# HW2
# PHYS4240: Solid State Physics

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## Question 1. Lattice Symmetries

a) What we are trying to show by this problem is that if we shift every Bravais lattice vector by the midpoint then taking any generic (shifted) lattice vector and inverting it yields another point on the lattice; this is the definition of an inversion point. So, we have that for a generic $\mathbf{R_a}$, shifting it yields:

$$\mathbf{R}_{\mathbf{a}'} = \sum_i \left[ a_i - \frac{1}{2}(n_i + m_i) \right] \boldsymbol{\alpha}_i, \tag{1}$$

where I've used $\boldsymbol{\alpha}_i$ for the primitive lattice vectors so that I can free $a$ and $b$ as indices.

Now, we need to show that inverting this gives back a point on the shifted lattice. That is, $-\mathbf{R}_{\mathbf{a}'} = \mathbf{R}_{\mathbf{b}'}$ where $\mathbf{R}_{\mathbf{b}'}$ is another shifted lattice vector. This lattice vector must have been retrieved due to an identical shift of some other point on the original Bravais lattice, meaning that $\mathbf{R_b}$ must be a point on the original Bravais lattice.

So, we first have the relation

$$-\mathbf{R}_{\mathbf{a}'} = \mathbf{R_b} \tag{2}$$

$$\sum_i \left[ -a_i + \frac{1}{2}(n_i + m_i) \right] \boldsymbol{\alpha}_i = \sum_i \left[ b_i - \frac{1}{2}(n_i + m_i) \right] \boldsymbol{\alpha}_i. \tag{3}$$

Equating the coefficients, we find

$$-a_i + \frac{1}{2}(n_i + m_i) = b_i - \frac{1}{2}(n_i + m_i), \tag{4}$$

so

$$b_i = n_i + m_i - a_i. \tag{5}$$

For $\mathbf{R_b}$ to be a point on the original, non-shifted lattice, we must have

$$\mathbf{R_b} = \sum_i b_i \boldsymbol{\alpha}_i, \quad \text{where } b_i \in \mathbb{Z}. \tag{6}$$

Since $n_i, m_i, a_i \in \mathbb{Z}$, so too must $b_i$. Thus, the lattice vector $\mathbf{R_b}$ is a valid lattice vector in the original lattice. Hence, the midpoint of two lattice points in a Bravais lattice is also an inversion center.

b) I just used my tablet to draw these, I'm not going to figure out how to LaTeX it... The drawing is in Fig. 1.

There are six mirror lines: one horizontal/vertical pair that aligns with the lattice sites, one on their midpoint, and a diagonal pair.

c) This one is in Fig. 2. The red dot corresponds to the six-fold rotation axis and the green to the three-fold axis.

In the case of the A and B sites not being identical (like I drew in Fig. 3), the six-fold rotation axis becomes the same as the three-fold rotation axis for a triangular lattice.

