

The background features a gradient from red at the top to blue at the bottom, overlaid with faint, semi-transparent circular patterns and a scale. The scale is a large arc on the left side, with numerical markings from 140 to 260 in increments of 10. Several smaller circles with arrows indicate clockwise or counter-clockwise rotation, suggesting a theme of waves or circular motion.

PHONONS

The wave nature of light is the same as that which makes sound echo.

- Richard P. Feynman

THIS LECTURE

- Harmonic approximation
- Vibrational dynamics, periodicity, phonons
- Simple model example
- *Ab initio* results for bulk phonons
- *Ab initio* results for surface phonons and inelastic HAS

HARMONIC APPROXIMATION

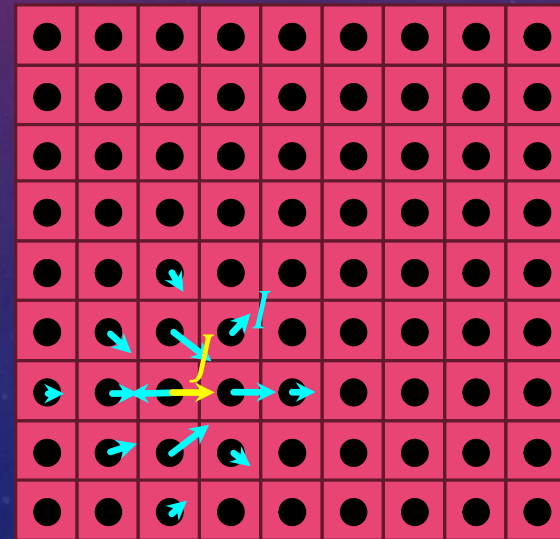
- For small displacements ($T \lesssim \frac{1}{3} T_{\text{melt}}$), $E_0(\vec{r}_1, \vec{r}_2, \dots)$ is in harmonic/linear:

$$\begin{aligned} E_0(\vec{r}_1, \vec{r}_2, \dots) &= E_0 + \sum_I \cancel{\frac{\partial E_0}{\partial \vec{r}_I}} \cdot \delta \vec{r}_I + \frac{1}{2} \sum_{IJ} \delta \vec{r}_I \cdot \frac{\partial^2 E_0}{\partial \vec{r}_I \partial \vec{r}_J} \cdot \delta \vec{r}_J + \dots \\ &= E_0 + \frac{1}{2} \sum_{IJ} \delta \vec{r}_I \cdot K_{IJ} \cdot \delta \vec{r}_J \end{aligned}$$

$$\vec{F}_I = - \frac{\partial E_0(\vec{r}_1, \vec{r}_2, \dots)}{\partial \vec{r}_I} = - \sum_J K_{IJ} \delta \vec{r}_J$$

- K_{IJ} , the “spring-constant matrix” can be computed from

$$\text{For all } J: \cup K_{IJ} = - \frac{\vec{F}_I(\{\vec{r}_I + \hat{e}_J \cdot \Delta r\}) - \vec{F}_I(\{\vec{r}_I - \hat{e}_J \cdot \Delta r\})}{2 \cdot \Delta r}$$



VIBRATIONAL DYNAMICS

- Vibrational modes:

$$\vec{F}_I = M_I \ddot{\vec{r}}_I$$

$$-\sum_J K_{IJ} \cdot \delta \vec{r}_J = -M_I \omega^2 \vec{r}_I$$

$$\sum_J K_{IJ} \cdot \delta \vec{r}_J^{(v)} = M_I \omega_{(v)}^2 \cdot \delta \vec{r}_I^{(v)} \quad (\text{eigenvalue problem})$$

- Translational symmetry:

- Each atom at location $\vec{r}_I = \vec{R}_I + \vec{\tau}_{n_I}$

- $K_{IJ} = K_{\vec{R}_I, n_I; \vec{R}_J, n_J} = K_{\vec{R}_J - \vec{R}_I, n_I; \vec{0}, n_J}$, $M_I = M_{\vec{R}_I, n_I} = M_{n_I}$

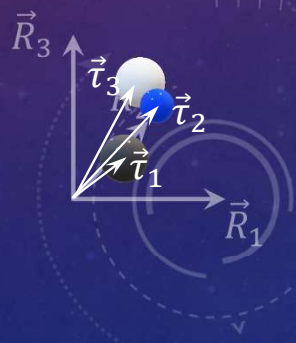
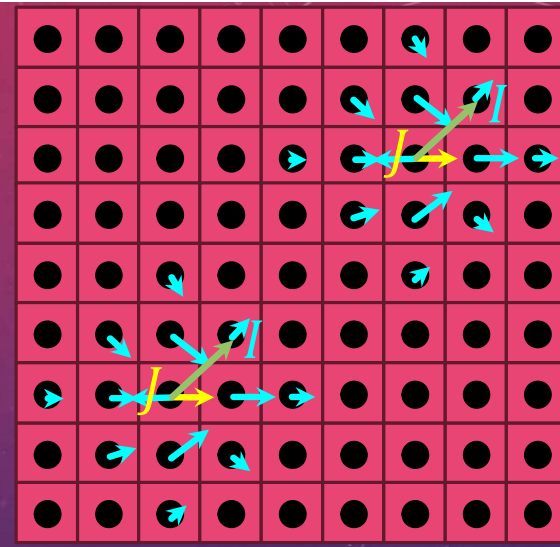
- $\delta \vec{r}_I = \delta \vec{r}_{\vec{R}, n} = e^{i\vec{q} \cdot \vec{R}} \vec{\mathcal{E}}_n$ (like Bloch's Theorem: envelope \times "polarization")

