Chapter 2

Ex. 2.1

(i)

The radiated electric field is

$$\vec{\epsilon}_a \approx r_{\rm e} \frac{e^{ikR_D}}{R_D} \left[\hat{n} \times (\hat{n} \times \vec{E}_{\rm in})\right] \; e^{-i\omega t} e^{-i\vec{q}\cdot\vec{r}}. \tag{1}$$

Replace $e^{-i\vec{q}\cdot\vec{r}}$ by $\langle e^{-i\vec{q}\cdot\vec{r}}\rangle = f(\vec{q})$. The vector $(\hat{n} \times \vec{E}_{\rm in})$ is perpendicular to both $\hat{n}$ and to $\vec{E}_{\rm in}$ and has length $|E_{\rm in} \sin\theta|$. Hence $|\hat{n} \times (\hat{n} \times \vec{E}_{\rm in})|^2 = E_{\rm in}^2 \sin^2\theta$. Thus

$$|\epsilon_a|^2 = E_{\rm in}^2 \frac{r_{\rm e}^2}{R_{\rm D}^2} \sin^2\theta |f(\vec{q})|^2. \tag{2}$$

The total radiated power passing through a sphere of radius $R_{\rm D}$ is

$$P = cR_{\rm D}^2 \int d\Omega \left(\frac{\epsilon_a^2}{8\pi} \times 2\right) \tag{3}$$

$$= \frac{c}{4\pi} r_{\rm e}^2 E_{\rm in}^2 \int d\Omega \, \sin^2\theta |f(\vec{q})|^2. \tag{4}$$

Let us normalize the incident electric field to that associated with a single photon in the normalization volume L^3

$$\frac{E_{\rm in}^2}{4\pi} = \frac{\hbar\omega}{L^3} = \frac{\hbar ck}{L^3} \tag{5}$$

which yields

$$P = \hbar c^2 k \frac{r_{\rm e}^2}{L^3} \int d\Omega \, \sin^2\theta |f(\vec{q})|^2. \tag{6}$$

(ii)

Now compare this to the quantum result using the photon scattering matrix element in Eq. (2.28)

$$M = r_{\rm e} f(\vec{q}) \wedge_k^2 \hat{\epsilon}_{\vec{k}\lambda} \cdot \hat{\epsilon}_{\vec{k}'\lambda}. \tag{7}$$

Fermi's Golden Rule for the transition rate is

$$\Gamma = \frac{2\pi}{\hbar}\sum_{\lambda'}\frac{L^3}{(2\pi)^3}\int d^3k'\, r_{\rm e}^2 \wedge_k^4 [\hat{\epsilon}_{\vec{k}\lambda}\cdot\hat{\epsilon}_{\vec{k}'\lambda}]^2\delta(\hbar\omega-\hbar ck')|f(\vec{q})|^2. \tag{8}$$

Noting that the two polarization vectors $\hat{\epsilon}_{\vec{k}'\lambda'}$ and the vector $\hat{k}'$ are all mutually perpindicular, we find $\sum_{\lambda'}[\hat{\epsilon}_{\vec{k}\lambda}\cdot\hat{\epsilon}_{\vec{k}'\lambda}]^2 = 1-[\hat{\epsilon}_{\vec{k}\lambda}\cdot\hat{k}']^2 = 1-\cos^2\theta = \sin^2\theta$. The radiated power is

$$P = \hbar c^2 k\frac{r_{\rm e}^2}{L^3}\int d\Omega\, \sin^2\theta |f(\vec{q})|^2, \tag{9}$$

in agreement with the result from the semiclassical calculation.

Ex. 2.2

$$S(\vec{q}) = \frac{1}{N}<|W(\vec{q})|^2> = \frac{1}{N}<\sum_{i=1}^{N}e^{i\vec{q}.\vec{r}_i}\sum_{j=1}^{N}e^{-i\vec{q}.\vec{r}_j}> \tag{10}$$

$$= \frac{1}{N}<\sum_{i=j}^{N}e^{i\vec{q}.\vec{r}_i-i\vec{q}.\vec{r}_j}> + \frac{1}{N}<\sum_{i\neq j}^{N}\int d^3\vec{r}d^3\vec{r'}e^{i\vec{q}.\vec{r}_i-i\vec{q}.\vec{r}_j}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r'}-\vec{r}_j)> \tag{11}$$

$$= \frac{1}{N}N + \frac{1}{N}\int d^3\vec{r}d^3\vec{r'}e^{i\vec{q}\cdot(\vec{r}-\vec{r'})}<\sum_{i\neq j}^{N}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r'}-\vec{r}_j)> \tag{12}$$

