FYS-MENA4111 oblig 2

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1. The face-centered cubic crystal structure of Silicon

   (a) Figure 1 shows the face-centered cubic crystal structure of Silicon with the three primitive lattice vectors Where

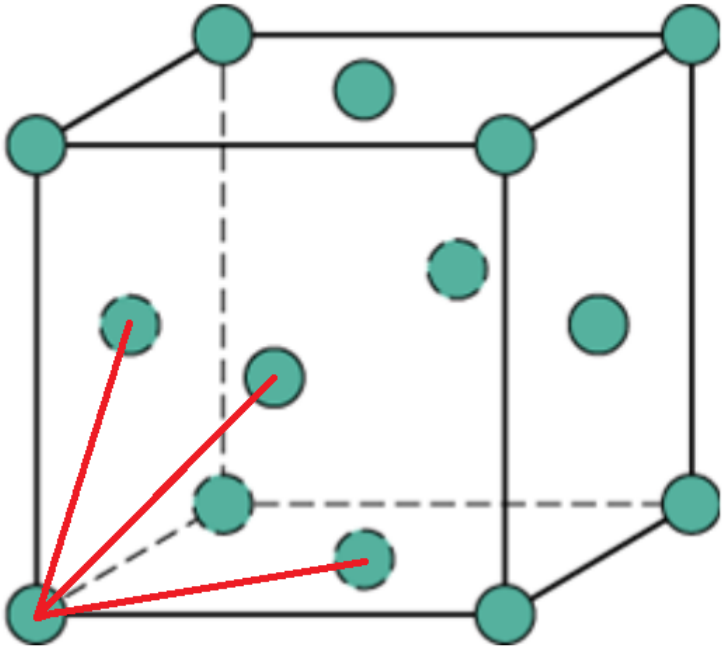

Figure 1: fcc-Si with the three primitive lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$

$$\mathbf{a}_1 = \tfrac{a}{2}(\mathbf{e}_y + \mathbf{e}_z)$$
$$\mathbf{a}_2 = \tfrac{a}{2}(\mathbf{e}_x + \mathbf{e}_z)$$
$$\mathbf{a}_3 = \tfrac{a}{2}(\mathbf{e}_x + \mathbf{e}_y)$$

(b) The length of these vectors is

$$|\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3| = |\mathbf{a}_\alpha| = \tfrac{a}{2}|(\mathbf{e}_y + \mathbf{e}_z)| = \tfrac{\sqrt{2}}{2}a$$

(c) The reciprocal lattice vectors are defined so that $\mathbf{a}_i \cdot \mathbf{a}_j$ is 2π if $i = j$ and 0 otherwise. This choice means that

$$\mathbf{b_1} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$
$$\mathbf{b_2} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

If we substitute with the expressions for the primitive lattice vectors we can find the primitive reciprocal lattice vectors explicitly.

$$\mathbf{b}_1 = \frac{2\pi}{a}(-1, 1, 1)$$
$$\mathbf{b}_2 = \frac{2\pi}{a}(1, -1, 1)$$
$$\mathbf{b}_3 = \frac{2\pi}{a}(1, 1, -1)$$

(d) It is possible to calculate the length of the primitive reciprocal lattice vectors

$$|\mathbf{b}_1| = |\mathbf{b}_2| = |\mathbf{b}_3| = \frac{2\pi\sqrt{3}}{a}$$

2. Relation between real and reciprocal lattice

   (a) It can be shown that $\mathbf{b}_\alpha \mathbf{a}_\beta = 2\pi\delta_{\alpha\beta}$. I.e. the dot product between a primitive and real reciprocal lattice vector is 2π when the indexes are the same and zero otherwise. Let's first assume that $\alpha = \beta$. And let's introduce

$$c = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1) = \mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)$$

   The general expression becomes

$$\mathbf{b}_\alpha \mathbf{a}_\alpha = \frac{2\pi}{c}(\mathbf{a}_\beta \times \mathbf{a}_\gamma)\mathbf{a}_\alpha = 2\pi$$

   In the other case, when $\alpha \neq \beta$ the dot product can be one of two things

$$\frac{2\pi}{c}(\mathbf{a}_\beta \times \mathbf{a}_\gamma)\mathbf{a}_\beta, \qquad \frac{2\pi}{c}(\mathbf{a}_\gamma \times \mathbf{a}_\beta)\mathbf{a}_\beta$$

   Which one is the case does not really matter at this point, as the result is the same. Now, we can use the following relation

$$\begin{aligned} \mathbf{a}_\alpha \times \mathbf{a}_\beta &= -\mathbf{a}_\beta \times \mathbf{a}_\alpha \\ (\mathbf{a}_\beta \times \mathbf{a}_\gamma)\mathbf{a}_\beta &= -(\mathbf{a}_\gamma \times \mathbf{a}_\beta)\mathbf{a}_\beta \end{aligned}$$

