Homework 4

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December 1, 2023

1 Phonons and IR Active Modes

1.1

Phononic dispersion of a linear diatomic chain and discrete Floquet modes: Consider a 1D linear chain of atoms that are constrained to move along the x-axis, as seen in Fig. 1. The system has two atoms per unit cell with inter-atomic spacing b and c such that $a = (b + c)$. To keep things more general, we assume that each atom can have a distinct mass (M, m) and spring constant (k_1, k_2) and we use u_n (v_n) to represents the displacement of the blue (red) atom of the n^{th} unit cell from equilibrium.

(a) Find the coupled finite-difference equations that describe the motion of the diatomic system.

The EOM of v_n is

$$M\ddot{v}_n = k_2(u_{n+1} - v_n) - k_1(v_n - u_n), \tag{1}$$

and the EOM of u_n is

$$m\ddot{u}_n = k_1(v_n - u_n) - k_2(u_n - v_{n-1}). \tag{2}$$

Discrete Floquet modes: One can show that the time-harmonic wave solutions of such discrete periodic systems take the form

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = \begin{bmatrix} g_n \\ h_n \end{bmatrix} e^{iqx}, \text{ where } \begin{bmatrix} g_{n+1} \\ h_{n+1} \end{bmatrix} = \begin{bmatrix} g_n \\ h_n \end{bmatrix} \text{ such that } \begin{bmatrix} u_{n+1} \\ v_{n+1} \end{bmatrix} = \begin{bmatrix} u_n \\ v_n \end{bmatrix} e^{qa}.$$

In other words, our wave solution is a discrete version of a Floquet mode; remember that advancing from index n to $n+1$ translates our system by a unit cell, corresponding to a distance $x_{n+1} - x_n = a$. Above we use q to represent the wave-vector.

(b) Use a trial solution of this form to find a dispersion relation for this system. [In this case, it is sufficient to find an expression for $\omega_\pm^2(q)$.]

The two EOMs becomes

$$-M\omega^2 v_n = k_2(\mathrm{e}^{\mathrm{i}qa} u_n - v_n) - k_1(v_n - u_n), \tag{3}$$

and

$$-m\omega^2 u_n = k_1(v_n - u_n) - k_2(u_n - v_n \mathrm{e}^{-\mathrm{i}qa}), \tag{4}$$

and therefore

$$\begin{pmatrix} m\omega^2 - k_1 - k_2 & k_1 + k_2 \mathrm{e}^{-\mathrm{i}qa} \\ k_1 + \mathrm{e}^{\mathrm{i}qa} k_2 & M\omega^2 - k_1 - k_2 \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = 0. \tag{5}$$

Taking the determinant to be zero, we get

$$(m\omega^2 - k_1 - k_2)(M\omega^2 - k_1 - k_2) - (k_1 + k_2 \mathrm{e}^{-\mathrm{i}qa})(k_1 + k_2 \mathrm{e}^{\mathrm{i}qa}) = 0, \tag{6}$$

and hence

$$\omega_\pm(q)^2 = \frac{(M + m)(k_1 + k_2) \pm \sqrt{(M + m)^2 (k_1 + k_2)^2 - 16 M m k_1 k_2 \sin^2(qa/2)}}{2Mm}. \tag{7}$$

(c) From this relatively simple expression, we can learn a lot about band gap formation within phononic lattices. Use this result to find size of the band gap in the situations tabulated below.

The band gap is expected to appear when $qa = \pm\pi$; therefore

$$\Delta\omega = \frac{\omega_+^2 - \omega_-^2}{\omega_+ + \omega_-} = \frac{\sqrt{(M+m)^2(k_1+k_2)^2 - 16Mmk_1k_2}}{Mm(\omega_+ + \omega_-)}. \tag{8}$$

It can be seen that b and c are irrelevant in the band gap, so below we only care about k and m.

- When $M = m$ but $k_1 \neq k_2$ we have

$$\Delta\omega = \frac{4m^2(k_1+k_2)^2 - 16m^2k_1k_2}{m^2(\omega_+ + \omega_-)} = \frac{2|k_1 - k_2|}{m(\omega_+ + \omega_-)} > 0. \tag{9}$$

- When $M \neq m$ and $k_1 = k_2 = k$, we have

$$\Delta\omega = \frac{(M+m)^2 \cdot 4k^2 - 16Mmk^2}{Mm(\omega_+ + \omega_-)} = \frac{2k|M-m|}{Mm(\omega_+ + \omega_-)} > 0. \tag{10}$$

- When $M = m$ and $k_1 = k_2 = k$, $\Delta\omega = 0$.

