^{\pm i 2\pi \frac{m_j n_j}{N_j}} = \frac{1 - e^{\pm i 2\pi m_j n_j}}{1 - e^{\pm i 2\pi m_j n_j / N_j}} \quad \Bigg\} \text{ By geometric series.}$$

$$\propto \; 1 - 1 = 0.$$

- Conclude that:

$$\sum_{\vec{n}}^{(\text{system})} e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = \begin{cases} N & \text{if } \vec{q}_{\vec{m}} = \vec{G} \\ 0 & \text{if not.} \end{cases}$$

$$\sum_{\vec{m}}^{\text{B.Z}} e^{\pm i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} = \begin{cases} N & \text{if } \vec{T}_{\vec{n}} = \vec{J} \\ 0 & \text{if not.} \end{cases}$$

- Now we can show that the $Q_{\vec{n}}$ and $F_{\vec{m}}$ mutually imply each other.

Recall equations (1) & (2):

$$Q_{\vec{n}} = \sum_{\vec{m}}^{\text{B.Z.}} e^{i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} F_{\vec{m}} \frac{1}{\sqrt{N}}$$

$$F_{\vec{m}} = \sum_{\vec{n}}^{(\text{sys.})} e^{-i \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}} Q_{\vec{n}} \frac{1}{\sqrt{N}}$$

• Multiply ② by $N^{-1/2}\, e^{i\vec{q}_{\vec{m}}\cdot\vec{T}_{\vec{n}_0}}$ & $\sum_{\vec{m}}$.

$$\underbrace{\sum_{\vec{m}}^{B.Z.} F_{\vec{m}}\,\frac{1}{\sqrt{N}}\, e^{i\vec{q}_{\vec{m}}\cdot\vec{T}_{\vec{n}_0}}}_{\equiv\, Q_{\vec{n}_0}} = \sum_{\vec{n}}^{(SYS)}\sum_{\vec{m}}^{B.Z.} \frac{Q_{\vec{n}}}{\sqrt{N}\,\sqrt{N}}\, e^{i\vec{q}_{\vec{m}}(\vec{T}_{\vec{n}_0}-\vec{T}_{\vec{n}})}$$

$$= \frac{1}{N}\sum_{\vec{n}}^{(SYS)} Q_{\vec{n}} \underbrace{\sum_{\vec{m}}^{B.Z.} e^{i\vec{q}_{\vec{m}}(\vec{T}_{\vec{n}_0}-\vec{T}_{\vec{n}})}}_{\text{Non-zero iff } \vec{T}_{\vec{n}_0}-\vec{T}_{\vec{n}} = \vec{J}_{\vec{n}_0}}$$

$$Q_{\vec{n}_0} = \frac{1}{N}\sum_{\vec{n}}^{(SYS)} Q_{\vec{n}}\, e^{i\vec{q}_{\vec{m}}\cdot\vec{J}_{\vec{n}_0}} = \frac{N}{N}\, Q_{\vec{n}_0}$$

$$Q_{\vec{n}_0} = Q_{\vec{n}_0}$$

• By a similar procedure, $F_{\vec{m}_0}$ can be recovered, and thus the fourier transform is consistent.

II) Summation in wavevector space

• A summation in wavevector space is to be replaced w/ an integration.

• First note that $\vec{q}_{\vec{m}} = \frac{m_1\vec{b}_1}{N_1} + \frac{m_2\vec{b}_2}{N_2} + \frac{m_3\vec{b}_3}{N_3}$

changes very little when any of the m_j are changed by one unit.

