

Electron energy in crystal potential

$$\sqrt{(pc)^2 + (m_0c^2)^2} = mc^2$$

where: $E = e \cdot V_0$

$$\sqrt{[p(\mathbf{r})c]^2 + (m_0c^2)^2} = mc^2 + e\Phi(\mathbf{r})$$

$$mc^2 = E + m_0c^2$$

$$mc^2 \gg |e\Phi(\mathbf{r})|$$

Expand:

$$[mc^2 + e\Phi(\mathbf{r})]^2 \approx (mc^2)^2 + 2(mc^2) \cdot e\Phi(\mathbf{r})$$

$$[p(\mathbf{r})c]^2 + (m_0c^2)^2 \approx (mc^2)^2 + 2(mc^2) \cdot e\Phi(\mathbf{r})$$

$$\frac{[p(\mathbf{r})]^2}{2m} - e\Phi(\mathbf{r}) = \frac{m^2 - m_0^2}{2m} = \left(\frac{m + m_0}{2m}\right) \cdot E \equiv E_{nr}$$

$$\Rightarrow \frac{p(\mathbf{r})^2}{2m} - e\Phi(\mathbf{r}) = E_{nr}$$

Wave equation

Hamiltonian:
$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - e\Phi(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 - e\Phi(\mathbf{r})$$

Time-Independent Schrodinger Eqn:
$$\left[-\frac{\hbar^2}{2m}\nabla^2 - e\Phi(\mathbf{r}) \right] \psi(\mathbf{r}) = E_{nr} \cdot \psi(\mathbf{r})$$

Rearrange:
$$\left\{ \nabla^2 + 4\pi^2 \left[\frac{2mE_{nr}}{h^2} + \frac{2me}{h^2} \Phi(\mathbf{r}) \right] \right\} \psi(\mathbf{r}) = 0$$

Previously defined:
$$\lambda = \frac{h}{\sqrt{2mE_{nr}}} \quad k^2 = \frac{2mE_{nr}}{h^2}$$

Structure Function:
$$U(\mathbf{r}) \equiv \frac{2me}{h^2} \Phi(\mathbf{r})$$

Wave Equation:
$$\left[\nabla^2 + 4\pi^2 (k^2 + U(\mathbf{r})) \right] \psi(\mathbf{r}) = 0$$

Bloch-wave solutions

The structure function is periodic: $U(\mathbf{r} + \mathbf{r}_{uvw}) = U(\mathbf{r})$

So:
$$U(\mathbf{r}) = \sum_{\mathbf{g}} U_{\mathbf{g}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}}$$

The coefficients of the structure function are:
$$U_{\mathbf{g}} = \frac{2me}{h^2} \Phi_{\mathbf{g}}$$

The wave equation looks like:

$$\left[\nabla^2 + 4\pi^2 \left(k^2 + \sum_{\mathbf{g}} U_{\mathbf{g}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right) \right] \psi(\mathbf{r}) = 0$$

Consider solutions of the form:

$$\psi^{(j)}(\mathbf{r}) = u^{(j)}(\mathbf{r}) \cdot e^{2\pi i \mathbf{k}^{(j)} \cdot \mathbf{r}}$$

where:

$$u^{(j)}(\mathbf{r}) = \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi i \mathbf{g} \cdot \mathbf{r}}$$

These solutions are Bloch waves:

$$\psi^{(j)}(\mathbf{r}) = \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi i [\mathbf{k}^{(j)} + \mathbf{g}] \cdot \mathbf{r}}$$

Structure Function

The coefficients of the structure function are:

$$U_{\mathbf{g}} = \frac{2me}{h^2} \Phi_{\mathbf{g}} = \frac{2me}{h^2} \cdot \phi(\mathbf{g}) \cdot X_{\mathbf{g}}$$

Let's relate these to the structure factors.

$$\phi(\mathbf{g}) = \sum_{m \text{ atoms}} \phi^{(m)}(g) e^{-2\pi i \mathbf{g} \cdot \mathbf{d}^{(m)}}$$

//Fourier transform of unit cell

$$f^{(m)}(\mathbf{g}) \equiv \frac{2\pi m e}{h^2} \int_{\mathbf{r}} \phi^{(m)}(\mathbf{r}) e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \cdot d^3 r$$

//atomic form factors

$$f^{(m)}(g) = \frac{2\pi m e}{h^2} \phi^{(m)}(g)$$

//spherical symmetry

$$F_{\mathbf{g}} = \sum_{m \text{ atoms}} f^{(m)}(g) e^{-2\pi i \mathbf{g} \cdot \mathbf{d}^{(m)}}$$

//crystal structure factors

$$F_{\mathbf{g}} = \frac{2\pi m e}{h^2} \phi(\mathbf{g})$$

—————>

$$U_{\mathbf{g}} = \frac{F_{\mathbf{g}} \cdot X_{\mathbf{g}}}{\pi}$$

Properties of Bloch waves (I)

The Bloch waves are quantum states:

$$|\psi^{(j)}\rangle = \begin{pmatrix} C_0^{(j)} \\ C_{\mathbf{g}_1}^{(j)} \\ C_{\mathbf{g}_2}^{(j)} \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} \quad \langle \psi^{(j)} | = \left\{ [C_0^{(j)}]^* \quad [C_{\mathbf{g}_1}^{(j)}]^* \quad [C_{\mathbf{g}_2}^{(j)}]^* \quad \cdot \quad \cdot \quad \cdot \right\}$$

We can normalize them:

$$1 = \langle \psi^{(j)} | \psi^{(j)} \rangle = \sum_{\mathbf{g}} |C_{\mathbf{g}}^{(j)}|^2$$