(d) Assuming $k_1 = k_2$, find the form of the Floquet modes in the limit when $q \ll \pi/a$. [Hint: You should find a Floquet mode that has a similar character to the displacement field sketched out by Fox in Fig. 10.3 of Chapter 10.]

When $k_1 = k_2 =: k$ and $qa \ll \pi$, we have

$$\omega_\pm(q)^2 \approx \frac{2(M+m)k \pm (2(M+m)k - 8Mm \cdot k^2(qa/2)^2/2(M+m)k)}{2Mm}, \tag{11}$$

$$\omega_- = \sqrt{\frac{k}{2(M+m)}}qa, \quad \omega_+ = \sqrt{\frac{2(M+m)k}{Mm}}. \tag{12}$$

Putting $\omega_\pm$ into

$$\begin{pmatrix} m\omega^2 - 2k & k + k\mathrm{e}^{-\mathrm{i}qa} \\ k + k\mathrm{e}^{\mathrm{i}qa} & M\omega^2 - 2k \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = 0, \tag{13}$$

and ignoring the $(qa)^2$ terms, for ω_-, we get

$$-2u_n + (1 + \mathrm{e}^{-\mathrm{i}qa})v_n = 0, \tag{14}$$

and when q is truly very small, we get

$$u_n = v_n, \tag{15}$$

which means the atoms are moving "as a whole"; when qa is not that small but is still small, we still find that the two types of atoms roughly move in the same direction, and therefore in the ω_- mode – the acoustic phonon branch – when $qa \ll \pi$ we just get ordinary sound wave. For ω_+, we get

$$\frac{m}{M}u_n + \frac{1}{2}(1 + \mathrm{e}^{-\mathrm{i}qa})v_n = 0, \tag{16}$$

and when qa is truly small we get

$$mu_n + Mv_n = 0. \tag{17}$$

That's to say, the vibration mode, when qa is small, doesn't really "propagate": in this mode primitive unit cells are essentially independent to each other, and we have the momentum conservation equation.

(e) Next, we assume that the red and blue atoms carry differing sign of charge. According to the criteria described by Fox, does this system support any IR active-phonon modes? In other words, if a plane wave propagates along the x-axis will it couple to the couple to these lattice vibration? (Explain why we do/don't have coupling.)

When the red and blue atoms have opposite charges, since as is mentioned before, in the optical branch the two atoms in one primitive unit cell move in directions, we have vibrating dipoles; but for a plane wave propagates along the x-axis, its polarization directions are orthogonal to the x axis, while the dipoles are parallel to the x axis, and $-\boldsymbol{d}\cdot\boldsymbol{E}$ vanishes. So the optical mode is not IR active, and therefore the system doesn't support IR active phonon modes.

2 Periodic systems

2.1

Perturbative treatment of Bragg scattering: In Lecture 22, we treated a periodic modulation of dielectric constant as a perturbation on a uniform dielectric background to introduce Bragg scattering and photonic bandgap formation. Here, we fill in some of the steps that we skipped in class (for further context, see Lecture 22.N3). Since we we draw heavily on methods from solid state physics, you may find it helpful to consult Simon's book "The Oxford solid state basics," (2013).

Assuming 1D wave propagation in the z-direction and a dielectric distribution of the form $\varepsilon(z) = \bar{\varepsilon} + \Delta\varepsilon(z)$, we found that the wave equation, $\nabla \times \nabla \times \mathbf{E} = \varepsilon_r(r)(\omega/c)^2\mathbf{E}$, can be reduced to $\left[-\left(c^2/\bar{\varepsilon}\right)\partial_z^2 - \omega^2\Delta\varepsilon_r(z)/\bar{\varepsilon}\right]\phi(z) = \omega^2\phi(z)$ given a wave solution of the form $\mathbf{E}(r,t) = \hat{y}\phi(z)e^{-i\omega t}$. Here, $\Delta\varepsilon_r(z)$ is a perturbation with very small amplitude.

