Applications of Quantum Mechanics: Example Sheet 2

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1. Two choices of primitive vectors for a 3-dimensional Bravais lattice Λ 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 Λ is basis independent.

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

3. 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.

4. 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 Λ. 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.

5. In the extended zone scheme, a point in $\mathbf{R}^3$ is in the n^{th} Brillouin zone ($n > 1$) if the origin is the n^{th} closest point of the reciprocal lattice Λ^*. 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* $\mathbf{k}$ *being in the subregion labelled by* $\mathbf{q} \in \Lambda^\star$ *if* $\mathbf{q}$ *is the the* n^{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.*]

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

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

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 $w_{\mathbf{r}}(\mathbf{x}) = w_0(\mathbf{x} - \mathbf{r})$ and conclude that $w_{\mathbf{r}}(\mathbf{x})$ is localised around the lattice site $\mathbf{r}$. Show that

$$\int d^3x\; w^\star_{\mathbf{r}'}(\mathbf{x}) w_{\mathbf{r}}(\mathbf{x}) = \delta(\mathbf{r} - \mathbf{r}')$$

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.

7. 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

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

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.*

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

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

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 $A > \hbar^2\gamma^2/24m$.

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

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

where τ 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 3×3 matrix.

The electrons are subjected to an oscillating electric field of the form $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}(\omega)e^{-i\omega t}$. The electric current is defined as $\mathbf{J} = -ne\mathbf{v}$ 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*, $\mathbf{J}(\omega) = \sigma(\omega)\boldsymbol{\mathcal{E}}(\omega)$ with the conductivity matrix

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

10. The semi-classical equations of motion for an electron of charge $-e$ and energy $E(\mathbf{k})$ moving in a magnetic field $\mathbf{B}$ are

$$\hbar\frac{d\mathbf{k}}{dt} = -e\mathbf{v}\times\mathbf{B} \quad \text{and} \quad \mathbf{v} = \frac{1}{\hbar}\frac{\partial E}{\partial \mathbf{k}}$$

Show that, in momentum space, the electrons orbit the Fermi surface $E(k_F)$ in a plane perpendicular to $\mathbf{B}$. Show that the orbit of the electron in position space, projected onto the plane perpendicular to $\mathbf{B}$, traces out the perimeter of a cross-section of the Fermi surface. [*Hint: Consider the evolution of the position* $\mathbf{r}_\perp = \mathbf{r} - (\hat{\mathbf{B}}\cdot\mathbf{r})\hat{\mathbf{B}}$, *perpendicular to the magnetic field.*]

A free electron has $E(k) = \hbar^2k^2/2m$. Use the results above to show that, for any value of $\mathbf{k}\cdot\mathbf{B}$, the electron orbits the Fermi surface with cyclotron frequency $\omega_B = eB/m$. Show that the time taken to orbit the Fermi surface can be written as

$$T = \frac{2\pi}{\omega_B} = \frac{\hbar^2}{eB}\left.\frac{\partial A(E)}{\partial E}\right|_{\mathbf{k}\cdot\mathbf{B}}$$

where $A(E)$ is the cross-sectional area of the Fermi surface with Fermi energy E.

[An Aside: This formula is important because it holds for Fermi surfaces of any shape.]

11. A one-dimensional crystal comprises a chain of atoms of mass m equally spaced by a distance a when in equilibrium. The forces between the atoms are such that the effective spring constants are alternately λ and $\alpha\lambda$. Show that the dispersion relation for phonons has the form

$$\omega_\pm(k)^2 = \frac{\lambda}{m}\left[(1+\alpha) \pm \sqrt{1 + 2\alpha\cos 2ka + \alpha^2}\right]$$

where the wavenumber k satisfies $-\pi/2a \le k \le \pi/2a$. What is the speed of sound in this crystal?