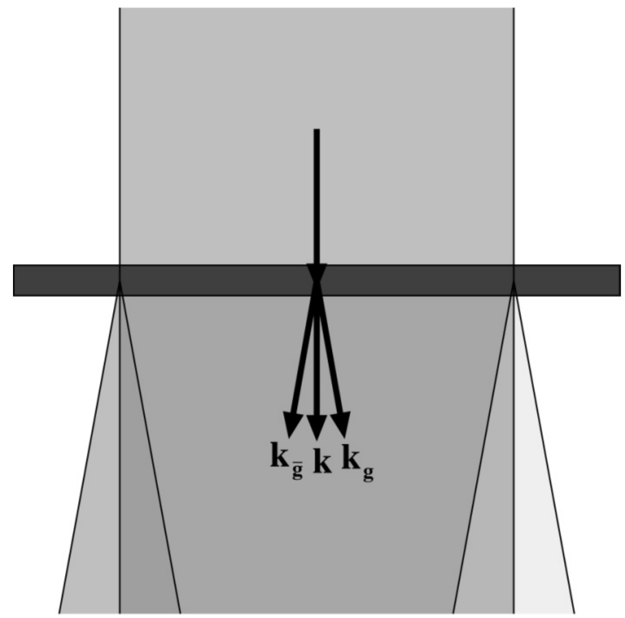
Total Wave Function

Wave function above sample is a plane wave:

$$\psi(\mathbf{r}) = e^{2\pi i \mathbf{k}\cdot\mathbf{r}}$$ //incident beam



Wave function below sample is a collection of diffracted beams (and **0**):

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

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

Intensities:

$$I_{\mathbf{g}} = \left|\Psi_{\mathbf{g}}\right|^2$$

We need to know the values of the $\Psi_{\mathbf{g}}$.

Electron energy in crystal potential

$$\sqrt{(pc)^2 + (m_0 c^2)^2} = mc^2$$

where: $E = e \cdot V_0$

$$mc^2 = E + m_0 c^2$$

$$\sqrt{\left[p(\mathbf{r})c\right]^2 + (m_0 c^2)^2} = mc^2 + e\Phi(\mathbf{r})$$

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

Expand:

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

$$\left[p(\mathbf{r})c\right]^2 + (m_0 c^2)^2 \approx (mc^2)^2 + 2(mc^2) \cdot e\Phi(\mathbf{r})$$

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

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

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:

$$\lambda = \frac{h}{\sqrt{2mE_{nr}}} \qquad k^2 = \frac{2mE_{nr}}{h^2}$$

Structure Function:

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

Wave Equation:

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

Bloch-wave solutions

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

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

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

The wave equation looks like:

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

Consider solutions of the form:

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

where:

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

These solutions are Bloch waves:

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

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:

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

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

Where: $\boldsymbol{\gamma}^{(j)} \equiv \mathbf{k}^{(j)} - \mathbf{k}$

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

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

Properties of Bloch waves (I)

The Bloch waves are quantum states:

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

We can normalize them:

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

Any two Bloch states are orthogonal:

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

Properties of Bloch waves (II)

The Bloch waves form an orthonormal set:

$$V=\begin{pmatrix} C_{\mathbf{g}_1}^{(1)} & C_{\mathbf{g}_1}^{(2)} & \cdots \\ C_{\mathbf{g}_2}^{(1)} & C_{\mathbf{g}2}^{(2)} & \\ \vdots & & \ddots \end{pmatrix}=\left(\left|\psi^{(1)}\right\rangle \quad \left|\psi^{(2)}\right\rangle \quad \ldots\right) \qquad V^{\dagger}=\begin{pmatrix} \left\langle\psi^{(1)}\right| \\ \left\langle\psi^{(2)}\right| \\ \vdots \end{pmatrix} \qquad V^{\dagger}V=I$$

Also: $\left(V^{T}\right)^{\dagger}V^{T}=I$

$$V^{T}=\begin{pmatrix} C_{\mathbf{g}_1}^{(1)} & C_{\mathbf{g}_2}^{(1)} & \cdots \\ C_{\mathbf{g}_1}^{(2)} & C_{\mathbf{g}2}^{(2)} & \\ \vdots & & \ddots \end{pmatrix}=\left(\left|\psi_{g_1}\right\rangle \quad \left|\psi_{g_2}\right\rangle \quad \cdots\right) \qquad \left(V^{T}\right)^{\dagger}=\begin{pmatrix} \left\langle\psi_{\mathbf{g}_1}\right| \\ \left\langle\psi_{\mathbf{g}2}\right| \\ \vdots \end{pmatrix}$$