Any two Bloch states are orthogonal:

$$0 = \langle \psi^{(j)} | \psi^{(j')} \rangle; j \neq j'$$

Properties of Bloch waves (II)

The Bloch waves form an orthonormal set:

$$V = \begin{pmatrix} C_{\mathbf{g}_1}^{(1)} & C_{\mathbf{g}_1}^{(2)} & \dots \\ C_{\mathbf{g}_2}^{(1)} & C_{\mathbf{g}_2}^{(2)} & \\ \vdots & & \ddots \end{pmatrix} = (|\Psi^{(1)}\rangle \quad |\Psi^{(2)}\rangle \quad \dots) \quad V^\dagger = \begin{pmatrix} \langle \Psi^{(1)} | \\ \langle \Psi^{(2)} | \\ \vdots \end{pmatrix} \quad V^\dagger V = I$$

Also: $(V^T)^\dagger V^T = I$

$$V^T = \begin{pmatrix} C_{\mathbf{g}_1}^{(1)} & C_{\mathbf{g}_2}^{(1)} & \dots \\ C_{\mathbf{g}_1}^{(2)} & C_{\mathbf{g}_2}^{(2)} & \\ \vdots & & \ddots \end{pmatrix} = (|\Psi_{\mathbf{g}_1}\rangle \quad |\Psi_{\mathbf{g}_2}\rangle \quad \dots) \quad (V^T)^\dagger = \begin{pmatrix} \langle \Psi_{\mathbf{g}_1} | \\ \langle \Psi_{\mathbf{g}_2} | \\ \vdots \end{pmatrix}$$

The g -components of the Bloch waves also form an orthonormal set:

$$\langle \Psi_{\mathbf{g}} | \Psi_{\mathbf{g}} \rangle = \sum_j |C_{\mathbf{g}}^{(j)}|^2 = 1$$

$$\langle \Psi_{\mathbf{g}'} | \Psi_{\mathbf{g}} \rangle = \sum_j [C_{\mathbf{g}'}^{(j)}]^* \cdot C_{\mathbf{g}}^{(j)} = 0, \quad (\mathbf{g}' \neq \mathbf{g})$$

Total wave function

The total wave function is a linear combination of *Bloch waves*:

$$\Psi(\mathbf{r}) = \sum_j \varepsilon^{(j)} \psi^{(j)}(\mathbf{r})$$

The $\varepsilon^{(j)}$ are the *excitation amplitudes*.

They are found using the boundary conditions at the top (entrance) surface.

In terms of diffracted beams:

$$\begin{aligned} \Psi(\mathbf{r}) &= \sum_j \varepsilon^{(j)} \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi i[\mathbf{k}^{(j)} + \mathbf{g}] \cdot \mathbf{r}} \\ &= \sum_{\mathbf{g}} \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\boldsymbol{\gamma}^{(j)} - \mathbf{s}_{\mathbf{g}}] \cdot \mathbf{r}} e^{2\pi i(\mathbf{k} + \mathbf{g} + \mathbf{s}_{\mathbf{g}}) \cdot \mathbf{r}} \end{aligned} \quad \text{Where: } \boldsymbol{\gamma}^{(j)} \equiv \mathbf{k}^{(j)} - \mathbf{k}$$

$$\Psi(\mathbf{r}) = \sum_{\mathbf{g}} \Psi_{\mathbf{g}}(\mathbf{r}) e^{2\pi i \mathbf{k}_{\mathbf{g}} \cdot \mathbf{r}}$$

$$\Psi_{\mathbf{g}}(\mathbf{r}) \equiv \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\boldsymbol{\gamma}^{(j)} - \mathbf{s}_{\mathbf{g}}] \cdot \mathbf{r}}$$

Boundary condition(s) (I)

At the foil entrance surface, we must have:

$$i) \psi(\mathbf{r}) \text{ continuous} \quad \text{and} \quad ii) \hat{\mathbf{n}} \cdot \nabla \psi(\mathbf{r}) \text{ continuous}$$

We can pick the foil entrance surface to be the plane $z=0$, with $\hat{\mathbf{n}} = -\hat{\mathbf{z}}$

Assuming that above the sample: $\psi(\mathbf{r}) = e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$

we are only able to satisfy condition *i*).

(To satisfy both conditions, include back-scattered waves.)

Consider condition *i*) only (neglecting back-scattered waves):

$$e^{2\pi i \mathbf{k} \cdot \mathbf{r}} \Big|_{z=0} = \sum_j \varepsilon^{(j)} \left\{ \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi i [\mathbf{k}^{(j)} + \mathbf{g}] \cdot \mathbf{r}} \right\} \Big|_{z=0}$$
$$\Rightarrow 1 = \sum_j \varepsilon^{(j)} \left\{ \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} e^{2\pi i [\boldsymbol{\gamma}^{(j)} + \mathbf{g}] \cdot \mathbf{r}} \right\} \Big|_{z=0}$$

Boundary Condition(s) (II)

Condition *i*) is satisfied if: $1 = \sum_j \varepsilon^{(j)} C_0^{(j)} e^{2\pi i \boldsymbol{\gamma}^{(j)} \cdot \mathbf{r}} \Big|_{z=0}$

and $0 = \sum_j \varepsilon^{(j)} \left\{ \sum_{\mathbf{g} \neq \mathbf{0}} C_{\mathbf{g}}^{(j)} e^{2\pi i [\boldsymbol{\gamma}^{(j)} + \mathbf{g}] \cdot \mathbf{r}} \right\} \Big|_{z=0}$