- Reduced problem:

- $\sum_m D_{nm}(\vec{q}) \cdot \vec{\mathcal{E}}_m^{(v\vec{q})} = M_n \omega_{(v\vec{q})}^2 \cdot \vec{\mathcal{E}}_n^{(v\vec{q})}$

- Dynamical matrix $D_{nm}(\vec{q}) \equiv \sum_{\vec{R}} e^{-i\vec{q} \cdot \vec{R}} K_{\vec{R}, n; \vec{0}, m}$ (eigenvalue problem)

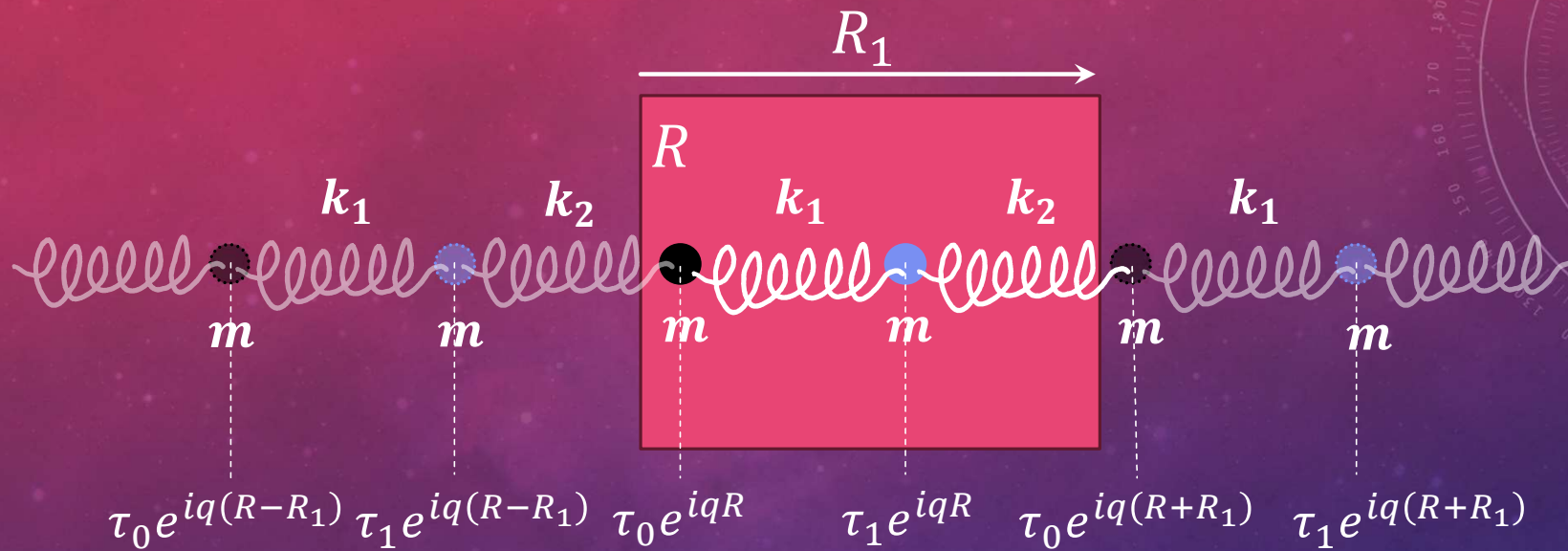
- Phonon modes: Frequencies $\omega_{(v\vec{q})}$, displacements/polarization $\vec{\mathcal{E}}_m^{(v\vec{q})}$