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

$$\left\langle\psi_{\mathbf{g}}\middle|\psi_{\mathbf{g}}\right\rangle=\sum_j\left|C_{\mathbf{g}}^{(j)}\right|^2=1$$

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

Boundary condition(s) (I)

At the foil entrance surface, we must have:

i) $\psi\left(\mathbf{r}\right)$ continuous and *ii*) $\hat{\mathbf{n}}\cdot\nabla\psi\left(\mathbf{r}\right)$ 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: $\psi\left(\mathbf{r}\right) = \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}}$

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

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

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

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

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

Boundary Condition(s) (II)

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

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

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

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

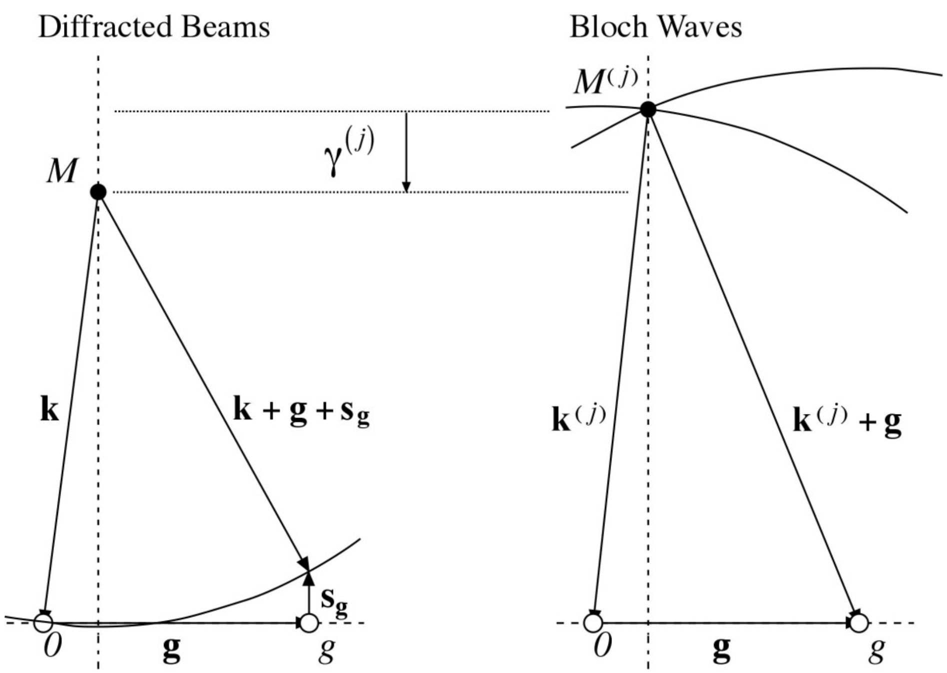
In other words:
$$\psi(\mathbf{r}) = \sum_j \left[C_{\mathbf{0}}^{(j)}\right]^* \psi^{(j)}(\mathbf{r})$$

Diffracted beam amplitudes

$$\psi(\mathbf{r}) = \sum_j \varepsilon^{(j)} \psi^{(j)}(\mathbf{r}) = \sum_{\mathbf{g}} \Psi_{\mathbf{g}}(\mathbf{r}) \mathrm{e}^{2\pi i(\mathbf{k}+\mathbf{g}+\mathbf{s_g})\cdot\mathbf{r}}$$

$$\Psi_{\mathbf{g}}(\mathbf{r}) = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} \mathrm{e}^{2\pi i\left[\mathbf{k}^{(j)}-\mathbf{k}-\mathbf{s_g}\right]\cdot\mathbf{r}} = \sum_j \varepsilon^{(j)} C_{\mathbf{g}}^{(j)} \mathrm{e}^{2\pi i\left[\gamma^{(j)}-\mathbf{s_g}\right]\cdot\mathbf{r}}$$

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



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

$$\mathbf{s_g} \cdot \mathbf{r} = s_g \cdot z$$

Solving for the Bloch-wave coefficients

Find the particular Bloch waves are solutions of:

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

$$K^2 \doteq k^2 + U_{\mathbf{0}} \left(\approx k^2\right)$$

The first term is:

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

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

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

Rearranging the sums

Break up the sum into two terms:

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

Reindex:

$$\mathbf{h}' = \mathbf{h} + \mathbf{g}'$$

$$\mathbf{h} = \mathbf{h}' - \mathbf{g}'$$

$$\mathbf{h} = \mathbf{0} \rightarrow \mathbf{h}' = \mathbf{g}'$$

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

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

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

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

Rewriting the sum

We want to simplify:

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

I.