- Because of this, to macroscopic accuracy, a sum in wavevector space can "smooth" into an integral.

$$\sum_{\vec{q}} (\cdots) \equiv \sum_{\vec{m}}^{B.Z.} (\cdots) = \int_{BZ} d^3m\, (\cdots)$$

... where $d^3m = dm_1 dm_2 dm_3$

- We want to integrate over the variable q, so introduce the corresponding Jacobian.

$$\int_{BZ} d^3m\, (\cdots) = \int_{BZ} d^3q\, |J|\, (\cdots)$$

$$J = \frac{\mathcal{D}(\vec{m})}{\mathcal{D}(\vec{q})} \quad \text{and} \quad J^{-1} = \frac{\mathcal{D}(\vec{q})}{\mathcal{D}(\vec{m})}$$

From $\vec{q}_{\vec{m}} = \frac{m_1 \vec{b}_1}{N_1} + \frac{m_2 \vec{b}_2}{N_2} + \frac{m_3 \vec{b}_3}{N_3}$,

$$J^{-1} = \begin{vmatrix} \frac{\partial q_x}{\partial m_1} & \frac{\partial q_y}{\partial m_1} & \frac{\partial q_z}{\partial m_1} \\ \frac{\partial q_x}{\partial m_2} & \frac{\partial q_y}{\partial m_2} & \frac{\partial q_z}{\partial m_2} \\ \frac{\partial q_x}{\partial m_3} & \frac{\partial q_y}{\partial m_3} & \frac{\partial q_z}{\partial m_3} \end{vmatrix}$$

$$J^{-1} = \begin{vmatrix} b_{1x}/N_1 & b_{1y}/N_1 & b_{1z}/N_1 \\ b_{2x}/N_2 & b_{2y}/N_2 & b_{2z}/N_2 \\ b_{3x}/N_3 & b_{3y}/N_3 & b_{3z}/N_3 \end{vmatrix} = \frac{V_c^{(R)}}{N}$$

- So far then,

$$\sum_{\vec{q}} (\cdots) = \int_{BZ} d^3q \, \frac{1}{J^{-1}} (\cdots) = \int_{BZ} d^3q \, \frac{N}{V_C^{(R)}} (\cdots)$$

$$= \frac{N V_c}{(2\pi)^3} \int_{BZ} d^3q \, (\cdots) \qquad \left(\begin{array}{c} \text{Note:} \\ V = N V_c \end{array} \right)$$

$$\sum_{\vec{q}} (\cdots) = \frac{V}{(2\pi)^3} \int_{BZ} d^3q \, (\cdots) \qquad (4)$$

- This proves what we set out to prove. Now, examine the quantity $\vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}}$.

$$\vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}} = \left(\frac{m_1 \vec{b}_1}{N_1} + \frac{m_2 \vec{b}_2}{N_2} + \frac{m_3 \vec{b}_3}{N_3} \right) \cdot \left(n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \right)$$

$$= 2\pi \left(\frac{m_1 n_1}{N_1} + \frac{m_2 n_2}{N_2} + \frac{m_3 n_3}{N_3} \right)$$

$$= \underbrace{\left(\frac{2\pi m_1}{N_1}, \frac{2\pi m_2}{N_2}, \frac{2\pi m_3}{N_3} \right)}_{\equiv \vec{g}_{\vec{m}}} \cdot \underbrace{(n_1, n_2, n_3)}_{\vec{n}}$$

$$\rightarrow \quad \vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}} = \vec{g}_{\vec{m}} \cdot \vec{n} \qquad (5)$$

- Now, the Fourier transform and its inverse can be represented with the dimensionless wavevector $\vec{g}_{\vec{m}}$ if the following replacement is made:

$$\vec{q}_{\vec{m}} \cdot \vec{T}_{\vec{n}} \longrightarrow \vec{g}_{\vec{m}} \cdot \vec{n}$$

- Repeating the previous analysis for a summation over the dimensionless wavevector $\vec{g}$.

$$\sum_{\vec{g}} (\cdots) \longrightarrow \int_{BZ} d^3g(\cdots) , \quad dg_j = dm_j \left(\frac{2\pi}{N_j}\right)$$

$$j = 1,2,3$$

- This produces a result identical to equation (4), except the volume term V is now absent in (6).

