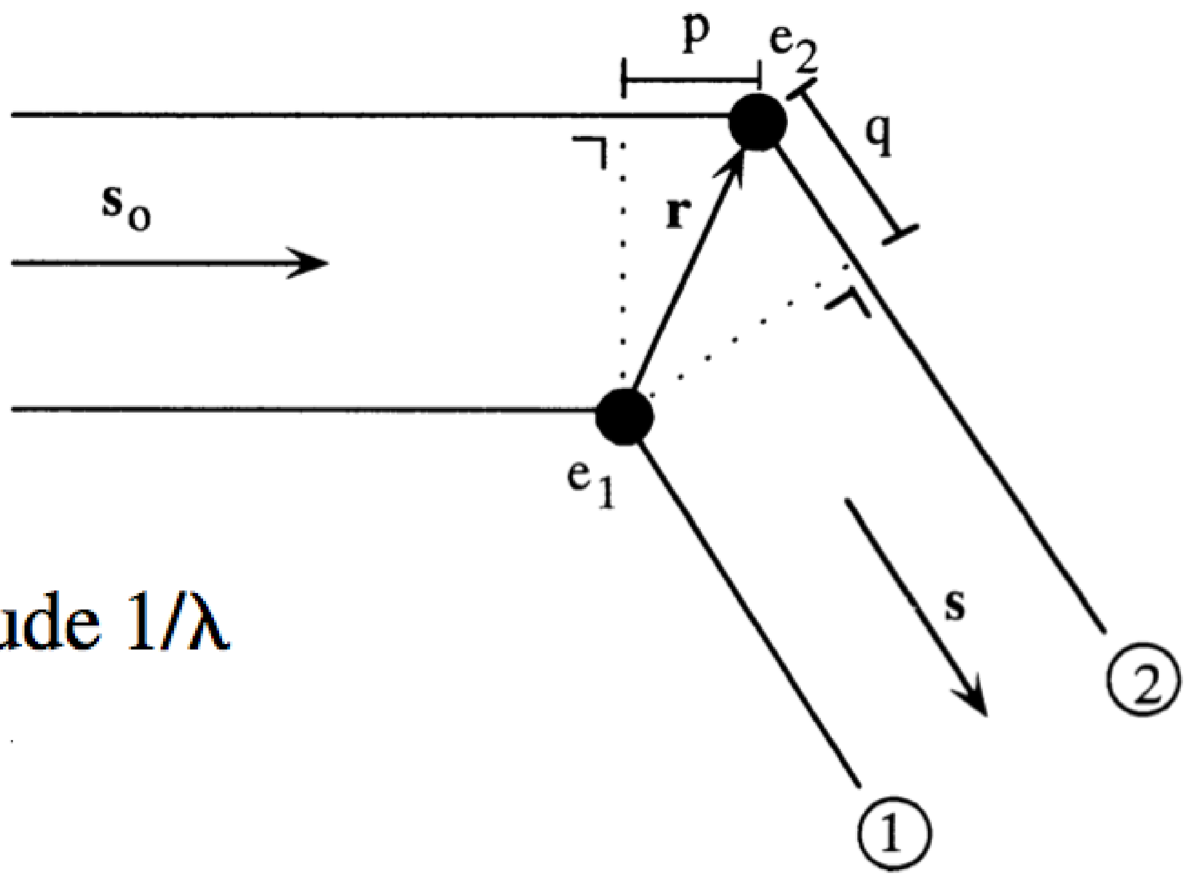
Structural Biology Methods

Fall 2022

Lecture #3

System of two electrons

Figure 4.4. A system of two electrons: e_1 and e_2. The path difference between the scattered waves 1 and 2 is $p + q$.



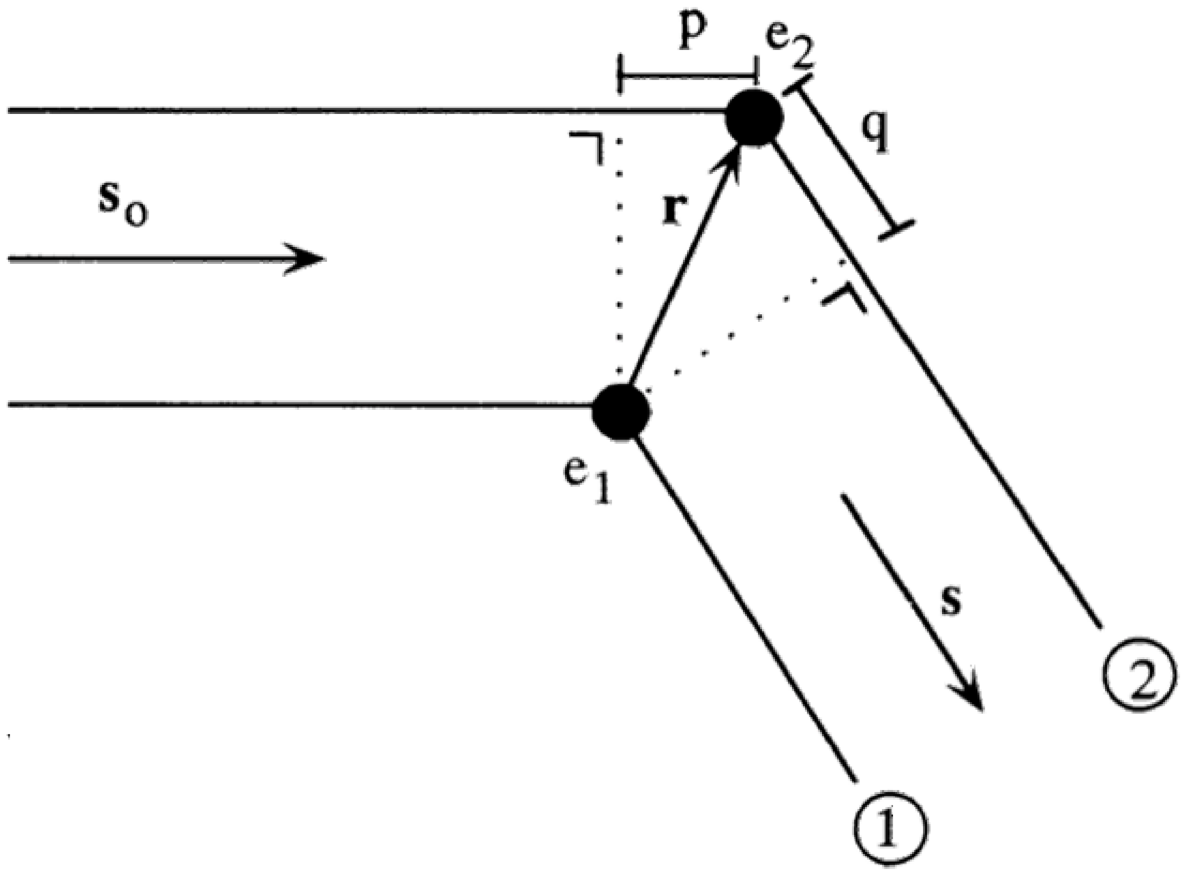
$\mathbf{s}_0$ and $\mathbf{s}$ are wave vectors of magnitude 1/λ

$$p = \lambda \cdot \mathbf{r} \cdot \mathbf{s}_0$$
$$q = -\lambda \cdot \mathbf{r} \cdot \mathbf{s}$$

minus sign is due to the fact that the projection of **r** on **s** has a direction opposite to s

$$p + q = \lambda \cdot \mathbf{r} \cdot (\mathbf{s}_0 - \mathbf{s}).$$

Figure 4.4. A system of two electrons: e_1 and e_2. The path difference between the scattered waves 1 and 2 is $p + q$.



The wave along electron e_2 is lagging behind in phase compared with the wave along e_1. With respect to wave 1, the phase of wave 2 is

$$-\frac{2\pi \mathbf{r} \cdot (\mathbf{s}_0 - \mathbf{s}) \cdot \lambda}{\lambda} = 2\pi \mathbf{r} \cdot \mathbf{S},$$

where

$$\mathbf{S} = \mathbf{s} - \mathbf{s}_0 \tag{4.1}$$

It is interesting to note that the wave can be regarded as being reflected against a plane with θ as the reflecting angle and $|S| = 2(\sin\theta)/\lambda$ (Figure 4.5). The physical meaning of vector **S** is the following: Because $\mathbf{S} = \mathbf{s} - \mathbf{s}_0$, with $|s| = |s_0| = 1/\lambda$, **S** is perpendicular to the imaginary "reflecting plane," which makes equal angles with the incident and reflected beam.