   But the only way for a constant to be equal to the negative of itself is if it is zero. So the product must be zero when $\alpha \neq \beta$

   (b) We can use this fact to show that

$$\begin{aligned} \exp(i\mathbf{G}\cdot\mathbf{R}) &= \exp(i(n_1 m_1 \mathbf{b}_1\mathbf{a}_1 + n_2 m_2 \mathbf{b}_2\mathbf{a}_2 + n_3 m_3 \mathbf{b}_3\mathbf{a}_3)) \\ &= \exp(i(n_1 m_1 2\pi + n_2 m_2 2\pi + n_3 m_3 2\pi)) \\ &= \exp(2i\pi l)) = 1 \end{aligned}$$

   where n, m and l are integers

   (c)

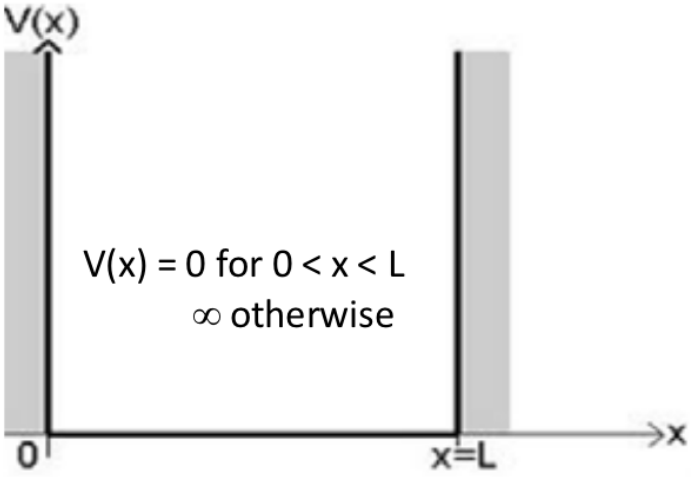

Figure 2: Schematic of an infinite square well potential

3. 1D system of particle in infinite square well

   (a) Finding the solution to the schrödinger equation in such a system is a common exercise

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

   (b) The three first eigenfunctions can be represented in the well

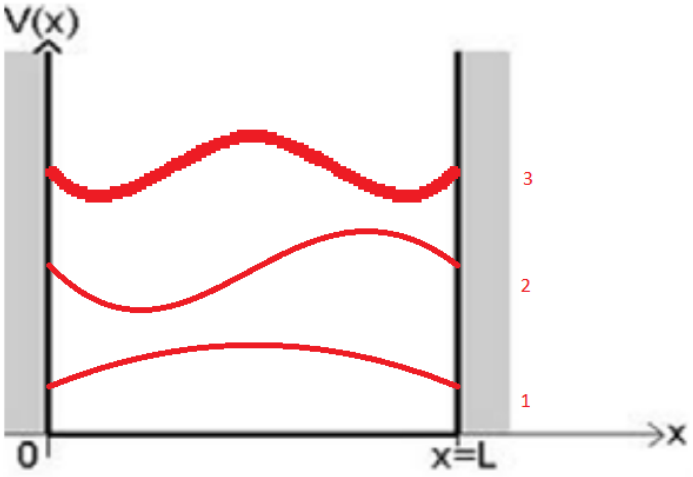

Figure 3: Eigenfunctions ψ_1, ψ_2 and ψ_3

(c) The eigenstates with corresponding energies are given by

$$k_n = \frac{n\pi}{a}, \qquad E_n = \frac{\hbar^2 k_n^2}{2m}$$

Where n are positive integers.

(d) For plane waves the common relation between wavenumber and wavelength is

$$k = \frac{2\pi}{\lambda}$$

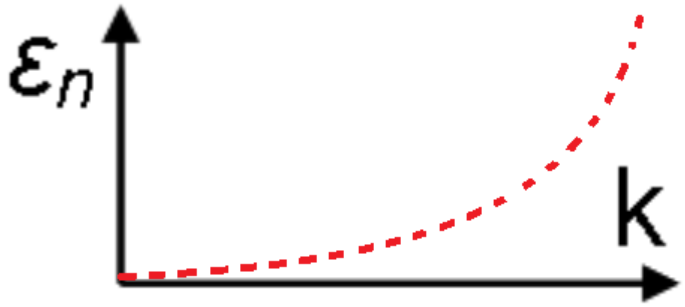

Figure 4: energies as function of the eigenstates k_n