III) Quantum Theory of Phonons

- Given: $H = \sum_\alpha \frac{P_\alpha^2}{2M_\alpha} + \frac{1}{2} \sum_{\alpha,\beta} A_{\alpha\beta} U_\alpha U_\beta$ (7)

... where U_γ is a scalar coordinate
P_μ is the momentum operator

- First get rid of mass terms. Let:

$$\tilde{P}_\alpha = \frac{P_\alpha}{\sqrt{M_\alpha}} \qquad \tilde{A}_{\alpha\beta} = \frac{A_{\alpha\beta}}{\sqrt{M_\alpha}\sqrt{M_\beta}} \qquad \tilde{U}_\alpha = \sqrt{M_\alpha}\, U_\alpha$$

$$H = \sum_\alpha \frac{1}{2} \tilde{P}_\alpha^2 + \frac{1}{2} \sum_{\alpha\beta} \tilde{A}_{\alpha\beta} \tilde{U}_\alpha \tilde{U}_\beta$$

... and now ignore the ~ symbol.

$$H = \frac{1}{2} \sum_\alpha P_\alpha^2 + \frac{1}{2} \sum_{\alpha\beta} A_{\alpha\beta} U_\alpha U_\beta$$

- Now make the following canonical transformation:

$$P_\alpha = \sum_s e_\alpha^{(s)} \mathcal{P}_s \qquad U_\alpha = \sum_s e_\alpha^{(s)} \mathcal{X}_s$$

... where the script "s" denotes a particular normal mode.

- The vectors $\vec{e}_s$ are the eigenvectors of the matrix $A_{\alpha\beta}$.

- Thus, we have the following properties:

$$\vec{e}^{(s_1)} \cdot \vec{e}^{(s_2)} = \delta_{s_1 s_2} \longrightarrow \sum_\alpha e_\alpha^{(s_1)} e_\alpha^{(s_2)} = \delta_{s_1 s_2}$$

$$A \vec{e}^{(s)} = \omega_s^2 \vec{e}^{(s)} \longrightarrow \sum_\beta A_{\alpha\beta} e_\beta^{(s)} = \omega_s^2 e_\alpha^{(s)}$$

and also, $\longrightarrow \sum_s e_\alpha^{(s)} e_\beta^{(s)} = \delta_{\alpha\beta}$

... The frequencies ω_s are real & positive.

- Now insert the transformed coordinates into the Hamiltonian.

* $$H = \frac{1}{2} \sum_\alpha P_\alpha^2 + \frac{1}{2} \sum_{\alpha\beta} A_{\alpha\beta} U_\alpha U_\beta$$

* $$H = \frac{1}{2} \sum_\alpha \sum_{s_1} \sum_{s_2} (e_\alpha^{(s_1)} P_{s_1})(e_\alpha^{(s_2)} P_{s_2}) + \frac{1}{2} \sum_\alpha \sum_\beta \sum_s (e_\alpha^{(s)} X_s)(e_\beta^{(s)} X_s) A_{\alpha\beta}$$

* $$H = \frac{1}{2} \sum_{s_1 s_2} \underbrace{\left(\sum_\alpha e_\alpha^{(s_1)} e_\alpha^{(s_2)} \right)}_{\delta_{s_1 s_2}} P_{s_1} P_{s_2} + \frac{1}{2} \sum_s \sum_\alpha \underbrace{\sum_\beta A_{\alpha\beta} e_\beta^{(s)}}_{\omega_s^2 e_\alpha^{(s)}} e_\alpha^{(s)} X_s^2$$

* $$H = \frac{1}{2} \sum_{s_1 s_2} \delta_{s_1 s_2} P_{s_1} P_{s_2} + \frac{1}{2} \sum_s \sum_\alpha \omega_s^2 e_\alpha^{(s)} e_\alpha^{(s)} X_s^2$$

$$H = \frac{1}{2}\sum_s P_s^2 + \frac{1}{2}\sum_s \omega_s^2 X_s^2 \overbrace{\sum_\alpha e_\alpha^{(s)} e_\alpha^{(s)}}^{1}$$

$$H = \frac{1}{2}\sum_s \left(P_s^2 + \omega_s^2 X_s^2\right)$$

- We want to write the Hamiltonian in terms of the creation & annihilation operators for the simple harmonic oscillator. Recall:

$$b_s = \frac{\omega_s X_s + i P_s}{\sqrt{2\omega_s}} \qquad b_s^\dagger = \frac{\omega_s X_s - i P_s}{\sqrt{2\omega_s}}$$

