PHYS4450 Solid State Physics

SAMPLE QUESTION FOR DISCUSSION in Week 5 EXERCISE CLASS on 20 February 2013

You may want to think about them before attending exercise class.

SQ7 For Chapter VI on lattice vibrations, the most important point is to know how many branches and the types of dispersion relations to be expected given a system.

TA: Let's consider graphene. If we only allow the carbon atoms to move up and down the plane, what does one expect for the dispersion relations and why? Next, if the carbon atoms are allowed to vibrate both within the graphene plane and off (up and down) the plane, what does one expect for the dispersion relations and why? Then search literature on possible dispersion relations from detailed calculations and/or measurements.

SQ8 (Related to the idea of phonons (Chapters VI and VII).) **Read me.** Introduction – We are discussing lattice vibrations in solids. In particular, we want to find the dispersion relation $\omega(\mathbf{q})$, which gives how the normal mode (angular) frequencies ω depends on the wavevector $\mathbf{q}$ (with $\mathbf{q} \in$ 1st B.Z).

From classical mechanics, the normal modes are independent of each other. That is to say, we have many **independent oscillators** (if we make the harmonic approximation). Each normal mode corresponds to an independent oscillator.

The idea of phonons – If we impose quantum mechanics on every independent oscillator, we will get the possible energies of $(n_{\mathbf{q}} + \frac{1}{2})\hbar\omega(\mathbf{q})$, where the quantum number $n_{\mathbf{q}}$ (with $\mathbf{q}$ labelling the particular normal mode and thus the particular independent oscillator under consideration) indicates the extent the oscillator is excited. One can show that the excitations behave like particles with energy $\hbar\omega(\mathbf{q})$ and a quantity that looks like a momentum $\hbar\mathbf{q}$.

Let's consider a particular normal mode. The state of no excitations corresponds to $n_q = 0$. The state of $n_q = 1$ corresponds to a state with one **phonon** that has the energy $\hbar\omega(\mathbf{q})$ and momentum $\hbar\mathbf{q}$. The state of $n_q \neq 0$ corresponds to a state with n_q **phonons** each of which has the energy $\hbar\omega(\mathbf{q})$ and momentum $\hbar\mathbf{q}$. Recall that in Statistical Mechanics, we know how to calculate the thermal average $\langle n_{\mathbf{q}} \rangle$ for a given temperature, and thus the averaged number of phonons of a normal mode excited at a temperature. This leads us to a different viewpoint on the system. In this new picture, we can simply forget the real stuffs that are oscillating (a huge number of atoms with chemical bonds among them). We simply focus on the **excitations**. No excitation (ground state or $n_q = 0$) can be taken as the **vacuum state**. See that such a vacuum is not "nothing", it has something, e.g., the zero point energy. Excited states are taken as the **creation** of a few phonons. This is the beginning of quantum field theory, which is a quantum theory that allows particles to be created and destroyed. If we turn the discrete coupled-atoms problem into a continuum problem, we will get a wave equation for the long wavelength oscillation (continuum means that the lattice spacing is always smaller than the wavelength). There are again normal modes. If we impose quantum mechanics on them, we see that a **vacuum** is just a state with no excitations. Excitations can be viewed as creating some particles. Therefore, we have a new viewpoint on what are particles (thus what is matter). Particles are excitations of a field. [Now, we get a sense on the Higgs' particle being an excitation of the Higgs field.]

TA: Start with a Lagrangian that will give the Hamiltonian as given in Appendix A to Chapter VI (see attached pages). Use the Lagrangian to identify the conjugate momentum. This is classical mechanics. To go from classical mechanics to quantum mechanics ("quantizing the harmonic oscillator"), the commutator is imposed on **a conjugate pair of coordinate and momentum**. Appendix A gives a summary of the key relationships in the quantum mechanics of a harmonic oscillator using the technique of introducing the creation operator $\hat{a}$ and annihilation operator $\hat{a}^\dagger$. This is an algebraic approach to the SHO problem in QM. TA will fill in the details. In your quantum physics course, the standard approach uses the differential equation form of the Schrödinger equation that amounts of a particular (position) representation of the position operator $\hat{X}$ (or $\hat{x}$) and momentum operator $\hat{P}$ (or $\hat{p}$). A further remark is that a similar approach is also convenient in treating angular momenta (orbital, spin, total angular momenta) in QM.

