Fundamentals of Neutron Diffraction

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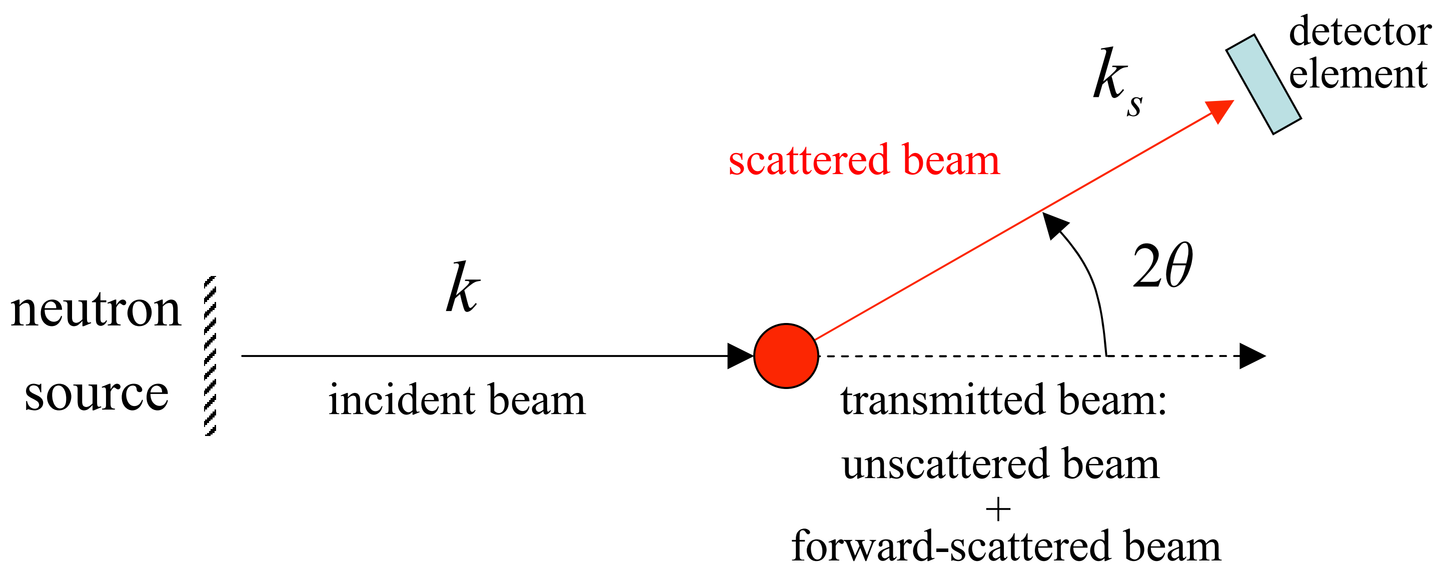
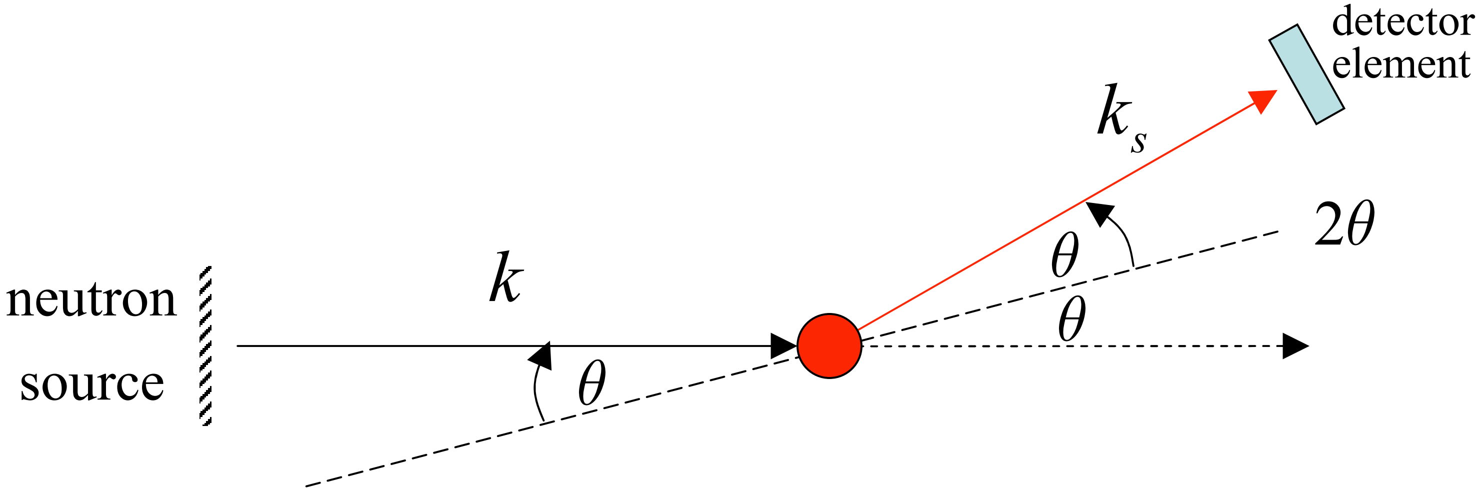
Basic Scattering Theory
SANS



detector
element
k_s
scattered beam
2θ
neutron
source
k
incident beam
transmitted beam:
unscattered beam
+
forward-scattered beam


detector
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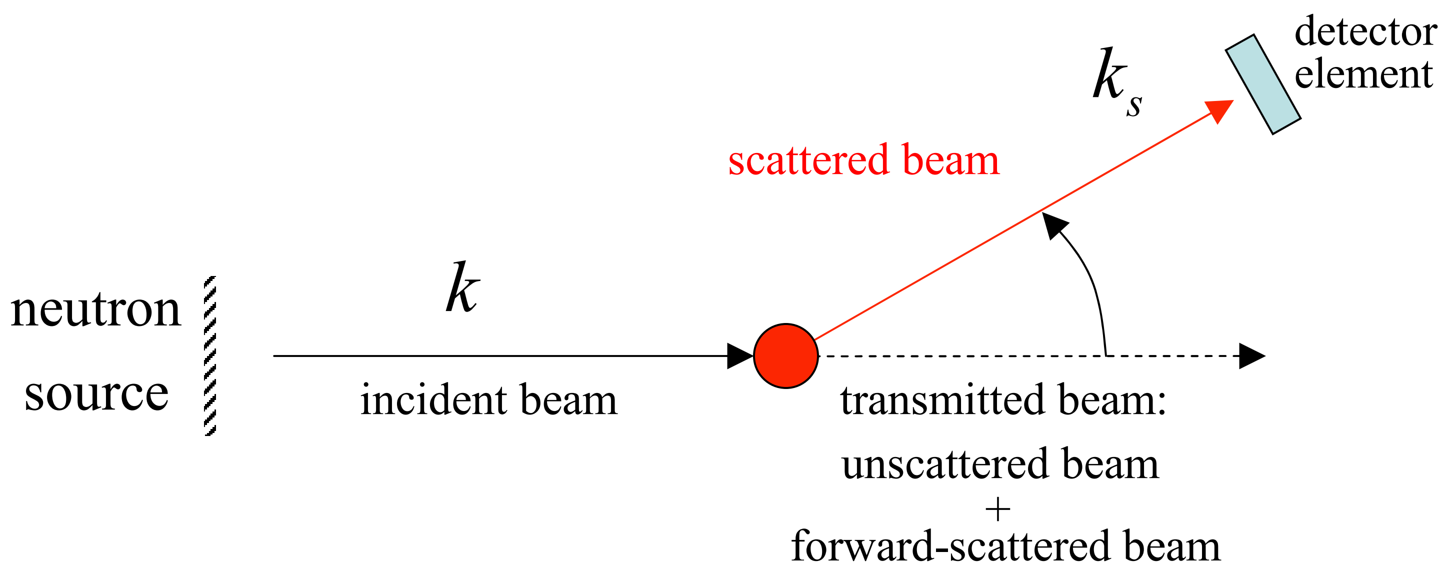
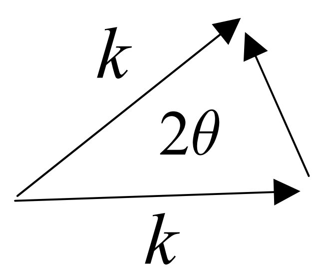