- Compute the quantity: $b_s^\dagger b_s + 1/2$.

$$b_s^\dagger b_s + \frac{1}{2} = \frac{(\omega_s X_s - i P_s)(\omega_s X_s + i P_s)}{2\omega_s} + \frac{1}{2}$$

$$= \frac{\omega_s^2 X_s^2}{2\omega_s} + \frac{i\omega_s}{2\omega_s}\left(X_s P_s - P_s X_s\right) + \frac{P_s^2}{2\omega_s} + \frac{1}{2}$$

commutation

$$= \frac{1}{2}\omega_s X_s^2 + \cancel{\frac{i}{2}(i)} + \frac{1}{2}\frac{P_s^2}{\omega_s} + \cancel{\frac{1}{2}}$$

$$= \frac{1}{2}\left(\omega_s X_s^2 + P_s^2/\omega_s\right)$$

$$\longrightarrow \quad \omega_s\left(b_s^\dagger b_s + \frac{1}{2}\right) = \frac{1}{2}\left(\omega_s^2 X_s^2 + P_s^2\right)$$

- Finally,

$$H = \frac{1}{2}\sum_s \omega_s\left(b_s^\dagger b_s + \frac{1}{2}\right)$$

- Now restore the mass term in U_α.

$$U_\alpha = \frac{1}{\sqrt{M_\alpha}} \sum_s e_\alpha^{(s)} X_s$$

- Express X_s in terms of b_s & $b_s^\dagger$.

$$U_\alpha = \frac{1}{\sqrt{2M_\alpha}} \sum_s e_\alpha^{(s)} \frac{b_s + b_s^\dagger}{\sqrt{\omega_s}}$$

- We want solutions to take the form of running plane waves, not sines & cosines. Plane wave solutions are generally complex, but our eigenvectors so far are considered real. To proceed, split the $|e_s\rangle$ into real and imaginary parts so that all $|e_s\rangle$ become:

$$|e_s\rangle = \frac{|e_{s_1}\rangle + i|e_{s_2}\rangle}{\sqrt{2}}$$

... where $|e_{s_1}\rangle$ and $|e_{s_2}\rangle$ are both REAL and correspond to the same eigenvalue.

- Note that $|e_s^*\rangle \neq |e_s\rangle$.
- Make the (purely notational) definition:

$$|e_s^*\rangle \equiv |e_{s'}\rangle$$

- The quantity $|e_s\rangle(b_s + b^\dagger_s)$ becomes:

$$|e_{s_1}\rangle(b_{s_1} + b^\dagger_{s_1}) + |e_{s_2}\rangle(b_{s_2} + b^\dagger_{s_2}) \equiv \vec{\mathcal{E}}$$

- From $|e_s\rangle = \frac{1}{\sqrt{2}}\left(|e_{s_1}\rangle + i|e_{s_1}\rangle\right)$, we see:

$$|e_s\rangle = \frac{1}{\sqrt{2}}\left(|e_{s_1}\rangle + i|e_{s_2}\rangle\right)$$

$$|e_{s'}\rangle = \frac{1}{\sqrt{2}}\left(|e_{s_1}\rangle - i|e_{s_2}\rangle\right)$$

$$|e_{s_1}\rangle = \frac{1}{\sqrt{2}}\left(|e_s\rangle + |e_{s'}\rangle\right)$$

$$|e_{s_2}\rangle = \frac{1}{i\sqrt{2}}\left(|e_s\rangle - |e_{s'}\rangle\right)$$

