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Applications of Quantum Mechanics: Example Sheet 3

Alejandra Castro, January 2025

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 nth Brillouin zone ($n > 1$) if the origin is the nth closest point of the reciprocal lattice Λ^*. Show that the various parts of the nth zone can be mapped into the first zone, without overlap except on bounding surfaces, to completely cover the first zone. Deduce that the nth 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.*]

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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.

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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

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

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