We must have $\boldsymbol{\gamma}^{(j)} = -\boldsymbol{\gamma}^{(j)} \hat{\mathbf{n}}$ so that $\boldsymbol{\gamma}^{(j)} \cdot \mathbf{r} \Big|_{z=0} = 0 \Rightarrow e^{2\pi i \boldsymbol{\gamma}^{(j)} \cdot \mathbf{r}} \Big|_{z=0} = 1$

$$\left. \begin{aligned} 1 &= \sum_j \varepsilon^{(j)} C_0^{(j)} \\ 0 &= \sum_{\mathbf{g} \neq \mathbf{0}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \Big|_{z=0} \left[\sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} \right] \end{aligned} \right\} \Rightarrow \boldsymbol{\varepsilon}^{(j)} = \left[C_0^{(j)} \right]^*$$

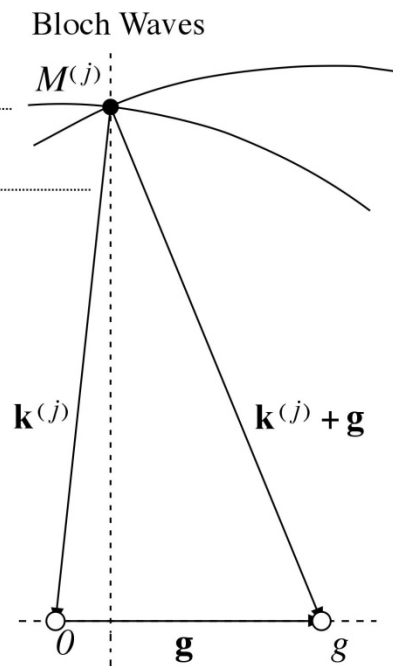
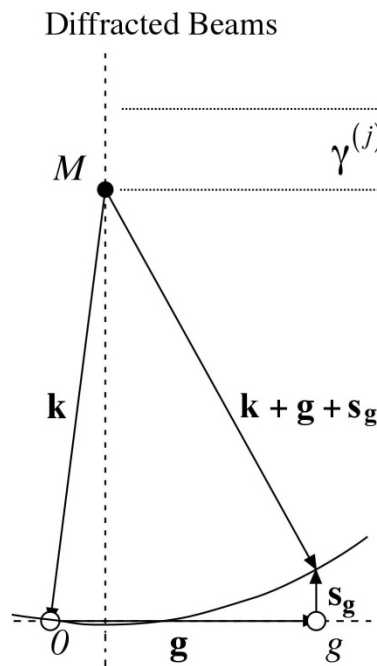
In other words: $\boldsymbol{\psi}(\mathbf{r}) = \sum_j \left[C_0^{(j)} \right]^* \boldsymbol{\psi}^{(j)}(\mathbf{r})$

Diffracted beam amplitudes

$$\Psi(\mathbf{r}) = \sum_j \varepsilon^{(j)} \Psi^{(j)}(\mathbf{r}) = \sum_{\mathbf{g}} \Psi_{\mathbf{g}}(\mathbf{r}) e^{2\pi i(\mathbf{k} + \mathbf{g} + \mathbf{s}_{\mathbf{g}}) \cdot \mathbf{r}}$$

$$\Psi_{\mathbf{g}}(\mathbf{r}) = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\mathbf{k}^{(j)} - \mathbf{k} - \mathbf{s}_{\mathbf{g}}] \cdot \mathbf{r}} = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\boldsymbol{\gamma}^{(j)} - \mathbf{s}_{\mathbf{g}}] \cdot \mathbf{r}}$$

We can pick: $\mathbf{s}_{\mathbf{g}} = -s_g \hat{\mathbf{n}} \quad \Rightarrow \quad \Psi_{\mathbf{g}}(\mathbf{r}) \rightarrow \Psi_{\mathbf{g}}(z) = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\boldsymbol{\gamma}^{(j)} - s_g] \cdot z}$



$$\boldsymbol{\gamma}^{(j)} \cdot \mathbf{r} = \boldsymbol{\gamma}^{(j)} \cdot z$$

$$\mathbf{s}_{\mathbf{g}} \cdot \mathbf{r} = s_g \cdot z$$

Solving for the Bloch-wave coefficients

Find the particular Bloch waves are solutions of:

$$\left[\nabla^2 + 4\pi^2 \left(K^2 + \sum_{\mathbf{g} \neq 0} U_{\mathbf{g}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right) \right] \psi(\mathbf{r}) = 0$$

$$K^2 \doteq k^2 + U_0 (\approx k^2)$$

The first term is:

$$\nabla^2 \psi^{(j)}(\mathbf{r}) = -4\pi^2 \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} (\mathbf{k}^{(j)} + \mathbf{g})^2 e^{2\pi i [\mathbf{k}^{(j)} + \mathbf{g}] \cdot \mathbf{r}}$$

We can find the $C_{\mathbf{g}}^{(j)}$ by solving:

$$\sum_{\mathbf{g}} \left\{ \left[k^2 - (\mathbf{k}^{(j)} + \mathbf{g})^2 \right] + \sum_{\mathbf{h} \neq 0} U_{\mathbf{h}} e^{2\pi i \mathbf{h} \cdot \mathbf{r}} \right\} C_{\mathbf{g}}^{(j)} e^{2\pi i (\mathbf{k}^{(j)} + \mathbf{g}) \cdot \mathbf{r}} = 0$$