- The vector quantity (labeled $\vec{\mathcal{E}}$) is:

$$= \frac{1}{\sqrt{2}}\left(|e_s\rangle + |e_{s'}\rangle\right)(b_{s_1} + b^\dagger_{s_1}) + \frac{1}{i\sqrt{2}}\left(|e_s\rangle - |e_{s'}\rangle\right)(b_{s_2} + b^\dagger_{s_2})$$

$$= \frac{1}{\sqrt{2}}|e_s\rangle\left(b_{s_1} + b^\dagger_{s_1} + \frac{b_{s_2}}{i} + \frac{b^\dagger_{s_2}}{i}\right) + \frac{1}{\sqrt{2}}|e_{s'}\rangle\left(b_{s_1} + b^\dagger_{s_1} - \frac{b_{s_2}}{i} - \frac{b^\dagger_{s_2}}{i}\right)$$

$$= \frac{1}{\sqrt{2}}|e_s\rangle\left(\underbrace{b_{s_1} - i b_{s_2}}_{\equiv \sqrt{2}\, b_s} + b^\dagger_{s_1} - i b^\dagger_{s_2}\right) + \frac{1}{\sqrt{2}}|e_{s'}\rangle\left(b_{s_1} + i b_{s_2} + b^\dagger_{s_1} + i b^\dagger_{s_2}\right)$$

- It makes natural sense to define (as above):

$$b_s = \frac{1}{\sqrt{2}}(b_{s_1} - i b_{s_2}) \qquad b_{s'} = \frac{1}{\sqrt{2}}(b_{s_1} + i b_{s_2})$$

$$b^\dagger_s = \frac{1}{\sqrt{2}}(b^\dagger_{s_1} + i b^\dagger_{s_2}) \qquad b^\dagger_{s'} = \frac{1}{\sqrt{2}}(b^\dagger_{s_1} - i b^\dagger_{s_2})$$

- The vector quantity $\vec{\varepsilon}$ is now:

$$= \cancel{\sqrt{2}}\,\frac{\cancel{\sqrt{2}}}{2}|e_s\rangle(b_s + b^{+}_{s'}) + \frac{\cancel{\sqrt{2}}}{2}|e_{s'}\rangle(b_{s'} + b^{+}_{s})$$

$$= |e_s\rangle b_s + \underset{\substack{\parallel\\ |e_s^{*\prime}\rangle}}{|e_s\rangle} b^{+}_{s'} + |e_{s'}\rangle b_{s'} + \underset{\substack{\parallel\\ |e_s^{*}\rangle}}{|e_{s'}\rangle} b^{+}_{s}$$

$$= \underbrace{|e_s\rangle b_s + |e_s^{*}\rangle b^{+}_{s}}_{} + \underbrace{|e_{s'}\rangle b_{s'} + |e_s^{*\prime}\rangle b^{+}_{s'}}_{\text{This term is the primed version of the term on the left.}}$$

- It follows that U_α can be written:

$$U_\alpha = \frac{1}{\sqrt{2M_\alpha}} \sum_s \frac{e_\alpha^{(s)} b_s + (e_\alpha^{(s)})^{*} b^{+}_{s}}{\sqrt{\omega_s}}$$

- Applying these developments to phonons, I clarify what α and s mean

$\alpha = \alpha(n, j, i)$

- $i \longrightarrow$ xyz components of disp.
- $j \longrightarrow$ basis atom #
- $n \longrightarrow$ primitive cell #

$s = s(q, \nu)$

- $\nu \longrightarrow$ branch subscript
- $q \longrightarrow$ dimensionless wave. vec.

- Recall the way $\vec{U}_{\vec{n}j}(t)$ looks for phonons:

$$\vec{U}_{\vec{n}j}(t) = Re \; \frac{\vec{V}_j(\vec{q})}{\sqrt{M_j}} \, e^{i\vec{q}\cdot\vec{T}_n - i\omega(\vec{q})t}$$

- Restoring this structure in our U_α, this gives:

$$\vec{U}_{\vec{n}j} = \frac{1}{\sqrt{2NM_j}} \sum_{\nu\vec{g}} \frac{\vec{V}_{j\nu}\, e^{i\vec{g}\cdot\vec{n}}\, b_{\nu\vec{g}} + \vec{V}^{*}_{j\nu}\, e^{-i\vec{g}\cdot\vec{n}}\, b^{\dagger}_{\nu g}}{\sqrt{\omega_\nu(\vec{g})}}$$

... where the time dependence is not written.