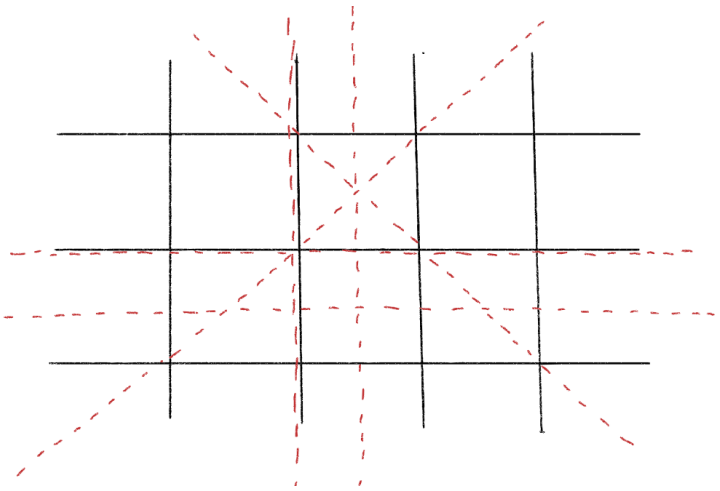

Figure 1

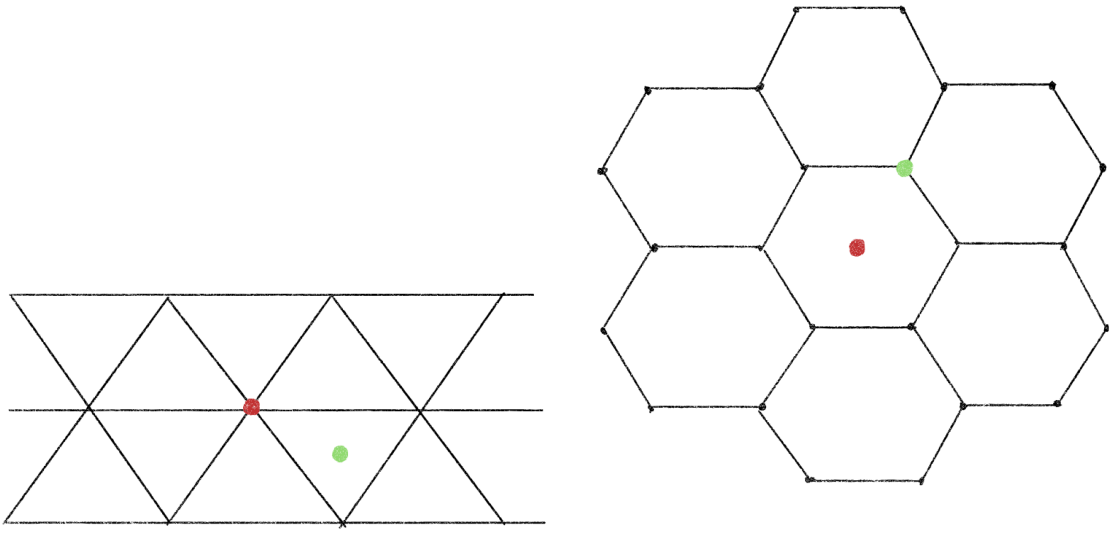

Figure 2

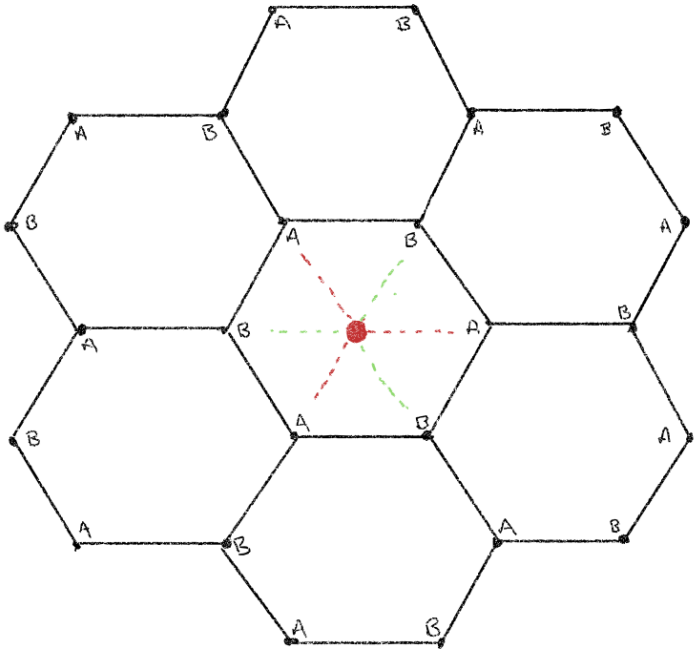


Figure 3

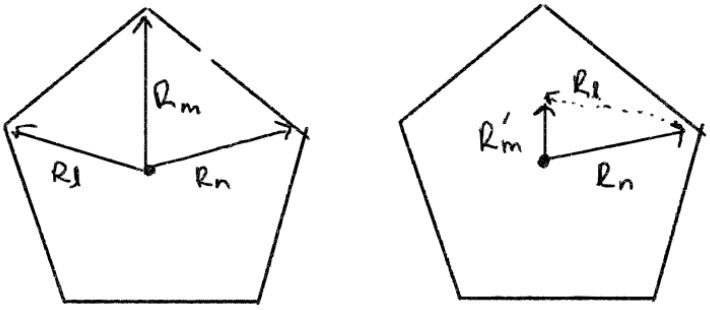


Figure 4

d) Let's say that we are in the center of a pentagonal unit cell, where we have five-fold rotational symmetry. We can consider one such lattice vector $\mathbf{R_n}$ that points from the center to one of the lattice sites. If we rotate once by $2\pi/5$, we get another lattice vector, say $\mathbf{R_m}$ by rotational symmetry that points at another lattice site. If we rotate again, i.e. by a total angle of $4\pi/5$, we have the same deal; call this vector $\mathbf{R_\ell}$.