Appendix A: QM of a harmonic Oscillator

$$H = \frac{P^2}{2M} + \frac{1}{2} M\omega^2 X^2 \quad (A1)$$

- From classical to quantum mechanics:

  Impose $[\hat{X}, \hat{P}] \equiv \hat{X}\hat{P} - \hat{P}\hat{X} = i\hbar \quad (A2)$

  (Note: Using $\hat{X} \to X$; $\hat{P} = \frac{\hbar}{i}\frac{\partial}{\partial X}$ is a possible representation)

  Solving the Schrödinger Equation $\Rightarrow \varepsilon_n = (n+\frac{1}{2})\hbar\omega$; $n = 0, 1, 2, \ldots$

- One can also proceed by defining

$$\left.\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2\hbar M\omega}}(M\omega\hat{X} + i\hat{P}) \\ \hat{a}^+ &= \frac{1}{\sqrt{2\hbar M\omega}}(M\omega\hat{X} - i\hat{P}) \end{aligned}\right\} (A3) \quad \text{Just replacing } \hat{X}, \hat{P} \text{ by } \hat{a}, \hat{a}^+$$

  $[\hat{a}, \hat{a}^+] = 1 \quad (A4)$ (followed from $[\hat{X}, \hat{P}] = i\hbar$)

- Expressing $\hat{X}$ and $\hat{P}$ in terms of $\hat{a}$ and $\hat{a}^+$:

$$\hat{X} = \sqrt{\frac{\hbar}{2M\omega}}(\hat{a}^+ + \hat{a}) \; ; \; \hat{P} = \frac{i}{2}\sqrt{2\hbar M\omega}(\hat{a}^+ - \hat{a}) \quad (A5)$$

- Then $\hat{H}$ can be expressed in terms of $\hat{a}$ and $\hat{a}^+$ as:

$$\hat{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right) \quad (A6)$$

- Defining $\hat{n} \equiv \hat{a}^+ \hat{a}$,

$$\hat{H} = \hbar\omega\left(\hat{n} + \frac{1}{2}\right) \qquad \text{(A7)}$$

- Energy eigenstates can be written as $|n\rangle$, which denotes the state with energy $(n+\frac{1}{2})\hbar\omega$
- $|n\rangle$ also denotes the state with <u>n excitations</u> ($n=0$, no excitation, i.e. ground state)
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$$\left.\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}\,|n-1\rangle \\ \hat{a}^+|n\rangle &= \sqrt{n+1}\,|n+1\rangle \end{aligned}\right\} \text{(A8)} \quad \begin{aligned} &(\therefore \hat{a} \text{ annihilates one excitation}) \\ &(\therefore \hat{a}^+ \text{ creates one excitation}) \end{aligned}$$

- It follows that $\hat{n}|n\rangle = n|n\rangle$
- $\underbrace{\text{Ground state}}_{|0\rangle}$: $\underbrace{\hat{a}|0\rangle = 0}$ (A9) (nothing to annihilate)

Use Eq. (A3) to write this as a differential equation, one can solve for the ground state wavefunction. Then Eq. (A8) gives the excited states.

- Applying Eq. (A8) repeatedly, the state $|n\rangle$ can be constructed from $|0\rangle$ as:

$$|n\rangle = \underset{\substack{\uparrow \\ \text{normalization} \\ \text{factor}}}{\frac{1}{\sqrt{n!}}} \underbrace{(\hat{a}^+)^n}_{\nwarrow \text{ creating } n \text{ excitations}} |0\rangle \qquad \text{(A10)}$$

- For a collection of <u>independent</u> Harmonic Oscillators:

$$\hat{H} = \sum_{\text{oscillators } i} \left(\frac{\hat{P}_i^2}{2M_i} + \frac{1}{2} M_i \omega_i^2 \hat{X}_i^2 \right) \qquad \text{(A11)}$$

- For normal modes in a crystal, the modes are labelled by $(s, \vec{q})$

which branch

$\vec{q} \in 1^{st}$ B.Z.

$$\hat{H} = \underbrace{\sum_s \sum_{\vec{q}}}_{\substack{\text{sum over} \\ \text{all independent} \\ \text{oscillators}}} \underbrace{\hbar\omega_s(\vec{q}) \left(\hat{a}_s^+(\vec{q})\, \hat{a}_s(\vec{q}) + \frac{1}{2} \right)}_{\substack{\text{carry out Eqs.(A1)-(A6) for each} \\ \text{independent oscillator}}} \qquad \text{(A12)}$$