Condensed Matter Physics 2023
Quiz 4 (Week 11)

1. In a powder diffraction experiment using a collimated beam of monochromatic X-rays with wavelength $\lambda = 1.62$ Å, diffraction peaks are observed at angles $2\theta = 42.3$, 49.2, 72.2 and 87.4°.
   (a) Identify the lattice type.
   (b) Calculate the lattice constant.

(a) Let's create a table as done in the lecture, where d is calculated using Bragg's law as $d = \lambda/(2\sin\theta)$.

Label	2θ (°)	d (Å)	d_a^2/d^2	$3d_a^2/d^2$	$h^2+k^2+l^2$	(h,k,l)
a	42.3	2.24	1	3	3	$(1,1,1)$
b	49.2	1.95	1.33	3.99	4	$(2,0,0)$
c	72.2	1.37	2.66	7.98	8	$(2,2,0)$
d	87.4	1.17	3.67	11.01	11	$(1,1,3)$

The (h,k,l) indices found are all even or all odd, hence the lattic is fcc.

(b) The lattice constant can be estimated from any of the rows as $a = d\sqrt{h^2+k^2+l^2} = 3.89$ Å.

2. Mainstream only. Given $E(k) = 3A\sin^2(\frac{ka}{2})$ is the energy of an electron band in a one-dimensional material, calculate the group velocity $v_g(k)$ and show that at the Brillouin zone boundary v_g is zero.

The group velocity is defined as $v_g = \frac{1}{\hbar}\frac{dE(k)}{dk}$. Given $E(k) = 3A\sin^2(\frac{ka}{2})$, we obtain:

$$v_g(k) = \frac{3A}{\hbar}\frac{d}{dk}\left[\sin^2\left(\frac{ka}{2}\right)\right] = \frac{3Aa}{\hbar}\sin\left(\frac{ka}{2}\right)\cos\left(\frac{ka}{2}\right) = \frac{3Aa}{2\hbar}\sin(ka)$$

where in the last relation we used $\sin(2x) = 2\sin(x)\cos(x)$.
At the Brillouin zone boundary $k = \pm\pi/a$, and $v_g(\pm\frac{\pi}{a}) = \frac{3Aa}{2\hbar}\sin(\pm\pi) = 0$.

3. Advanced only. Show that the effective mass of an electron in a one-dimensional crystal that travels with group velocity $v_g(k)$ and energy $E = \hbar\omega(k)$ is given by $m^* = \hbar^2(\partial^2E/\partial k^2)^{-1}$. Hint: consider the effective mass m^* as the quantity that satisfies Newton's second law; the force on the electron is given by $F = dp/dt = \hbar dk/dt$.

We consider Newton's second law $F = m^*a$, with

$$a = \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{\partial E}{\partial k}\right) = \frac{1}{\hbar}\frac{\partial^2E}{\partial k^2}\frac{dk}{dt}.$$

Using $F = \hbar dk/dt$, we obtain

$$m^* = Fa^{-1} = \hbar\frac{dk}{dt}\hbar\left(\frac{\partial^2E}{\partial k^2}\frac{dk}{dt}\right)^{-1} = \hbar^2\left(\frac{\partial^2E}{\partial k^2}\right)^{-1}$$

4. (a) Consider a simple square lattice (two dimensions). The kinetic energy of a free electron at a corner of the first Brillouin zone is higher than that of an electron at midpoint of a side face of the zone by a factor b. What is the value of b?
   (b) What is the corresponding factor for a simple cubic lattice in three dimensions?

(c) Consider now a two- or three-dimensional crystal formed by a divalent element, described within the nearly-free electron model. Given the results above, can you explain a scenario where this solid is a metal?

(a) The kinetic energy of a free electron is $E = \frac{\hbar^2 k^2}{2m}$. A corner of the first Brillouin zone is $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a})$, where a is the lattice parameter. Then $k^2 = \frac{2\pi^2}{a^2}$, which gives $E = \frac{\hbar^2 \pi^2}{ma^2}$. At midpoint of a side face, $\mathbf{k} = (\frac{\pi}{a}, 0)$, $k^2 = \frac{\pi^2}{a^2}$ and $E = \frac{\hbar^2 \pi^2}{2ma^2}$. The ratio between the two is 2, hence $b = 2$.

(b) In three dimensions, at the corner of the first Brillouin zone $\mathbf{k} = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$, $k^2 = \frac{3\pi^2}{a^2}$ and $E = \frac{3\hbar^2 \pi^2}{2ma^2}$. At $\mathbf{k} = (\frac{\pi}{a}, 0, 0)$, $k^2 = \frac{\pi^2}{a}$ corresponding to $E = \frac{\hbar^2 \pi^2}{2ma^2}$. The ratio is 3.

(c) Unless the band gap at the midpoint of a face is larger than the kinetic energy difference between this point and a corner, the electrons will start filling the second band instead of filling up the corner states in the first band. Under these conditions, divalent elements will be metals and not insulators.