Now, translational symmetry dictates that the sum of any two lattice vectors is itself a lattice vector. If we sum $\mathbf{R_n}$ and $\mathbf{R_\ell}$, we get a vector that is collinear with $\mathbf{R_m}$, call it $\mathbf{R_{m'}}$. I've done a little drawing in Fig. 4. However, we can easily tell that $\mathbf{R_{m'}}$ is significantly shorter than $\mathbf{R_m}$. We could begin to make the argument that, if it were to be *longer*, it could point at another lattice site outside the unit cell, thus making it a valid lattice vector. However, this one resides entirely within this unit cell. By construction of this problem, the chosen lattice vectors and their rotated counterparts consitute the "shortest paths" to the 5 surrounding lattice sites from our rotation point. Therefore, in our case, $\mathbf{R_{m'}}$ cannot be a lattice vector since it is shorter than any of the shortest paths to the lattice sites.

Hence, translational symmetry is violated, meaning that five-fold rotational symmetry cannot co-exist with translational invariance.

A rotation in 3D about an axis corresponds to the rotation of the (2D) plane perpendicular to the axis about a point in that plane. Since we know that five-fold rotational symmetry doesn't work in this 2D case, then by extension, it must also not work in the 3D case.

## Question 2. Lattice Sums

a) First, we note that we can apply periodic boundary conditions for our lattice, implying that we are able to do the following (in 1D):

$$\psi(x + Na) = \psi(x) = e^{iqNa}\psi(x), \tag{7}$$

where $N$ is the number of primitive cells and $a$ is the lattice constant. But this is saying that

$$e^{iqNa} = 1 \quad \rightarrow \quad qNa = 2\pi m,\ m \in \mathbb{Z}. \tag{8}$$

Rearranging:

$$q = \frac{m}{N}\left(\frac{2\pi}{a}\right). \tag{9}$$

With this in mind, we consider the sum in $(a)$:

$$\sum_q = e^{iqR_n}, \tag{10}$$

with $R_n$ a lattice vector. We know what $q$ has to be:

$$\rightarrow \sum_m e^{i2\pi nm/N}. \tag{11}$$

Via periodic boundary conditions, we know that the sum is finite, so we can consider it a geometric series. In general, we know

$$\sum_{k=0}^{n} ar^k = S_n = \begin{cases} a(n+1) & |r| = 1, \\ a\left(\frac{1-r^{n+1}}{1-r}\right) & \text{otherwise.} \end{cases} \tag{12}$$

In our case we know that $r = \exp i2\pi n/N$, and the quantity $(n+1)$ corresponds to the number of terms in the sum. We have $N$, not $(N+1)$, since the upper limit is not inclusive as it is equivalent to the lower limit (which is inclusive). Considering the case with $|r| \neq 1$:

$$S_n = a\left(\frac{1 - e^{i2\pi n}}{1 - e^{i2\pi n/N}}\right) = 0 \tag{13}$$

because $e^{i2\pi n} = 1$ for $n \in \mathbb{Z}$. So, the only terms we care about for this sum are those for which $|r| = 1$, when $n/N$ is an integer. However, $0 \leq n < N$, so the only possible value of $n$ that satisfies this condition is $n = 0$, meaning $R_n = 0$. So, from Eq. (12) (with $(n+1) \to N$ and $a = 1$:

$$\sum_q e^{iqR_n} = N\delta_{R_n,0}. \tag{14}$$

The generalization to 3D is pretty simple. We can collapse the exponential to look like

$$e^{i\mathbf{q}\cdot\mathbf{R_n}} = \prod_j e^{iq_j(R_n)_j}, \tag{15}$$

which is the product of three sums that are identical to the 1D case. So, defining $\prod N_i \equiv N$:

$$\boxed{\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R_n}} = N\delta_{\mathbf{R_n},\mathbf{0}}.} \tag{16}$$

Looking next at the sum in $(b)$, we have that

$$\sum_n e^{iqR_n} = \sum_n e^{i2\pi nm/N}. \tag{17}$$

This proceeds similarly to the previous case. In the case that $|r| \neq 1$, the sum vanishes, but if $|r| = 1$, then we get $N$ but this time the condition for $e^{iqR_n} = 1$ is on $m$, since it is the term that appears in the exponent of $r$. Hence, in this instance our total condition is that $q$ is a reciprocal lattice vector, as that is the only way to retrieve 1 from the exponential. Therefore:

$$\boxed{\sum_n e^{i\mathbf{q}\cdot\mathbf{R_n}} = N\delta_{\mathbf{q},\mathbf{G}}.} \tag{18}$$

These results make sense: this is the formula for the discrete Fourier transform, and we know the normal Fourier transform of the exponential is the Dirac delta.

