PHYSICS 211B: CONDENSED MATTER PHYSICS
HW ASSIGNMENT #1 PROBLEMS

These problems draw upon material that should have been covered in Physics 211A. If you encounter any difficulties, please consult chapters 3, 4, and 5 of the lecture notes.

(1) For each of the following structures, indicate whether or not it is a Bravais lattice. If it is, give the three primitive vectors. If not, describe it as a Bravais lattice with the smallest possible basis.

(a) Base-centered cubic (simple cubic with additional points in the centers of the two horizontal faces).

(b) Side-centered cubic (simple cubic with additional points in the centers of the four vertical faces).

(c) Edge-centered cubic (simple cubic with additional points at the midpoints of all nearest-neighbor links).

(2) Polycrystalline specimens of three different monatomic cubic crystals are analyzed with a Debye-Scherrer camera. It is known that one sample is fcc, one is bcc, and one has a diamond structure. The approximate angular position ϕ of the first four diffraction rings are found to be

$$\begin{aligned} \mathsf{A}: &\ 42.2^\circ, 49.2^\circ, 72.0^\circ, 87.3^\circ \\ \mathsf{B}: &\ 28.8^\circ, 41.0^\circ, 50.8^\circ, 59.6^\circ \\ \mathsf{C}: &\ 42.8^\circ, 73.2^\circ, 89.0^\circ, 115^\circ \end{aligned}$$

(a) Identify the crystal structures A, B, and C.

(b) If the wavelength of the incident X-ray is $\lambda = 1.5\text{Å}$, what is the length of the side of the cubic cell in each case?

(c) If the (monatomic) diamond structure were replaced by a (binary) zincblende structure, at what angles would the first four rings be observed?

(3) A monolayer of atoms is deposited on a surface. The atoms form a regular hexagonal lattice. This problem deals with the vibrations of these atoms.

(a) Suppose the surface is perfectly smooth. The atoms interact by a potential

$$\Phi = \tfrac{1}{2} \sum_{\boldsymbol{R},\boldsymbol{R}'} v\big(|\boldsymbol{R} + \boldsymbol{u}_\perp(\boldsymbol{R}) - \boldsymbol{R}' - \boldsymbol{u}_\perp(\boldsymbol{R}')|\big) + \tfrac{1}{2} K_z \sum_{\boldsymbol{R}} u_z^2(\boldsymbol{R})$$

where $\boldsymbol{u}_\perp = u_x\,\hat{\boldsymbol{x}} + u_y\,\hat{\boldsymbol{y}}$ is the displacement along the surface (perpendicular to the surface normal $\hat{\boldsymbol{z}}$), $\boldsymbol{R}$ and $\boldsymbol{R}'$ denote sites of the hexagonal Bravais lattice, and the last term describes the binding of the atoms to the surface (u^z is the displacement along the surface

normal). Show that the dynamical matrix for the lattice vibrations takes the form

$$\hat{\Phi}(\boldsymbol{k}) = \begin{pmatrix} \hat{\Phi}^{xx}(\boldsymbol{k}) & \hat{\Phi}^{xy}(\boldsymbol{k}) & 0 \\ \hat{\Phi}^{yx}(\boldsymbol{k}) & \hat{\Phi}^{yy}(\boldsymbol{k}) & 0 \\ 0 & 0 & \hat{\Phi}^{zz}(\boldsymbol{k}) \end{pmatrix}$$

where the upper left 2×2 block is given by

$$\Phi^{\alpha\beta}(\boldsymbol{k}) = 2 \sum_{\boldsymbol{R}} \sin^2(\tfrac{1}{2}\boldsymbol{k} \cdot \boldsymbol{R}) \Big\{ (\delta^{\alpha\beta} - \hat{R}^\alpha \hat{R}^\beta) R^{-1} v'(R) + \hat{R}^\alpha \hat{R}^\beta v''(R) \Big\}$$

with α, $\beta = 1$ or 2, and $\hat{\Phi}^{zz}(\boldsymbol{k}) = K_z$ independent of $\boldsymbol{k}$. You may find it useful to invoke Eqn. 3.54 of the lecture notes (you don't have to derive it!).