Remembering

$$<\sum_{i\neq j}^{N}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r'}-\vec{r}_j)> = n^{(2)}(\vec{r'}_i-\vec{r}_j),$$

then obviously

$$S(\vec{q}) = 1+\frac{1}{N}\int d^3\vec{r}d^3\vec{r'}e^{i\vec{q}\cdot(\vec{r}-\vec{r'})}n^{(2)}(\vec{r'}-\vec{r}) = 1+n\int d^3\vec{r}e^{i\vec{q}.\vec{r}}g(\vec{r})$$

where we used $N/V = n$ and $n^{(2)}(\vec{R}) = n^2 g(\vec{R})$.

P.S. " <> " indicates thermal average in liquid or amorphous materials. It is unnecessary only for perfect lattices. Generally " <> " must be in the formula.

Chapter 3

Ex. 3.1

•	SC	FCC	BCC
radius	$a/2$	$\frac{\sqrt{2}}{4}a$	$\frac{\sqrt{3}}{4}a$
volume of one sphere	$\frac{\pi}{6}a^3$	$\frac{\sqrt{2}\pi}{24}a^3$	$\frac{\sqrt{3}\pi}{16}a^3$
number of sites in unit cell	1	4	2
volume fraction	$\frac{\pi}{6}$	$\frac{\sqrt{2}}{6}\pi$	$\frac{\sqrt{3}}{8}\pi$

Ex. 3.2

FCC $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$
BCC $8 \times \frac{1}{8} + 1 = 2$

Ex. 3.3

(i)

Suppose the lattice spacing is a. The three primitive vectors are

$$\vec{a}_1 = a\,(0, \frac{1}{2}, \frac{1}{2})$$
$$\vec{a}_2 = a\,(\frac{1}{2}, 0, \frac{1}{2})$$
$$\vec{a}_3 = a\,(\frac{1}{2}, \frac{1}{2}, 0)$$

Thus, the coordinates of the four points of the tetrahedron spanned by the three vectors are

$$O = (0, 0, 0)$$
$$A = a(0, \frac{1}{2}, \frac{1}{2})$$
$$B = a(\frac{1}{2}, 0, \frac{1}{2})$$
$$C = a(\frac{1}{2}, \frac{1}{2}, 0)$$

By calculating the distance of any two points, we can prove that the edges of the tetrahedron are equal. So it is a regular tetrahedron.

(ii)

Another lattice site (on the opposite sublattice) locates at $P = \frac{a}{4}(1,1,1)$

The distance of P to each corner of the tetrahedron is

$$\overline{PO} = a|(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})|$$

$$\overline{PA} = a|(\frac{1}{4}, \frac{-1}{4}, \frac{-1}{4})|$$

$$\overline{PB} = a|(\frac{-1}{4}, \frac{1}{4}, \frac{-1}{4})|$$

$$\overline{PC} = a|(\frac{-1}{4}, \frac{-1}{4}, \frac{1}{4})|$$

We get $\overline{PO} = \overline{PA} = \overline{PB} = \overline{PC} = \frac{\sqrt{3}a}{4}$. Therefore, P is at the geometrical center of this tetrahedron.

Ex. 3.4

(i) $\vec{R}_{\vec{m}\pm\vec{n}} = (m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3) \pm (n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3) = (m_1 \pm n_1)\,\vec{a}_1 + (m_2 \pm n_2)\,\vec{a}_2 + (m_3 \pm n_3)\,\vec{a}_3$

Indeed have the form of (3.15) and are lattice vectors characterized by $\vec{m} \pm \vec{n}$.

(ii) Start in 1D. Pick the lattice site closest to the origin, whose distance from the origin is a. Claim: all sites satisfying 1D version of (3.16) can be written as $R_m = ma$ with m being an integer.

Proof: Assume $R' = \alpha\, a$ is a lattice site with α being a non-integer. $[\alpha]$ represents the integer part of α, and $\Delta\alpha = \alpha - [\alpha]$ is its fractional part. Thus $0 < \Delta\alpha < 1$.