Lastly, the sum in $(c)$ is the square of the above result. The square doesn't affect the delta function itself, it still indicates that the result is zero unless $\mathbf{q} = \mathbf{0}$:

$$|\sum_n e^{i\mathbf{q}\cdot\mathbf{R_n}}|^2 = N^2\delta_{\mathbf{q},\mathbf{G}}. \tag{19}$$

b) To start, we cannot do anything here really without a function of some variable; we shall stay in 1 dimension and consider some new function $g$ defined like (all sums are understood to be from $-\infty$ to $+\infty$; just to avoid typing and notational confusion)

$$g(x) = \sum_n f(x + na). \tag{20}$$

This function has the periodicity of the lattice; $g(x+ma) = \sum_n f(x+(n+m)a) = \sum_n f(x+a)$ based upon the fact that the sum is over infinity. Due to this, we know that we are able to express $g$ as a discrete Fourier series:

$$g(x) = \sum_\ell g_\ell e^{iG\ell x} = \sum_n f(x+na), \tag{21}$$

where $G = 2\pi/a$. We know that for such series, we can find $g_\ell$ like so:

$$g_\ell = \frac{1}{a}\int_0^a \mathrm{d}x \ \sum_n f(x+na)e^{-iG\ell x}. \tag{22}$$

In this case, we can move the sum outside the integral:

$$g_\ell = \frac{1}{a}\sum_n \int_0^a \mathrm{d}x \ f(x+na)e^{-ilGx}. \tag{23}$$

This looks almost like the Fourier transform of $f$; to make it look closer like one, we can define $z \equiv x+na$ so that we have $f(z)$ in the integrand. With this, we also have that the integration limits change (but not the differential): $a- > na+a$ and $0 \to na$. With all this:

$$g_\ell = \frac{1}{a}\sum_n \int_{na}^{na+a} f(z)e^{-ilG(z-na)}. \tag{24}$$

Obviously the term proportial to $na$ in the exponential will just be 1, so we are left with

$$g_\ell = \frac{1}{a}\sum_n \int_{na}^{na+a} f(z)e^{-ilGz}. \tag{25}$$

Now, the sum is over all $n$. The integrand goes from $na$ to $na+a$, so what we are essentially doing is summing an infinite number of integrals of size $a$ that fully covers the entire domain with no overlap or missing space. At the end of the day, then, this is just the integral with respect to $z$ over all space:

$$g_\ell = \frac{1}{a}\int_0^\infty f(z)e^{-ilGz}. \tag{26}$$

This is now precisely the Fourier transform of $f$:

$$g_\ell = \frac{1}{a}\tilde{f}(G\ell). \tag{27}$$

If we plug this back into our expression for $g$:

$$\sum_n f(x+na) = \frac{1}{a}\sum_\ell \tilde{f}(G\ell)e^{iG\ell x}. \tag{28}$$

If we now simple take $x \to 0$, the exponential is just 1 and we arrive at

$$\boxed{\sum_n f(na) = \frac{1}{a}\sum_\ell \tilde{f}(G\ell),} \tag{29}$$

which is Poisson's summation formula.

## Question 3. X-Ray Diffraction for a Diamond Lattice

We know that in the event we have an crystal with a multi-atom basis, the atomic form-factor is replaced with

$$f(\mathbf{q}) = \sum_{s=1}^{m} e^{-i\mathbf{q}\cdot\boldsymbol{\tau}_s} f_s(\mathbf{q}). \tag{30}$$

However, we know that diamond has two identical atoms in its unit cell, meaning $f_1 = f_2 = f_c$, so we can pull this factor out

$$f(\mathbf{q}) = f_c(\mathbf{q}) \sum_{s=1}^{2} e^{-i\mathbf{q}\cdot\boldsymbol{\tau}_s}. \tag{31}$$

