

# Applications of Quantum Mechanics: Example Sheet 3

David Tong, February 2018

1. Two choices of primitive vectors for a 3-dimensional Bravais lattice  $\Lambda$  are related by  $\mathbf{a}'_i = \sum_{n=1}^3 M_{ij} \mathbf{a}_j$ . Show that  $M$  and  $M^{-1}$  are matrices of integers, and deduce that  $\det M = \pm 1$ . Show that the volume of a unit cell of  $\Lambda$  is basis independent.

2. Find a basis of primitive vectors for the FCC lattice  $\Lambda$ . Find the reciprocal lattice  $\Lambda^*$  and show that it has BCC structure. [*Hint: consider the basis vectors for the primitive unit cell of  $\Lambda$  and construct the basis vectors for the primitive unit cell of  $\Lambda^*$  explicitly.*] Sketch or construct the Wigner-Seitz cell of the FCC lattice.

3. A particle is governed by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x})$$

where  $V$  has the periodicity of some 3-dimensional Bravais lattice  $\Lambda$ . Show that the matrix element of  $H$  vanishes if evaluated between Bloch states

$$\psi(\mathbf{x}) = u(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{and} \quad \tilde{\psi}(\mathbf{x}) = \tilde{u}(\mathbf{x})e^{i\tilde{\mathbf{k}}\cdot\mathbf{x}},$$

with  $\mathbf{k}$  and  $\tilde{\mathbf{k}}$  in the first Brillouin zone and unequal, and  $u$  and  $\tilde{u}$  periodic. [*Hint: you can show this for the kinetic and potential terms in  $H$  separately.*] Deduce that there is a complete set of energy eigenstates of  $H$  of the Bloch state form.

4. In the extended zone scheme, a point in  $\mathbf{R}^3$  is in the  $n^{\text{th}}$  Brillouin zone ( $n > 1$ ) if the origin is the  $n^{\text{th}}$  closest point of the reciprocal lattice  $\Lambda^*$ . Show that the various parts of the  $n^{\text{th}}$  zone can be mapped into the first zone, without overlap except on bounding surfaces, to completely cover the first zone. Deduce that the  $n^{\text{th}}$  zone has the same total volume as the first zone.

[*Hint 1: Consider a division of the first Brillouin zone into subregions labelled by non-zero reciprocal lattice vectors, with a point  $\mathbf{k}$  being in the subregion labelled by  $\mathbf{q} \in \Lambda^*$  if  $\mathbf{q}$  is the the  $n^{\text{th}}$  closest point lattice point to  $\mathbf{k}$ .*]

[*Hint 2: Start by sketching the first, second and third zones for the square lattice in 2-dimensions to see what is going on.*]

5. Let  $\psi_{\mathbf{k}}(\mathbf{x})$  be Bloch states in a Bravais lattice  $\Lambda$ . The *Wannier wavefunction* is defined to be

$$w_{\mathbf{r}}(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_{\mathbf{k}}(\mathbf{x}) \quad (1)$$

where the sum is over all  $\mathbf{k}$  in the first Brillouin zone,  $\mathbf{r} \in \Lambda$  and  $N$  is the number of lattice sites. Show that  $w_{\mathbf{r}}(\mathbf{x}) = w_0(\mathbf{x} - \mathbf{r})$ . Conclude that, if the phases of Bloch states are chosen such that  $w_0(\mathbf{x})$  is localised around the origin, then  $w_{\mathbf{r}}(\mathbf{x})$  is localised around the lattice site  $\mathbf{r}$ . Show that

$$\int d^3x w_{\mathbf{r}'}^*(\mathbf{x}) w_{\mathbf{r}}(\mathbf{x}) = \delta_{\mathbf{r},\mathbf{r}'}$$

Conversely, let  $\phi(\mathbf{x})$  be a state localised around an atom at the origin, not necessarily orthogonal to wavefunctions on other sites. Show that

$$\Psi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{r} \in \Lambda} e^{i\mathbf{k}\cdot\mathbf{r}} \phi(\mathbf{x} - \mathbf{r})$$

is a Bloch state.

6. An electron hops on a two-dimensional square lattice, with lattice spacing  $a$ . Use the tight-binding model, with nearest-neighbour hopping parameter  $t$ , to show that the dispersion relation is

$$E(\mathbf{k}) = -2t \left( \cos(k_x a) + \cos(k_y a) \right) + \text{constant}$$

Draw the energy contours in the Brillouin zone. Draw the Fermi surface if the atoms have valency  $Z = 1$ . Show that many electrons can change their momentum by the same wavevector  $\mathbf{q}$  at little cost of energy, a situation that is referred to as a *nested Fermi surface*.