Rearranging the sums

Break up the sum into two terms:

$$\sum_{\mathbf{g}} \left\{ \left[k^2 - (\mathbf{k}^{(j)} + \mathbf{g})^2 \right] C_{\mathbf{g}}^{(j)} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right\} + \sum_{\mathbf{g}'} \left\{ C_{\mathbf{g}'}^{(j)} \sum_{\mathbf{h} \neq 0} U_{\mathbf{h}} e^{2\pi i (\mathbf{h} + \mathbf{g}') \cdot \mathbf{r}} \right\} = 0$$

Reindex: $\mathbf{h}' = \mathbf{h} + \mathbf{g}'$
 $\mathbf{h} = \mathbf{h}' - \mathbf{g}'$
 $\mathbf{h} = \mathbf{0} \rightarrow \mathbf{h}' = \mathbf{g}'$

$$\sum_{\mathbf{h} \neq 0} U_{\mathbf{h}} e^{2\pi i (\mathbf{h} + \mathbf{g}') \cdot \mathbf{r}} = \sum_{\mathbf{h}' \neq \mathbf{g}'} U_{\mathbf{h}' - \mathbf{g}'} e^{2\pi i \mathbf{h}' \cdot \mathbf{r}}$$

$$\sum_{\mathbf{g}} \left\{ \left[k^2 - (\mathbf{k}^{(j)} + \mathbf{g})^2 \right] C_{\mathbf{g}}^{(j)} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right\} + \sum_{\mathbf{g}'} \left\{ C_{\mathbf{g}'}^{(j)} \sum_{\mathbf{h} \neq \mathbf{g}'} U_{\mathbf{h} - \mathbf{g}'} e^{2\pi i \mathbf{h} \cdot \mathbf{r}} \right\} = 0$$

Now we can group terms that have the same exponential function:

$$\left[k^2 - (\mathbf{k}^{(j)} + \mathbf{g})^2 \right] C_{\mathbf{g}}^{(j)} + \sum_{\mathbf{h} \neq \mathbf{g}} U_{\mathbf{g} - \mathbf{h}} C_{\mathbf{h}}^{(j)} = 0$$

Rewriting the sum

We want to simplify: $\left[(\mathbf{k}^{(j)} + \mathbf{g})^2 - k^2 \right] C_{\mathbf{g}}^{(j)} = \sum_{\mathbf{h} \neq \mathbf{g}} U_{\mathbf{g}-\mathbf{h}} C_{\mathbf{h}}^{(j)}$

I.

$$\mathbf{k}^{(j)} = \mathbf{k} + \boldsymbol{\gamma}^{(j)}$$

$$\begin{aligned} (\mathbf{k}^{(j)} + \mathbf{g})^2 &= \left[(\mathbf{k} + \mathbf{g}) + \boldsymbol{\gamma}^{(j)} \right]^2 \\ &= (\mathbf{k} + \mathbf{g})^2 + 2(\mathbf{k} + \mathbf{g}) \cdot \boldsymbol{\gamma}^{(j)} + \boldsymbol{\gamma}^{(j)2} \end{aligned}$$

II.

$$k = |\mathbf{k} + \mathbf{g} + \mathbf{s}_{\mathbf{g}}|$$

$$\begin{aligned} k^2 &= (\mathbf{k} + \mathbf{g} + \mathbf{s}_{\mathbf{g}})^2 \\ &= (\mathbf{k} + \mathbf{g})^2 + 2(\mathbf{k} + \mathbf{g}) \cdot \mathbf{s}_{\mathbf{g}} + s_{\mathbf{g}}^2 \end{aligned}$$

I. - II.

$$(\mathbf{k}^{(j)} + \mathbf{g})^2 - k^2 = 2(\mathbf{k} + \mathbf{g}) \cdot (\boldsymbol{\gamma}^{(j)} - \mathbf{s}_{\mathbf{g}}) + \boldsymbol{\gamma}^{(j)2} + s_{\mathbf{g}}^2$$

So now we have:

$$\left[2(\mathbf{k} + \mathbf{g}) \cdot (\boldsymbol{\gamma}^{(j)} - \mathbf{s}_{\mathbf{g}}) + \boldsymbol{\gamma}^{(j)2} + s_{\mathbf{g}}^2 \right] C_{\mathbf{g}}^{(j)} = \sum_{\mathbf{h} \neq \mathbf{g}} U_{\mathbf{g}-\mathbf{h}} C_{\mathbf{h}}^{(j)}$$

High-energy approximation

$$\begin{aligned}
 & (\mathbf{k}^{(j)} + \mathbf{g})^2 - k^2 \\
 &= 2(\mathbf{k} + \mathbf{g}) \cdot (\gamma^{(j)} - \mathbf{s}_g) + \gamma^{(j)2} - s_g^2 \\
 &\approx 2\mathbf{k} \cdot (\gamma^{(j)} - \mathbf{s}_g)
 \end{aligned}$$

