Applications of Quantum Mechanics: Example Sheet 3

Alejandra Castro, March 2024

1. Two choices of primitive vectors for a 3-dimensional Bravais lattice \( \Lambda \) are related by
\[
a'_i = \sum_{n=1}^{3} M_{ij} a_j.
\]
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
\[
H = -\frac{\hbar^2}{2m} \nabla^2 + V(x)
\]
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
\[
\psi(x) = u(x)e^{ik\cdot x} \quad \text{and} \quad \tilde{\psi}(x) = \tilde{u}(x)e^{i\tilde{k}\cdot x},
\]
with \( k \) and \( \tilde{k} \) 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 \( \mathbb{R}^3 \) is in the \( n \)th Brillouin zone \( (n > 1) \) if the origin is the \( n \)th closest point of the reciprocal lattice \( \Lambda^* \). Show that the various parts of the \( n \)th zone can be mapped into the first zone, without overlap except on bounding surfaces, to completely cover the first zone. Deduce that the \( n \)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 \( k \) being in the subregion labelled by \( q \in \Lambda^* \) if \( q \) is the the \( n \)th closest point lattice point to \( k \).]

[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 $\psi_k(x)$ be Bloch states in a Bravais lattice $\Lambda$. The Wannier wavefunction is defined to be

$$w_r(x) = \frac{1}{\sqrt{N}} \sum_k e^{-i k \cdot r} \psi_k(x) \quad (1)$$

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

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

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

$$\Psi_k(x) = \frac{1}{\sqrt{N}} \sum_{r \in \Lambda} e^{ik \cdot r} \phi(x - r)$$

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

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

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 $q$ 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 $k = (\gamma/2, 0)$, 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
\[
E_{++} = \frac{\hbar^2 \gamma^2}{4m} + 2A, \quad E_{--} = \frac{\hbar^2 \gamma^2}{4m} - 2A, \quad E_{+-} = E_{-+} = \frac{\hbar^2 \gamma^2}{4m}.
\]

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 \( A > \frac{\hbar^2 \gamma^2}{24m} \).

8. For an atom at the origin, the elastic scattering amplitude for incident waves with wavevector \( \mathbf{k} \) and outgoing waves with wavevector \( \mathbf{k}' = k \hat{r} \) is \( f(\hat{r}) \). Show that the scattering amplitude for an atom at \( \mathbf{d} \) is
\[
e^{i\mathbf{q} \cdot \mathbf{d}} f(\hat{r}) \quad \text{with} \quad \mathbf{q} = \mathbf{k} - \mathbf{k}'
\]
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 \( f_j, \ j = 1, \ldots, n \). Show that the scattering amplitude due to the whole crystal is
\[
\Delta(\mathbf{q}) \sum_{j=1}^n e^{i\mathbf{q} \cdot \mathbf{d}_j} f_j(\hat{r})
\]
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 \( \mathbf{r} = \sum_i n_i \mathbf{a}_i + \mathbf{d}, \ n_i \in \mathbb{Z} \) 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 \( \mathbf{b} \cdot \mathbf{r} \in 2\pi \mathbb{Z} \) for any \( \mathbf{r} = \sum_i n_i \mathbf{a}_i \) with \( n_i \in \mathbb{Z} \). 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

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

where $\tau$ is the scattering time. Describe the physical significance of the last term. Explain why, in general, the effective mass tensor $m^\star$ 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 $\mathbf{J} = -n e \mathbf{v}$ 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

$$\sigma(\omega) = \frac{n e^2 \tau}{1 - i\omega \tau} (m^\star)^{-1}$$