(a) We begin by identify an appropriate first order correction to our eigenvalue equation. Assuming that $\Delta\varepsilon_r(z)$ is first order in smallness [i.e. $\Delta\varepsilon_r(z) \to \gamma\Delta\varepsilon_r(z)$, where γ is a unitless order parameter] expand the eigenvalue $\left(\omega^2\right)$ and eigenfunction (ϕ) in orders of γ to properly formulate perturbation theory. Collect terms of order $(\gamma)^0$ and $(\gamma)^1$ and describe the general procedure by which you obtain the first order correction to the mode frequency.

[Hint: after subbing $\omega^2 = \left(\omega_0^2 + \gamma\omega_1^2 + \gamma^2\omega_2^2 \ldots\right)$ and $\phi(x) = (\phi_0(x) + \gamma\phi_1(x) + \gamma^2\phi_2(x) + \ldots)$ you should find that your zero- and first-order operators of the form $\hat{O}_0 = -\left(c^2/\bar{\varepsilon}\right)\partial_z^2$ and $\hat{O}_1 = -\omega_0^2\Delta\varepsilon_r(z)/\bar{\varepsilon}$, respectively.]

We have

$$\mathrm{LHS} = -\frac{c^2}{\bar{\epsilon}}\partial_z^2\phi_0 - \frac{\gamma c^2}{\bar{\epsilon}}\partial_z^2\phi_1 - \cdots - \frac{\gamma\omega_0^2\Delta\epsilon_{\mathrm{r}}(z)}{\bar{\epsilon}}\phi_0 - \cdots,$$

and

$$\mathrm{RHS} = \omega_0^2\phi_0 + \gamma\omega_0^2\phi_1 + \gamma\omega_1^2\phi_0 + \cdots,$$

and therefore

$$-\frac{c^2}{\bar{\epsilon}}\partial_z^2\phi_0 = \omega_0^2\phi_0, \tag{18}$$

and

$$-\frac{\gamma c^2}{\bar{\epsilon}}\partial_z^2\phi_1 - \frac{\gamma\omega_0^2\Delta\epsilon_{\mathrm{r}}(z)}{\bar{\epsilon}}\phi_0 = \gamma\omega_0^2\phi_1 + \gamma\omega_1^2\phi_0. \tag{19}$$

The second equation is not enough to decide ω_1 and ϕ_1; kind of arbitrarily, we dictate that (here we set γ back to 1)

$$\omega_1^2 = \int \mathrm{d}^3\boldsymbol{r}\,\phi_0^* \frac{-\omega_0^2\Delta\epsilon_{\mathrm{r}}(z)}{\bar{\epsilon}}\phi_0, \tag{20}$$

or its equivalence when there is degeneracy; and ϕ_1 can then be found if it's necessary.

Now we can just first find ϕ_0 and then ω_1.

(b) Next, we assume that our dielectric perturbation takes the form $\Delta\varepsilon_r(z) = (\Delta\varepsilon_{pp}/2)\cos(2\pi z/a)$, where $\Delta\varepsilon_{pp}$ is the peak-to-peak modulation of dielectric constant. Assuming that the unperturbed solutions are plane waves, use two such plane waves $(\pm k)$ to find a first order estimate energy splitting (or photonic band gap) at the zone boundary. [Hint: We need to use degenerate perturbation theory here! You should find a bandgap of $\Delta\omega_{gap} \cong (\omega_0/4)\left(\Delta\varepsilon_{pp}/\bar{\varepsilon}\right)$.]

Solving the problem regarding ϕ_0 and ω_0, we have

$$\phi_{0,\boldsymbol{q}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}, \quad \omega_0(\boldsymbol{q}) = \frac{c}{\sqrt{\bar{\epsilon}}}|\boldsymbol{q}|. \tag{21}$$

Now we consider the perturbation of O_1 to $\phi_{0,\pm\boldsymbol{q}}$. We have

$$\begin{aligned}
\int \mathrm{d}^3\boldsymbol{r}\,\phi_{0,-\boldsymbol{q}}^* O_1 \phi_{0,\boldsymbol{q}} &= \frac{1}{V}\int \mathrm{d}^3\boldsymbol{r}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\frac{-\omega_0^2\Delta\epsilon_{\mathrm{r}}(z)}{\bar{\epsilon}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \\
&= -\frac{\omega_0^2}{\bar{\epsilon}}\cdot\frac{1}{L}\int \mathrm{d}z\,\mathrm{e}^{2\mathrm{i}qz}\cdot\frac{\Delta\epsilon_{\mathrm{pp}}}{2}\cos(2\pi z/a) \\
&= -\frac{\omega_0^2}{\bar{\epsilon}}\cdot\frac{\Delta\epsilon_{\mathrm{pp}}}{4}\cdot\frac{1}{L}\int \mathrm{d}z\,\mathrm{e}^{\mathrm{i}2qz}\left(\mathrm{e}^{\mathrm{i}\frac{2\pi z}{a}} + \mathrm{e}^{-\mathrm{i}\frac{2\pi z}{a}}\right) \\
&= -\frac{\omega_0^2}{\bar{\epsilon}}\cdot\frac{\Delta\epsilon_{\mathrm{pp}}}{4}(\delta_{2q,2\pi/a} + \delta_{2q,-2\pi/a}).
\end{aligned} \tag{22}$$

