The Chinese University of Hong Kong

PHYS4061 Computational Physics, 1st semester, 2019-2020

Homework 1

Definition of reciprocal lattices:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},$$

1. Prove that reciprocal lattice primitive vectors defined above satisfy

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{8\pi^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

   Hint: Write $\vec{b}_1$ (but not $\vec{b}_2$ or $\vec{b}_3$) in terms of $\vec{a}_i$, and use the orthogonality relations of $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$.

2. Show that the reciprocal vectors of $\vec{b}_i$ are the original direct lattice primitive vector $\vec{a}_i$, i.e., show that

   $a_1 = 2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}$, etc.

   Hint: Write $\vec{b}_3$ in the numerator (but not $\vec{b}_2$) in terms of $\vec{a}_i$, and use the vector identity $A \times (B \times C) = B(A \cdot C) - C(A \cdot B)$, and appeal to the orthogonality relations and results from problem 1.

3. Show the packing fraction in the following crystal structures: bcc $= \frac{\sqrt{3}}{8}\pi$, fcc $= \frac{\sqrt{2}}{6}\pi$, diamond structure $= \frac{\sqrt{3}}{16}\pi$

4. Write a small program to integrate $f(x) = x^4$ from $[-1, +1]$ using

   1) trapezoidal rule with M slices, and

   2) random sampling with M sample points.

   Calculate the squared deviation from the analytic value as a function of M, compare the difference of these two algorithms.

(If you used $f(x) = x^2$ and submitted the HW, you don't need to correct it. No mark will be deducted)

Due date: 24 Sept 2019

Submit your code and a brief report of this problem. Please write all the step clearly for all written questions or marks will be deducted.