VIBRATIONAL DYNAMICS: 1D EXAMPLE



VIBRATIONAL DYNAMICS: 1D EXAMPLE

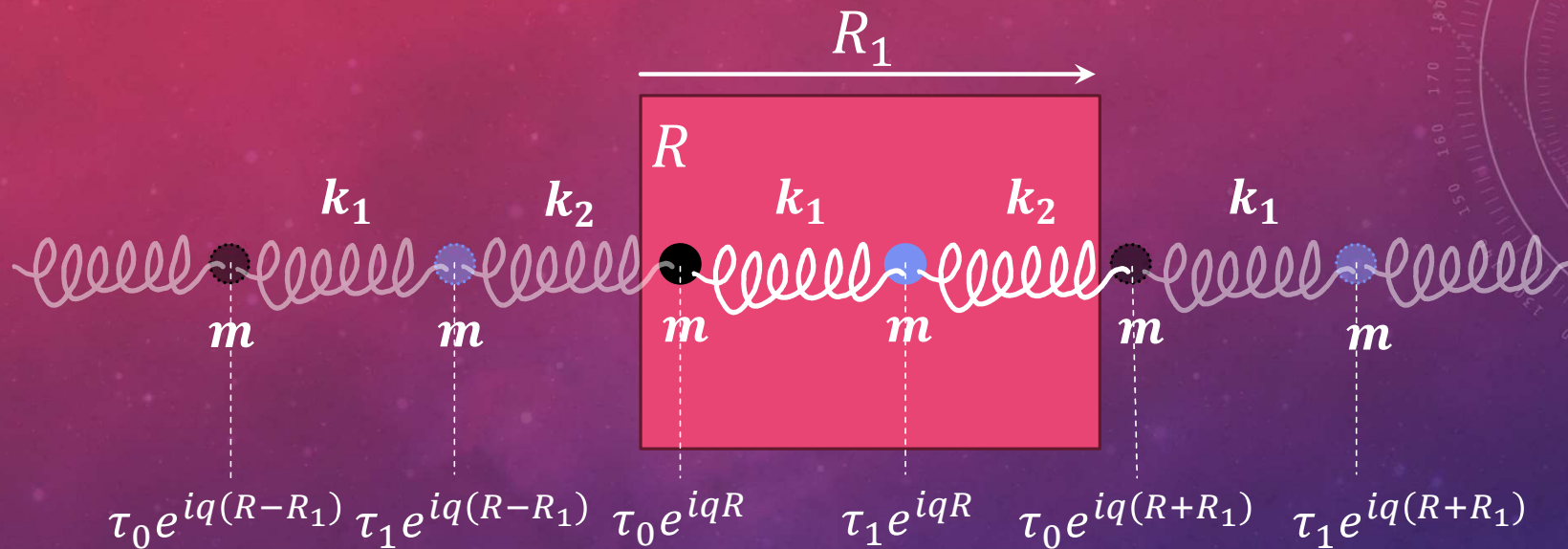


$ma = F:$

$$\begin{aligned}
 -m\omega^2 \tau_0 e^{iqR} &= k_1 (\tau_1 e^{iqR} - \tau_0 e^{iqR}) - k_2 (\tau_0 e^{iqR} - \tau_1 e^{iq(R-R_1)}) \\
 -m\omega^2 \tau_1 e^{iqR} &= k_2 (\tau_0 e^{iq(R+R_1)} - \tau_1 e^{iqR}) - k_1 (\tau_1 e^{iqR} - \tau_0 e^{iqR})
 \end{aligned}$$