<u>Elastic scattering</u>

$$k_s = k = \frac{2\pi}{\lambda}$$

$$\mathbf{Q} = \mathbf{k}_s - \mathbf{k}$$



$$Q = 2k \sin\theta \simeq \frac{4\pi}{\lambda}\theta$$

Shrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{k},\mathbf{r})+V(\mathbf{r})\psi(\mathbf{k},\mathbf{r})=\frac{\hbar^2k^2}{2m}\psi(\mathbf{k},\mathbf{r})$$

$$V(\mathbf{r})=\frac{2\pi\hbar^2}{m}\sum_i b_i\delta(\mathbf{r}-\mathbf{R}_i)+g\boldsymbol{\mu}\bullet\mathbf{B}(\mathbf{r})$$

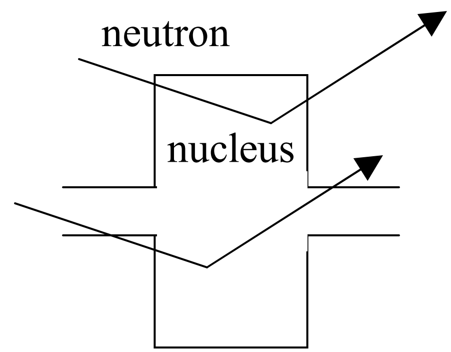
nuclear interaction:
Fermi "contact"

magnetic interaction:
nucleus spin
electron spins

$b_i =$ Fermi scattering length

sum over all nucleii at positions $\mathbf{R}_i$

$$b_i=\begin{cases}\text{positive (repulsive interaction)}\\ \text{negative (attractive interaction)}\end{cases}$$



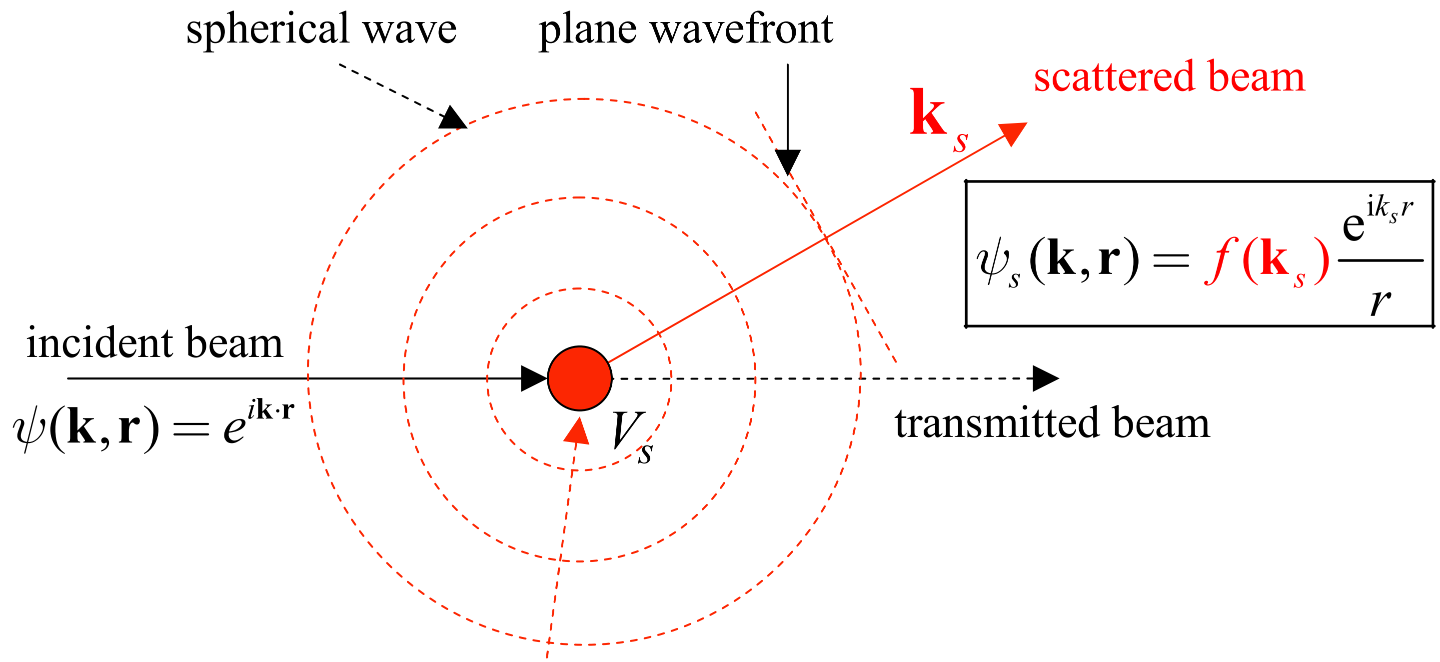
$$\frac{\hbar^2}{2m}\left[-\nabla^2\psi(\mathbf{k},\mathbf{r})+4\pi\rho(\mathbf{r})\psi(\mathbf{k},\mathbf{r})=k^2\psi(\mathbf{k},\mathbf{r})\right]$$

$$-\nabla^2\psi(\mathbf{k},\mathbf{r})+4\pi\rho(\mathbf{r})\psi(\mathbf{k},\mathbf{r})=k^2\psi(\mathbf{k},\mathbf{r})$$

$$\rho(\mathbf{r})=\sum_i b_i\delta(\mathbf{r}-\mathbf{R}_i)=\text{scattering length density (SLD)}$$

$$\left[L^{-2}\right] \qquad \left[L\right] \quad \left[L^{-3}\right]$$

$$-\nabla^2\psi(\mathbf{k},\mathbf{r})+4\pi\rho(\mathbf{r})\psi(\mathbf{k},\mathbf{r})=k^2\psi(\mathbf{k},\mathbf{r})$$



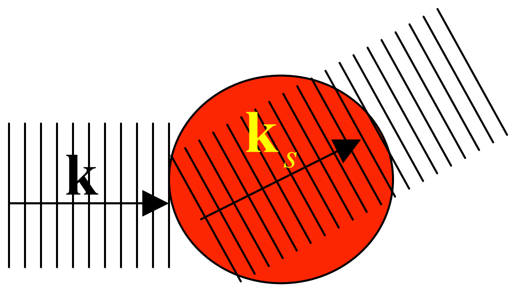
$$\boxed{\psi_s(\mathbf{k},\mathbf{r})=f(\mathbf{k}_s)\frac{\mathrm{e}^{ik_s r}}{r}}$$

$$f(\mathbf{k}_s)=\int_{V_s}\psi(\mathbf{k},\mathbf{r})\rho(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}d^3r$$