We can make another clever choice and define $\boldsymbol{\tau}_1 = \mathbf{0}$ for instance, meaning that we have

$$f(\mathbf{q}) = f_c(\mathbf{q})(1 + e^{-i\mathbf{q}\cdot\boldsymbol{\tau}_2}). \tag{32}$$

In this particular case, we know that in diamond (and silicon which shares this same property) certain values of $\mathbf{G}$, destructive interference occurs and $f(\mathbf{G})$ vanishes. This leads to

$$f_c(\mathbf{Q})(1 + e^{-i\mathbf{Q}\cdot\boldsymbol{\tau}_2}) = 0. \tag{33}$$

This is zero only if the quantity in parentheses is zero, or the exponential equals -1. This corresponds to the condition that $\mathbf{Q}\cdot\boldsymbol{\tau}_2 = \pi n$ where $n$ is an odd number. We now consider having the reciprocal lattice vectors given in the problem, and from the lecture notes we know that given our choice of $\boldsymbol{\tau}_1$ we have that

$$\boldsymbol{\tau}_2 = \frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}). \tag{34}$$

Simplifying the reciprocal lattice vector:

$$\mathbf{G} = \frac{2\pi}{a}\left[h(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}) + k(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}) + \ell(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})\right] \tag{35}$$

$$= \frac{2\pi}{a}\left[(-h + k + \ell)\hat{\mathbf{x}} + (h - k + \ell)\hat{\mathbf{y}} + (h + k - \ell)\hat{\mathbf{z}}\right]. \tag{36}$$

Doing the dot product:

$$\mathbf{G}\cdot\boldsymbol{\tau}_2 = \frac{\pi}{2}[-h + k + \ell + h - k + \ell + h + k - \ell] = \pi n, \tag{37}$$

$$\rightarrow \boxed{h + k + \ell = 2n.} \tag{38}$$

Again, $n$ is an odd integer. Hence, for such a choice of our reciprocal lattice vectors, we achieve perfect destructive interference.

## Question 4. Reciprocal Lattices

a) The reciprocal lattice of a 1D lattice with lattice constant $a$ is defined simply by

$$G = m\left(\frac{2\pi}{a}\right). \tag{39}$$

I have drawn a picture of what this looks like in Fig. 5, where the distance between reciprocal lattice points is given by $(2\pi/a)$. We can pretty easily determine a relation for the $n$th Brillouin zone:

$$-\frac{2n\pi}{a} \leq G < -\frac{2(n-1)\pi}{a} \;\cup\; \frac{2(n-1)\pi}{a} \leq G < \frac{2n\pi}{a}. \tag{40}$$

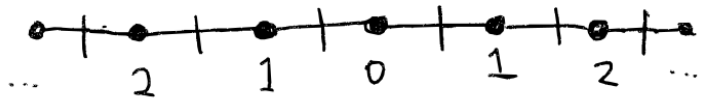


Figure 5

b) We know that the relation between the primitive reciprocal lattice vectors and the primite lattice vectors is given by

$$\mathbf{g}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{|(\mathbf{a}_1 \times \mathbf{a}_2| \cdot \mathbf{a}_3}. \tag{41}$$

If we dot this with a primitive lattice vector $\mathbf{a}_\ell$, we get

$$\mathbf{a}_\ell \cdot \mathbf{g}_i = 2\pi \frac{\mathbf{a}_\ell(\mathbf{a}_j \times \mathbf{a}_k)}{|(\mathbf{a}_1 \times \mathbf{a}_2| \cdot \mathbf{a}_3}. \tag{42}$$

The cross product between two vectors yields a new vector that is perpendicular to both original vectors. A therefore, the dot product in the numerator is only satisfied when $\ell = i$, which leads is simply the volume of the unit cell in real space, $\Omega_p$. Therefore,

$$\mathbf{a}_\ell \cdot \mathbf{g}_i = 2\pi\delta_{\ell,i}. \tag{43}$$

Dotting the full reciprocal and real lattice vectors we therefore find

$$\mathbf{G}_m \cdot \mathbf{R}_n = 2\pi \sum_i m_n n_i \equiv 2\pi\nu. \tag{44}$$

c) The primitive lattice vectors for a FCC lattice are

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}),\ \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}),\ \text{and}\ \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{45}$$

We will need the cross products of these vectors to continue. First,

$$\mathbf{a}_1 \times \mathbf{a}_2 = \frac{a^2}{4}\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}). \tag{46}$$