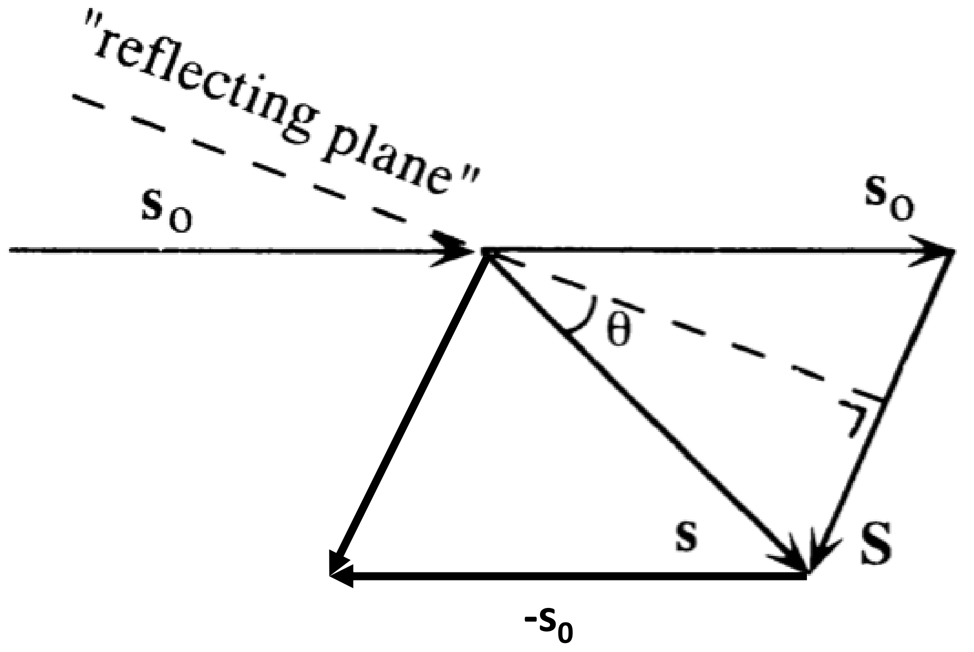
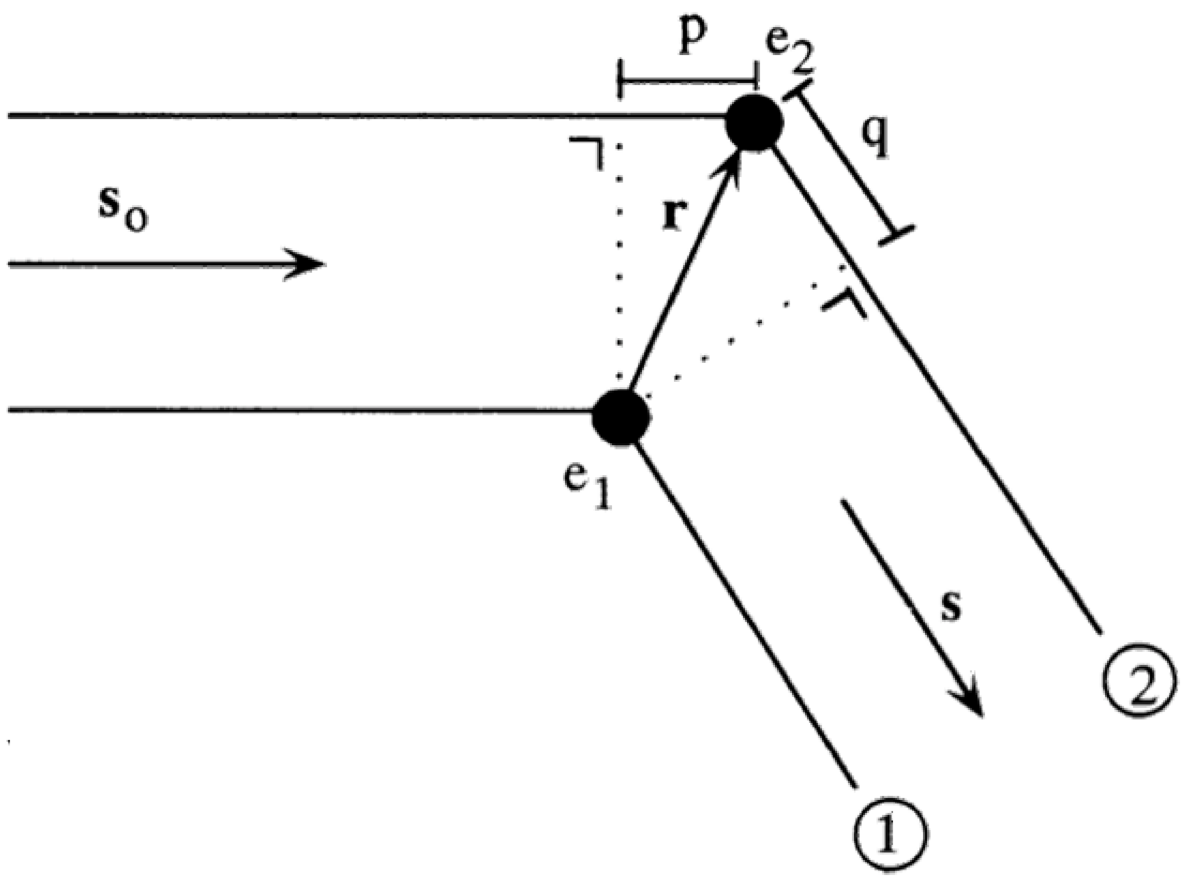


Figure 4.5. The primary wave, represented by $\mathbf{s}_0$, can be regarded as being reflected against a plane. θ is the reflecting angle. Vector **S** is perpendicular to this plane.

Figure 4.4. A system of two electrons: e_1 and e_2. The path difference between the scattered waves 1 and 2 is $p + q$.



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where

$$\mathbf{S} = \mathbf{s} - \mathbf{s}_0 \qquad (4.1)$$

If we add the waves 1 and 2 in Figure 4.4, the Argand diagram shows two vectors, **1** and **2**, with equal length (amplitude) and a phase of $2\pi\mathbf{r} \cdot \mathbf{S}$ for wave **2** with respect to wave **1** (Figure 4.6). Vector **T** represents the sum of the two waves. In mathematical form: $\mathbf{T} = 1 + 2 = 1 + 1\,\exp[2\pi i\mathbf{r} \cdot \mathbf{S}]$ if the length of the vectors equals 1. So far we had the origin of this two-electron system in e_1.

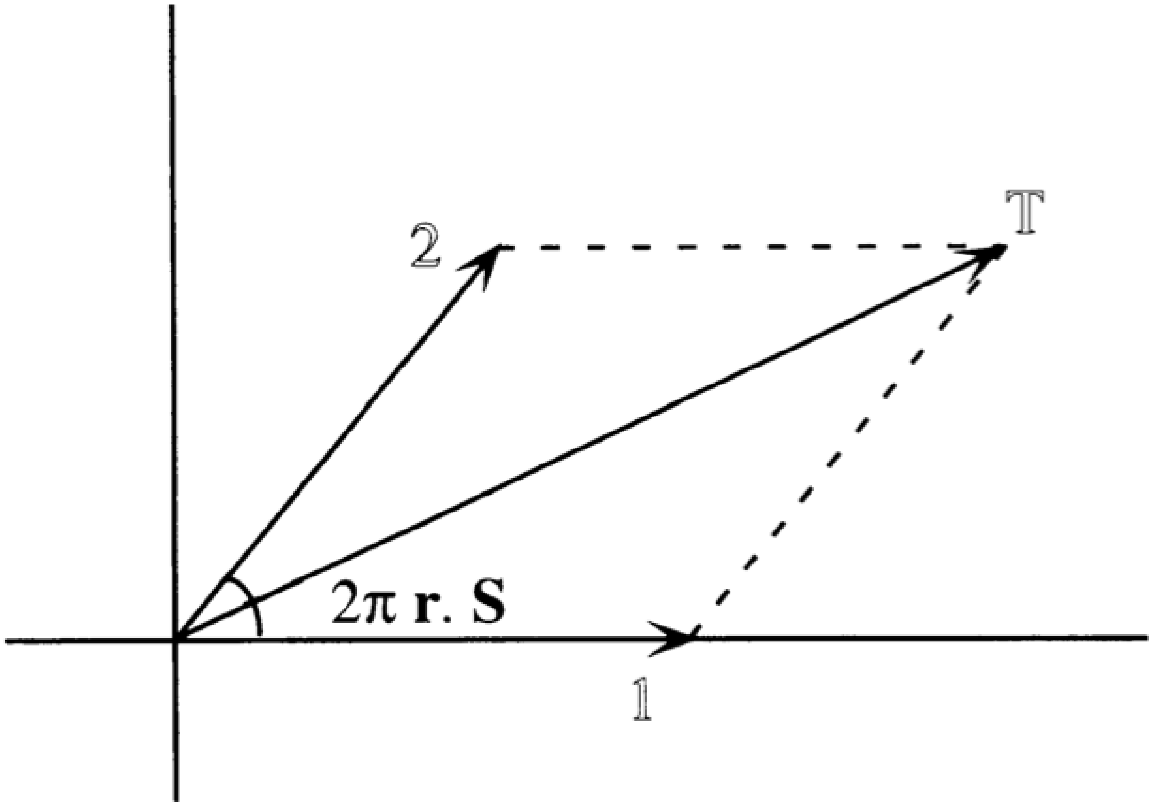

Figure 4.6. The summation of the two scattered waves in Figure 4.4 with the origin in electron e_1.

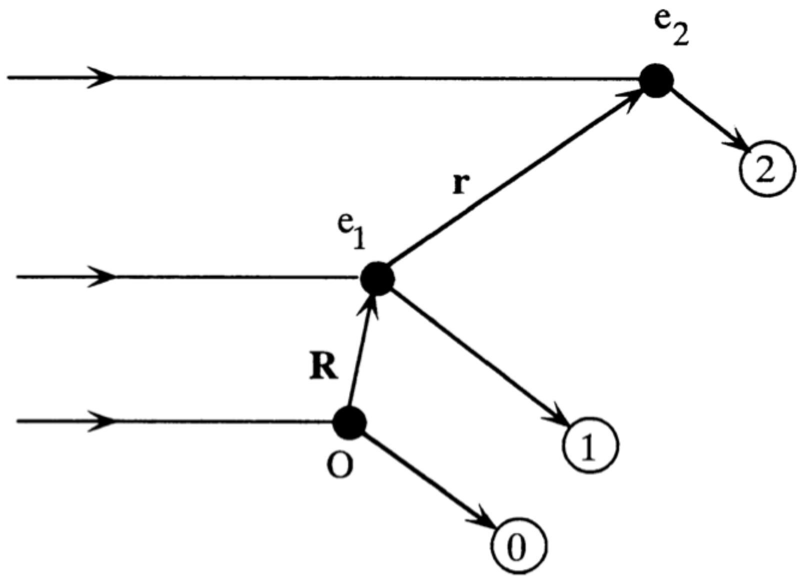

Figure 4.7. The origin, or reference point, for the scattered waves of the two-electron system is now located at O.

Suppose we move the origin over $-\mathbf{R}$ from e_1 to point O (Figure 4.7). Then we obtain the following: With respect to a wave **0**, wave **1** has a phase of $2\pi\mathbf{R}\cdot\mathbf{S}$, and wave **2** has a phase of $2\pi(\mathbf{r}+\mathbf{R})\cdot\mathbf{S}$ (Figure 4.8)

$$\begin{aligned}\mathbf{T} &= 1+2 = \exp[2\pi i\mathrm{R}\cdot\mathbf{S}] + \exp[2\pi i(\mathbf{r}+\mathrm{R})\cdot\mathbf{S}] \\ &= \exp[2\pi i\mathrm{R}\cdot\mathbf{S}]\{1+\exp[2\pi i\mathbf{r}\cdot\mathbf{S}]\}\end{aligned}$$

Conclusion: A shift of the origin by $-\mathbf{R}$ causes an increase of all phase angles by $2\pi\mathbf{R}\cdot\mathbf{S}$. The amplitude and intensity (which is proportional to the square of the amplitude) of wave **T** do not change.

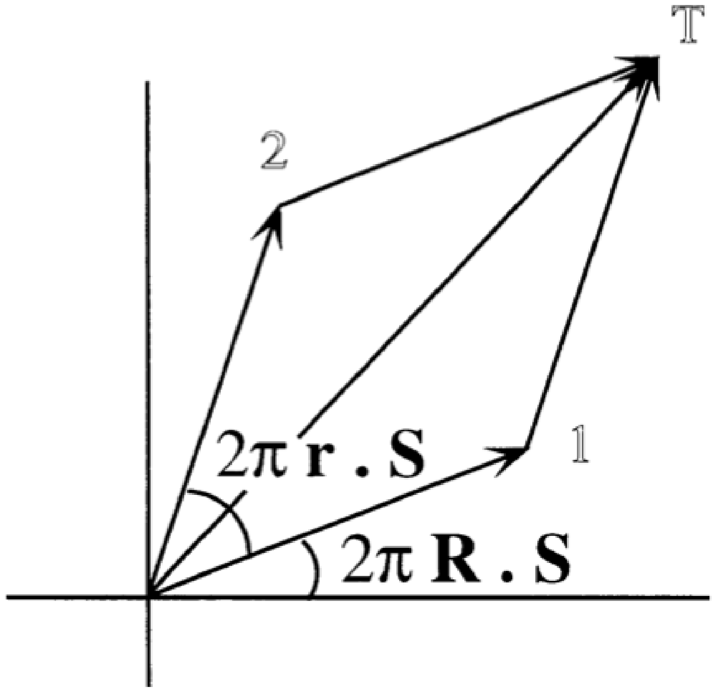

Figure 4.8. The summation of waves **1** and **2** with the origin of the two-electron system in position O.

