# Oblig 2 / Assignment 2

**Name:** ................................................

**Repetition of solid state physics**

**1)** <u>Read</u> Chapt. 2.2-2.6 (p.6-16) in Lecture Notes "FYSMENA4111_LectNotes_2018", or corresponding text about crystal structure, reciprocal space, and electronic structure in a solid state book, e.g. C. Kittel, "*Introduction to Solid State Physics*".

Be sure that you understand the following concepts after lesson 3, Oct. 3rd.
(You do not have to write it down in this oblig):

- Reciprocal lattice vectors, Brillouin zone,
- **k**-space (reciprocal space) and **k**-points/states?
- Why we can present all eigenstates in only the first Brillouin zone.
- Electronic structure: Band structure and band folding.
- Plane waves, and how an eigenfunction is described in terms of plane waves.
- Why k-space is useful for describing wavefunction, and for solving Schrödinger-eq.
- Why we use <u>two</u> periodicities in the Bloch's theorem.
- $V(\mathbf{r}) = e^{i\mathbf{kr}} \Sigma_{\mathbf{G}} V_{\mathbf{G}} \cdot e^{i\mathbf{Gr}}$ and $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} \cdot u_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} \Sigma_{\mathbf{G}} u_{\mathbf{k+G}} \cdot e^{i\mathbf{Gr}} = \Sigma_{\mathbf{G}} u_{\mathbf{k+G}} \cdot e^{i(\mathbf{k+G})\mathbf{r}}$

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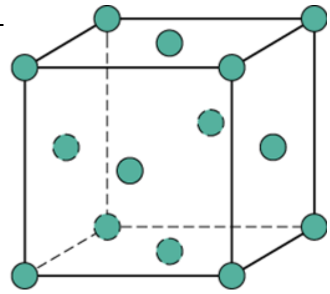


**2)** Consider fcc-Si with lattice constant $a$ = 5.43 Å.
Its primitive lattice vectors are

$\mathbf{a}_1 = 0.5 \cdot a \cdot (e_y + e_z)$
$\mathbf{a}_2 = 0.5 \cdot a \cdot (e_x + e_z)$
$\mathbf{a}_3 = 0.5 \cdot a \cdot (e_x + e_y)$, where $e_\alpha$ are unit vectors $|e_\alpha|=1$ in Cartesian coord.

2a) Draw these primitive lattice vectors in the crystal structure figure.
2b) Calculate the length $|\mathbf{a}_\alpha|$ of the vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$.
2c) Derive the primitive vectors of the reciprocal lattice: $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$.
2d) Calculate the length $|\mathbf{b}_\alpha|$ of the vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$?

*<u>Hint:</u> Be careful, so that you include $e_x$, $e_y$, and $e_z$ in the expressions.*
*<u>Hint:</u> use $e_\alpha \cdot e_\beta = \delta_{\alpha\beta}$ and $e_\alpha \times e_\beta = \pm(1-\delta_{\alpha\beta}) \cdot e_\gamma$ where the $\pm$–sign depends on $\alpha$ and $\beta$.*

**3)** Relation between real and reciprocal space:
3b) Show that $\mathbf{b}_\alpha \mathbf{a}_\beta = 2\pi\delta_{\alpha\beta}$.
Hint: $\mathbf{a}_\alpha \times \mathbf{a}_\beta = -\mathbf{a}_\beta \times \mathbf{a}_\alpha$ and $\mathbf{b}_\alpha \mathbf{a}_\beta = \mathbf{a}_\beta \mathbf{b}_\alpha$ and $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1) = \mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)$.

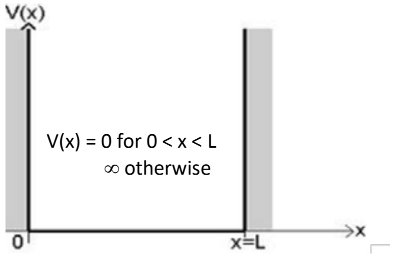
3b) $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ and $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$ (where $n_\alpha$ and $m_\alpha$ are integers).
Show that $exp(i\mathbf{G} \cdot \mathbf{R}) = 1$.
Hint: use results from 3a).

3c) Show that $\psi_{\mathbf{k+G}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r})$, where $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} \cdot u_{\mathbf{k}}(\mathbf{r})$ with $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$.
Hint: because $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})$, then $u_{\mathbf{k}}(\mathbf{r}) = \Sigma_{\mathbf{G}} u_{\mathbf{k+G}} \cdot e^{i\mathbf{Gr}}$.

**4)** Particle in a 1D box with infinite square well (e.g., see Griffiths, or similar).

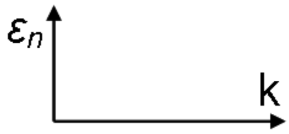
4a) <u>Write down</u> the solution $\psi_n(x)$ to the Schrödinger eq.

$$\left\{-\frac{\hbar^2\nabla^2}{2m_e}+V(x)\right\}\psi_n(x)=\varepsilon_n\psi_n(x)\,.$$




4b) <u>Sketch</u> in the figure the 3 first eigenfunctions. That is, the 3 solutions with lowest energies ($n$ = 1, 2, and 3).
<u>Sketch</u> the density $n_n(x)=|\psi_n(x)|^2$ of these 3 eigenfunctions.

4c) <u>Write down</u> the relation between the energy $\varepsilon_n$ and the wave number k. <u>Sketch</u> this relation in the $\varepsilon_n$-k-figure.
<u>Write down</u> the relation between k and the wave length λ.




4d) Assume that there are $N_e$(1D) electrons in the 1D-box with length L = 1 cm. Assume that $N_e(\text{1D})= {}^3\sqrt{N_e(\text{3D})}$, where $N_e$(3D) is the number of electrons for the 3D crystal of 1×1×1 cm = 1 cm$^3$ for Si, from in assignment/oblig #1.

<u>Calculate</u> k and $\varepsilon_n$ for $n$=1, 2, 3, and $N_e$(1D), in units of 1/m and eV, respectively.
*Hint:* $m_e$ = 9.11×10$^{-31}$ kg; $\hbar$ = 1.05×10$^{-34}$ J·s; 1 (J·s)$^2$/(m$^2$·kg) = 1 J = 6.24×10$^{18}$ eV.

4e) <u>Argue</u> that $\psi_n(x)$ from the particle-in-a-box problem <u>can</u> actually describe also electrons in a true crystal. That is, what physical properties of a material do particle-in-a-box capture.
<u>Argue</u> that $\psi_n(x)$ from the particle-in-a-box problem <u>cannot</u> represent electrons in a crystal That is, what is missing?
<u>Discuss:</u> for which type of materials and/or for which type of eigenstates can we expect that $\psi_n(x)$ from the particle-in-a-box problem is a reasonable approximation to electrons in a true crystal?

**5)** Assume cubic primitive cell with $a$ = 2.50 Å, thus $\mathbf{a}_1 = a\cdot e_x$, $\mathbf{a}_2 = a\cdot e_y$, and $\mathbf{a}_3 = a\cdot e_z$.
Assume wavefunction periodicity of $L_1 = L_2 = L_3$ = 1 cm: $\psi(\mathbf{r}+\mathbf{L}) = \psi(\mathbf{r})$.

5a) How many primitive cells are there in the volume $\Omega = L_1L_2L_3$ ?
5b) Write down the allowed **k**-vectors (ie, the **k**-states) that generate the proper periodic boundary condition for the wavefunctions.