Exact ψ in scatterer

$$f(\mathbf{k}_s) = \int_{V_s} \psi(\mathbf{k},\mathbf{r})\rho(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} d^3r$$

$\boxed{\text{Born approximation ("Kinematic theory")}}$

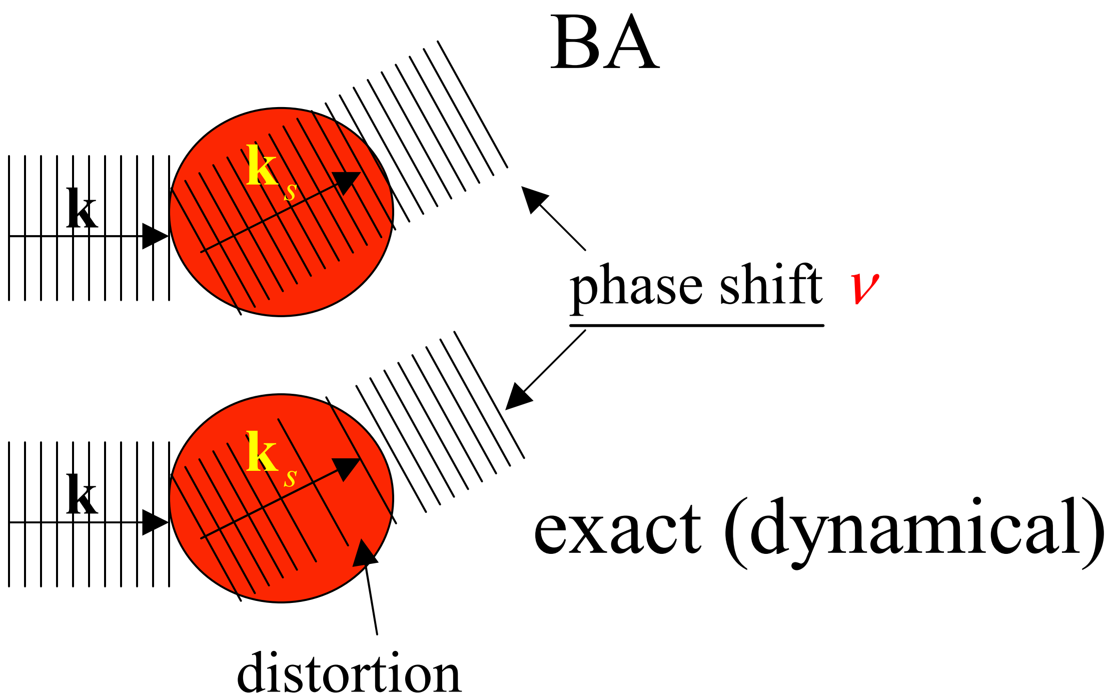


$\psi(\mathbf{k},\mathbf{r}) \approx \mathrm{e}^{\mathrm{i}\mathbf{k}_s\cdot\mathbf{r}}$ inside scatterer

$$\therefore f(\mathbf{k}_s) \approx \int_{V_s} \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}}\rho(\mathbf{r})\, d^3r$$

$$= \hat{\rho}(\mathbf{Q}) = \mathrm{FT}_{\mathbf{Q}}\rho(\mathbf{r})$$

When is the BA valid?



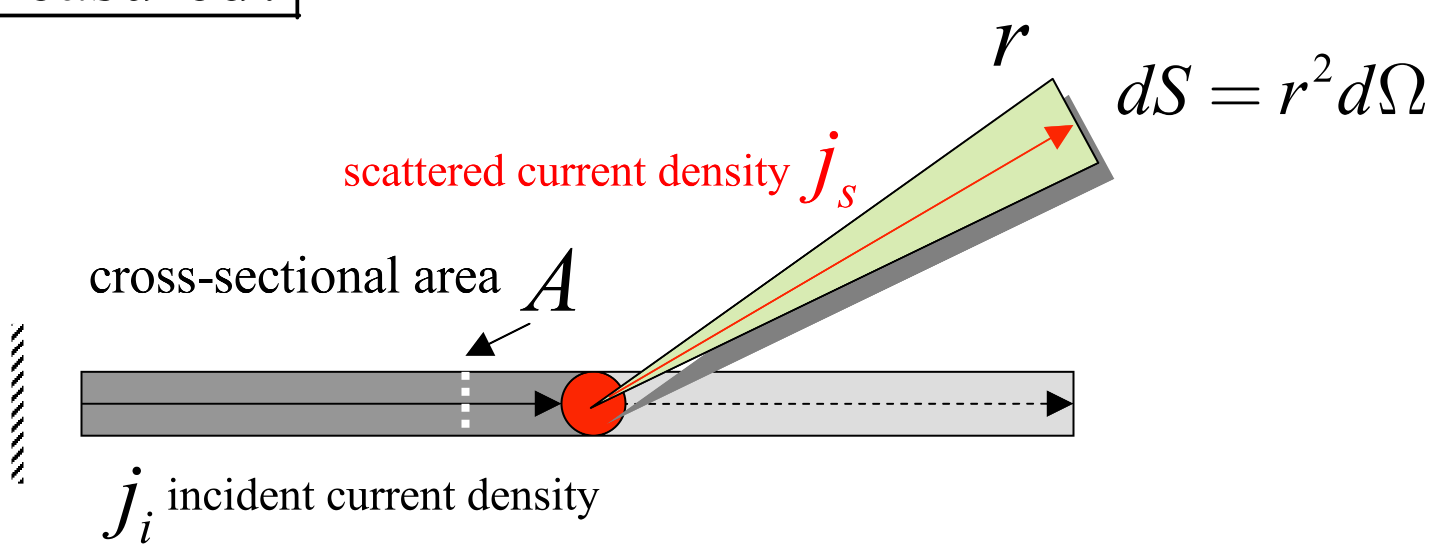
For a uniform sphere of radius R:

$$\therefore \nu_{\max} = 2R\rho\lambda = \frac{R[\mu m]\rho\left[10^{-4}nm^{-2}\right]\lambda[nm]}{5} \quad \left(\rho\left[10^{-4}nm^{-2}\right] = \rho\left[10^{-6}\text{Å}^{-2}\right]\right)$$

$e.g.$, for representative $\rho\left[10^{-4}nm^{-2}\right]\lambda[nm] = 5\times 1$, $\boxed{\nu_{\max} = R[\mu m]}$

BA exact as $\nu \to 0$; good for $\nu < 1$ (particles not too large)

What's measured?