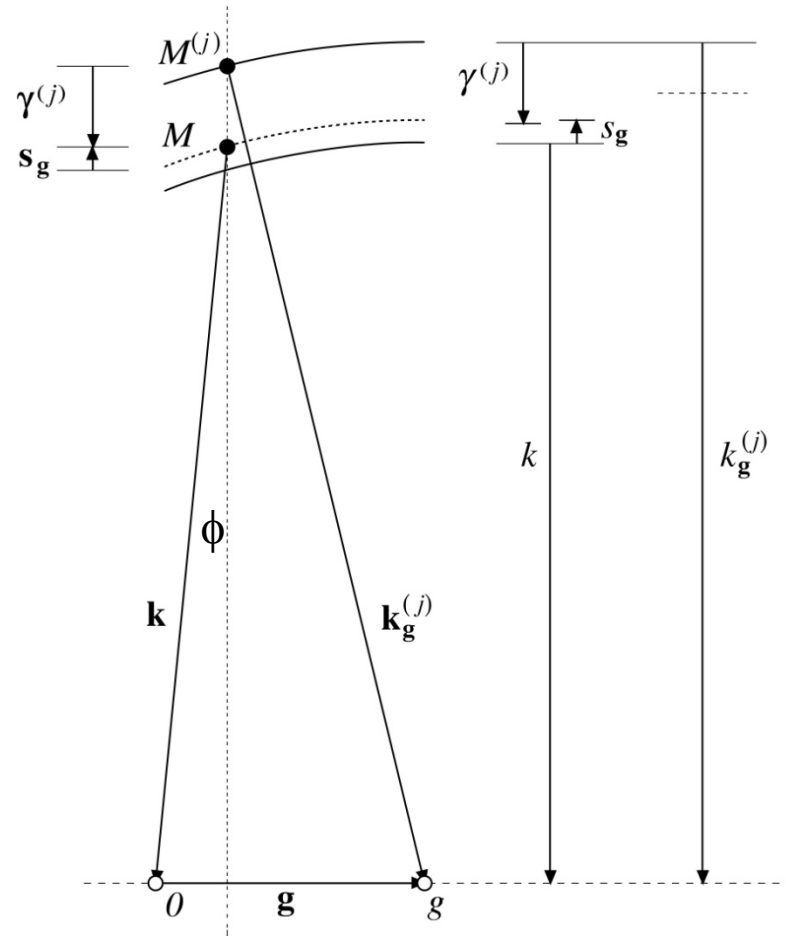
$$\mathbf{k} \cdot \hat{\mathbf{n}} = k \cdot \cos \phi$$

$$2\mathbf{k} \cdot (\gamma^{(j)} - \mathbf{s}_g) = 2k \cdot \cos \phi \cdot (\gamma^{(j)} - s_g)$$

Assume $\phi = 0$

This gives:

$$2k \cdot (\gamma^{(j)} - s_g) C_g^{(j)} = \sum_{\mathbf{h} \neq \mathbf{g}} U_{\mathbf{g}-\mathbf{h}} C_h^{(j)}$$



Extinction distance

We can now write:

$$s_{\mathbf{g}} C_{\mathbf{g}}^{(j)} + \sum_{\mathbf{h} \neq \mathbf{g}} \left(\frac{U_{\mathbf{g}-\mathbf{h}}}{2k} \right) C_{\mathbf{h}}^{(j)} = \gamma^{(j)} C_{\mathbf{g}}^{(j)}$$

Define the *extinction distance*:

$$\xi_{\mathbf{g}-\mathbf{h}} \equiv \frac{k}{U_{\mathbf{g}-\mathbf{h}}} = \frac{\pi\nu}{\lambda F_{\mathbf{g}-\mathbf{h}}}$$

The characteristic length over which 100% of beam diffracts from one particular channel into another (if no other effects are present).

$$\xi_{\mathbf{g}} \equiv \frac{\pi\nu}{\lambda F_{\mathbf{g}}}$$

$$s_{\mathbf{g}} C_{\mathbf{g}}^{(j)} + \sum_{\mathbf{h} \neq \mathbf{g}} \left(\frac{1}{2\xi_{\mathbf{g}-\mathbf{h}}} \right) C_{\mathbf{h}}^{(j)} = \gamma^{(j)} C_{\mathbf{g}}^{(j)}$$

Eigenvalue Problem

This has the form of an eigenvalue problem. $\tilde{A}|\psi^{(j)}\rangle = \gamma^{(j)}|\psi^{(j)}\rangle$

Where \tilde{A} is a matrix:

$$|\psi^{(j)}\rangle = \begin{pmatrix} C_0^{(j)} \\ C_{\mathbf{g}_1}^{(j)} \\ C_{\mathbf{g}_2}^{(j)} \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

$$\tilde{A} = \begin{pmatrix} s_0 & \frac{1}{2\xi_{\mathbf{g}_1}} & \cdot & \frac{1}{2\xi_{\mathbf{g}_{n-1}}} \\ \frac{1}{2\xi_{\mathbf{g}_1}} & s_{\mathbf{g}_1} & \cdot & \frac{1}{2\xi_{\mathbf{g}_{n-1}-\mathbf{g}_1}} \\ \cdot & \cdot & \cdot & \cdot \\ \frac{1}{2\xi_{\mathbf{g}_{n-1}}} & \frac{1}{2\xi_{\mathbf{g}_1-\mathbf{g}_{n-1}}} & \cdot & s_{\mathbf{g}_{n-1}} \end{pmatrix}$$

This system of equations can be solved for the $\gamma^{(j)}$ and the $C_{\mathbf{g}}^{(j)}$

Two-beam condition

Only 0 and g are significant: $\psi(\mathbf{r}) = \left[\Psi_0(z) + \Psi_g(z) \cdot e^{2\pi i(\mathbf{g}+\mathbf{s})\cdot\mathbf{r}} \right] \cdot e^{2\pi i\mathbf{k}\cdot\mathbf{r}}$