(b) Assuming that the above sum for $\hat{\Phi}^{\alpha\beta}(\boldsymbol{k})$ is dominated by the nearest neighbor terms, compute the phonon dispersions along the $(1, 0)$ axis in reciprocal space. You should use M for the ionic mass, a for the lattice constant, and abbreviate $A \equiv a^{-1} v'(a)$ and $B \equiv v''(a)$.

(c) Find the general form of the dynamical matrix for arbitrary phonon wavevector $\boldsymbol{k}$. For the acoustic modes, find the sound velocities $c_\pm$ for $\boldsymbol{k} \approx 0$.

(4) Consider a one-dimensional chain of s-orbitals separated by a distance a_0, with

$$H = \sum_n \Big(\varepsilon_{\mathsf{A}} \, | \, \mathsf{A}_n \rangle\langle \, \mathsf{A}_n \, | + \varepsilon_{\mathsf{B}} \, | \, \mathsf{B}_n \rangle\langle \, \mathsf{B}_n \, | \\ - t \sum_n \Big(| \, \mathsf{A}_n \rangle\langle \, \mathsf{B}_n \, | + | \, \mathsf{B}_n \rangle\langle \, \mathsf{A}_{n+1} \, | + | \, \mathsf{B}_n \rangle\langle \, \mathsf{A}_n \, | + | \, \mathsf{A}_{n+1} \rangle\langle \, \mathsf{B}_n \, | \Big) \quad .$$

(a) How many atoms are there per unit cell? What is the length of the Wigner-Seitz cell?

(b) Find the dispersions $E_a(k)$ of the energy bands.

(c) Sketch the band structure over the one-dimensional Brillouin zone.

(d) Show that for $\varepsilon_{\mathsf{A}} = \varepsilon_{\mathsf{B}}$ that you recover the correct energy band for the uniform one-dimensional nearest-neighbor chain.

(5) Hexagonal boron nitride, BN, has a honeycomb lattice structure, with boron atoms at A sites and nitrogen atoms at B sites. The tight binding Hamiltonian is

$$H = \sum_{\boldsymbol{R}} \Big(\varepsilon_{\mathsf{A}} \, | \, \mathsf{A}_{\boldsymbol{R}} \rangle\langle \, \mathsf{A}_{\boldsymbol{R}} \, | + \varepsilon_{\mathsf{B}} \, | \, \mathsf{B}_{\boldsymbol{R}} \rangle\langle \, \mathsf{B}_{\boldsymbol{R}} \, | \Big) \\ - t \sum_{\boldsymbol{R}} \Big(| \, \mathsf{A}_{\boldsymbol{R}} \rangle\langle \, \mathsf{B}_{\boldsymbol{R}} \, | + | \, \mathsf{A}_{\boldsymbol{R}} \rangle\langle \, \mathsf{B}_{\boldsymbol{R}+\boldsymbol{a}_1} \, | + | \, \mathsf{A}_{\boldsymbol{R}} \rangle\langle \, \mathsf{B}_{\boldsymbol{R}-\boldsymbol{a}_2} \, | + \text{H.c.} \Big) \quad .$$

(a) Find the 2×2 Hamiltonian matrix $\hat{H}(\boldsymbol{k})$. You may find it convenient to write the wavevector as $\boldsymbol{k} = \frac{\theta_1}{2\pi} \boldsymbol{b}_1 + \frac{\theta_2}{2\pi} \boldsymbol{b}_2$ and express your answer in terms of $\theta_{1,2}$.

(b) Find expressions for the band energies at high symmetry points Γ, K, and M.

(c) Find an expression for the band gap Δ. Is the gap direct or indirect?