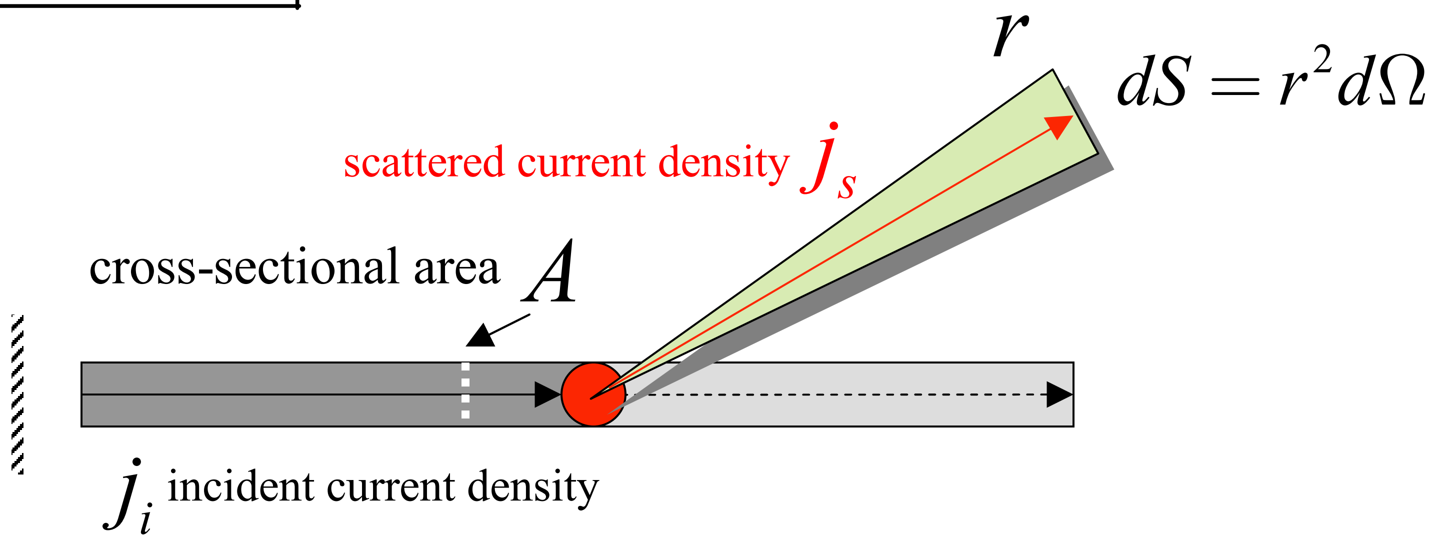
current: $J = \dfrac{dN}{dt} = jA$

current density: $j = \dfrac{dN}{dt} / A =$ "flux"

Differential Cross Section : $d\sigma$

$$j_s dS = j_i d\sigma$$

What's measured?



$$\therefore d\sigma = j_s dS / j_i = \frac{dN_s}{dN_i} A$$

$$d\sigma = \frac{\partial \sigma}{\partial \Omega} d\Omega = \frac{"d\sigma"}{d\Omega} d\Omega$$

What's calculated?

$$j = \frac{\hbar}{2mi}\left[\psi^* \nabla \psi - \psi \nabla \psi^*\right]$$

incident: $\psi_i = \mathrm{e}^{ikz}, \; j_i = \hbar k / m$

scattered: $\psi_s = f(\mathbf{k}_s)\dfrac{e^{ik_s r}}{r}, \; j_s = \dfrac{\hbar k_s}{m}\dfrac{\left|f(\mathbf{k}_s)\right|^2}{r^2}$

$$\therefore d\sigma = \frac{j_s(dS = r^2 d\Omega)}{j_i} = \frac{\cancel{k_s r^2}\left|f(\mathbf{k}_s)\right|^2}{\cancel{kr^2}}$$

$$\frac{\partial \sigma}{\partial \Omega} = \left|f(\mathbf{k}_s)\right|^2$$

What's measured/calulated?

NOTE: we want to know $f(\mathbf{k}_s)$, since $f(\mathbf{k}_s) \approx \hat{\rho}(\mathbf{Q})$,

and then $\rho(\mathbf{r}) \approx \mathrm{FT}^{-1}\hat{\rho}(\mathbf{Q})$;

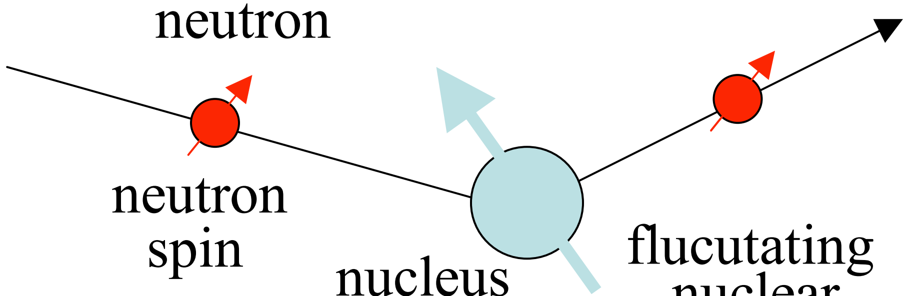
… but we directly measure $\left|\hat{\rho}(\mathbf{Q})\right|^2$.

The "phase problem": can we get $\hat{\rho}(\mathbf{Q})$ from $\left|\hat{\rho}(\mathbf{Q})\right|^2$?

$$\frac{\partial\sigma}{\partial\Omega} = \left|f(\mathbf{k}_s)\right|^2 \rightarrow \left\langle \left|f(\mathbf{k}_s)\right|^2 \right\rangle$$

thermal motions
random configurations
random orientations
spin degrees of freedom
...other uncontrolled DOF

Coherent & Incoherent Scattering



$$b_{\mathrm{coh},n} = \langle b_n \rangle_{\substack{\mathrm{nuc}\\ \mathrm{spin}}}$$ coherent

$$b_{\mathrm{inc},n} = \sqrt{\langle b_n^2 \rangle_{\substack{\mathrm{nuc}\\ \mathrm{spin}}} - \langle b_n \rangle^2_{\substack{\mathrm{nuc}\\ \mathrm{spin}}}}$$ incoherent (fluctuation variance)

$$4\pi b_{\mathrm{inc},n}^2 = \sigma_{\mathrm{inc},n}$$

Coh/Inc Rule:

$$\boxed{\langle b_m b_n \rangle = b_{\mathrm{inc,n}}^2 \delta_{m,n} + b_{\mathrm{coh},m} b_{\mathrm{coh},n}}$$

$$\frac{\partial\sigma}{\partial\Omega} = \left\langle \left| f(\mathbf{k}_s) \right|^2 \right\rangle \to \left\langle \left| \hat{\rho}(\mathbf{Q}) \right|^2 \right\rangle$$

$$= \left\langle \left| \mathrm{FT}_{\mathbf{Q}} \sum_n b_n \delta(\mathbf{r} - \mathbf{R}_n) \right|^2 \right\rangle = \left\langle \left| \sum_n b_n \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet\mathbf{R}_n} \right|^2 \right\rangle$$ (Rayleigh-Gans construction)

$$= \left\langle \sum_{m,n} \left\langle b_m b_n \right\rangle_{\substack{\text{nuc}\\ \text{spin}}} \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m - \mathbf{R}_n)} \right\rangle = \left\langle \sum_{m,n} \left(b_{\mathrm{inc,n}}^2 \delta_{m,n} + b_{\mathrm{coh},m} b_{\mathrm{coh},n} \right) \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m - \mathbf{R}_n)} \right\rangle$$

$$= \sum_n b_{\mathrm{inc},n}^2 + \left\langle \sum_{m,n} b_{\mathrm{coh},m} b_{\mathrm{coh},n} \; \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m - \mathbf{R}_n)} \right\rangle$$

$$\frac{\partial\sigma}{\partial\Omega} = \sum_n \frac{\sigma_{\mathrm{inc},n}}{4\pi} + \left\langle \sum_{m,n} b_{\mathrm{coh},m} b_{\mathrm{coh},n}\, \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m - \mathbf{R}_n)} \right\rangle$$

$$\left.\frac{\partial\sigma}{\partial\Omega}\right|_{\mathrm{inc}} \qquad \left.\frac{\partial\sigma}{\partial\Omega}\right|_{\mathrm{coh}}$$

structure <u>in</u>dependent (a major contribution to background)

structure dependent

$$\sigma_{\mathrm{coh}} / V = \Sigma, \text{ "macroscopic" cross-section}$$

$$\left[L^2\right] / \left[L^3\right] \quad \left[L^{-1}\right]$$

Notation alert: $\left.\frac{\partial\sigma}{\partial\Omega}\right|_{\mathrm{coh}} \to \frac{d\Sigma}{d\Omega}$, etc.