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

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

$$=\left(\mathbf{k}+\mathbf{g}\right)^2+2\left(\mathbf{k}+\mathbf{g}\right)\cdot\boldsymbol{\gamma}^{(j)}+\gamma^{(j)2}$$

II.

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

$$k^2=\left(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}}\right)^2$$

$$=\left(\mathbf{k}+\mathbf{g}\right)^2+2\left(\mathbf{k}+\mathbf{g}\right)\cdot\mathbf{s}_{\mathbf{g}}-s_{\mathbf{g}}{}^2$$

I. - II.

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

So now we have:

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

High-energy approximation

$$\left(\mathbf{k}^{(j)}+\mathbf{g}\right)^2-k^2$$

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

$$\approx 2\mathbf{k}\cdot\left(\boldsymbol{\gamma}^{(j)}-\mathbf{s}_{\mathbf{g}}\right)$$

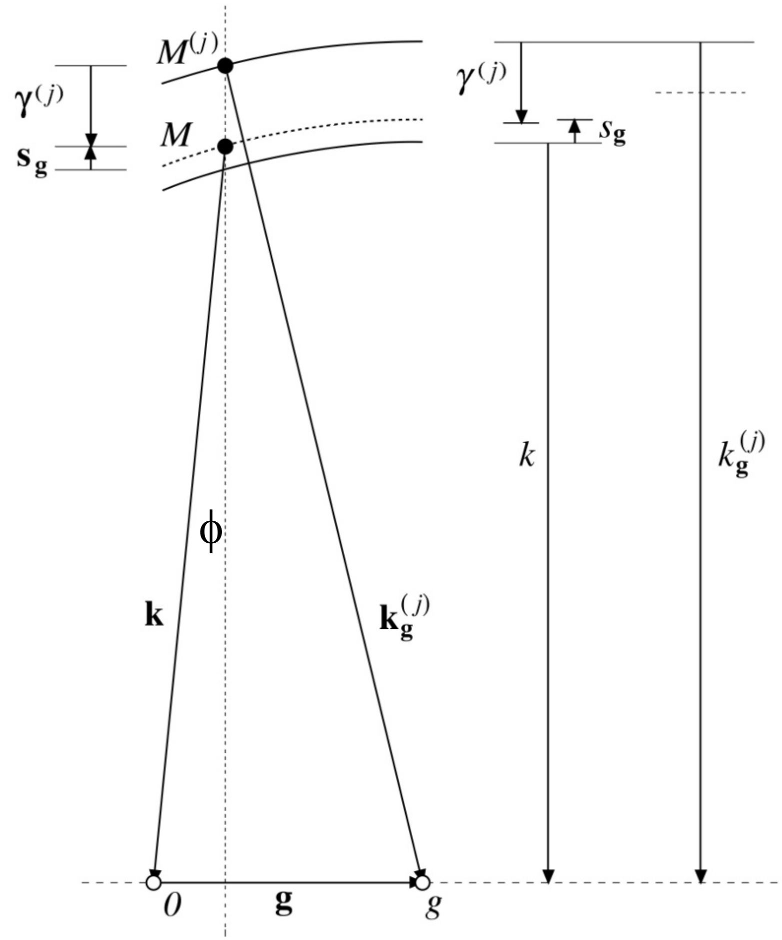
$$\mathbf{k}\cdot\hat{\mathbf{n}}=k\cdot\cos\phi$$

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

Assume $\phi=0$

This gives:

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



Structure Function

$$\Phi_{\mathbf{g}} = \phi(\mathbf{g}) \cdot X_{\mathbf{g}}$$ //Fourier coefficients of the crystal potential

$$U_{\mathbf{g}} = \frac{2me}{h^2}\Phi_{\mathbf{g}} = \frac{2me}{h^2} \cdot \phi(\mathbf{g}) \cdot X_{\mathbf{g}}$$ //Fourier coefficients of the structure function

$$\phi(\mathbf{g}) = \sum_{m \text{ atoms}} \phi^{(m)}(g) \mathrm{e}^{-2\pi i \mathbf{g} \cdot \mathbf{d}^{(m)}}$$ //Fourier transform of unit cell

$$f^{(m)}(g) = \frac{2\pi me}{h^2}\phi^{(m)}(g)$$ //atomic form factors

$$F_{\mathbf{g}} = \frac{2\pi me}{h^2} \cdot \phi(\mathbf{g}) = \sum_{m \text{ atoms}} f^{(m)}(g) \mathrm{e}^{-2\pi i \mathbf{g} \cdot \mathbf{d}^{(m)}}$$ //crystal structure factors