(6) Consider a tight binding model of (p_x, p_y) orbitals on a triangular lattice. The hopping is restricted to nearest neighbor links. Recall that the hopping matrix elements are given by

$$t_{\mu\nu}(\hat{\boldsymbol{\eta}}) = t_{\rm w}\,\delta_{\mu\nu} - (t_{\rm s} + t_{\rm w})\,\hat{\eta}_\mu\,\hat{\eta}_\nu \quad ,$$

where the link direction is $\hat{\boldsymbol{\eta}}$.

(a) Find the matrix $\hat{t}_{\mu\nu}(\boldsymbol{k})$. You may find it convenient to write $\boldsymbol{k} = \frac{\theta_1}{2\pi}\,\boldsymbol{b}_1 + \frac{\theta_2}{2\pi}\,\boldsymbol{b}_2$ and express your answer in terms of $\theta_{1,2}$.

(b) Find expressions for the band energies at the high symmetry points Γ, K, and M.

(c) For $t_{\rm s} = 1$ and $t_{\rm w} = \frac{1}{2}$, plot the dispersions $E_\pm(\boldsymbol{k})$ along the path $\Gamma{\rm M}{\rm K}\Gamma$.

(7) Make a sketch of the extended Brillouin zones like in Fig. 5.2 of the lecture notes, but for the triangular lattice. Then make plots the free electron Fermi surface for valences $Z = 2$ and $Z = 3$, such as in Fig. 2.3.

(8) *Cyclotron resonance in Si and Ge* – This problem is based on the following figures:

Both Si and Ge are indirect gap semiconductors with anisotropic conduction band minima and doubly degenerate valence band maxima. In Si, the conduction band minima occur along the $\langle 100\rangle$ ($\langle \Gamma{\rm X}\rangle$) directions, and are six-fold degenerate. The equal energy surfaces are cigar-shaped, and the effective mass along the $\langle \Gamma{\rm X}\rangle$ principal axes (the 'longitudinal' effective mass) is $m_{\rm l}^* \simeq 1.0\,m_{\rm e}$, while the effective mass in the plane perpendicular to this axis (the 'transverse' effective mass) is $m_{\rm t}^* \simeq 0.20\,m_{\rm e}$. The valence band maximum occurs at the unique Γ point, and there are two isotropic hole branches: a 'heavy' hole with $m_{\rm hh}^* \simeq 0.49\,m_{\rm e}$, and a 'light' hole with $m_{\rm lh}^* \simeq 0.16\,m_{\rm e}$.

In Ge, the conduction band minima occur at the fourfold degenerate L point (along the eight $\langle 111\rangle$ directions) with effective masses $m_{\rm l}^* \simeq 1.6\,m_{\rm e}$ and $m_{\rm t}^* \simeq 0.08\,m_{\rm e}$. The valence band maximum again occurs at the Γ point, where the hole masses are $m_{\rm hh}^* \simeq 0.34\,m_{\rm e}$ and $m_{\rm lh}^* \simeq 0.044\,m_{\rm e}$. Use the following figures to interpret the cyclotron resonance data shown below. Verify whether the data corroborate the quoted values of the effective masses in Si and Ge.