Isotropic scattering

... average over random orientations

$$\left.\frac{\partial\sigma}{\partial\Omega}\right|_{\text{coh}} = \left\langle \sum_{m,n} b_{\text{coh},m} b_{\text{coh},n}\, \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m-\mathbf{R}_n)} \right\rangle_{\text{random orientation}}$$

$$= \left\langle \sum_{m,n} b_{\text{coh},m} b_{\text{coh},n}\, \mathrm{e}^{\mathrm{i}\mathbf{Q}\bullet(\mathbf{R}_m-\mathbf{R}_n)} \right\rangle_{\text{direction of } \mathbf{Q}}$$

$$= \sum_{m,n} b_{\text{coh},m} b_{\text{coh},n}\, \mathrm{sinc}\left[\frac{Q\left|\mathbf{R}_m-\mathbf{R}_n\right|}{\pi}\right]$$

$$\mathrm{sinc}(\mathrm{x}) = \frac{\sin(\pi x)}{\pi x} = j_0(\pi x)$$

"Fundamental Theorem of Diffraction"

1. Born Approximation

2. Convolution-product theorem:

$$(2\pi)^{-3}\int\left\langle\left|\hat{\rho}(\mathbf{Q})\right|^{2}\right\rangle \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}}d^{3}Q=\int_{V}\rho(\mathbf{r}+\mathbf{r}')\rho(\mathbf{r}')d^{3}r'$$

3. $$\left.\frac{\partial\sigma}{\partial\Omega}\right|_{\mathrm{coh}}=\left\langle\left|\hat{\rho}(\mathbf{Q})\right|^{2}\right\rangle=\mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}}\Gamma(\mathbf{r})\int_{V}\mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}}\Gamma(\mathbf{r})d^{3}r'$$

4. $$\Gamma(\mathbf{r})=\int_{V}\left\langle\rho(\mathbf{r}+\mathbf{r}')\rho(\mathbf{r}')\right\rangle d^{3}r'$$

$$\Gamma(0)=V\left\langle\rho^{2}\right\rangle$$

$$\Gamma(\infty)=\int_{V}\left\langle\rho(\infty+\mathbf{r}')\right\rangle\left\langle\rho(\mathbf{r}')\right\rangle d^{3}r'=V\left\langle\rho\right\rangle^{2}$$

asymptotic independence

4. $\Gamma(\mathbf{r}) = \int \left\langle \rho(\mathbf{r}+\mathbf{r}')\rho(\mathbf{r}') \right\rangle d^3r'$

$$\Gamma(0) = V\left\langle \rho^2 \right\rangle$$

$$\Gamma(\infty) = V\left\langle \rho \right\rangle^2$$

<u>Debye-Porod correlation function</u>

5. $\boxed{\gamma(\mathbf{r}) = \dfrac{\Gamma(\mathbf{r}) - \Gamma(\infty)}{\Gamma(0) - \Gamma(\infty)}}$ $\quad \therefore \gamma(\mathbf{r}) = \int \left\langle \Delta\rho(\mathbf{r}+\mathbf{r}')\Delta\rho(\mathbf{r}') \right\rangle d^3r'$

<u>fluctuation correlation function</u>

$$\gamma(0) = 1$$

$$\gamma(\infty) = 0$$

$$\Gamma(\mathbf{r}) = V\left\langle \rho \right\rangle^2 + V\left\langle (\Delta\rho)^2 \right\rangle \gamma(\mathbf{r}),$$

$\left\langle (\Delta\rho)^2 \right\rangle = \left\langle \rho^2 \right\rangle - \left\langle \rho \right\rangle^2$ = <u>contrast</u>

3. $$\left.\frac{\partial\sigma}{\partial\Omega}\right|_{\mathrm{coh}} = \int \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}}\,\Gamma(\mathbf{r})\,d^3r'$$

6.

incoherent background | forward scattering

$$\boxed{\begin{aligned}\frac{\partial\sigma}{\partial\Omega} &= N\left\langle b_{\mathrm{inc}}^2\right\rangle + (2\pi)^3 V\left\langle \rho_{\mathrm{coh}}^2\right\rangle \delta(\mathbf{Q}) \\ &\quad + V\left\langle(\Delta\rho)^2\right\rangle \int \mathrm{e}^{i\mathbf{Q}\cdot\mathbf{r}}\,\gamma(\mathbf{r})\,d^3r'\end{aligned}}$$

coherent scattering from microstructure (needs contrast)

In 2-phase (A-B) system: $\left\langle(\Delta\rho)^2\right\rangle = \varphi_A\varphi_B\left(\rho_A-\rho_B\right)^2,\ \varphi_A+\varphi_B=1$

$$\boxed{\begin{aligned}\frac{\partial\sigma}{\partial\Omega} &= N\left\langle b_{\text{inc}}^2\right\rangle + (2\pi)^3 V\left\langle \rho_{\text{coh}}^2\right\rangle \delta(\mathbf{Q}) \\ &\quad + V\left\langle (\Delta\rho)^2\right\rangle \int \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}}\gamma(\mathbf{r})\,d^3r'\end{aligned}}$$

Notation alert: $\frac{\partial\sigma}{\partial\Omega} \triangleq V\left\langle (\Delta\rho)^2\right\rangle \int \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}}\gamma(\mathbf{r})\,d^3r'$

$$\therefore \quad \boxed{\frac{\partial\sigma}{\partial\Omega} = V\left\langle (\Delta\rho)^2\right\rangle S(\mathbf{Q})}$$

where

$S(\mathbf{Q}) = \int \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}}\gamma(\mathbf{r})\,d^3r'$ "scattering function"

Aside: more generally:

$$S(\mathbf{Q}) = \int S(\mathbf{Q},\omega)\,d\omega$$

The scattering function

$$S(\mathbf{Q}) = \quad \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}} \gamma(\mathbf{r})\, d^3 r'$$

$$\boxed{\begin{array}{l} \dfrac{1}{(2\pi)^3} \displaystyle\int S(\mathbf{Q})\, d^3Q = \gamma(0) = 1 \\ \therefore \dfrac{1}{(2\pi)^3} \displaystyle\int \left.\dfrac{\partial\sigma(\mathbf{Q})}{\partial\Omega}\right|_{\mathrm{coh}} d^3Q = V\left\langle (\Delta\rho)^2 \right\rangle \ \underline{\text{Porod invariant}} \end{array}}$$

Isotropic scattering:

$$S(\mathbf{Q}) = \int \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}} \gamma(r)\, d^3 r, \ \ S(Q) = \int_0^\infty r\gamma(r)\sin(Qr)\, dr$$

$$= \frac{4\pi}{Q}\int_0^\infty r\gamma(r)\sin(Qr) dr = 4\pi\int_0^\infty r^2\gamma(r)\,\mathrm{sinc}(Qr/\pi) dr$$

$$\boxed{p(r) = r^2\gamma(r) / \int_0^\infty r^2\gamma(r)\,\mathrm{sinc}(Qr/\pi)\, dr, \ \ \text{Distance distribution function}}$$

