Solid State Physics Homework 2

Jinyuan Wu

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Problem 2
Solution

(a) Since

$$\boldsymbol{a} \cdot \boldsymbol{b}_j = 2\pi\delta_{ij},$$

suppose $\{x_i\}$ are the coordinates based on $\{\boldsymbol{a}_i\}$, i.e.

$$\boldsymbol{r} = \sum_{i=1}^{3} x_i \boldsymbol{a}_i, \tag{1}$$

we have

$$x_i = \frac{1}{2\pi}\boldsymbol{b}_i \cdot \boldsymbol{r}. \tag{2}$$

So

$$\boldsymbol{\nabla} x_i = \frac{1}{2\pi}\boldsymbol{b}_i. \tag{3}$$

The equation of a (hkl) plane is

$$hx_1 + kx_2 + lx_3 = \text{const}, \tag{4}$$

so one of the normal vector of the plane is given by

$$\boldsymbol{\nabla}(hx_1 + kx_2 + lx_3) = \frac{h}{2\pi}\boldsymbol{b}_1 + \frac{k}{2\pi}\boldsymbol{b}_2 + \frac{l}{2\pi}\boldsymbol{b}_3, \tag{5}$$

and of course this is parallel to $\boldsymbol{G}$, so $\boldsymbol{G}$ is perpendicular to the plane.

(b) There has to be a lattice vector connecting two (hkl) planes. The distance between the two planes is therefore

$$d = \frac{|\boldsymbol{G}' \cdot \boldsymbol{G}|}{|\boldsymbol{G}|} = \frac{2\pi|hx'_1 + kx'_2 + lx'_3|}{|\boldsymbol{G}|}, \quad \boldsymbol{G}' = \sum_{i=1}^{3} x'_i \boldsymbol{b}_i. \tag{6}$$

For two adjacent planes, we should take the non-zero minimum value of d. Of course

$$|hx'_1 + kx'_2 + lx'_3| \in \mathbb{N},$$

and a elementary number theory theorem tells us that 1 is a linear combination of any coprime integers, so the non-zero minimum of $|hx'_1 + kx'_2 + lx'_3|$ is 1, and thus

$$d_{\min} = \frac{2\pi}{|\boldsymbol{G}|}. \tag{7}$$

(c) For a simple cubic lattice, $\boldsymbol{a}_i$ vectors are orthogonal to each other, and so are $\boldsymbol{b}_i$ vectors. The condition $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$ means the length of all $\boldsymbol{b}_i$ vectors is $2\pi/a$, so

$$|\boldsymbol{G}| = \sqrt{\left(\frac{2\pi}{a}\right)^2 (h^2 + k^2 + l^2)},$$

and therefore

$$d^2 = \frac{a^2}{h^2 + k^2 + l^2}. \tag{8}$$

Problem 3
Solution

Problem 4

Solution Since the volume of all primitive cells of the same lattice is the same, we can just calculate the volume of the parallelepiped spanned by $\{\boldsymbol{b}_i\}$. The condition $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$ can be rewritten as

$$\begin{pmatrix} \boldsymbol{b}_1^\top \\ \boldsymbol{b}_2^\top \\ \boldsymbol{b}_3^\top \end{pmatrix} \begin{pmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \boldsymbol{a}_3 \end{pmatrix} = 2\pi I_{3\times 3},$$

and by taking the determinant of the equation we get

$$\det \begin{pmatrix} \boldsymbol{b}_1^\top \\ \boldsymbol{b}_2^\top \\ \boldsymbol{b}_3^\top \end{pmatrix} \det \begin{pmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \boldsymbol{a}_3 \end{pmatrix} = (2\pi)^3 = \det \begin{pmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \boldsymbol{b}_3 \end{pmatrix} \det \begin{pmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \boldsymbol{a}_3 \end{pmatrix},$$

so

$$V$$