Suppose we move the origin over $-\mathbf{R}$ from e_1 to point O (Figure 4.7). Then we obtain the following: With respect to a wave **0**, wave **1** has a phase of $2\pi\mathbf{R}\cdot\mathbf{S}$, and wave **2** has a phase of $2\pi(\mathbf{r}+\mathbf{R})\cdot\mathbf{S}$ (Figure 4.8)

$$\mathbf{T} = 1 + 2 = \exp[2\pi i \mathrm{R}\cdot\mathbf{S}] + \exp[2\pi i(\mathbf{r}+\mathrm{R})\cdot\mathbf{S}]$$
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Scattering by an atom

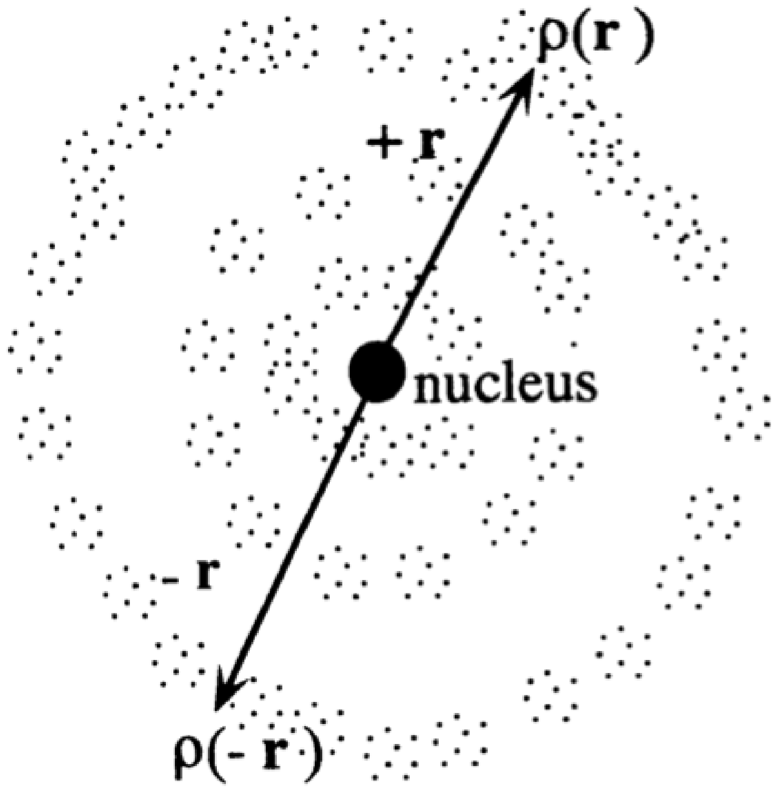


Figure 4.9. The electron cloud of an atom. $\rho(\mathbf{r})$ is the electron density. Because of the centrosymmetry, $\rho(\mathbf{r}) = \rho(-\mathbf{r})$.

$$f = \int_{\mathbf{r}} \rho(\mathbf{r}) \exp[2\pi i \mathbf{r} \cdot \mathbf{S}]\, d\mathbf{r}, \tag{4.2}$$

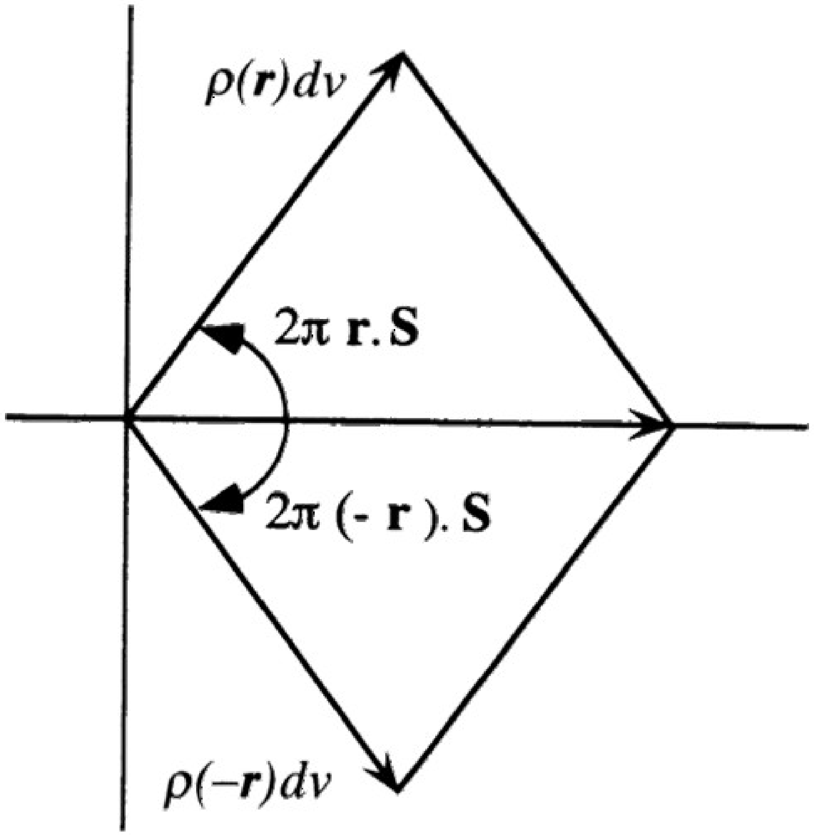
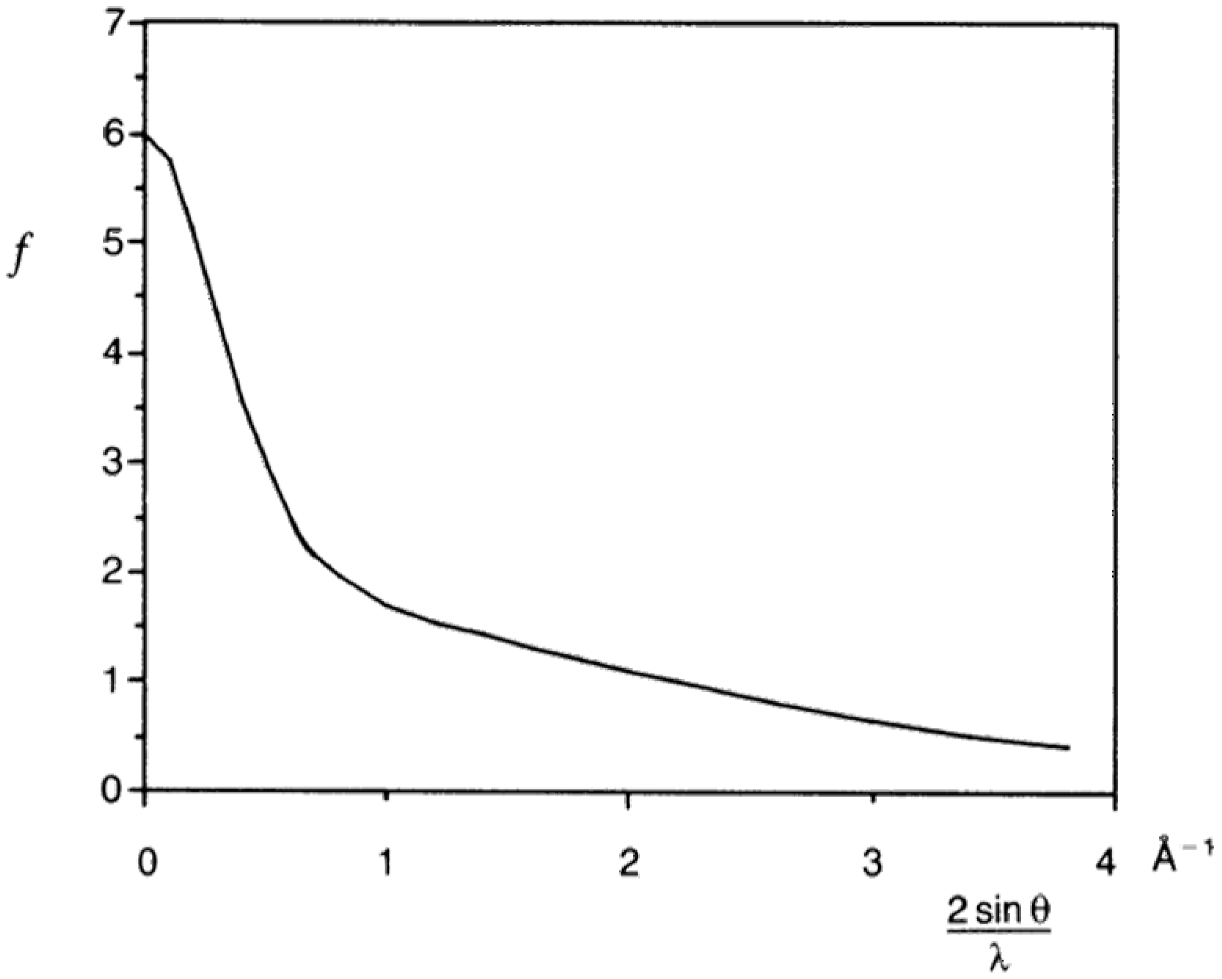


Figure 4.10. The scattering factor f of an atom is always real if we assume centrosymmetry of the electron cloud. The imaginary part of every scattering vector is compensated by the imaginary part of a vector with equal length but a phase angle of opposite sign.

$$f = \int_{\mathbf{r}} \rho(\mathbf{r}) \{\exp[2\pi i \mathbf{r} \cdot \mathbf{S}] + \exp[-2\pi i \mathbf{r} \cdot \mathbf{S}]\} \, d\mathbf{r}$$

$$= 2 \int_{\mathbf{r}} \rho(\mathbf{r}) \cos[2\pi \mathbf{r} \cdot \mathbf{S}] \, d\mathbf{r}.$$

Scattering by an atom depends of the length of |S| (resolution)



$$= \frac{2\sin\theta}{\lambda}.$$

Figure 4.11. The scattering factor f for a carbon atom as a function of $2(\sin\theta)/\lambda$. f is expressed as electron number, and for the beam with $\theta = 0$, $f = 6$.