<u>**The Laws**</u>

for <u>small</u> Q, expand the $\mathrm{Sin}(Qr)$:

$$S(Q) = \frac{4\pi}{Q} \int_0^\infty r\gamma(r) \; Qr - \frac{1}{3!}(Qr)^3 + \cdots \; dr$$

$$= S(0) \; 1 - \frac{1}{6} Q^2 \langle r^2 \rangle + \cdots \;, \quad \langle r^n \rangle = \int_0^\infty r^n p(r) \, dr$$

$$\therefore S(Q) = S(0) \; 1 - \frac{1}{3} \underline{Q^2} R_{\mathrm{G}}^2 + \cdots$$

$$R_{\mathrm{G}}^2 = \int_0^\infty r^2 p(r) \, d^3 r, \; R_{\mathrm{G}} = \text{Guinier radius (radius of gyration)}$$

<u>**Guinier's "Law"**</u>

$$S(Q) \approx S(0) \mathrm{e}^{-Q^2 R_{\mathrm{G}}^2 / 3}$$

Note: this implies $S(Q) \approx S(Q)$ only for $QR_{\mathrm{G}} \le \pi$.

The Laws

for large Q, first expand $\gamma(r)$ for small r:

for a scatterer of volume V and surface area S,

$\gamma(r) = [1 - r/\xi + \cdots]$, $\xi = 4V/S$ Porod correlation length

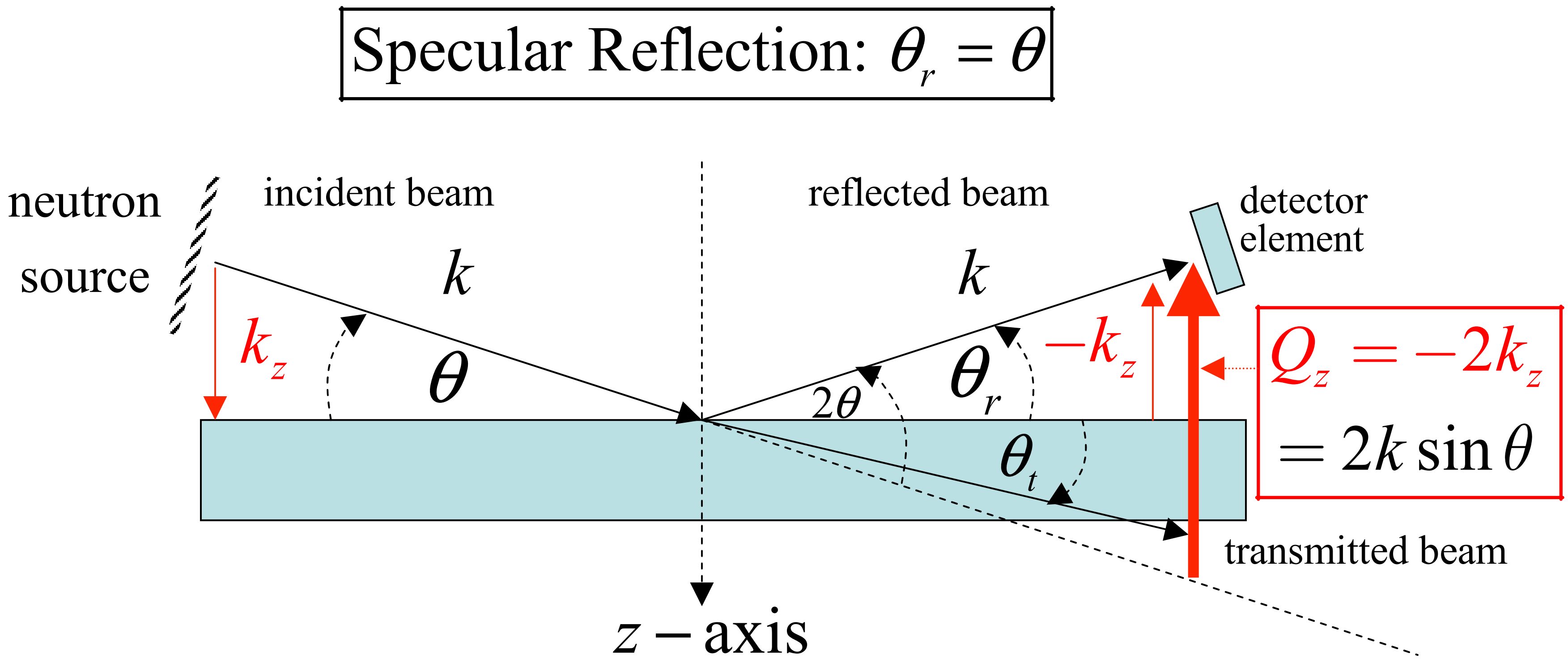
Then from a basic theorem about Fourier transforms,

$$S(Q) \sim \frac{S/V}{Q^4} = \frac{4/\xi}{Q^4}$$

Porod's Law

$$\left.\frac{\partial\sigma(\mathbf{Q})}{\partial\Omega}\right|_{\text{coh}} = \frac{\left\langle(\Delta\rho)^2\right\rangle S}{Q^4}, \text{ for } Q\xi >> 1.$$

Basic Scattering Theory
NSR



Specular Reflection: $\theta_r = \theta$
neutron source
incident beam
reflected beam
detector element
k
k
k_z
θ
2θ
θ_r
θ_t
$-k_z$
$Q_z = -2k_z = 2k \sin\theta$
transmitted beam
$z-$axis

Shrödinger Equation

$$-\nabla^2\psi(\mathbf{k},\mathbf{r})+4\pi\rho(\mathbf{r})\psi(\mathbf{k},\mathbf{r})=k^2\psi(\mathbf{k},\mathbf{r})$$

Specular paradigm

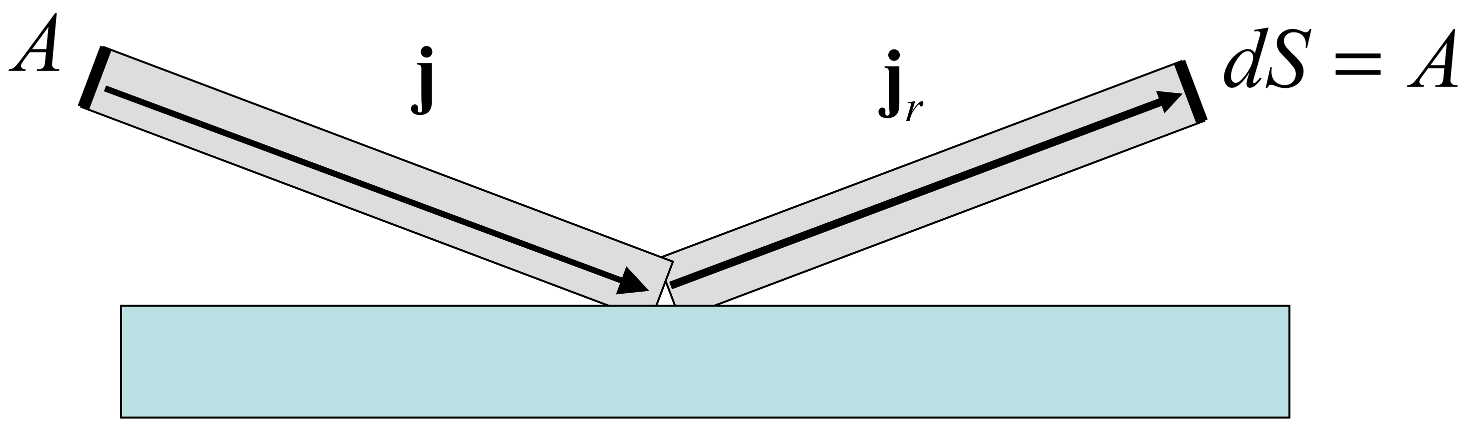
$$\rho(\mathbf{r})=\langle\rho(x,y,z)\rangle_{xy}\triangleq\rho(z)$$

$$\psi(\mathbf{k},\mathbf{r})=\mathrm{e}^{\mathrm{i}k_x x}\mathrm{e}^{\mathrm{i}k_y y}\psi(k_z,z)$$

$$\boxed{-\partial_z^2\psi(k_z,z)+4\pi\rho(z)\psi(k_z,z)=k_z^2\psi(k_z,z)}$$

$1-D$ wave equation

What's measured?