Expand

VIBRATIONAL DYNAMICS: 1D EXAMPLE

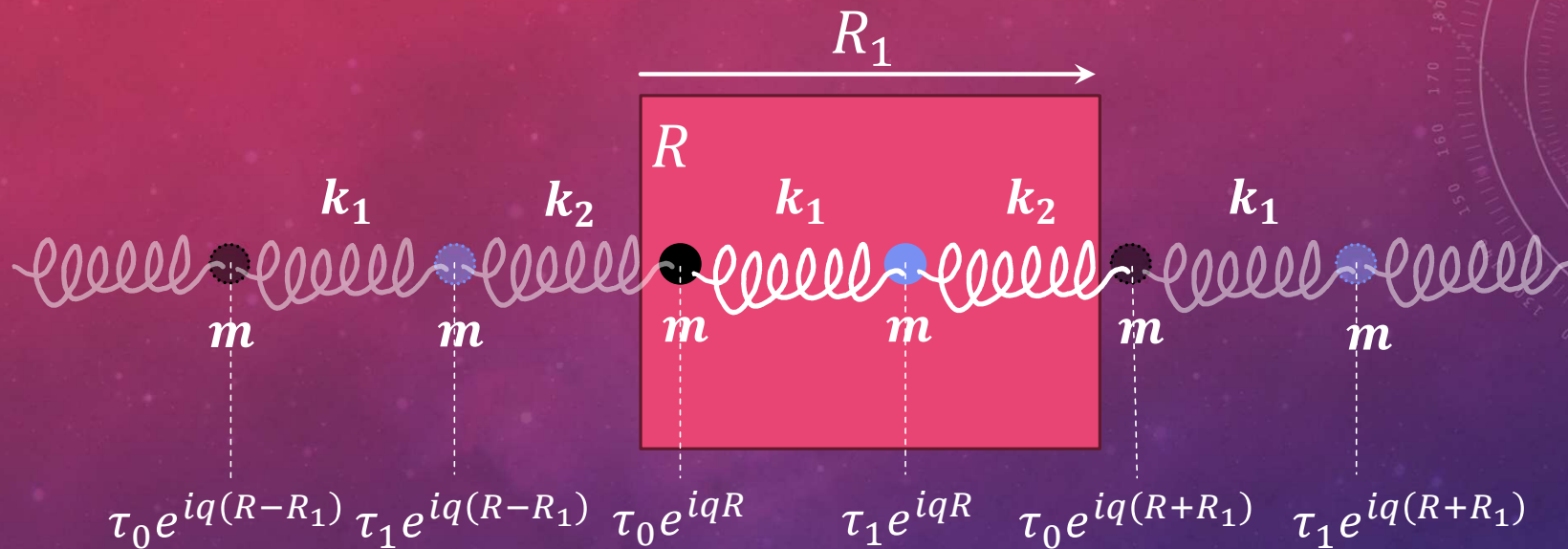


$ma = F:$

$$\begin{aligned}
 -m\omega^2 \tau_0 e^{iqR} &= k_1 (\tau_1 e^{iqR} - \tau_0 e^{iqR}) - k_2 (\tau_0 e^{iqR} - \tau_1 e^{iqR} e^{-iqR_1}) \\
 -m\omega^2 \tau_1 e^{iqR} &= k_2 (\tau_0 e^{iqR} e^{iqR_1} - \tau_1 e^{iqR}) - k_1 (\tau_1 e^{iqR} - \tau_0 e^{iqR})
 \end{aligned}$$

Cancel

VIBRATIONAL DYNAMICS: 1D EXAMPLE

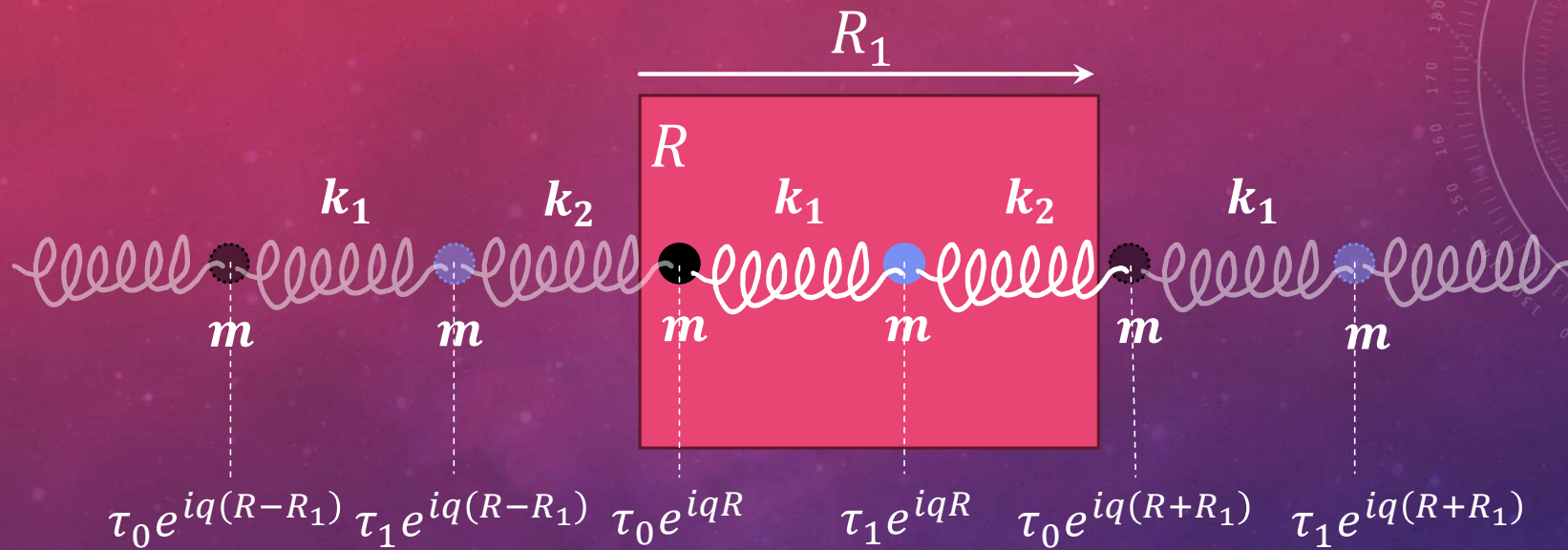


$ma = F$:

$$-m\omega^2\tau_0 = k_1(\tau_1 - \tau_0) - k_2(\tau_0 - \tau_1 e^{-iqR_1})$$

$$-m\omega^2\tau_1 = k_2(\tau_0 e^{iqR_1} - \tau_1) - k_1(\tau_1 - \tau_0)$$

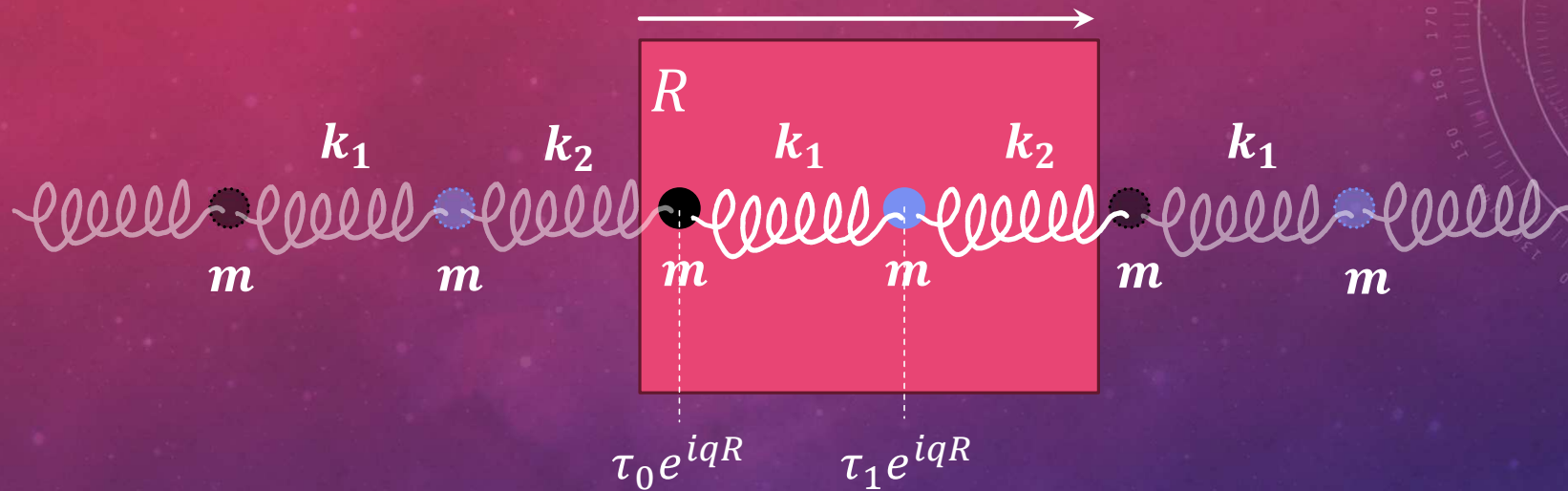
VIBRATIONAL DYNAMICS: 1D EXAMPLE



$$ma = F:$$

$$-m\omega^2 \begin{pmatrix} \tau_0 \\ \tau_1 \end{pmatrix} = - \overbrace{\begin{pmatrix} k_1 + k_2 & -(k_1 + k_2 e^{-iqR_1}) \\ -(k_1 + k_2 e^{iqR_1}) & k_1 + k_2 \end{pmatrix}}^{D(q)} \begin{pmatrix} \tau_0 \\ \tau_1 \end{pmatrix}$$

VIBRATIONAL DYNAMICS: 1D EXAMPLE

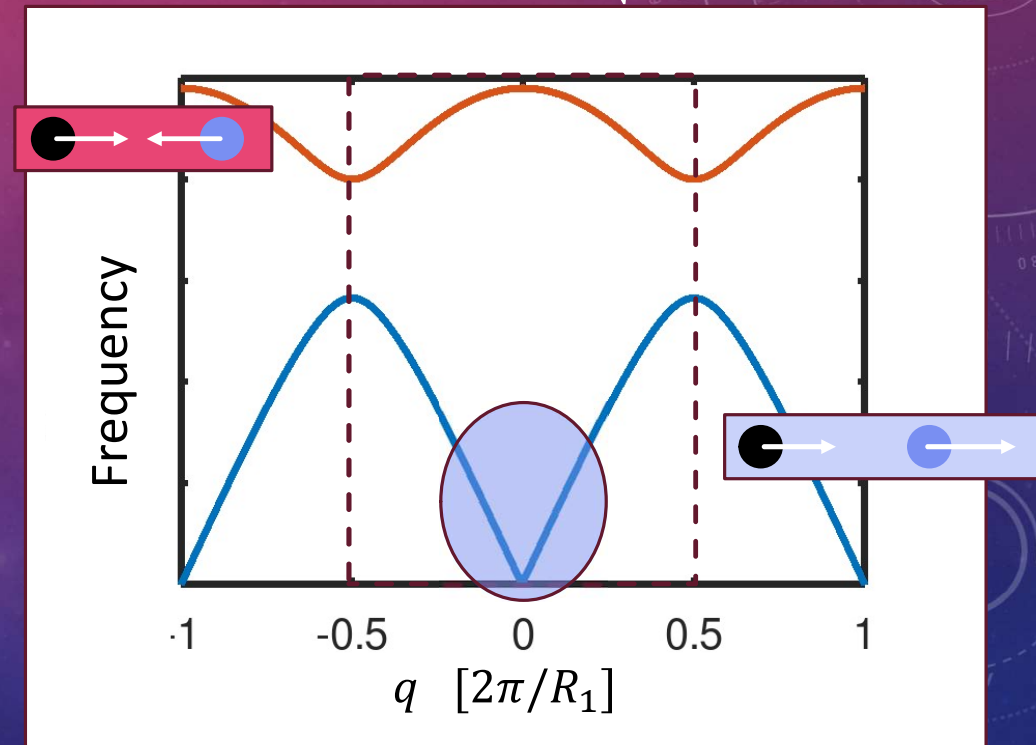


$$-D(q) = e^{-iq(-R_1)} \begin{pmatrix} 0 & 0 \\ k_2 & 0 \end{pmatrix} + \begin{pmatrix} -(k_1 + k_2) & k_1 \\ k_1 & -(k_1 + k_2) \end{pmatrix} + e^{-iq(+R_1)} \begin{pmatrix} 0 & k_2 \\ 0 & 0 \end{pmatrix}$$