Scattering by a unit cell

Suppose a unit cell has n atoms at positions $\mathbf{r}_j$ ($j = 1, 2, 3, \ldots, n$) with respect to the origin of the unit cell (Figure 4.12). With their own nuclei as origins, the atoms diffract according to their atomic scattering factor f. If the origin is now transferred to the origin of the unit cell, the phase angles change by $2\pi\mathbf{r}_j \cdot \mathbf{S}$. With respect to the new origin, the scattering is given by

$$\mathbf{f}_j = f_j \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}],$$

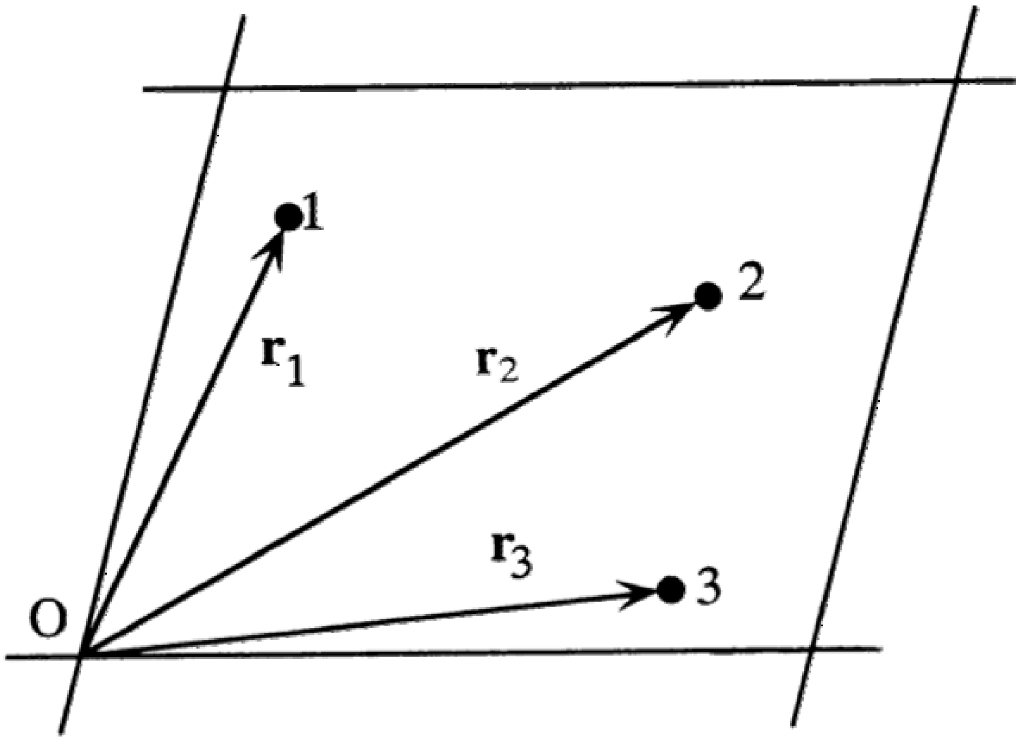


Figure 4.12. A unit cell with three atoms (1, 2, and 3) at positions $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$.

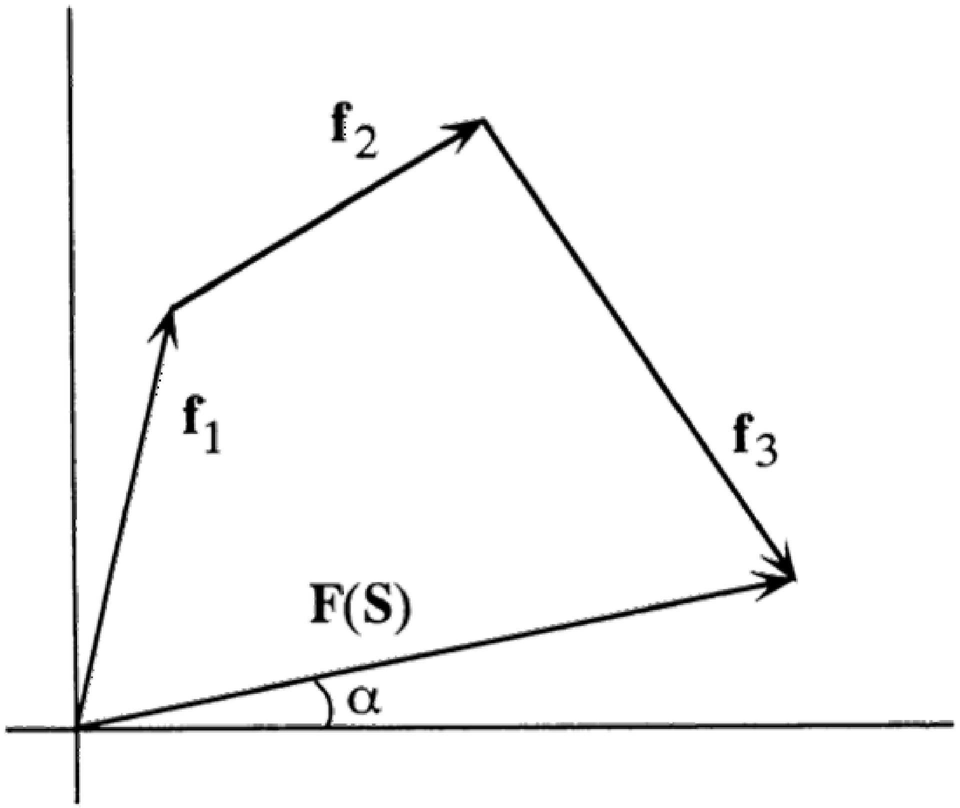


Figure 4.13. The structure factor **F(S)** is the sum of the scattering by the separate atoms in the unit cell.

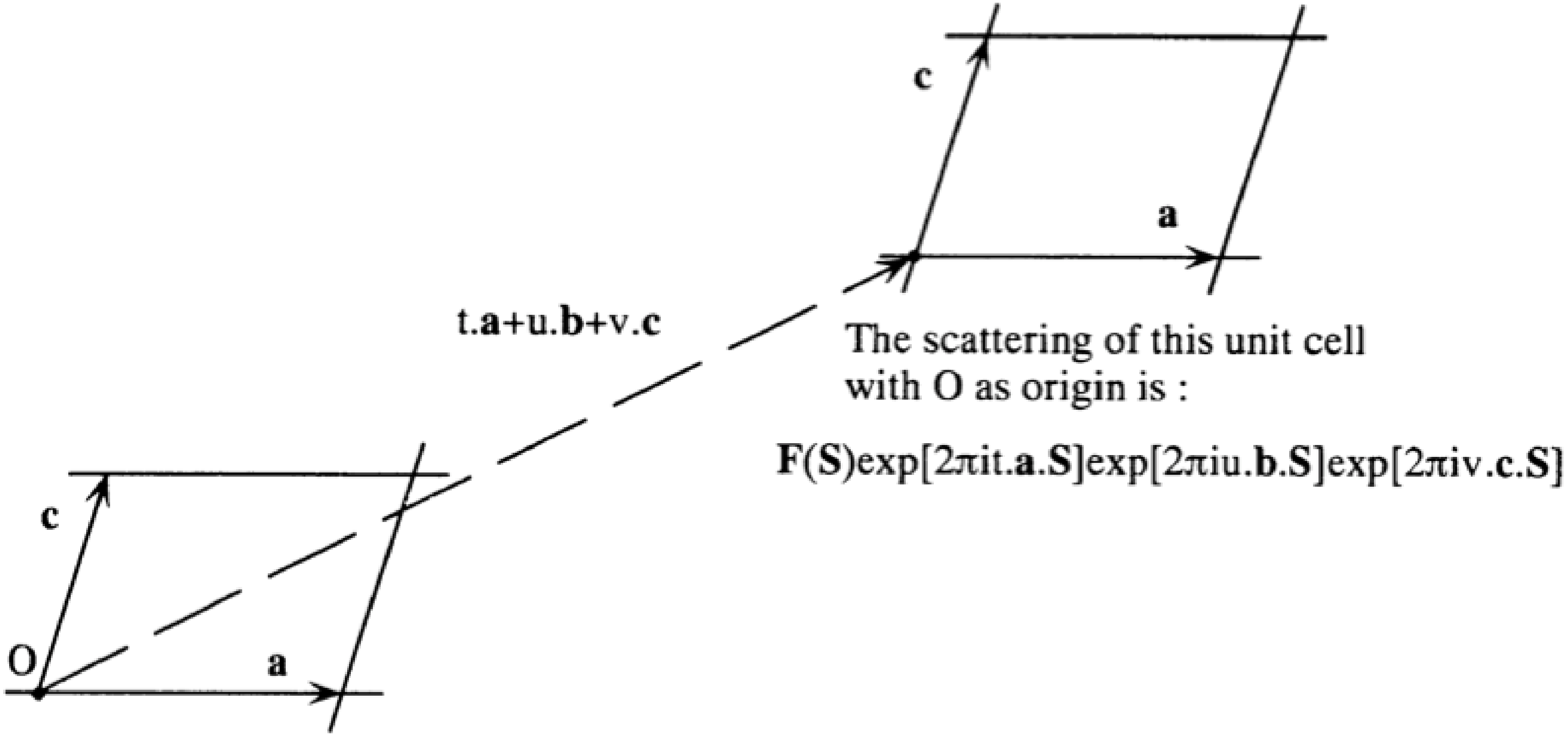
unit cell is

$$\mathbf{F}(\mathbf{S}) = \sum_{j=1}^{n} f_j \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}]. \tag{4.3}$$

F(S) is called the *structure factor* because it depends on the arrangement (structure) of the atoms in the unit cell (Figure 4.13).

Scattering by a crystal

Suppose that the crystal has translation vectors **a**, **b**, and **c** and contains a large number of unit cells: n_1 in the **a** direction, n_2 in the **b** direction, and n_3 in the **c** di



The scattering of this unit cell

with O as origin is **F**(**S**)

Figure 4.14. A crystal contains a large number of identical unit cells. Only two of them are drawn in this figure.

To obtain the scattering by the crystal, we must add the scattering by all unit cells with respect to a single origin. We choose the origin O in Figure 4.14. For a unit cell with its own origin at position $t \cdot \mathbf{a} + u \cdot \mathbf{b} + v \cdot \mathbf{c}$, in which t, u, and v are whole numbers, the scattering is

$$\mathbf{F}(\mathbf{S}) \times \exp[2\pi i t \mathbf{a} \cdot \mathbf{S}] \times \exp[2\pi i u \mathbf{b} \cdot \mathbf{S}] \times \exp[2\pi i v \mathbf{c} \cdot \mathbf{S}].$$

The total wave **K(S)** scattered by the crystal is obtained by a summation over all unit cells:

$$\mathbf{K}(\mathbf{S}) = \mathbf{F}(\mathbf{S}) \times \sum_{t=0}^{n_1} \exp[2\pi i t \mathbf{a} \cdot \mathbf{S}] \times \sum_{u=0}^{n_2} \exp[2\pi i u \mathbf{b} \cdot \mathbf{S}] \times \sum_{v=0}^{n_3} \exp[2\pi i v \mathbf{c} \cdot \mathbf{S}].$$

The total wave **K(S)** scattered by the crystal is obtained by a summation over all unit cells:

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Because n_1, n_2, and n_3 are very large, the summation $\sum_{t=0}^{n_1} \exp[2\pi i t\mathbf{a} \cdot \mathbf{S}]$ and the other two over u and v are almost always equal to zero unless $\mathbf{a} \cdot \mathbf{S}$ is an integer h, $\mathbf{b} \cdot \mathbf{S}$ is an integer k, and $\mathbf{c} \cdot \mathbf{S}$ is an integer l. This is easy to understand if we regard $\exp[2\pi i t\mathbf{a} \cdot \mathbf{S}]$ as a vector in the Argand diagram with a length of 1 and a phase angle $2\pi t\mathbf{a} \cdot \mathbf{S}$ (see Figure 4.15).