So we only need two Bloch waves: $\psi(\mathbf{r}) = \varepsilon^{(1)}\psi^{(1)}(\mathbf{r}) + \varepsilon^{(2)}\psi^{(2)}(\mathbf{r})$

$$\psi^{(1)}(\mathbf{r}) = C_0^{(1)}e^{2\pi i\mathbf{k}^{(1)}\cdot\mathbf{r}} + C_g^{(1)}e^{2\pi i[\mathbf{k}^{(1)}+\mathbf{g}]\cdot\mathbf{r}} = \left(C_0^{(1)} + C_g^{(1)}e^{2\pi i\mathbf{g}\cdot\mathbf{r}} \right) e^{2\pi i\gamma^{(1)}z} e^{2\pi i\mathbf{k}\cdot\mathbf{r}} \quad \varepsilon^{(1)} = \left[C_0^{(1)} \right]^*$$

$$\psi^{(2)}(\mathbf{r}) = C_0^{(2)}e^{2\pi i\mathbf{k}^{(2)}\cdot\mathbf{r}} + C_g^{(1)}e^{2\pi i[\mathbf{k}^{(2)}+\mathbf{g}]\cdot\mathbf{r}} = \left(C_0^{(2)} + C_g^{(2)}e^{2\pi i\mathbf{g}\cdot\mathbf{r}} \right) e^{2\pi i\gamma^{(2)}z} e^{2\pi i\mathbf{k}\cdot\mathbf{r}} \quad \varepsilon^{(2)} = \left[C_0^{(2)} \right]^*$$

Assume the structure factor is real: $F_{-\mathbf{g}} = (F_{\mathbf{g}})^* = F_{\mathbf{g}}$

Then: $U_{\mathbf{g}} = U_{-\mathbf{g}} \quad \xi_{\mathbf{g}} = \xi_{-\mathbf{g}} (= \xi) \quad s_{\mathbf{g}} = s$

The problem becomes:

$$\tilde{A} = \begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & s \end{pmatrix} \quad |\psi^{(1)}\rangle = \begin{pmatrix} C_0^{(1)} \\ C_g^{(1)} \end{pmatrix} \quad |\psi^{(2)}\rangle = \begin{pmatrix} C_0^{(2)} \\ C_g^{(2)} \end{pmatrix}$$

Solving the two-beam condition

We need to solve a 2×2 eigenvalue problem:

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & s \end{pmatrix} \begin{pmatrix} C_0 \\ C_g \end{pmatrix} = \gamma \begin{pmatrix} C_0 \\ C_g \end{pmatrix}$$

Here's how to do it:

$$\begin{aligned} (\tilde{A} - \gamma \tilde{1}) \cdot \begin{pmatrix} C_0 \\ C_g \end{pmatrix} = 0 \cdot \begin{pmatrix} C_0 \\ C_g \end{pmatrix} &\Rightarrow \det \begin{pmatrix} -\gamma & \frac{1}{2\xi} \\ \frac{1}{2\xi} & s - \gamma \end{pmatrix} = 0 & \begin{aligned} -\gamma(s - \gamma) - \left(\frac{1}{2\xi}\right)^2 &= 0 \\ \gamma^2 - s\gamma - \left(\frac{1}{2\xi}\right)^2 &= 0 \end{aligned} \end{aligned}$$

Two eigenvalues:

$$\gamma^{(1,2)} = \frac{s \pm \sqrt{s^2 + \frac{1}{\xi^2}}}{2}$$

and two eigenfunctions:

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & s \end{pmatrix} \begin{pmatrix} C_0^{(1,2)} \\ C_g^{(1,2)} \end{pmatrix} = \gamma^{(1,2)} \begin{pmatrix} C_0^{(1,2)} \\ C_g^{(1,2)} \end{pmatrix}$$

Special case, strong beam ($s=0$)

$$\gamma^{(1)} = \frac{1}{2\xi}, \quad \gamma^{(2)} = -\frac{1}{2\xi}$$

Now find the C 's:

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & 0 \end{pmatrix} \begin{pmatrix} C_0^{(1)} \\ C_g^{(1)} \end{pmatrix} = \frac{1}{2\xi} \begin{pmatrix} C_0^{(1)} \\ C_g^{(1)} \end{pmatrix}, \quad |\psi^{(1)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & 0 \end{pmatrix} \begin{pmatrix} C_0^{(2)} \\ C_g^{(2)} \end{pmatrix} = -\frac{1}{2\xi} \begin{pmatrix} C_0^{(2)} \\ C_g^{(2)} \end{pmatrix}, \quad |\psi^{(2)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Finally, find the $\varepsilon^{(j)}$'s: $\varepsilon^{(1)} = \frac{1}{\sqrt{2}}, \quad \varepsilon^{(2)} = \frac{1}{\sqrt{2}}$

The strong, two-beam solution

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{2}}\psi^{(1)}(\mathbf{r}) + \frac{1}{\sqrt{2}}\psi^{(2)}(\mathbf{r})$$

$$\psi^{(1)}(\mathbf{r}) = \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right) \cdot e^{\pi i z / \xi} \cdot e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$$

$$\psi^{(2)}(\mathbf{r}) = \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right) e^{-\pi i z / \xi} \cdot e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$$