So the transition matrix element is non-zero when $q = \pm\pi/a$, and the two wave vector points are connected by a G vector and are equivalent. What we need to do then is to diagonalize

$$\begin{pmatrix} \omega_0^2 & -\frac{\omega_0^2}{\bar{\epsilon}} \cdot \frac{\Delta\epsilon_{\rm pp}}{4} \\ -\frac{\omega_0^2}{\bar{\epsilon}} \cdot \frac{\Delta\epsilon_{\rm pp}}{4} & \omega_0^2 \end{pmatrix} \tag{23}$$

and the eigenvalues are

$$\omega_\pm^2 = \omega_0^2 \pm \frac{\omega_0^2}{\bar{\epsilon}} \cdot \frac{\Delta\epsilon_{\rm pp}}{4}, \tag{24}$$

where

$$\omega_0 = \frac{c}{\sqrt{\bar{\epsilon}}}\frac{\pi}{a}. \tag{25}$$

The gap then is

$$\Delta\omega = \omega_+ - \omega_- = \omega_0(\sqrt{1 + \Delta\epsilon_{\rm pp}/4\bar{\epsilon}} - \sqrt{1 - \Delta\epsilon_{\rm pp}/4\bar{\epsilon}}) \approx \frac{\omega_0}{4}\frac{\Delta\epsilon_{\rm pp}}{\bar{\epsilon}}. \tag{26}$$

2.2 The Coherent-State and Classical Correspondence

In this problem we examine some general properties of a coherent state. The coherent state, $|\alpha\rangle$, is defined as $|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0} \alpha^n (n!)^{-1/2} |n\rangle$, where α is a complex number that has a similar significance to our classical complex mode amplitude. Remember that $|n\rangle$ are eigenstates of the Hamiltonian, $H = \hbar\omega \left(a^\dagger a + \frac{1}{2}\right)$.

(a) Show that the lowering operator, a, produces $a|\alpha\rangle = \alpha|\alpha\rangle$.

We have

$$\begin{aligned} a\,|\alpha\rangle &= \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n}\,|n-1\rangle \\ &= \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^{n+1}}{\sqrt{(n+1)!}} \sqrt{n+1}\,|n\rangle \\ &= \alpha \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n\rangle \\ &= \alpha\,|\alpha\rangle\,. \end{aligned} \tag{27}$$

(b) Use your result from (a) to find the time-evolution of a coherent state, $\frac{d}{dt}\langle\alpha(t)|a|\alpha(t)\rangle$, where $|\alpha(t)\rangle \equiv e^{-i\omega t} e^{-|\alpha|^2/2} \sum_{n=0} \alpha^n (n!)^{-1/2} |n\rangle$. [Hint: Remember that $\frac{d}{dt}\langle\psi|a|\psi\rangle = \frac{i}{\hbar}\langle\psi|[H,a]|\psi\rangle$.]

Actually we have

$$|\alpha(t)\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha \mathrm{e}^{-\mathrm{i}\omega n t})^n}{\sqrt{n!}}\,|n\rangle\,. \tag{28}$$

We have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\alpha|a|\alpha\rangle &= \frac{\mathrm{i}}{\hbar}\langle\alpha|[H,a]\,|\alpha\rangle \\ &= \frac{\mathrm{i}}{\hbar}\langle\alpha|-\hbar\omega a|\alpha\rangle = -\mathrm{i}\omega\alpha\,\langle\alpha|\alpha\rangle \\ &= -\mathrm{i}\omega\alpha. \end{aligned} \tag{29}$$

So we find the time evolution of α is

$$\alpha(t) = \alpha \mathrm{e}^{-\mathrm{i}\omega t}. \tag{30}$$