Since the $\mathbf{a}$ vectors are cyclic, so too will these cross products. Now, the area of the real-space unit cell $\Omega_p$ is given by

$$\Omega_p = (\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = \frac{a^3}{8}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \cdot (\hat{\mathbf{x}} + \hat{\mathbf{y}}) = \frac{a^3}{4}. \tag{47}$$

Therefore,

$$\mathbf{g}_1 = 2\pi \frac{4}{a^3} \cdot \frac{a^2}{4}(\mathbf{a}_2 \times \mathbf{a}_3) = \frac{2\pi}{a}(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}). \tag{48}$$

Again, since the cross products of the $\mathbf{a}$ vectors are cyclic, we can go ahead and find that

$$\mathbf{g}_2 = \frac{2\pi}{a}(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}), \text{ and} \tag{49}$$

$$\mathbf{g}_3 = \frac{2\pi}{a}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}). \tag{50}$$

These are directly proportional to the primitive lattice vectors for the BCC lattice; hence, the reciprocal lattice of the FCC lattice is a BCC lattice in reciprocal space.

We now will show the inverse of the above statement; i.e. that the reciprocal lattice of the BCC lattice is an FCC lattice in reciprocal space. Following the same steps, we need the cross products of the BCC primitive lattice vectors:

$$\mathbf{a}_1 \times \mathbf{a}_2 = \frac{a^2}{4}\begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{51}$$

These are cyclic for the same reason as with the previous part. So,

$$\Omega_p = \frac{a^2}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \cdot (\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) = \frac{a^3}{2}. \tag{52}$$

We can now find

$$\mathbf{g}_1 = 2\pi\frac{2}{a^3}\frac{a^2}{4}(\mathbf{a}_2 \times \mathbf{a}_3) = \frac{2\pi}{a} \cdot \frac{2}{a^2} \cdot \frac{a^2}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) = \frac{2\pi}{a}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \tag{53}$$

so

$$\mathbf{g}_2 = \frac{2\pi}{a}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \text{ and} \tag{54}$$

$$\mathbf{g}_3 = \frac{2\pi}{a}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{55}$$

These are proportional to the primitive lattice vectors for the FCC lattice.

d) We have the identity (in any dimension)

$$\mathbf{G}_\mathbf{m} \cdot \mathbf{R}_\mathbf{n} = 2\pi\nu, \ \nu \in \mathbb{Z}. \tag{56}$$

where $\mathbf{G}_\mathbf{m}$ is a reciprocal lattice vector. If we consider a $\mathbf{V}_{\mathbf{n}'}$ in the reciprocal space of $\mathbf{G}$, we must also have the condition

$$\mathbf{V}_{\mathbf{n}'} \cdot \mathbf{G}_\mathbf{m} = 2\pi\nu', \ \nu' \in \mathbb{Z}. \tag{57}$$

However, since the dot product is commutative, this is saying that $\mathbf{V}_{\mathbf{n}'}$ is proportional to $\mathbf{R}_\mathbf{n}$ up to an integer (which itself is proportional to $n$), meaning that $\mathbf{V}_{\mathbf{n}'}$ is an element of the original lattice. Hence, the reciprocal space of the reciprocal space of a lattice comes back to the real space of the lattice.

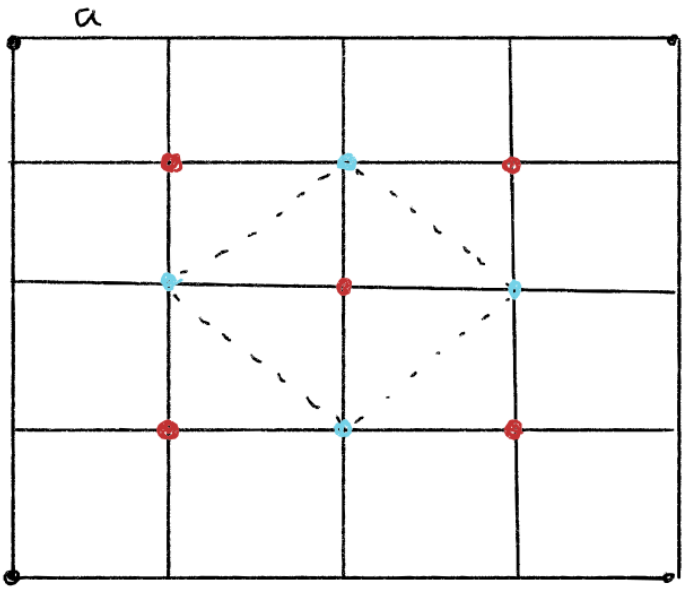


Figure 6

## Question 5. More About Lattices

a) We don't even really need to draw anything for the first case. In the ferromagnetic case, all lattice sites are equivalent, so the unit cell is simply a single unit square of length $a$, meaning

$$A_0 = a^2, \text{ and } A_{\text{BZ}} = \frac{(2\pi)^2}{A_0} = \left(\frac{2\pi}{a}\right)^2. \tag{58}$$