$$\textit{recall}\ \text{current: } J = \frac{dN}{dt} = \mathbf{j} \bullet \mathbf{A}$$

Reflectivity $R \triangleq \mathbf{j}_r \bullet \mathbf{A} \,/\, \mathbf{j} \bullet \mathbf{A}$

What's calculated?

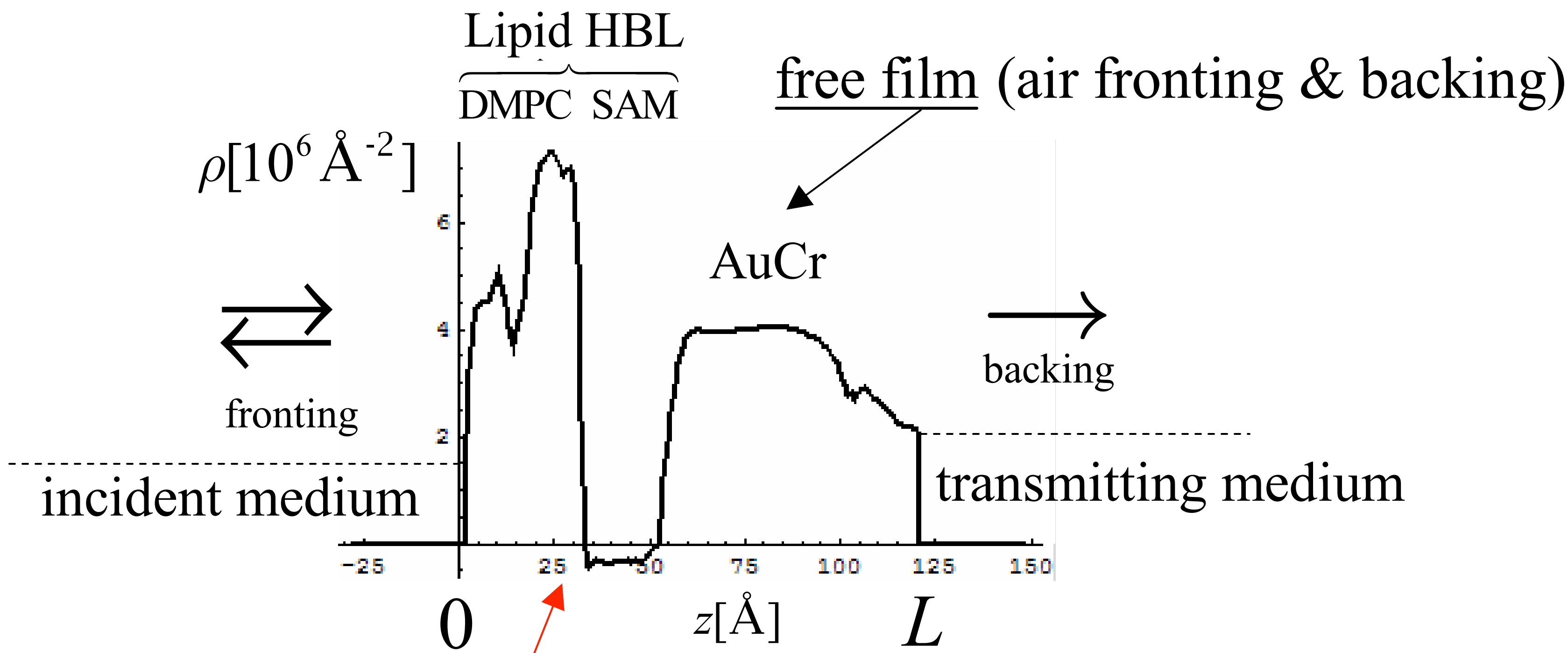
$$j = \frac{\hbar}{2mi}\left[\psi^{*}\nabla\psi - \psi\nabla\psi^{*}\right]$$

incident: $\psi_i = \mathrm{e}^{\mathrm{i}\mathbf{k}\bullet\mathbf{r}}, \; j_i = \hbar\mathbf{k}/m$

reflected : $\psi_r = r\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\bullet\mathbf{r}}, \; j_r = \frac{\hbar\mathbf{k}}{m}r$

$$\boxed{\therefore R = \mathbf{j}_r\bullet\mathbf{A}/\mathbf{j}\bullet\mathbf{A} = \left|r(Q_z)\right|^2 \rightarrow \left\langle \left|r(Q_z)\right|^2 \right\rangle}$$

$$\boxed{\mathbf{NOTE}: R \leq 1}$$



for the free film

$$\boxed{r(Q_z) = \frac{4\pi}{\mathrm{i}Q_z}\int_0^L \psi(k_z, z)\rho(z)\mathrm{e}^{\mathrm{i}k_z z}dz}, \quad \left(Q_z \triangleq 2k_z\right)$$

$$\textit{recall}\;\; f(\mathbf{k}_s) = \int_{V_s} \psi(\mathbf{k},\mathbf{r})\rho(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}d^3r \text{ for point scatterers}$$

$$\boxed{r(Q_z) = \frac{4\pi}{\mathrm{i}Q_z}\int_0^L \psi(k_z, z)\rho(z)\mathrm{e}^{\mathrm{i}k_z z}dz}$$

Born Approximation: $\psi(k_z, z) \rightarrow \mathrm{e}^{\mathrm{i}k_z z}$

$$r^{\mathrm{BA}}(Q_z) = \frac{4\pi}{\mathrm{i}Q_z}\int_0^L \rho(z)\mathrm{e}^{\mathrm{i}2k_z z}dz = \frac{4\pi}{\mathrm{i}Q_z}\hat{\rho}(Q_z)$$

Q_z

WARNING: BA breaks down as $Q_z \rightarrow 0$ (unlike SANS case)

Free film

Transfer Matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

Real numbers

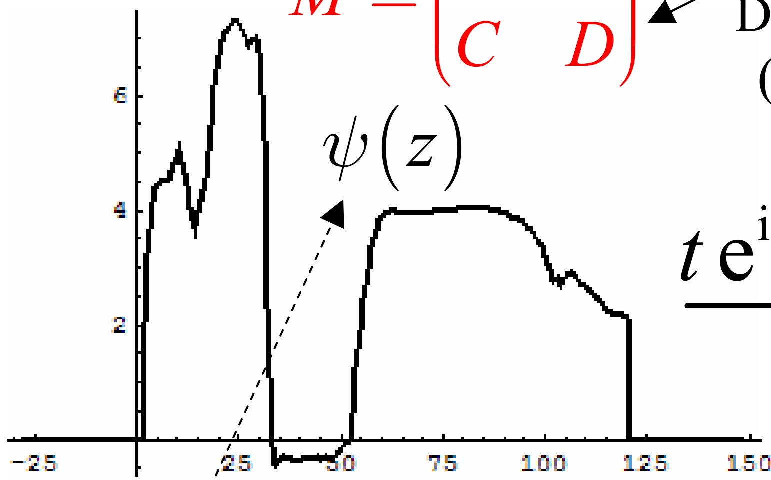
Det $M = (AD - BC) = 1$

(M is unimodular)