From (3.16), we know $[\alpha]\, a$ and thus $R' - [\alpha]\, a = \Delta\alpha\, a$ is also a lattice site, but its distance to the origin is less than a, leading to a contradiction.

For 2D, let us look for the closest site to the origin, located at $\vec{a}_1$. This immediately gives us a lattice line, $m\vec{a}_1$, with m being an integer. Any lattice site $\vec{R} \neq m\vec{a}_1$, gives us a parallel lattice line, $\vec{R} + m\vec{a}_1$. Look for $\vec{R} = \vec{a}_2$ such that $\vec{a}_2 + m\vec{a}_1$ is the lattice line closest to the line $m\vec{a}_1$. Then $m\vec{a}_1 + m_2\vec{a}_2$ are all lattice sites. Now assume $\alpha_1\,\vec{a}_1 + \alpha_2\vec{a}_2$ is also a lattice site, with $\Delta\alpha_1 > 0$ and $\Delta\alpha_2 > 0$. Then we know $(m_1 + \Delta\alpha_1)\,\vec{a}_1 + [\alpha_2]\,\vec{a}_2$ forms a lattice line, which is closer to the $m\vec{a}_1$ line than the $\vec{a}_2 + m\vec{a}_1$ line! Contradiction again. It is now obvious how to generalize this to 3D.

Ex. 3.5

For a Bravais lattice, it has a set of primitive vectors, $\vec{a}_i$. The locations of all lattice points could be expressed as

$$\vec{R}_{\vec{c}} = \sum_i c_i \vec{a}_i, \qquad c_i \in Z(\text{integer}).$$

The mid-point of any two lattice sites, say $\vec{R}_{\vec{m}}$ and $\vec{R}_{\vec{n}}$ is

$$\begin{aligned}\vec{R}_{mid} &= \frac{1}{2}\left(\vec{R}_{\vec{m}} + \vec{R}_{\vec{n}}\right) \\ &= \sum_i \frac{1}{2}\left(m_i + n_i\right)\vec{a}_i\end{aligned}$$

where m_i and n_i are integers.

We can always shift the origin of the coordinate of the lattice to this mid-point so that all lattice points have new coordinates as

$$\vec{R}'_{\vec{c}} = \vec{R}_{\vec{c}} - \vec{R}_{mid} = \sum_i \left[c_i - \frac{1}{2}\left(m_i + n_i\right)\vec{a}_i\right] \tag{13}$$

If $\vec{R}_{mid}$ is an inversion center, given a lattice site $\vec{R}'_{\vec{c}}$, $-\vec{R}'_{\vec{c}}$ must be a lattice point as well. Namely, there exists a set of p_i which are integers such that

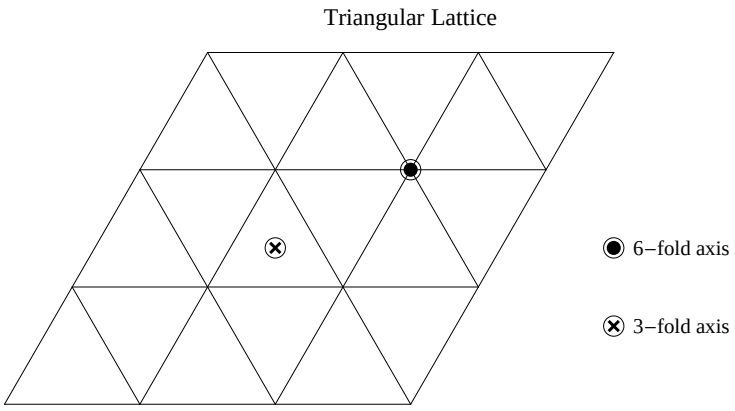
$$-\vec{R}'_{\vec{c}} = \vec{R}'_{\vec{p}} = \sum_i \left[p_i - \frac{1}{2}\left(m_i + n_i\right)\right]\vec{a}_i \tag{14}$$