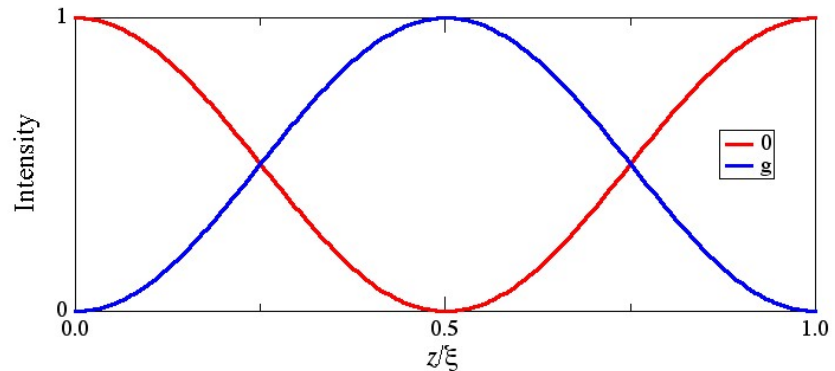
$$\psi(\mathbf{r}) = \left[\cos(\pi z / \xi) + i \sin(\pi z / \xi) e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right] e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$$

$$\Psi_0(z) = \cos(\pi z / \xi)$$

$$\Psi_g(z) = i \sin(\pi z / \xi)$$

$$|\Psi_0(z)|^2 = \cos^2(\pi z / \xi)$$

$$|\Psi_g(z)|^2 = \sin^2(\pi z / \xi)$$



The general two-beam solution

The amplitudes are related by:

$$i) \frac{1}{2\xi} C_{\mathbf{g}}^{(1,2)} = \gamma^{(1,2)} C_0^{(1,2)}$$

$$ii) \frac{1}{2\xi} C_0^{(1,2)} + s C_{\mathbf{g}}^{(1,2)} = \gamma^{(1,2)} C_{\mathbf{g}}^{(1,2)}$$

Define: $w \equiv s\xi$

$$\Rightarrow 2\xi\gamma^{(1,2)} = w \pm \sqrt{w^2 + 1}$$

$$2\gamma^{(1,2)} = s \pm \sqrt{s^2 + \frac{1}{\xi^2}}$$

Normalize:

$$\left(C_0^{(1,2)}\right)^2 + \left(C_{\mathbf{g}}^{(1,2)}\right)^2 = 1$$

$$\Rightarrow \left(C_0^{(1,2)}\right)^2 \left[1 + \left(w \pm \sqrt{w^2 + 1}\right)^2\right] = 1$$

Now define: $\cot \beta \doteq w$

$$\Rightarrow \left(C_0^{(1,2)}\right)^2 = \frac{\sin^2 \beta}{2 \pm 2 \cos \beta}$$

Combine:

$$\left(C_0^{(1)}\right)^2 = \sin^2 (\beta/2)$$

$$\left(C_0^{(2)}\right)^2 = \cos^2 (\beta/2)$$

We can pick:

$$C_0^{(1)} = \sin (\beta/2)$$

$$C_0^{(2)} = \cos (\beta/2)$$

Finding the Bloch waves

Now find the \mathbf{g} coefficient of the Bloch wave: $C_{\mathbf{g}}^{(1,2)} = 2\xi\gamma^{(1,2)}C_0^{(1,2)}$

The factor in front can be written as:

$$2\xi\gamma^{(1,2)} = \frac{\cos(\beta) \pm 1}{\sin(\beta)}$$

$$C_{\mathbf{g}}^{(1)} = \cos(\beta/2)$$

$$C_{\mathbf{g}}^{(2)} = -\sin(\beta/2)$$

$$|\psi^{(1)}\rangle = \begin{pmatrix} C_0^{(1)} \\ C_{\mathbf{g}}^{(1)} \end{pmatrix} = \begin{pmatrix} \sin(\beta/2) \\ \cos(\beta/2) \end{pmatrix}$$

$$|\psi^{(2)}\rangle = \begin{pmatrix} C_0^{(2)} \\ C_{\mathbf{g}}^{(2)} \end{pmatrix} = \begin{pmatrix} \cos(\beta/2) \\ -\sin(\beta/2) \end{pmatrix}$$

$$\psi^{(1)}(\mathbf{r}) = \left[\sin(\beta/2) + \cos(\beta/2) \cdot e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right] \cdot e^{\pi i (s+s_{eff})z} \cdot e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$$

$$\psi^{(2)}(\mathbf{r}) = \left[\cos(\beta/2) - \sin(\beta/2) \cdot e^{2\pi i \mathbf{g} \cdot \mathbf{r}} \right] \cdot e^{\pi i (s-s_{eff})z} \cdot e^{2\pi i \mathbf{k} \cdot \mathbf{r}}$$

$$\psi(\mathbf{r}) = \sin(\beta/2) \cdot \psi^{(1)}(\mathbf{r}) + \cos(\beta/2) \cdot \psi^{(2)}(\mathbf{r})$$

Two-beam result

Define: $s_{eff} \equiv \sqrt{s^2 + \left(\frac{1}{\xi^2}\right)}$ $\gamma^{(1,2)} \equiv \frac{s \pm s_{eff}}{2}$ ($s_{eff} \geq 0$)

Using diffracted beams: $\psi(\mathbf{r}) = \left[\Psi_0(z) + \Psi_g(z) \cdot e^{2\pi i(\mathbf{g}+\mathbf{s})\cdot\mathbf{r}} \right] \cdot e^{2\pi i\mathbf{k}\cdot\mathbf{r}}$

$$\Psi_0(z) = \left[\sin^2(\beta/2) e^{\pi i s_{eff} z} + \cos^2(\beta/2) e^{-\pi i s_{eff} z} \right] e^{\pi i s z} = \left[\cos(\pi s_{eff} z) - i \cos(\beta) \sin(\pi s_{eff} z) \right] e^{\pi i s z}$$

$$\Psi_g(z) = \frac{1}{2} \sin \beta \cdot (e^{\pi i s_{eff} z} - e^{-\pi i s_{eff} z}) \cdot e^{-2\pi i s z} \cdot e^{\pi i s z} = i \sin(\beta) \sin(\pi s_{eff} z) e^{-\pi i s z}$$

$$w = s\xi = \cot(\beta)$$

$$\sin(\beta) = \frac{1}{\sqrt{1 + \cot^2(\beta)}} = \frac{1}{\sqrt{1 + w^2}} = \frac{1}{s_{eff} \xi}$$

$$\cos(\beta) = \frac{1}{\sqrt{1 + \tan^2(\beta)}} = \frac{w}{\sqrt{1 + w^2}} = \frac{s}{s_{eff}}$$