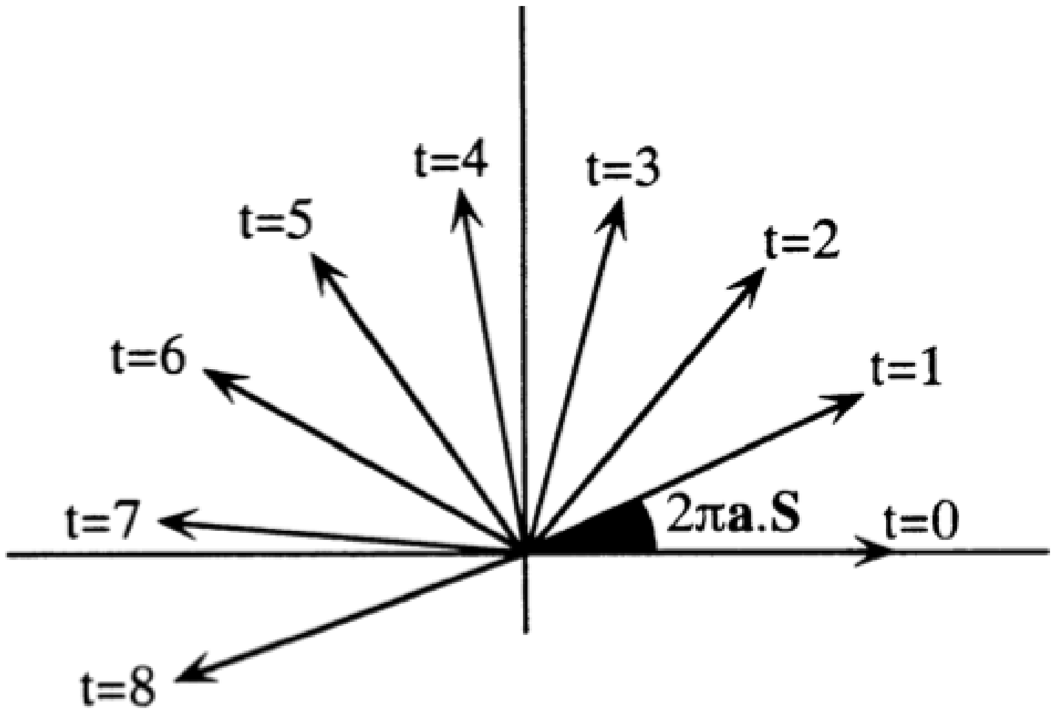
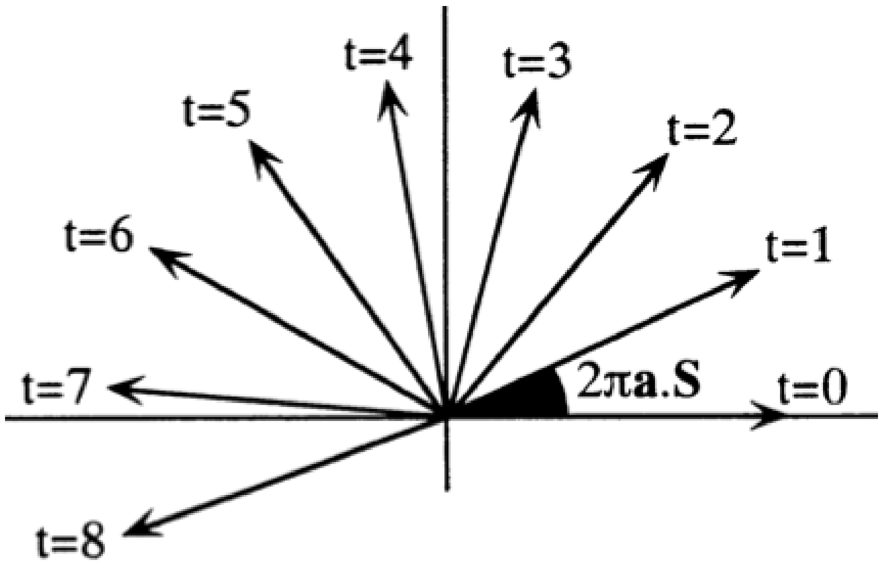


Figure 4.15. Each arrow represents the scattering by one unit cell in the crystal. Because of the huge number of unit cells and because their scattering vectors are pointing in different directions, the scattering by a crystal is, in general, zero. However, in the special case that $\mathbf{a} \cdot \mathbf{S}$ is an integer h, all vectors point to the right and the scattering by the crystal can be of appreciable intensity.



Conclusion: A crystal does not scatter X-rays, unless

$$\begin{aligned} \mathbf{a} \cdot \mathbf{S} &= h, \\ \mathbf{b} \cdot \mathbf{S} &= k, \\ \mathbf{c} \cdot \mathbf{S} &= l. \end{aligned} \tag{4.4}$$

These are known as the Laue conditions. h, k, and l are whole numbers, either positive, negative, or zero. The amplitude of the total scattered wave is proportional to the amplitude of the structure factor **F(S)** and the number of unit cells in the crystal.

Calculation of electron density

The structure factor is a function of the electron density distribution in the unit cell:

$$\mathbf{F}(\mathbf{S}) = \sum_{i} f_j \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}]. \qquad (4.3)$$

$$\mathbf{F}(\mathbf{S}) = \int_{\text{cell}} \rho(\mathbf{r}) \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}]\, dv. \qquad (4.8)$$

where $\rho(\mathbf{r})$ is the electron density at position $\mathbf{r}$ in the unit cell. If x, y, and z are fractional coordinates in the unit cell ($0 \leq x < 1$; the same for y and z) and V is the volume of the unit cell, we have

$$dv = V \cdot dx\, dy\, dz$$

and

$$\mathbf{r} \cdot \mathbf{S} = (\mathbf{a} \cdot x + \mathbf{b} \cdot y + \mathbf{c} \cdot z) \cdot \mathbf{S} = \mathbf{a} \cdot \mathbf{S} \cdot x + \mathbf{b} \cdot \mathbf{S} \cdot y + \mathbf{c} \cdot \mathbf{S} \cdot z$$
$$= hx + ky + lz.$$

Scattering by a unit cell

Suppose a unit cell has n atoms at positions $\mathbf{r}_j$ ($j = 1, 2, 3, \ldots, n$) with respect to the origin of the unit cell (Figure 4.12). With their own nuclei as origins, the atoms diffract according to their atomic scattering factor f. If the origin is now transferred to the origin of the unit cell, the phase angles change by $2\pi\mathbf{r}_j \cdot \mathbf{S}$. With respect to the new origin, the scattering is given by

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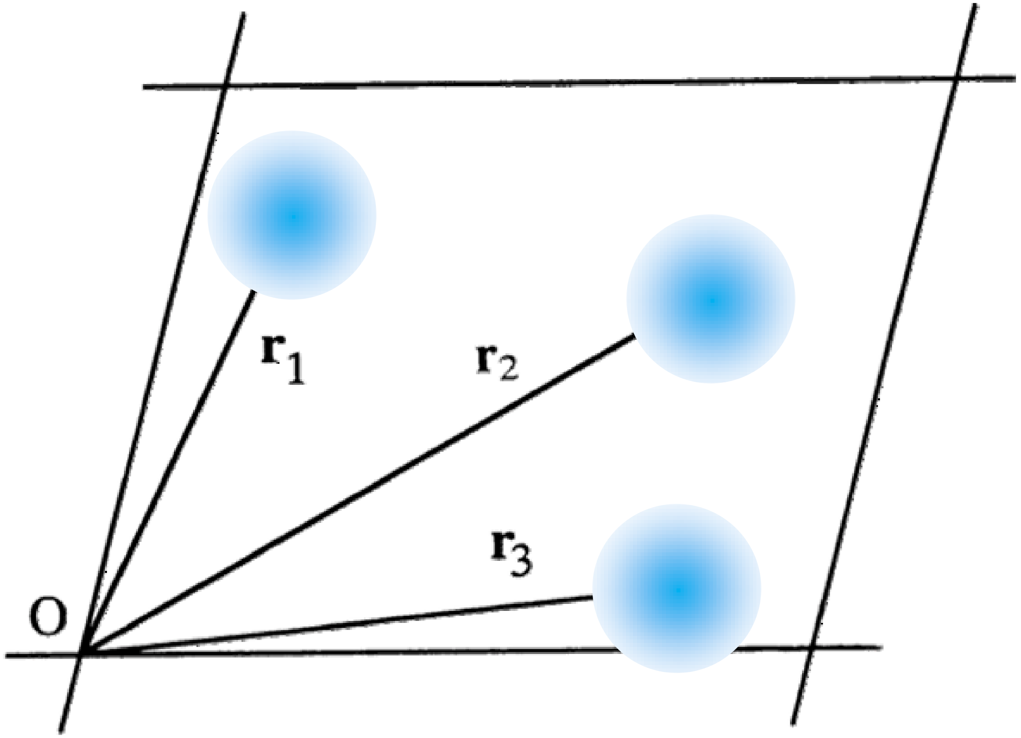

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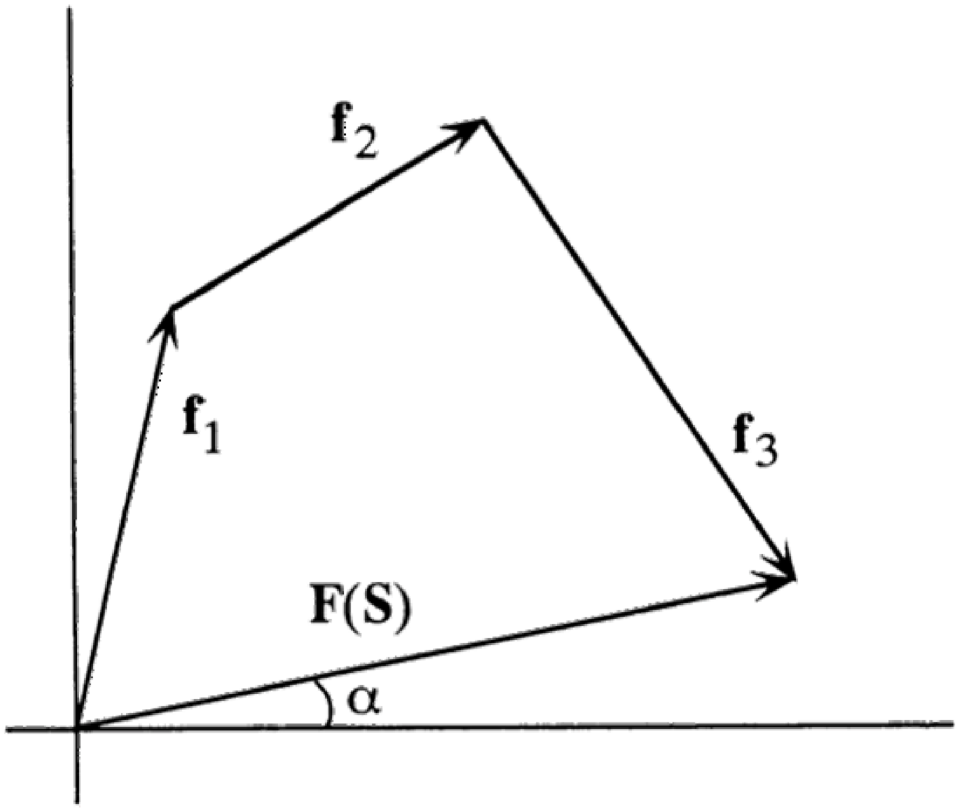