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

Extinction distance

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

Define the *extinction distance*: $$\xi_{\mathbf{g-h}} \equiv \frac{k}{U_{\mathbf{g-h}}} = \frac{\pi v}{\lambda F_{\mathbf{g-h}}}$$

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

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

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

Eigenvalue Problem

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

Where $\tilde{A}$ is a matrix:

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

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

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

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

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

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

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

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

The problem becomes:

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

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:

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

$$-\gamma\left(s - \gamma\right) - \left(\frac{1}{2\xi}\right)^2 = 0$$

$$\gamma^2 - s\gamma - \left(\frac{1}{2\xi}\right)^2 = 0$$

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)

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

Now find the C's:

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & 0 \end{pmatrix} \begin{pmatrix} C_0^{(1)} \\ C_{\mathbf{g}}^{(1)} \end{pmatrix} = \frac{1}{2\xi} \begin{pmatrix} C_0^{(1)} \\ C_{\mathbf{g}}^{(1)} \end{pmatrix},\ \left|\psi^{(1)}\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & \frac{1}{2\xi} \\ \frac{1}{2\xi} & 0 \end{pmatrix} \begin{pmatrix} C_0^{(2)} \\ C_{\mathbf{g}}^{(2)} \end{pmatrix} = -\frac{1}{2\xi} \begin{pmatrix} C_0^{(2)} \\ C_{\mathbf{g}}^{(2)} \end{pmatrix},\ \left|\psi^{(2)}\right\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

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

The strong, two-beam solution

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

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

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

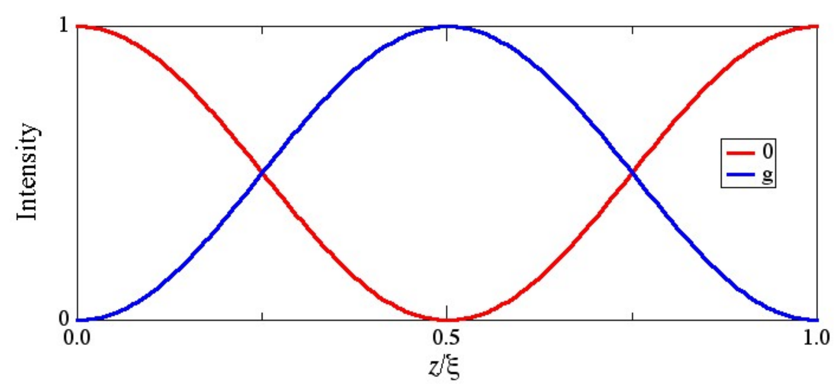
$$\psi(\mathbf{r}) = \left[\cos(\pi z/\xi) + i\sin(\pi z/\xi) e^{2\pi i \mathbf{g}\cdot\mathbf{r}}\right] e^{2\pi i \mathbf{k}\cdot\mathbf{r}}$$

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

$$\Psi_{\mathbf{g}}(z) = i\sin(\pi z/\xi)$$

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

$$\left|\Psi_{\mathbf{g}}(z)\right|^2 = \sin^2(\pi z/\xi)$$



The general two-beam solution

The amplitudes are related by:

$$i)\ \frac{1}{2\xi}C_{\mathbf{g}}^{(1,2)} = \gamma^{(1,2)}C_{\mathbf{0}}^{(1,2)}$$

$$ii)\ \frac{1}{2\xi}C_{\mathbf{0}}^{(1,2)} + sC_{\mathbf{g}}^{(1,2)} = \gamma^{(1,2)}C_{\mathbf{g}}^{(1,2)}$$

Define: $w \equiv s\xi$

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

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

Normalize:

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

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

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

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

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 **g** coefficient of the Bloch wave: $C_{\mathbf{g}}^{(1,2)} = 2\xi\gamma^{(1,2)} C_{\mathbf{0}}^{(1,2)}$

The factor in front can be written as:

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

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

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

$$\left|\psi^{(1)}\right\rangle = \begin{pmatrix} C_{\mathbf{0}}^{(1)} \\ C_{\mathbf{g}}^{(1)} \end{pmatrix} = \begin{pmatrix} \sin(\beta/2) \\ \cos(\beta/2) \end{pmatrix}$$

$$\left|\psi^{(2)}\right\rangle = \begin{pmatrix} C_{\mathbf{0}}^{(2)} \\ C_{\mathbf{g}}^{(2)} \end{pmatrix} = \begin{pmatrix} \cos(\beta/2) \\ -\sin(\beta/2) \end{pmatrix}$$