VIBRATIONAL DYNAMICS: 1D EXAMPLE

- Results periodic in q ...
 - because e^{iqR_1} , $D(q)$ are periodic
- Relevant range is $[-0.5, 0.5]$
 - “Brillouin zone”
- Two “bands” (—, —)
 - because two degrees of freedom
- **Lower band** is \approx linear, $\omega = c q$
 - Corresponds to acoustic waves
- **Higher band** has non-zero ω
 - Corresponds to optical activity
- Displacements longitudinal
 - 1 LA and 1 LO mode

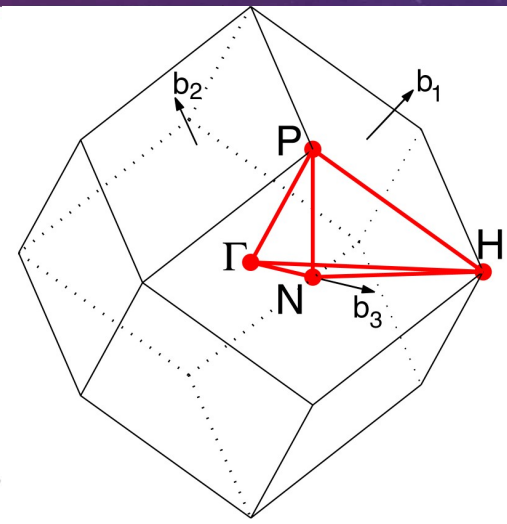
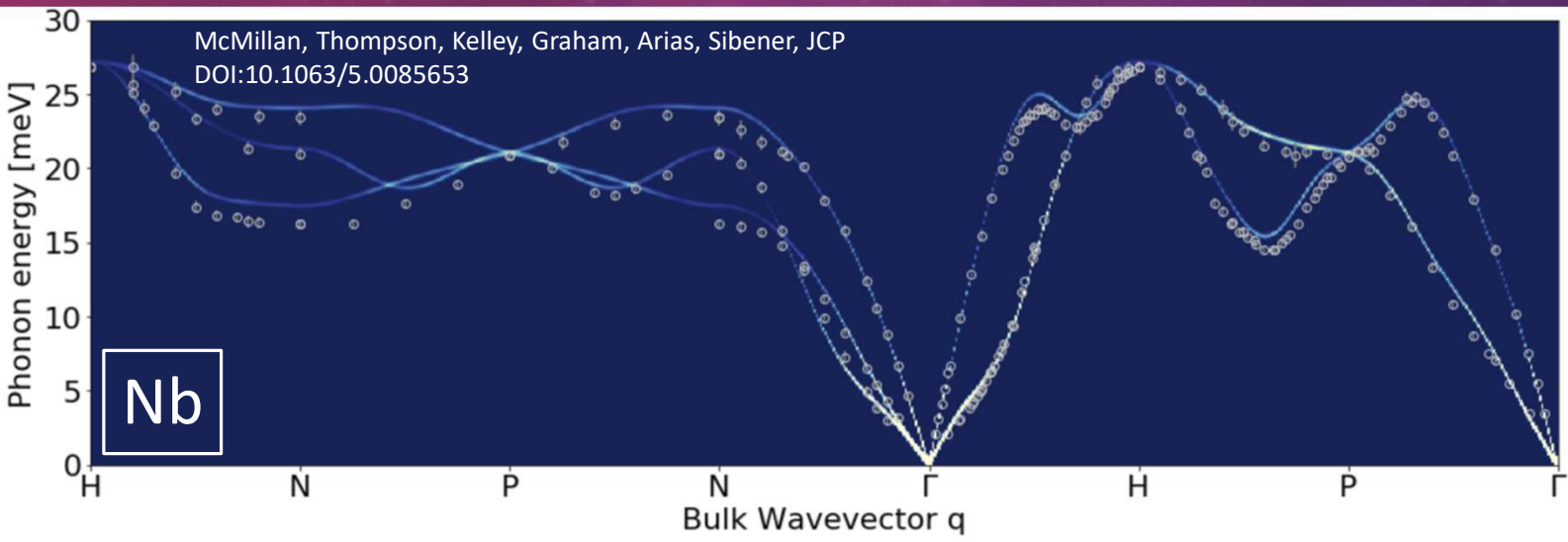
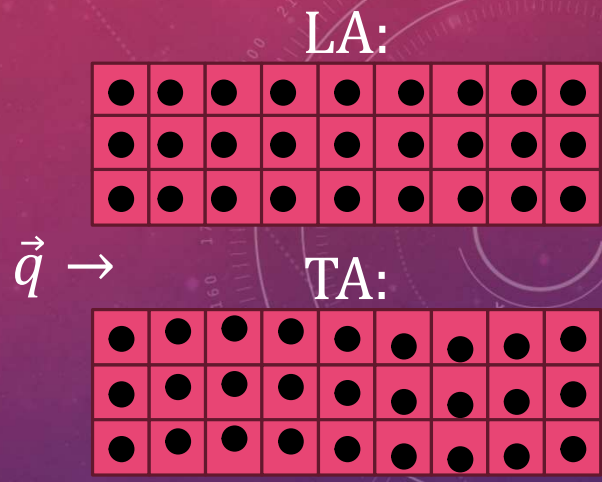
$$D(q)\vec{\mathcal{E}} = m\omega^2\vec{\mathcal{E}} \Rightarrow \omega = \sqrt{\text{eig}(D(q))/m}$$