Figure 4.13. The structure factor **F(S)** is the sum of the scattering by the separate atoms in the unit cell.

unit cell is

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$$\mathbf{F}(\mathbf{S}) = \int_{\text{cell}} \rho(\mathbf{r}) \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}]\, dv. \quad (4.8)$$

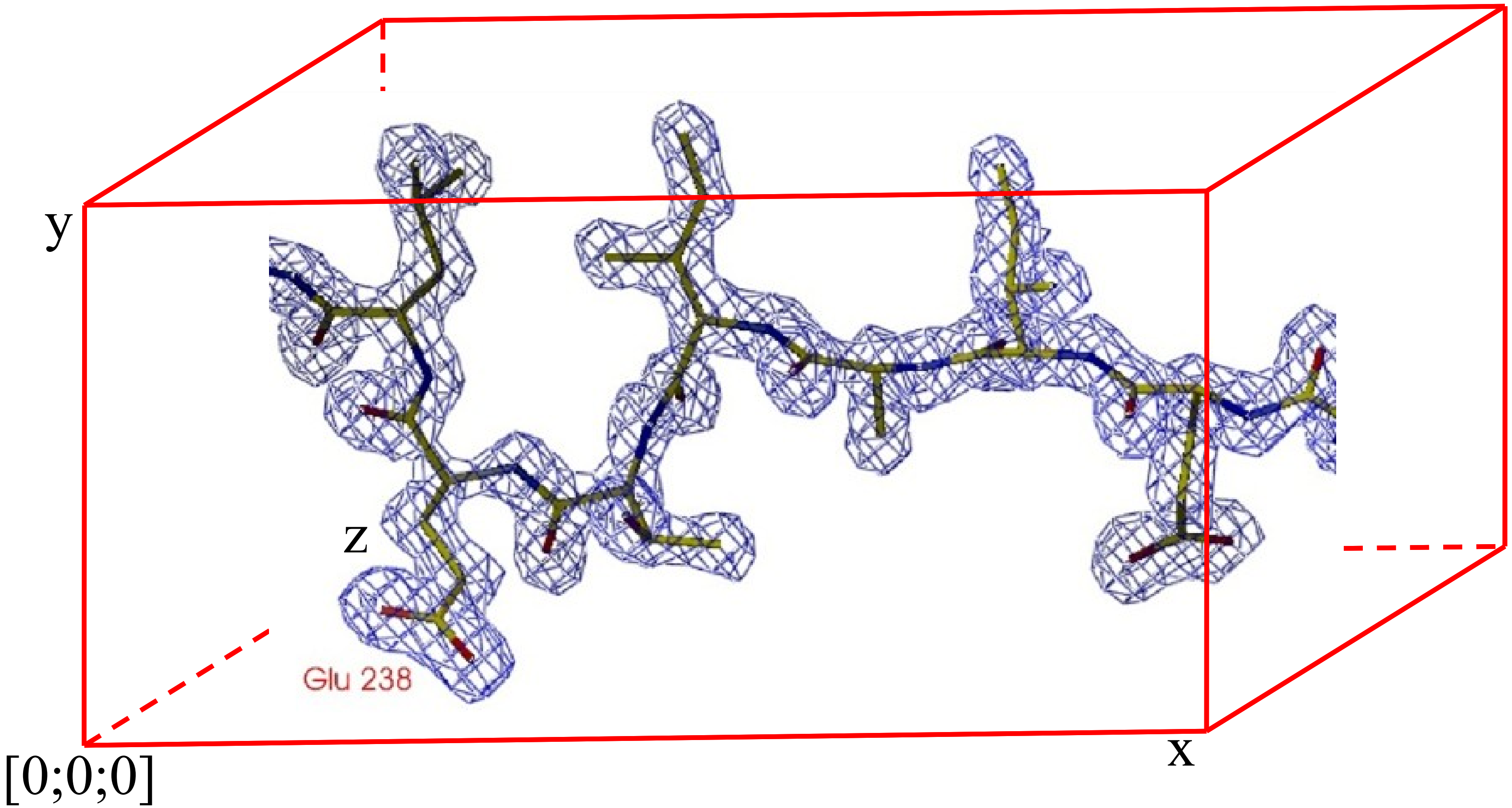
where $\rho(\mathbf{r})$ is the electron density at position $\mathbf{r}$ in the unit cell. If x, y, and z are fractional coordinates in the unit cell ($0 \leq x < 1$; the same for y and z) and V is the volume of the unit cell, we have

$$dv = V \cdot dx\, dy\, dz$$

and

$$\begin{aligned}\mathbf{r} \cdot \mathbf{S} &= (\mathbf{a} \cdot x + \mathbf{b} \cdot y + \mathbf{c} \cdot z) \cdot \mathbf{S} = \mathbf{a} \cdot \mathbf{S} \cdot x + \mathbf{b} \cdot \mathbf{S} \cdot y + \mathbf{c} \cdot \mathbf{S} \cdot z \\ &= hx + ky + lz.\end{aligned}$$

Information from X-ray diffraction experiment



$$\rho(x\,y\,z) = \frac{1}{V} \sum_h \sum_k \sum_l \left| F(h\,k\,l) \right| \exp\left[-2\pi i(hx + ky + lz) + i\alpha(h\,k\,l)\right]$$

Temperature (B) factor

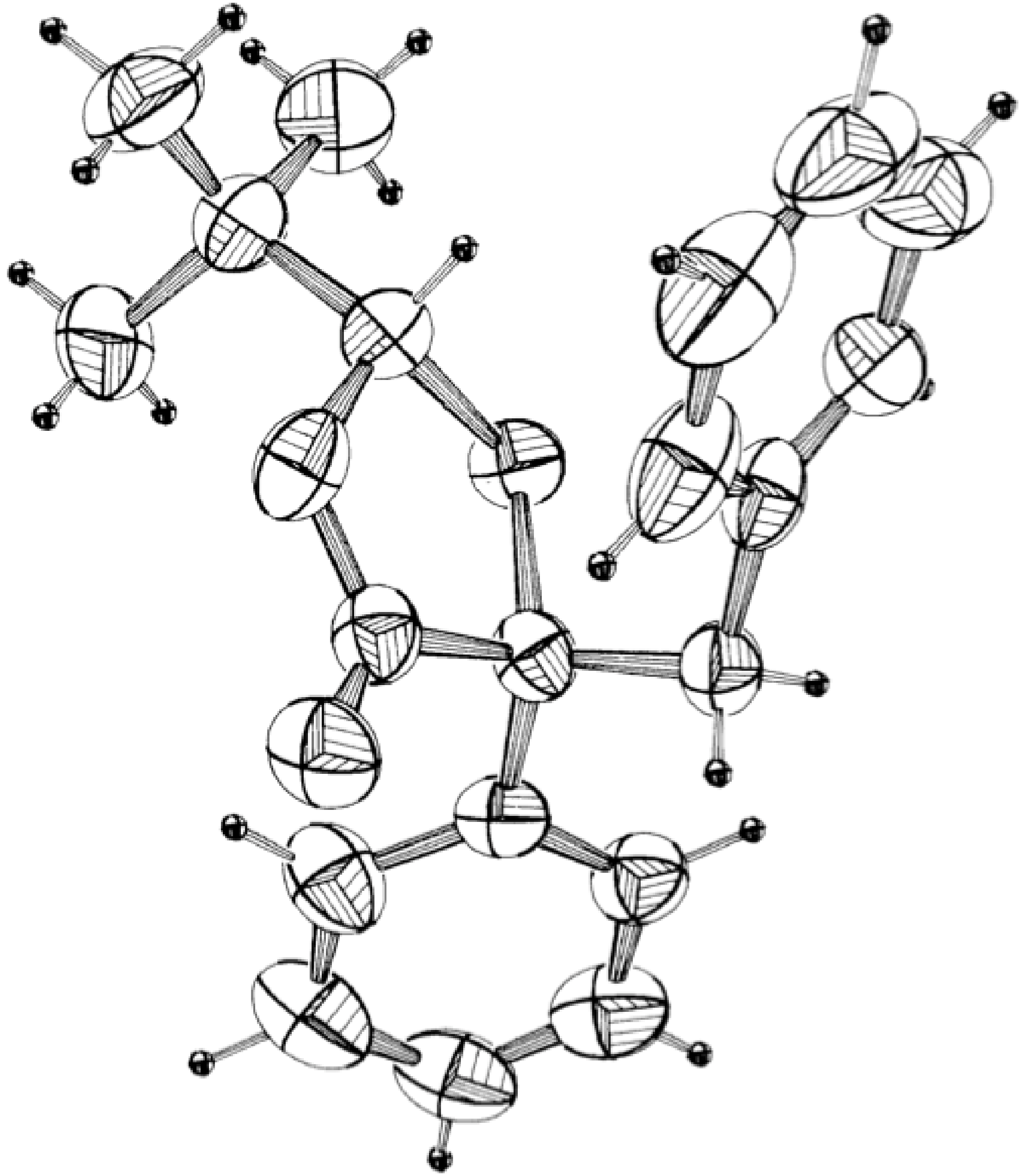


Figure 4.22. The plot of an organic molecule with 50% probability of thermal ellipsoids. (Reproduced with permission from Strijtveen and Kellogg © 1987 Pergamon Press PLC.)

$$\mathbf{F}(\mathbf{S}) = \int_{\text{cell}} \rho(\mathbf{r}) \exp[2\pi i \mathbf{r}_j \cdot \mathbf{S}] \, dv. \tag{4.8}$$

$$F(h\,k\,l) = V \int_{x=0}^{1} \int_{y=0}^{1} \int_{z=0}^{1} \rho(x\,y\,z) \exp[2\pi i(hx + ky + lz)] \, dx\, dy\, dz. \tag{4.9}$$

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$\mathbf{F}(h\,k\,l)$ is the Fourier transform of $\rho(x\,y\,z)$, but the reverse is also true: $\rho(x\,y\,z)$ is the Fourier transform of $\mathbf{F}(h\,k\,l)$ and, therefore, $\rho(x\,y\,z)$ can be written as a function of all $\mathbf{F}(h\,k\,l)$:

$$\rho(x\,y\,z) = \frac{1}{V} \sum_h \sum_k \sum_l \mathbf{F}(h\,k\,l) \exp[-2\pi i(hx + ky + lz)]. \qquad (4.10)$$

The Laue conditions tell us that diffraction occurs only in discrete directions and, therefore, in Eqation (4.10), the integration has been replaced by a summation. Because $\mathbf{F} =$ [redacted] $\exp[i$ [redacted], we can also write

$$\rho(x\,y\,z) = \frac{1}{V} \sum_h \sum_k \sum_l \left| \text{[redacted]} \right| \exp[-2\pi i \text{[redacted]} + i \text{[redacted]}] \qquad (4.11)$$

Notes

1. $\mathbf{F}(h\,k\,l)$ is the Fourier transform of the electron density $\rho(x\ y\ z)$ in the entire unit cell. Often the unit cell contains more than one molecule. Then $\mathbf{F}(h\,k\,l)$ is composed of the sum of the transforms of the separate molecules at position $(h\,k\,l)$ in reciprocal space.
2. Because of the crystallographic repeat of the unit cells, the value of the transform $\mathbf{F}(h\,k\,l)$ is zero in between the reciprocal space positions $(h\,k\,l)$. If there were no crystallographic repeat, the transform would be spread over the entire reciprocal space and its value is not restricted to reciprocal space positions $(h, k\,\ell)$.

