Applications of Quantum Mechanics: Example Sheet 3

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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 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.

4. 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.*]

5. 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 $w_{\mathbf{r}}(\mathbf{x}) = w_0(\mathbf{x} - \mathbf{r})$. Conclude that, if the phases of the 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

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

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.

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

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

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.*

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

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, $j = 1, \ldots, n$. Show that the scattering amplitude due to the whole crystal is

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

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 $\boldsymbol{\mathcal{E}}$ 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

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