PHONON MODES I

BCC Nb:

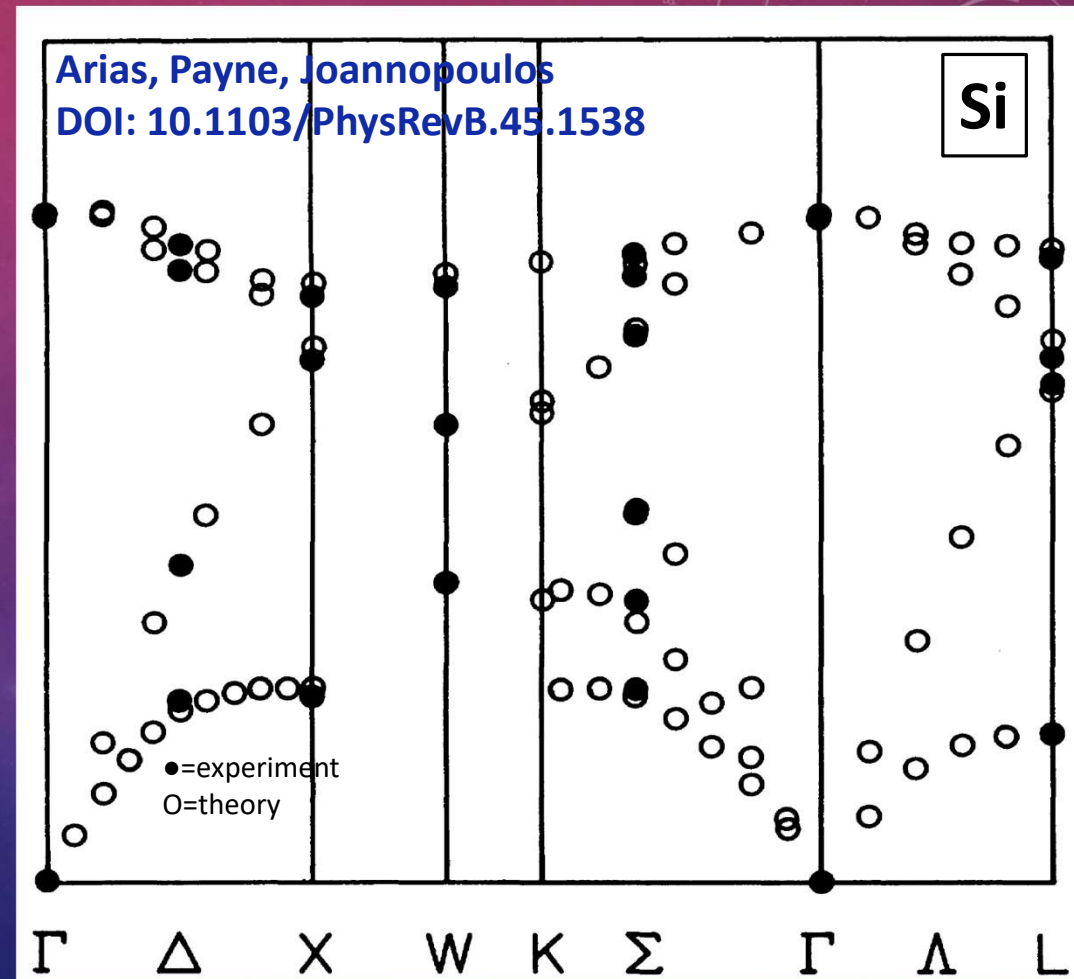
- 1 atom/cell \Rightarrow acoustic modes only
- 3 D of F / unit cell \Rightarrow 3 bands
- 1 longitudinal (LA) and 2 transverse (TA) bands