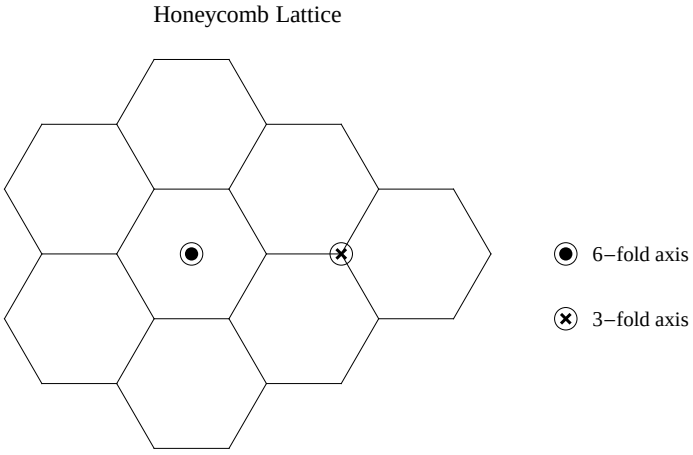
Combining Eq. (13) and Eq. (14), we get

$$p_i = \left(m_i + n_i\right) - c_i \in Z.$$

This tells us that $\vec{R}_{mid}$ is indeed an inversion center.

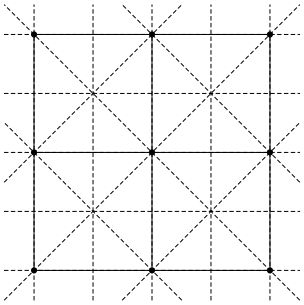
Ex. 3.6





If the atoms on A and B sublattice are different, C_6 symmetry will be broken. The original 6-fold axis will become a 3-fold axis. And the original 3-fold axis is still 3-fold.

Ex. 3.7



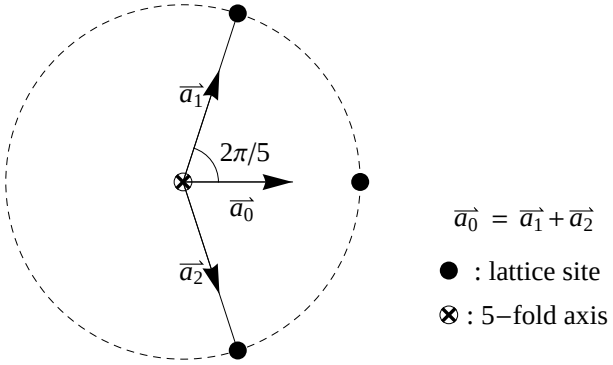
Ex. 3.8

A diamond structure could be viewed as a FCC lattice with a basis containing two atoms called A and B. A and B have a $\frac{a}{4}(1,1,1)$ shift where a is the lattice constant. If we take the mid-point of A and B as an inversion center, the positions of the sublattices will exchange applying to all the lattice sites. As a result, the lattice is unchanged if the atoms on different sublattice sites are the same; otherwise, the lattice is not centrosymmetric. Therefore, diamond structures are centrosymmetric, but Zincblende lattices are not.

Ex. 3.9

Suppose the lattice has n-fold symmetry. Then rotating by $\alpha = \frac{2\pi}{n}$ about the origin (assumed to be a lattice site) should leave the lattice invariant. Assume $\vec{a}_0$ is the shortest lattice vector connecting

the origin to one of its neighbors. After a rotation of $\alpha = \pm\frac{2\pi}{5}$, it becomes $\vec{a}_1$ and $\vec{a}_2$ respectively, which should be lattice vectors themselves (see figure). Then $\vec{a}_1 + \vec{a}_2$ should also be a lattice vector. But simple trigonometry finds it is shorter than $\vec{a}_0$ (see figure), which leads to contradiction. Thus 5-fold symmetry is not allowed in 2D. Since 3D lattices are made of parallel 2D planes, this implies such symmetry is impossible in 3D as well.



Ex. 3.10

The construction of 1D resiprocal lattice $\{\vec{b}_j\}$ with $\vec{b}_j \cdot \vec{a}_m = 2\pi\delta_{mj}$:

$$\vec{b} \cdot \vec{a} = 2\pi \Rightarrow \vec{b} = \frac{2\pi}{a}\hat{x}.$$

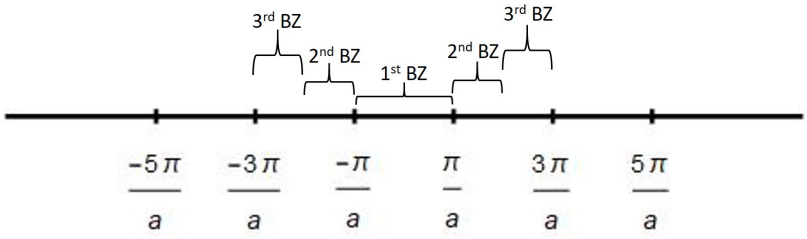
The reciprocal lattice vectors are

$$\vec{G} = m\vec{b} = m\frac{2\pi}{a}\hat{x}. \quad (m\text{=integer})$$

1st BZ: $[-\pi/a, \pi/a)$

2nd BZ: $[-3\pi/a, -\pi/a), [\pi/a, 3\pi/a)$

nth BZ: $[(1-2n)\pi/a, (3-2n)\pi/a), [(2n-3)\pi/a, (2n-1)\pi/a)$



Ex. 3.11

1) FCC

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}) = (0, a/2, a/2)$$
$$\vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z}) = (a/2, 0, a/2)$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}) = (a/2, a/2, 0)$$

$$w = \vec{a}_1.(\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{8} + \frac{a^3}{8} = \frac{a^3}{4}$$

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

This is indicative that $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ forms a BCC lattice with lattice constant $\frac{4\pi}{a}$.
2) BCC

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x}) = (-a/2, a/2, a/2)$$
$$\vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z} - \hat{y}) = (a/2, -a/2, a/2)$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) = (a/2, a/2, -a/2)$$

$$w = \vec{a}_1.(\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{2}$$

$$\vec{b}_1 = \frac{2\pi}{w}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(0, 1, 1)$$
$$\vec{b}_2 = \frac{2\pi}{w}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}(1, 0, 1)$$
$$\vec{b}_3 = \frac{2\pi}{w}(\vec{a}_1 \times \vec{a}_2) = \frac{2\pi}{a}(1, 1, 0)$$

$(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ constructs a FCC lattice with lattice constant $\frac{4\pi}{a}$.

Ex. 3.12

For a direct lattice $\vec{R} = \sum_i n_i \vec{a}_i$ whose reciprocal lattice $\vec{K} = \sum_i k_i \vec{b}_i$, we have

$$e^{i\vec{R}\cdot\vec{K}} = e^{\sum n_i \vec{a}_i \cdot \sum k_j \vec{b}_j} = 1.$$

Let us call the reciprocal lattice of $\vec{K}$ $\vec{R}'$, then we have $e^{i\vec{K}\cdot\vec{R}'} = 1$, thus $\vec{R}' = \vec{R}$.

Ex. 3.13

(a)

Begin with a 1D array of disks of radius r_0. If the centers of the disks are on the 1D lattice $\{\vec{R}_j = jd(1,0,0); j \in Z\}$ where $d = 2r_0$, then the disks are just touching as shown in Fig. 1a.

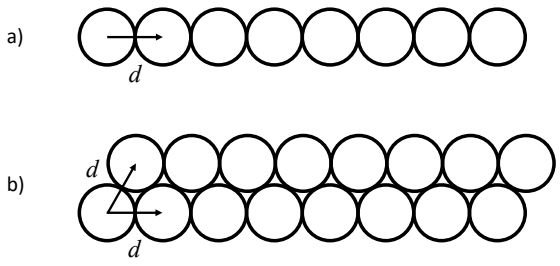


Figure 1

Now consider adding a second line of atoms as shown in Fig. 1b with lattice positions $\{\vec{R}_j = d(j+\delta, y, 0); j \in Z\}$. The lowest possible allowed value of y (and hence the densest lattice) occurs for horizontal displacement $\delta = 1/2$. At $y_{\min} = \frac{\sqrt{3}}{2}$ each disk in the second row touches two disks in the first row. Extending this to an arbitrary number of rows yields the triangular lattice with lattice vectors $\vec{a}_1 = d(1,0,0)$ and $\vec{a}_2 = d(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$.

(b)

Now consider the triangular lattice A defined by points $\vec{R}_{jk} = j\vec{a}_1 + k\vec{a}_2$ as shown in the left panel of Fig. 2.

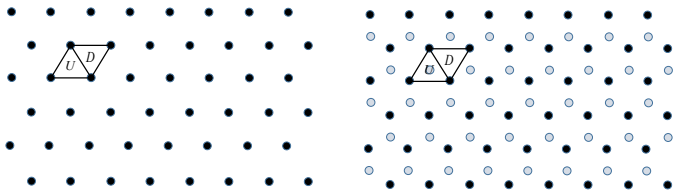


Figure 2