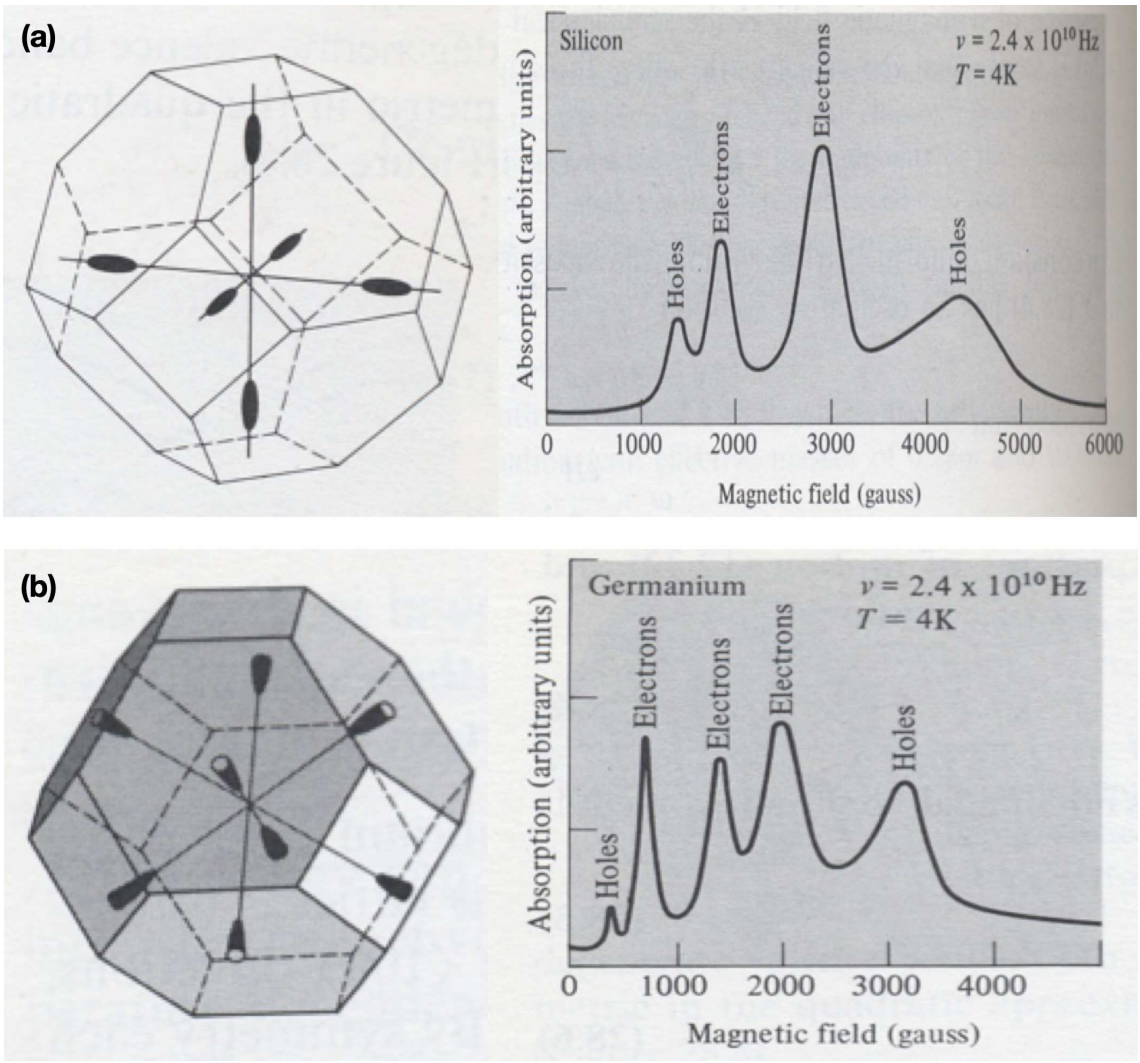

Figure 1: (a) Left: Constant energy surfaces near the conduction band minima in silicon. There are six symmetry-related ellipsoidal pockets whose long axes run along the $\langle 100 \rangle$ directions. Right: Cyclotron resonance data in Si (G. Dresselhaus *et al.*, *Phys, Rev,* **98**, 368 (1955).) The field lies in a (110) plane and makes an angle of 30° with the $[001]$ axis. (b) Left: Constant energy surfaces near the conduction band minima in germanium. There are eight symmetry-related half-ellipsoids whose long axes run along the $\langle 111 \rangle$ directions, and are centered on the midpoints of the hexagonal zone faces. With a suitable choice of primitive cell in $\boldsymbol{k}$-space, these can be represented as four ellipsoids, the half-ellipsoids on opposite faces being joined together by translations through suitable reciprocal lattice vectors. Right: Cyclotron resonance data in Ge (G. Dresselhaus *et al.*, *Phys, Rev,* **98**, 368 (1955).) The field lies in a (110) plane and makes an angle of 60° with the $[001]$ axis.