- Note that vectors $\vec{V}$ and frequencies ω are found from solving:

$$\tilde{C}\,\vec{V} = \omega^2 \vec{V}$$

... where many of the details are not explicitly written. The full version reads:

$$\sum_{i'j'} \tilde{C}^{ii'}_{jj'}(\vec{g})\, V^{i'}_{j'\nu}(\vec{g}) = \omega^2_\nu(\vec{g})\, V^{i}_{j\nu}(\vec{g})$$

- Note the normalization of $\vec{V}$'s account for the $\sqrt{N}$ in the denominator of $\vec{U}_{\vec{n}j}$. That is, $\sum_{ij} \left(V^{i}_{j\nu_1}(\vec{g})\right)^{*} V^{i}_{j\nu_2}(\vec{g}) = \delta_{\nu_1\nu_2}$.

- Since we are dealing with simple harmonic oscillators, the average displacement of an oscillator is zero. The quantity of interest is the expectation value of ${U^i_{\vec{n}j}}^2$.

Start w/ $\vec{U}_{\vec{n}j} = \frac{1}{\sqrt{2m_j N}} \sum_{\nu \vec{g}} \frac{\vec{V}_{j\nu} e^{i\vec{g}\cdot\vec{n}} b_{\nu\vec{g}} + \vec{V}^{\star}_{j\nu} e^{-i\vec{g}\cdot\vec{n}} b^+_{\nu\vec{g}}}{\sqrt{\omega_\nu}}$

$$(\vec{U}_{\vec{n}j})^2 = \frac{1}{2m_j N} \times$$

$$\sum_{\nu_1 g_1 \nu_2 g_2} \frac{\left(\vec{V}_{j\nu_1} e^{i\vec{g}_1\cdot\vec{n}} b_{\nu_1 g_1} + \vec{V}^{\star}_{j\nu_1} e^{-i\vec{g}_1\cdot\vec{n}} b^+_{\nu_1 g_1}\right)\left(\vec{V}_{j\nu_2} e^{i\vec{g}_2\cdot\vec{n}} b_{\nu_2 g_2} + \vec{V}^{\star}_{j\nu_2} e^{-i\vec{g}_2\cdot\vec{n}} b^+_{\nu_2 g_2}\right)}{\sqrt{\omega_{\nu_1}\omega_{\nu_2}}}$$

- Then,

$$\left\langle (U^i_{\vec{n}j})^2 \right\rangle = \frac{1}{2m_j N} \sum \frac{1}{\sqrt{\omega_{\nu_1}\omega_{\nu_2}}} \times$$

$$\left(\cancel{\propto \langle b_{s_1} b_{s_2} \rangle} + |V^i_{j\nu_1}|^2 \delta_{s_1 s_2} \langle b_{s_1} b^+_{s_1} \rangle + |V^i_{j\nu_1}|^2 \langle b^+_{\nu_1} b_{\nu_1} \rangle \delta_{s_1 s_2} + \cancel{\propto \langle b^+_{s_1} b^+_{s_2} \rangle} \right)$$

$$\langle (U^i_{\vec{n}j})^2 \rangle = \frac{1}{2m_j N} \sum_{\nu\vec{g}} \frac{1}{\omega_\nu(\vec{g})} |V^i_{j\nu}|^2 \left(\propto \langle b^+_s b_s \rangle + \propto \langle b_s b^+_s \rangle \right)_{s=\nu g}$$

$$\langle (U^i_{\vec{n}j})^2 \rangle = \frac{1}{m_j N} \sum_{\nu\vec{g}} |V^i_{j\nu}(\vec{g})|^2 \frac{\bar{n}_{\nu g} + \frac{1}{2}}{\omega_\nu(\vec{g})}$$

(8)

- The result for part (II) turns $\sum_g \to \int d^d g$. Done.

100