7. An electron of mass  $m$ , moving in a two-dimensional square lattice with lattice spacing  $a$ , experiences the potential

$$V = 2A \left( \cos(\gamma x) + \cos(\gamma y) \right) \quad \text{with} \quad \gamma = \frac{2\pi}{a}$$

Throughout this question, we work in the nearly-free electron model.

a. Show that at the edge of the Brillouin zone, with  $\mathbf{k} = (\gamma/2, 0)$ , there are two eigenstates with energy

$$E_{\pm} = \frac{\hbar^2 \gamma^2}{8m} \pm A$$

b. Show that at the corner of the Brillouin zone, with  $\mathbf{k} = (\gamma/2, \gamma/2)$ , there are four eigenstates, with energy

$$E_{++} = \frac{\hbar^2 \gamma^2}{4m} + 2A \quad , \quad E_{--} = \frac{\hbar^2 \gamma^2}{4m} - 2A \quad , \quad E_{+-} = E_{-+} = \frac{\hbar^2 \gamma^2}{4m}$$

c. Sketch the energy contours in the first Brillouin zone. If the atoms have valency  $Z = 2$ , show that the material is an insulator when  $A > \hbar^2 \gamma^2 / 24m$ .

8. For an atom at the origin, the elastic scattering amplitude for incident waves with wavevector  $\mathbf{k}$  and outgoing waves with wavevector  $\mathbf{k}' = k\hat{\mathbf{r}}$  is  $f(\hat{\mathbf{r}})$ . Show that the scattering amplitude for an atom at  $\mathbf{d}$  is

$$e^{i\mathbf{q}\cdot\mathbf{d}} f(\hat{\mathbf{r}}) \quad \text{with} \quad \mathbf{q} = \mathbf{k} - \mathbf{k}'$$

A crystal has  $n$  atoms in each unit cell, located relative to the origin of the unit cell at  $\mathbf{d}_j$ , for which the scattering amplitudes are  $f_j$ ,  $j = 1, \dots, n$ . Show that the scattering amplitude due to the whole crystal is

$$\Delta(\mathbf{q}) \sum_{j=1}^n e^{i\mathbf{q}\cdot\mathbf{d}_j} f_j(\hat{\mathbf{r}})$$

with  $|\Delta(\mathbf{q})|$  sharply peaked where  $\mathbf{q}$  is equal to a reciprocal lattice vector.

9. A diamond is a lattice of identical carbon atoms located at  $\mathbf{r} = \sum_i n_i \mathbf{a}_i$  and  $\mathbf{r} = \sum_i n_i \mathbf{a}_i + \mathbf{d}$ ,  $n_i \in \mathbf{Z}$  where

$$\mathbf{a}_1 = \frac{a}{2} (0, 1, 1), \quad \mathbf{a}_2 = \frac{a}{2} (1, 0, 1), \quad \mathbf{a}_3 = \frac{a}{2} (1, 1, 0), \quad \mathbf{d} = \frac{a}{4} (1, 1, 1).$$

Show that the nearest neighbours of each atom form a regular tetrahedron and that there are two atoms in each unit cell.

The reciprocal lattice vectors  $\{\mathbf{b}\}$  are defined by  $\mathbf{b} \cdot \mathbf{r} \in 2\pi\mathbf{Z}$  for any  $\mathbf{r} = \sum_i n_i \mathbf{a}_i$  with  $n_i \in \mathbf{Z}$ . Show that the scattering amplitude for scattering of waves on a diamond is proportional to

$$(1 + e^{i\mathbf{q}\cdot\mathbf{d}}) \Delta(\mathbf{q})$$

where  $\Delta(\mathbf{q})$  is strongly peaked on the reciprocal lattice. Determine the four lowest values of  $|\mathbf{q}|$  for which there is non-zero scattering.

10. In the semi-classical approximation, the motion of an electron of charge  $-e$  in an external electric field  $\mathcal{E}$  is determined by the *Drude model*

$$m^* \frac{d\mathbf{v}}{dt} = -e\mathcal{E} - \frac{1}{\tau} m^* \mathbf{v}$$

where  $\tau$  is the scattering time. Describe the physical significance of the last term. Explain why, in general, the effective mass tensor  $m^*$  should be viewed as a  $3 \times 3$  matrix.

The electrons are subjected to an oscillating electric field of the form  $\mathcal{E} = \mathcal{E}(\omega)e^{-i\omega t}$ . The electric current is defined as  $\mathbf{J} = -nev$  where  $n$  is the density of electrons. Show that the electric current takes the form  $\mathbf{J} = \mathbf{J}(\omega)e^{-i\omega t}$  where  $\mathbf{J}(\omega)$  is given by *Ohm's law*,  $\mathbf{J}(\omega) = \sigma(\omega)\mathcal{E}(\omega)$  with the conductivity matrix

$$\sigma(\omega) = \frac{ne^2\tau}{1 - i\omega\tau} (m^*)^{-1}$$