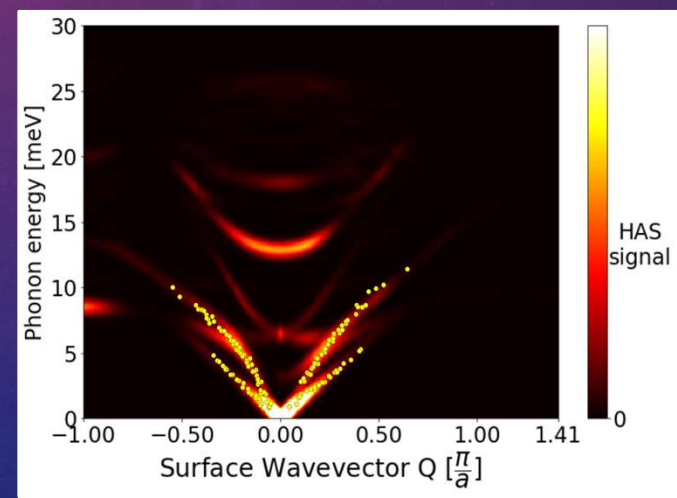
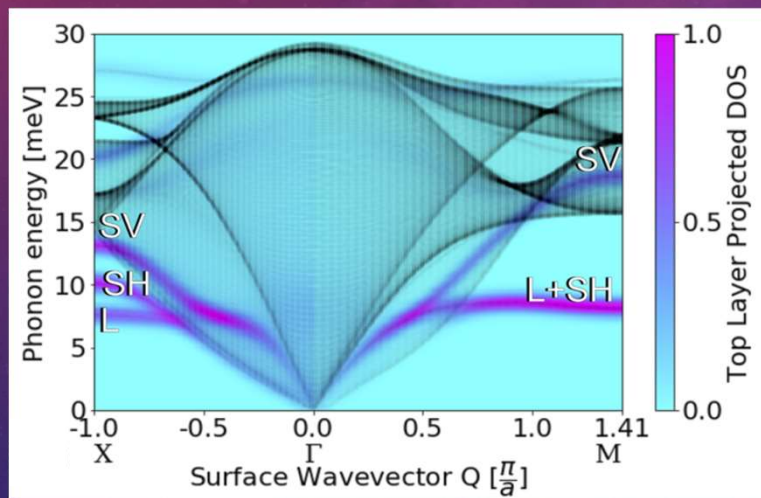
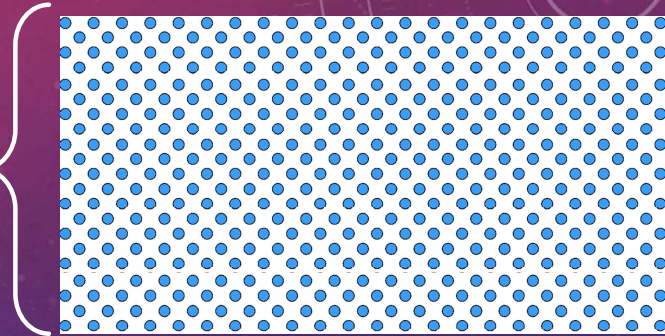
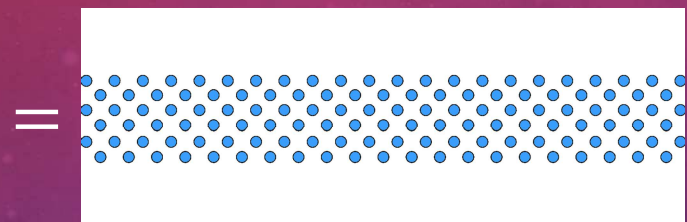
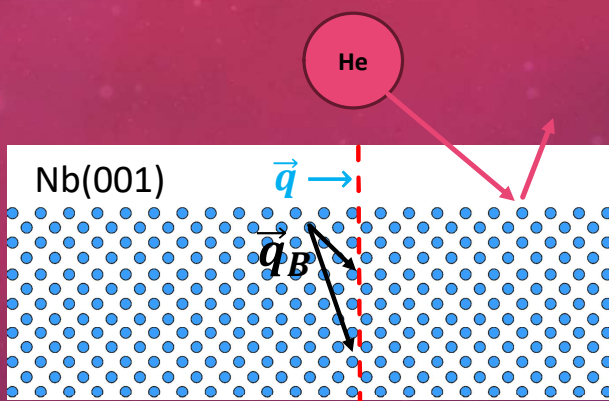
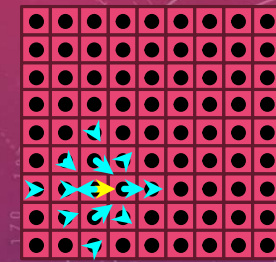
PHONON MODES I: BULK PHONONS

Si:

- 2 atoms/cell \Rightarrow A and 0 modes
- 6 D of F / unit cell \Rightarrow 6 bands
- 1 LA and 2 TA bands
- 1 LO and 2 TO bands



PHONON MODES II: QUANTIZED SURFACE PHONONS



Kelley, Sundararaman, Arias DOI: 10.48550/arXiv.2306.01892

The background is a gradient from dark purple at the top to dark blue at the bottom. It features numerous out-of-focus circular bokeh lights in shades of purple and blue. On the left side, there are several semi-transparent technical diagrams, including circular gauges with numerical scales (140, 150, 160, 170, 180, 190, 200, 210, 220, 230, 240, 250, 260) and various circular patterns with arrows and dashed lines.

THANK YOU!

TAA2@CORNELL.EDU