$$F(h\,k\,l) = V \int_{x=0}^{1} \int_{y=0}^{1} \int_{z=0}^{1} \rho(x\,y\,z) \exp[2\pi i(hx + ky + lz)]\, dx\, dy\, dz. \tag{4.9}$$

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Intensity diffracted by a crystal

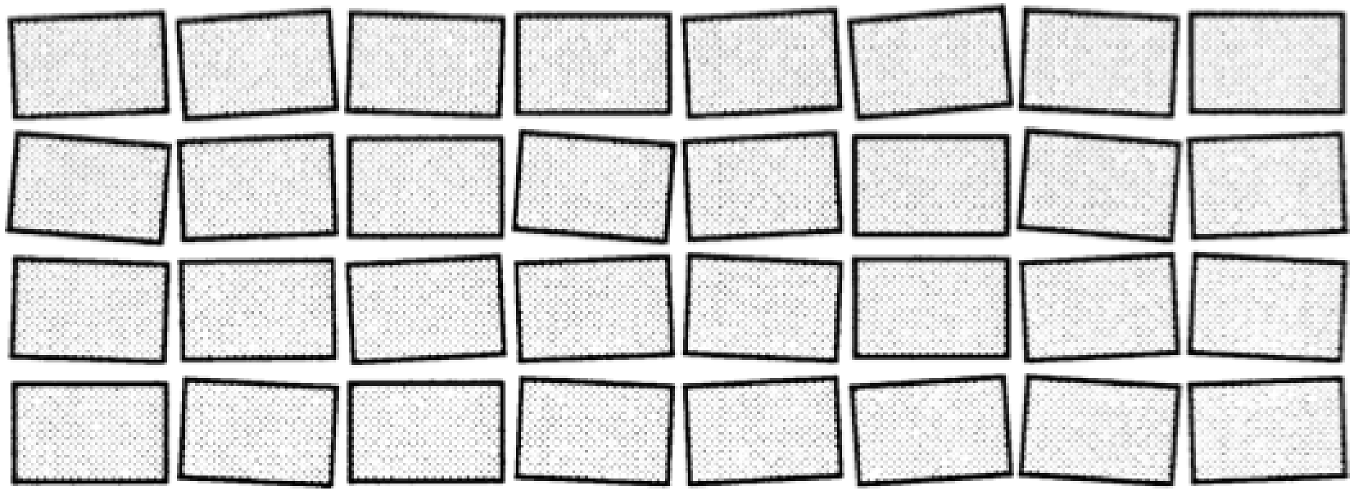


Figure 4.29. Most crystals are imperfect and can be regarded as being composed of small mosaic blocks.

We have the following assumptions:

1. Apart from ordinary absorption, the intensity I_0 of the incident beam is the same throughout the crystal.
2. The mosaic blocks are so small that a scattered wave is not scattered again (i.e., multiple scattering does not occur).
3. The mosaic blocks scatter independently of each other.

With these assumptions, the expression for I (int., $h\,k\,l$), if the crystal is rotated with an angular velocity ω through the reflection position, is

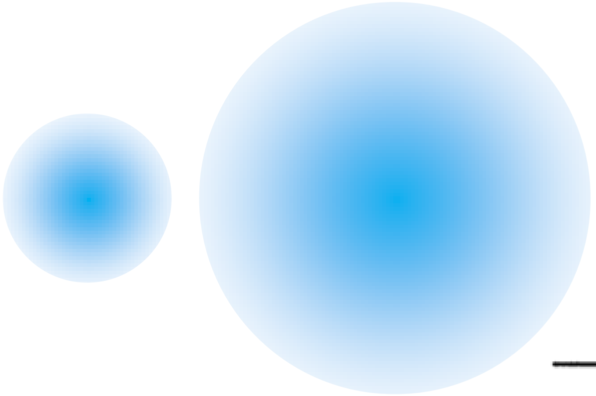
$$I(\text{int.},\ h\,k\,l) = \frac{\lambda^3}{\omega \cdot V^2} \times \left(\frac{e^2}{mc^2}\right)^2 \times V_{\mathrm{cr}} \times I_0 \times L \times P \times T_{\mathrm{r}} \times |F(h\,k\,l)|^2 . \tag{4.32}$$

λ – wavelength
ω – angular velocity of crystal rotation
V – unit cell volume
e – electron charge
m – electron mass
c – speed of light
V_{cr} – crystal volume

I_0 – intensity of the excitation beam
L – Lorentz coefficient
P – polarization coefficient
T_r – transmission coefficient
|F(hkl)| - structure factor amplitude

Effect of the unit cell size on the diffraction intensity

$$I(\text{int.},\ h\,k\,l) = \frac{\lambda^3}{\omega \cdot V^2} \times \left(\frac{e^2}{mc^2}\right)^2 \times V_{\text{cr}} \times I_0 \times L \times P \times T_{\text{r}} \times |F(h\,k\,l)|^2$$



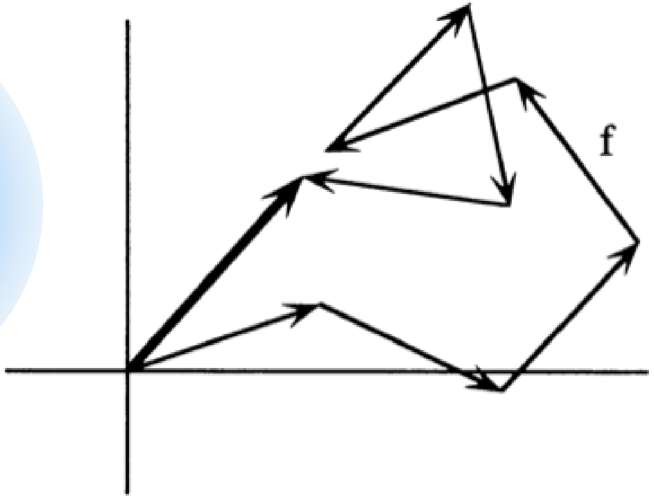


Figure 4.36. The displacement of a particle under the influence of Brownian motion. For n steps, where n is very large and each step has a length f, the final distance to the origin is $f\sqrt{n}$.

$$\sqrt{\overline{|F(h\,k\,l)|^2}} = f \times \sqrt{n} \quad \text{and} \quad \overline{|F(h\,k\,l)|^2} = f^2 \times n.$$

Combining the effect of the unit cell volume V and $|F(h\,k\,l)|$ in the scattering equation (4.32) leads to

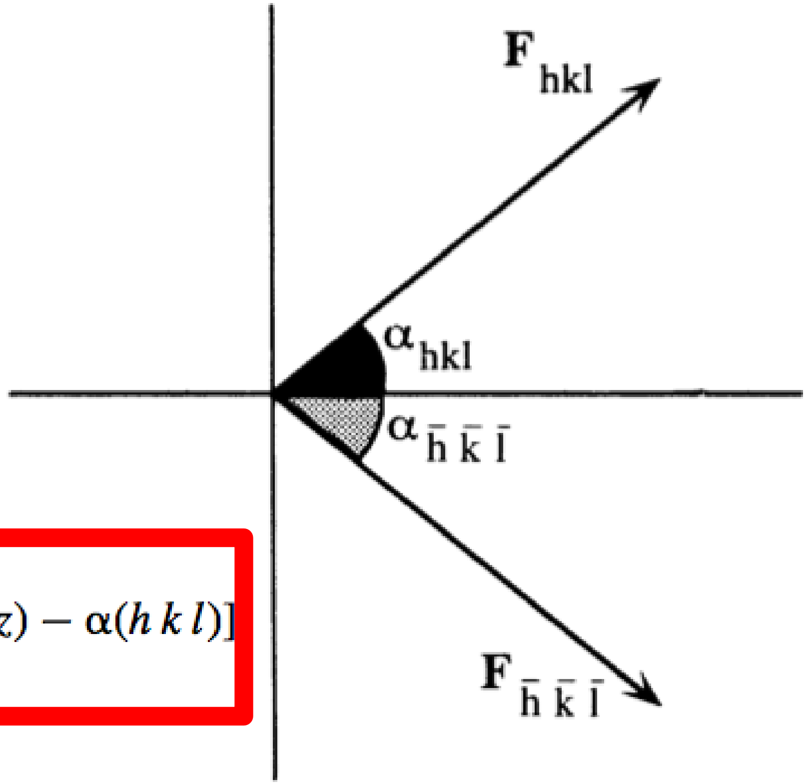
$$\overline{I(int.,\ h\,k\,l)} \text{ is proportional to } \frac{\overline{|F(h\,k\,l)|^2}}{V^2} = \frac{f^2}{V^2} \times n. \qquad (4.36)$$

Friedel pairs

$$\mathbf{F}(h\,k\,l) = V \int_{\text{cell}} \rho(x\,y\,z) \exp[2\pi i(hx + ky + lz)]\,dx\,dy\,dz$$

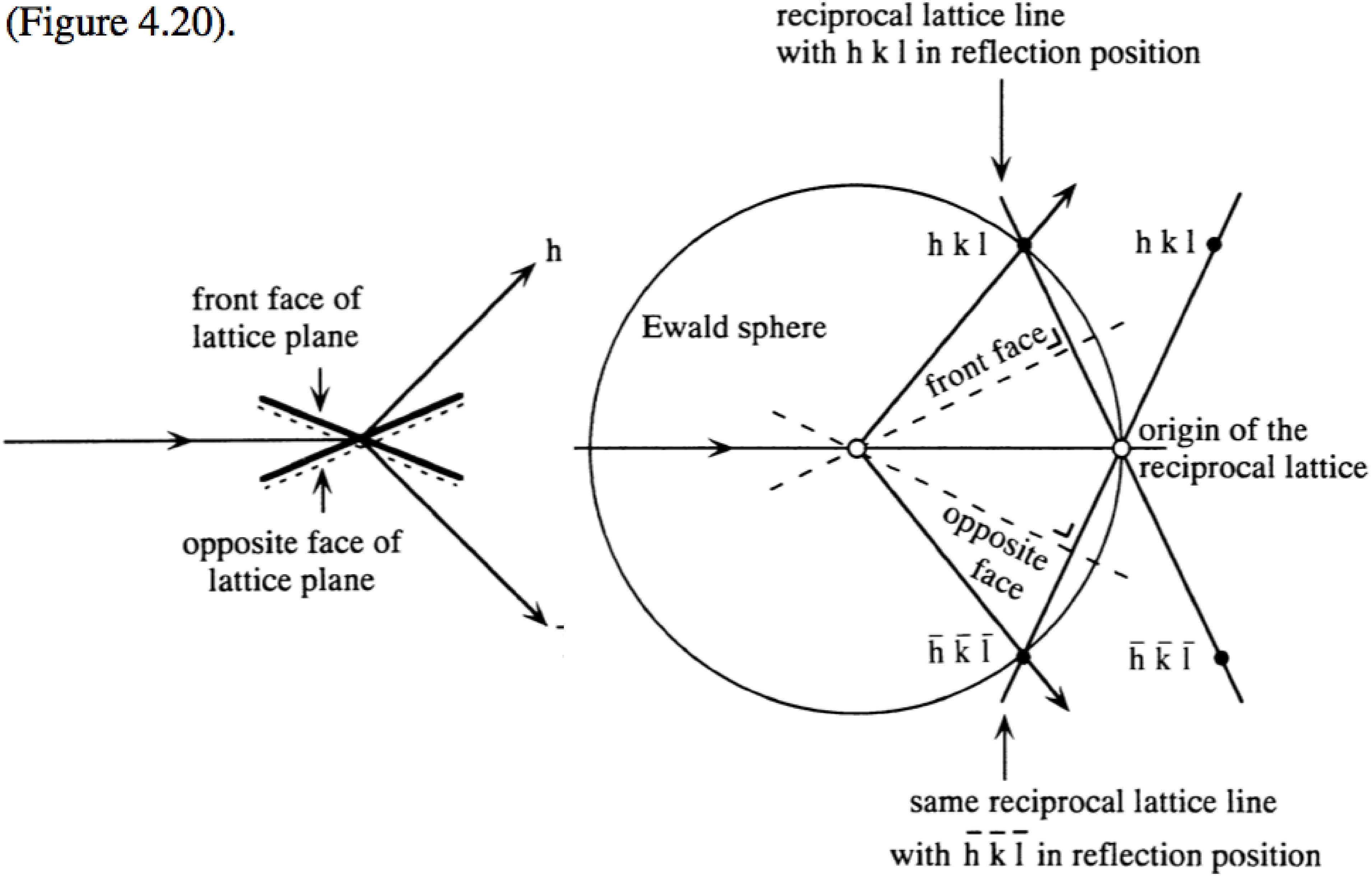
$$\mathbf{F}(\bar{h}\,\bar{k}\,\bar{l}) = V \int_{\text{cell}} \rho(x\,y\,z) \exp[2\pi i(-hx - ky - lz)]\,dx\,dy\,dz. \qquad (4.25)$$