In the anti-ferromagnatic case, the lattice sites are not equivalent – they look like Fig. 6. In this case, then, are unit cell looks a bit different. In particular, it is another square connecting identical lattice sites, but the side length is $a\sqrt{2}$ this time. Therefore,

$$A_0 = 2a^2, \text{ and } A_{\text{BZ}} = \frac{(2\pi)^2}{A_0} = \frac{1}{2}\left(\frac{2\pi}{a}\right). \tag{59}$$

As we would expect, the area of the primitive cells in this case are larger, so the corresponding area in the reciprocal space is smaller.

b) This part is drawn in Fig. 7.

c) The atomic packing factor is defined as

$$\text{APF} = \frac{N_{ac} V_a}{V_c}, \tag{60}$$

where $N_{a/c}$ is the number of atoms in a unit cell, $V_a$ is the volume of the atom, and $V_c$ is the volume of the unit cell. We first note that we can approximate our atoms as spheres of radius $r$, so $V_c = 4\pi r^3/3$ for each lattice. Also, I am using the visuals from the lecture notes to assist with my determination of some lengths.

First, for the SC lattice, in our unit cell, we grab 1/8th of each atom at each corner, of which there are 8, meaning we have 1 atom per unit cell. The length of the unit cell is two halfs of each atom, so it is simply $2r$. Thus:

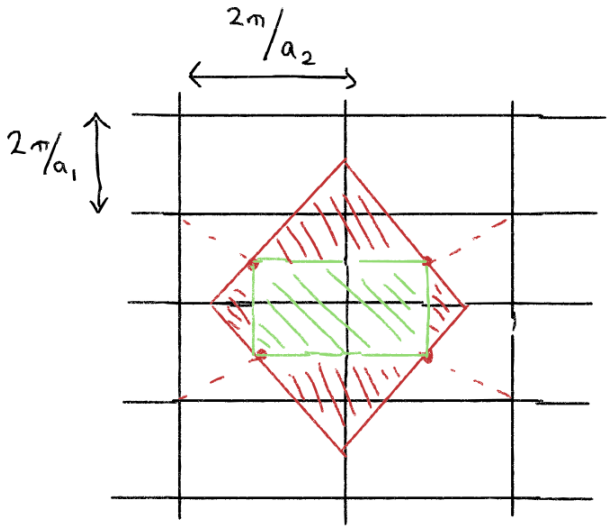


Figure 7

$$\mathrm{APF}_{\mathrm{SC}} = \frac{1 \cdot 4\pi r^3/3}{(2r)^3} = \frac{4}{3 \cdot 8}\pi = \frac{\pi}{6}. \tag{61}$$

For the BCC, we have an additional atom in the center of the unit cell, so there are 2 atoms per unit cell. The length of the diagonal from the center of the unit cell to the center of the call a corner is $2r$, so the total diagonal is $4r$, meaning the length of the side is $4r/\sqrt{3}$. With this:

$$\mathrm{APF}_{\mathrm{BCC}} = \frac{2 \cdot 4\pi r^3/3}{(4r/\sqrt{3})^3} = \frac{8}{3} \cdot \frac{3\sqrt{3}}{64}\pi = \frac{\pi\sqrt{3}}{8}. \tag{62}$$

Lastly, for the FCC, instead of an atom at the center, we have half of an atom on each face, so an additional 3 atoms compared to the SC for a total of 4 atoms in the unit cell. From this, we have that the diagonal of one of the sides is $4r$, meaning a side length is $4r/\sqrt{2} = 2r\sqrt{2}$, so

$$\mathrm{APF}_{\mathrm{FCC}} = \frac{4 \cdot 4\pi r^3/3}{(2r\sqrt{2})^3} = \frac{16}{3}\frac{1}{16\sqrt{2}}\pi = \frac{\pi\sqrt{2}}{6}. \tag{63}$$