**PHYS4450 Solid State Physics**

## SAMPLE QUESTIONS FOR DISCUSSION IN Week 7 EXERCISE CLASS (6 March 2013)

You may want to think about them before attending exercise class. SQ12 summarizes all the results related to density of normal mode frequencies (also called density of states unfortunately) $D(\omega)$ for a linear phonon dispersion relation (Ch.VI-VII) and the density of states $g(E)$ for a parabolic free electron dispersion relation (Ch.VIII). SQ13 gives some sense about metal physics. SQ14 is a **must-try** problem on the simplest possible math problem (2×2 matrices).

SQ12 (Related to Ch.VI,VII,VIII.) In discussing phonons, we made use of the phonon density of states $D(\omega)$ (see Ch.VII), where $D(\omega)d\omega$ is the number of normal modes with frequencies in the interval $\omega$ to $\omega+d\omega$.

The idea can be extended to consider the density of electronic states $g(E)$ (see Ch.VIII). Here, $g(E)dE$ is the number of electronic states with energies in the interval $E$ to $E+dE$, including spin degeneracy.

To show the similarity of the two problems, the TA will prepare a TABLE in which the left hand column is 1D, 2D, 3D, and the top row is (i) linear $\omega(q)$ phonon dispersion relation ($\omega(q) = v_s q$) and (ii) parabolic $E(k)$ dispersion relation ($E(k) = \hbar^2 k^2/2m$). The elements in the table give the DOS for each of the six cases, in particular on how $D(\omega)$ depends on $\omega$ and how $g(E)$ depends on $E$ in different dimensions. Discuss how one can get at some of these results.

SQ13 **Typical numbers of "Fermi something" in a metal.** The early sections in Ch.VIII showed that an important quantity that determines many properties of a metal is its conduction electron number density (number of free electrons per unit volume). Take sodium as an example. It is bcc structure. Find the lattice constant from data book. Knowing that the outmost 3s electron will be freed in a metal to become a conduction electron, find the conduction electron number density $n$.

First, it will be useful to work out the combination $\hbar^2/m$ for an electron in units of $eV\cdot$ Å$^2$. Memorizing this number (and its unit) will be convenient in doing solid state physics.

Hence, find the Fermi energy, Fermi temperature, Fermi velocity, and Fermi wavevector (magnitude). Find the density of states per unit volume at the Fermi energy, which is related to the proportionality constant in the heat capacity. Find also the plasma frequency $\omega_p = \sqrt{ne^2/m\epsilon_0}$. The latter frequency $\omega_p$ is of importance in the optical properties of a metal. For example, for EM waves of $\omega < \omega_p$, the metal is reflective (so you can use copper as a mirror); but for $\omega > \omega_p$, the same metal is transparent.

SQ14 **(Simple Math of 2×2 matrices contains much physics – Essential ideas of perturbation theory and preparation for band theory.)**

We need to know some results on time-independent perturbation theory in quantum mechanics to proceed to band theory. Sounds scary!? Relax! In fact, much of these topics has to do with 2×2 matrices and nothing more! Although students may have learned basic perturbation theory in other courses, it will be useful to **review** the key results. Here, it is more important to **know what the perturbation problem is and what the key results mean** than to know how to derive the results.

(i) In non-degenerate perturbation theory, what is the first and second order corrections in the energy due to a perturbative term $H'$ in the Hamiltonian $H = H_0 + H'$. What is the first order correction to the wave function? In particular, if $\psi_{a,0}$ and $\psi_{b,0}$ are two eigenstates of $H_0$ corresponding to different eigenvalues $\epsilon_{a,0}$ and $\epsilon_{b,0}$, how does state $b$ influence state $a$ in the presence of $H'$, and vice versa? [TA: It is **more important to illustrate the meaning** of the results, instead of deriving the results. Give a good reference where derivation can be found will be OK.] The point here is to illustrate the physical picture below.

(ii) Find the exact eigenvalues of a matrix of the form

$$\begin{pmatrix} \epsilon_{upper} & \Delta \\ \Delta^* & \epsilon_{lower} \end{pmatrix}$$

where $\epsilon_{upper} > \epsilon_{lower}$.

If $|\Delta| \ll \epsilon_{upper} - \epsilon_{lower}$, one can expand the square root in the exact results of the eigenvalues. Hence, obtain approximate expressions for the eigenvalues. Relate the results to (i). Point out that the case of $\epsilon_{upper} = \epsilon_{lower}$ will be problematic for the approximated expressions.

(iii) Find the eigenvalues of a matrix of the form

$$\begin{pmatrix} \epsilon_0 & \Delta \\ \Delta^* & \epsilon_0 \end{pmatrix}$$

This corresponds to the case of $\epsilon_{upper} = \epsilon_{lower} = \epsilon_0$. Note that the exact results in (ii) are still applicable, but the approximate expressions don't.

(iv) In degenerate perturbation theory (assume two degenerate states), illustrate how to set up a $2 \times 2$ matrix to handle a perturbative term $H'$. In particular, illustrate how the two eigenvalues behave as the perturbative term $H'$ increases in strength. The answer in (ii) may be useful.

(v) Apply the idea in (iii) to molecular formation and illustrate how the bonding and anti-bonding molecular orbitals are related to the results of a degenerate perturbation calculation, e.g., in $H_2^+$ molecular ion. (This is a topic in Quantum Physics II.) Molecular orbitals in HF, for example, can be handled by the approximation in (ii).