Figure 4.24. Argand diagram for the structure factors of the reflections $\mathbf{F}(h\,k\,l)$ and $\mathbf{F}(\bar{h}\,\bar{k}\,\bar{l})$.



$$\rho(x\,y\,z) = \frac{2}{V} \sum_{hkl=0}^{+\infty} |F(h\,k\,l)| \cos[2\pi(hx + ky + lz) - \alpha(h\,k\,l)]$$

One more comment on lattice planes: If the beam $h\,k\,l$ corresponds to reflection against one face (let us say the front) of a lattice plane, then $(\bar{h}\bar{k}\,\bar{l})$ [or $(-h, -k, -l)$ corresponds to the reflection against the opposite face (the back) of the plane (Figure 4.20).



Symmetry in the diffraction pattern

4.12.1. A 2-Fold Axis Along *y*

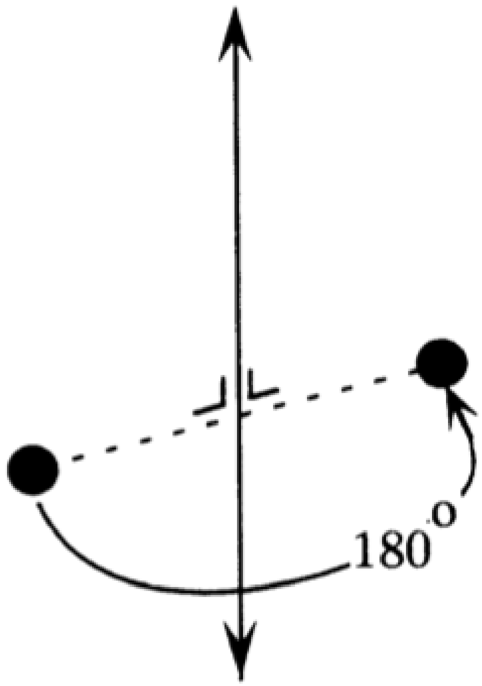
If a 2-fold axis through the origin and along y is present, then the electron density $\rho(x\,y\,z) = \rho(\bar{x}\,y\,\bar{z})$ (Figure 4.25). Therefore,

$$\mathbf{F}(h\,k\,l) = V \int_{\substack{\text{asymm}\\ \text{unit}}} \rho(x\,y\,z)\{\exp[2\pi i(hx + ky + lz)] + \exp[2\pi i(-hx + ky - lz)]\}\,dx\,dy\,dz \qquad (4.26)$$

The integration in Eq. (4.26) is over one asymmetric unit (half of the cell), because the presence of the second term under the integral takes care of the other half of the cell.

$$\mathbf{F}(\bar{h}\,k\,\bar{l}) = V \int_{\substack{\text{asymm}\\ \text{unit}}} \rho(x\,y\,z)\{\exp[2\pi i(-hx + ky - lz)] + \exp[2\pi i(hx + ky + lz)]\}\,dx\,dy\,dz \qquad (4.27)$$

It follows that $\mathbf{F}(h\,k\,l) = \mathbf{F}(\bar{h}\,k\,\bar{l})$ and also $I(h\,k\,l) = I(\bar{h}\,k\,\bar{l})$,


180°

4.12.2. A 2-Fold Screw Axis Along y

For a 2-fold screw axis along y (Figure 4.26),

$$\rho(x\,y\,z) = \rho\{\bar{x}(y + 1/2)\bar{z}\}$$

$$\mathbf{F}(h\,k\,l) = V \int_{\substack{\text{asymm}\\ \text{unit}}} \rho(x\,y\,z)\{\underbrace{\exp[2\pi i(hx + ky + lz)]}_{\text{term I}\ \downarrow} + \underbrace{\exp[2\pi i(-hx + k(y + 1/2) - lz)]}_{\text{term II}\ \uparrow}\}\,dx\,dy\,dz \qquad (4.28)$$

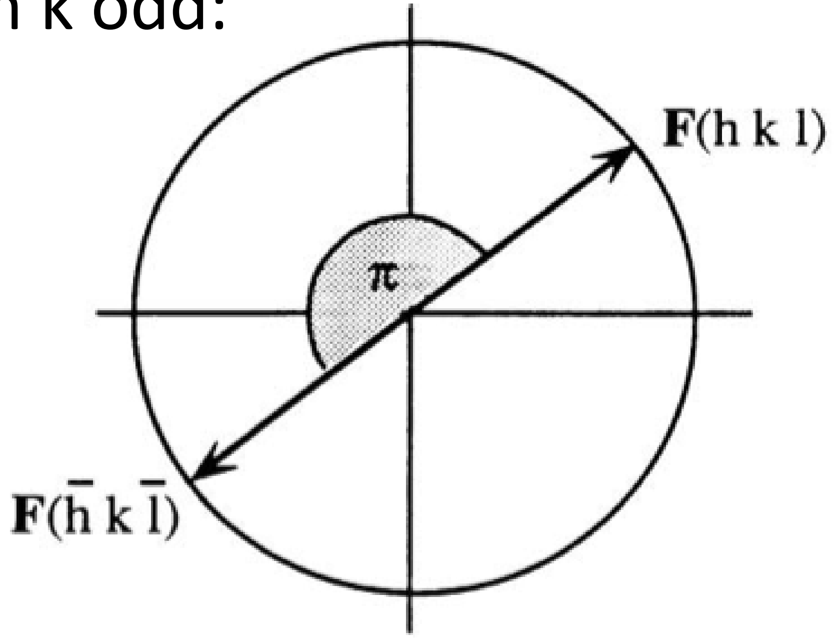
$$\mathbf{F}(\bar{h}\,k\,\bar{l}) = V \int_{\substack{\text{asymm}\\ \text{unit}}} \rho(x\,y\,z)\{\underbrace{\exp[2\pi i(-hx + ky - lz)]}_{\text{term III}\ \downarrow} + \underbrace{\exp[2\pi i(hx + k(y + 1/2) + lz)]}_{\text{term IV}\ \uparrow}\}\,dx\,dy\,dz. \qquad (4.29)$$

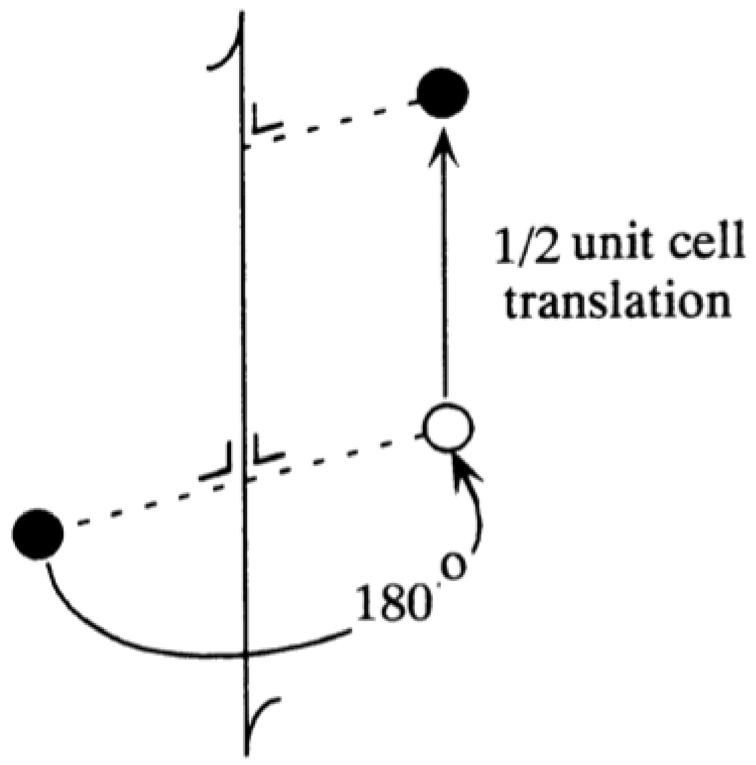
In Equation (4.28), term II is

$$\exp\{2\pi i[-hx + k(y + 1/2) - lz]\} = \exp[2\pi i(-hx + ky - lz + 1/2k)].$$

For k even, this is equal to term III in Equation (4.29). The same is true for term IV in Equation (4.29) and term I in Equation (4.28). Therefore, when k is even, $\mathbf{F}(h\,k\,l) = \mathbf{F}(\bar{h}\,k\,\bar{l})$ and $I(h\,k\,l = I(\bar{h}\,k\,\bar{l})$. When k is odd, terms I and IV have a difference of π in their phase angles: $2\pi(hx + ky + lz)$ and $2\pi(hx + ky + lz + 1/2k)$.

For F(hkl) with k odd:




1/2 unit cell
translation
180°

Systematic absences in P2(1)

$$\mathbf{F}(0\,k\,0) = V \int_{\substack{\text{asymm}\\\text{unit}}} \rho(x\,y\,z)\{\exp[2\pi iky] + \exp[2\pi ik(y + 1/2)]\}\,dx\,dy\,dz. \tag{4.30}$$

When k is even, this is $2 \times V \int \rho(x\,y\,z) \exp[2\pi iky]\,dx\,dy\,dz$. However, when k is odd, the two terms in Equation (4.30) cancel and $\mathbf{F}(0\,k\,0) = 0$