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

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

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

Two-beam result

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

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

$$\Psi_{\mathbf{0}}(z) = \left[\sin^2(\beta/2)\mathrm{e}^{\pi i s_{eff} z} + \cos^2(\beta/2)\mathrm{e}^{-\pi i s_{eff} z}\right]\mathrm{e}^{\pi i s z} = \left[\cos\left(\pi s_{eff} z\right) - i\cos(\beta)\sin\left(\pi s_{eff} z\right)\right]\mathrm{e}^{\pi i s z}$$

$$\Psi_{\mathbf{g}}(z) = \frac{1}{2}\sin\beta\cdot\left(\mathrm{e}^{\pi i s_{eff} z} - \mathrm{e}^{-\pi i s_{eff} z}\right)\cdot \mathrm{e}^{-2\pi i s z}\cdot \mathrm{e}^{\pi i s z} = i\sin(\beta)\sin\left(\pi s_{eff} z\right)\mathrm{e}^{-\pi i s z}$$

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

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

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

$$\Psi_{\mathbf{0}}(z) = \left[\cos\left(\pi s_{eff} z\right) - i\left(\frac{s}{s_{eff}}\right)\sin\left(\pi s_{eff} z\right)\right]\mathrm{e}^{\pi i s z}$$

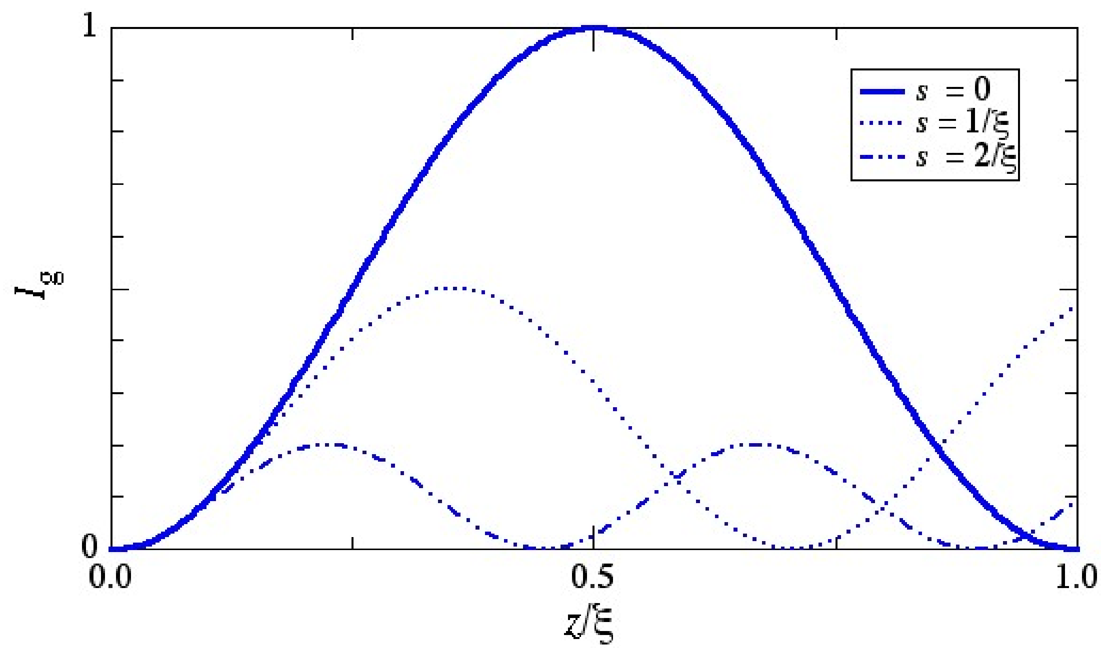
$$\Psi_{\mathbf{g}}(z) = \frac{i\sin\left(\pi s_{eff} z\right)}{s_{eff}\,\xi}\mathrm{e}^{-\pi i s z}$$

Two-beam intensity

Now find the diffracted intensity:

$$I_{\mathbf{g}} = \left|\psi_{\mathbf{g}}\right|^2 = \left[\frac{\sin\left(\pi s_{eff} z\right)}{s_{eff}\xi}\right]^2$$

$$s_{eff} \equiv \sqrt{s_{\mathbf{g}}{}^2 + \left(\frac{1}{\xi_{\mathbf{g}}{}^2}\right)}$$



Howie-Whelan Equations

Diffracted Beam Amplitude:

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

Take the Derivative:

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

Condition on Block-Waves:

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

Substitute and Group:

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

Substitute again:

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

Beam amplitudes are expressed without any reference to Bloch waves.