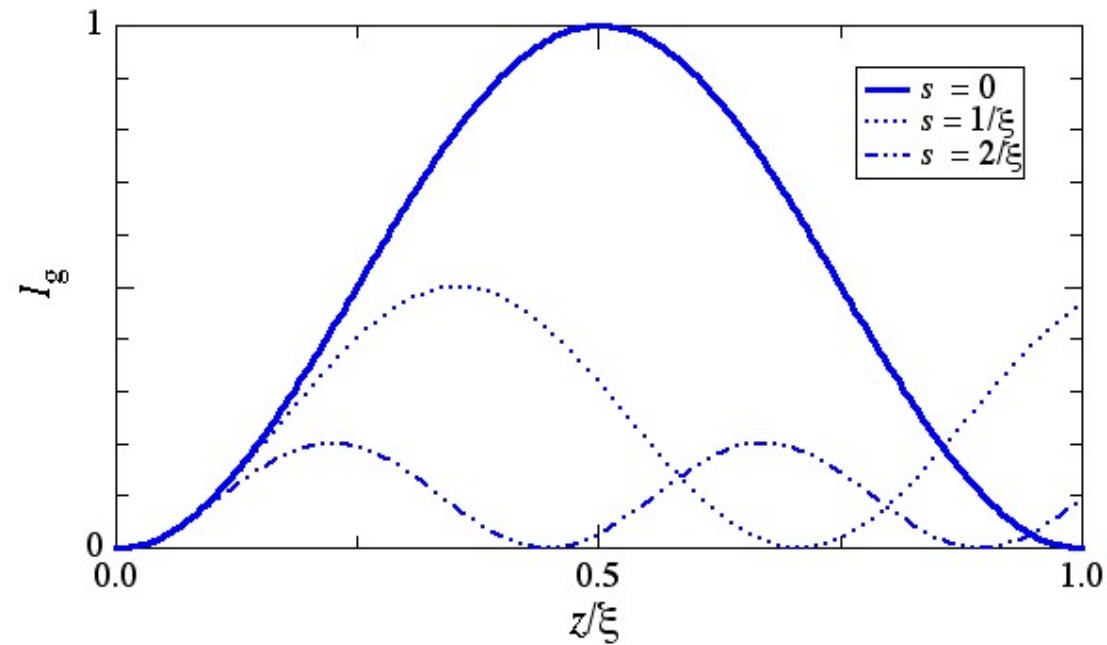
$$\Psi_0(z) = \left[\cos(\pi s_{eff} z) - i \left(\frac{s}{s_{eff}} \right) \sin(\pi s_{eff} z) \right] e^{\pi i s z}$$

$$\Psi_g(z) = \frac{i \sin(\pi s_{eff} z)}{s_{eff} \xi} e^{-\pi i s z}$$

Two-beam intensity

Now find the diffracted intensity:

$$I_{\mathbf{g}} = |\psi_{\mathbf{g}}|^2 = \left[\frac{\sin(\pi s_{\text{eff}} z)}{s_{\text{eff}} \xi} \right]^2 \quad s_{\text{eff}} \equiv \sqrt{s_{\mathbf{g}}^2 + \left(\frac{1}{\xi_{\mathbf{g}}^2} \right)}$$



Howie-Whelan Equations

Diffracted Beam Amplitude:

$$\Psi_{\mathbf{g}}(z) = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\gamma^{(j)} - s_{\mathbf{g}}]z}$$

Take the Derivative:

$$\frac{d\Psi_{\mathbf{g}}}{dz} = \sum_j \left\{ 2\pi i[\gamma^{(j)} - s_{\mathbf{g}}] \right\} \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} e^{2\pi i[\gamma^{(j)} - s_{\mathbf{g}}]z}$$

Condition on Block-Waves:

$$(\gamma^{(j)} - s_{\mathbf{g}}) C_{\mathbf{g}}^{(j)} = \sum_{\mathbf{h} \neq \mathbf{g}} \left(\frac{1}{2\xi_{\mathbf{g}-\mathbf{h}}} \right) C_{\mathbf{h}}^{(j)}$$

Substitute and Group:

$$\frac{d\Psi_{\mathbf{g}}}{dz} = \sum_{\mathbf{h} \neq \mathbf{g}} \left(\frac{\pi i}{\xi_{\mathbf{g}-\mathbf{h}}} \right) \left[\sum_j \varepsilon^{(j)} C_{\mathbf{h}}^{(j)} e^{2\pi i(\gamma^{(j)} - s_{\mathbf{h}})z} \right] \cdot e^{2\pi i(s_{\mathbf{h}} - s_{\mathbf{g}})z}$$

Substitute again:

$$\frac{d\Psi_{\mathbf{g}}}{dz} = \sum_{\mathbf{h} \neq \mathbf{g}} \left(\frac{\pi i}{\xi_{\mathbf{g}-\mathbf{h}}} \right) \Psi_{\mathbf{h}} e^{2\pi i(s_{\mathbf{h}} - s_{\mathbf{g}})z}$$

Beam amplitudes are expressed without any reference to Bloch waves.