$\overrightarrow{e^{ik_z z}}$

$\overleftarrow{r\, e^{-ik_z z}}$

$\psi(z)$



$\overrightarrow{t\, e^{ik_z z}}$

0 $\quad z$[Å] $\quad L$

M "transfers" $\psi(z)$ and $\psi'(z)$ from $z = 0$ to $z = L$

$$M \begin{pmatrix} 1 + r \\ i(1 - r) \end{pmatrix} = \begin{pmatrix} 1 \\ i \end{pmatrix} t\, e^{ik_z L}$$

$\cdots$giving two equations for r and t

$$\begin{pmatrix} 1+r \\ \mathrm{i}(1-r) \end{pmatrix} = M \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} t$$

$$\boxed{\begin{aligned} r &= \frac{B+C+\mathrm{i}(D-A)}{B-C+\mathrm{i}(D+A)} \\ &= -\frac{\alpha-\beta+2\mathrm{i}\gamma}{\alpha+\beta} \end{aligned}}$$

$$\boxed{\begin{aligned} \alpha &= A^2+C^2 \\ \beta &= B^2+D^2 \\ \gamma &= AB-CD \\ \gamma^2 &= \alpha\beta-1 \end{aligned}}$$

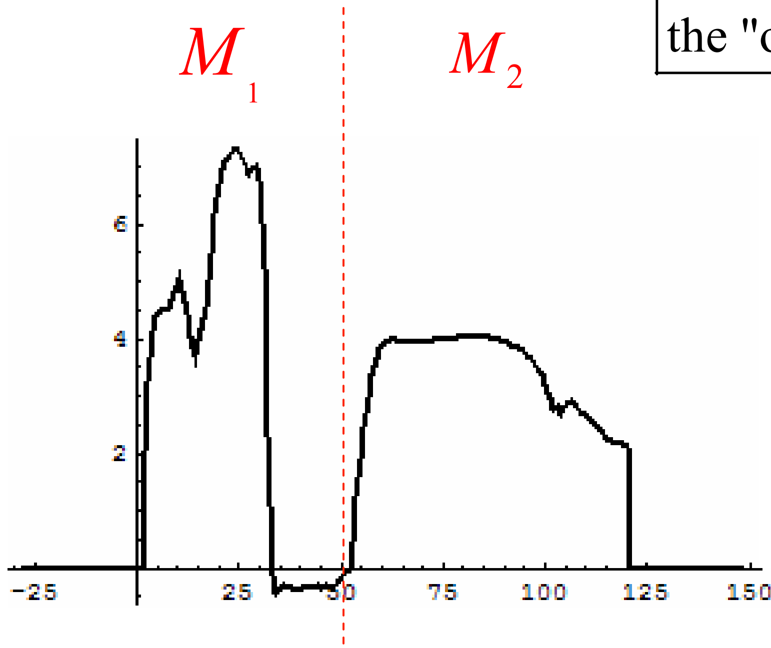
$$\boxed{R = |r|^2 = \frac{\Sigma-2}{\Sigma+2}, \quad \Sigma = A^2+B^2+C^2+D^2 = \alpha+\beta}$$

The phase problem: $R[\alpha+\beta]$ doesn't determine α, β and γ.

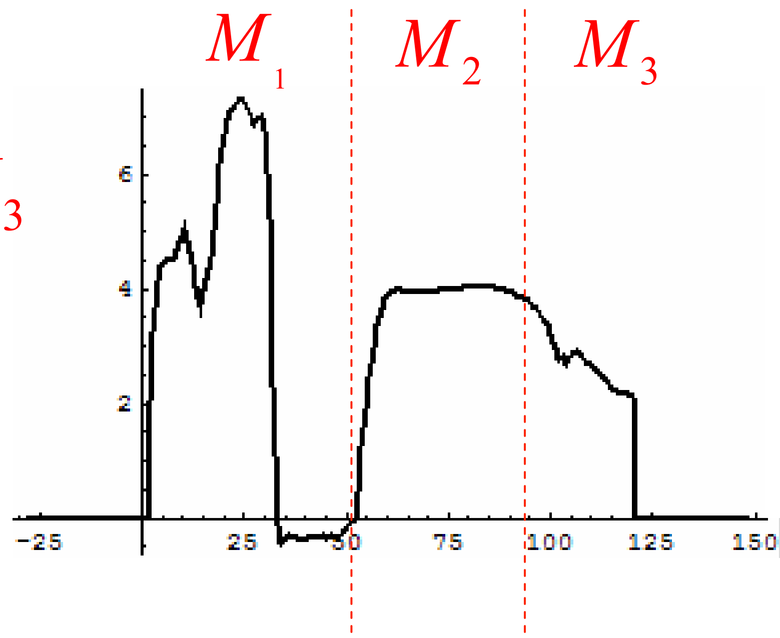
Transfer Matrix

Aside: historically, M also is called the "optical" matrix.

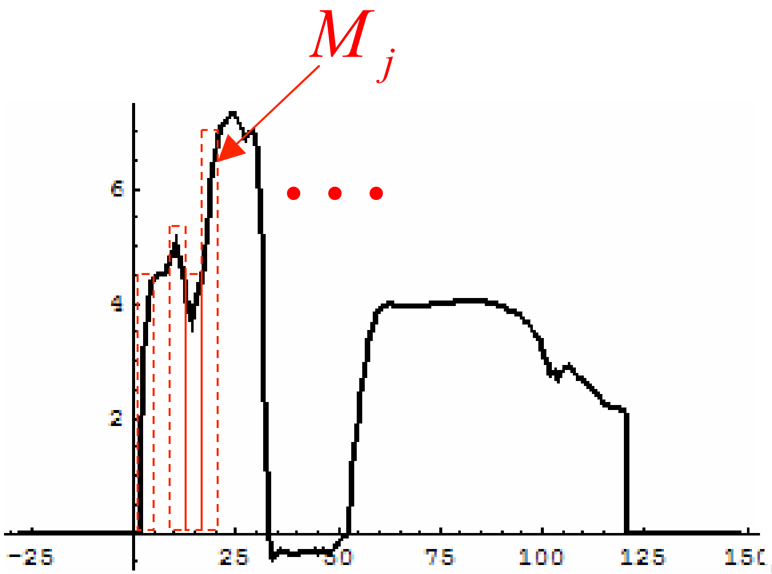
$$M = M_1 M_2$$



$$M = M_1 M_2 M_3$$



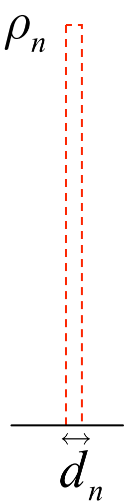
Transfer Matrix



$$M = M_1 M_2 \cdots M_N$$

Exact in $\lim\limits_{\mathrm{N}\to\infty}$

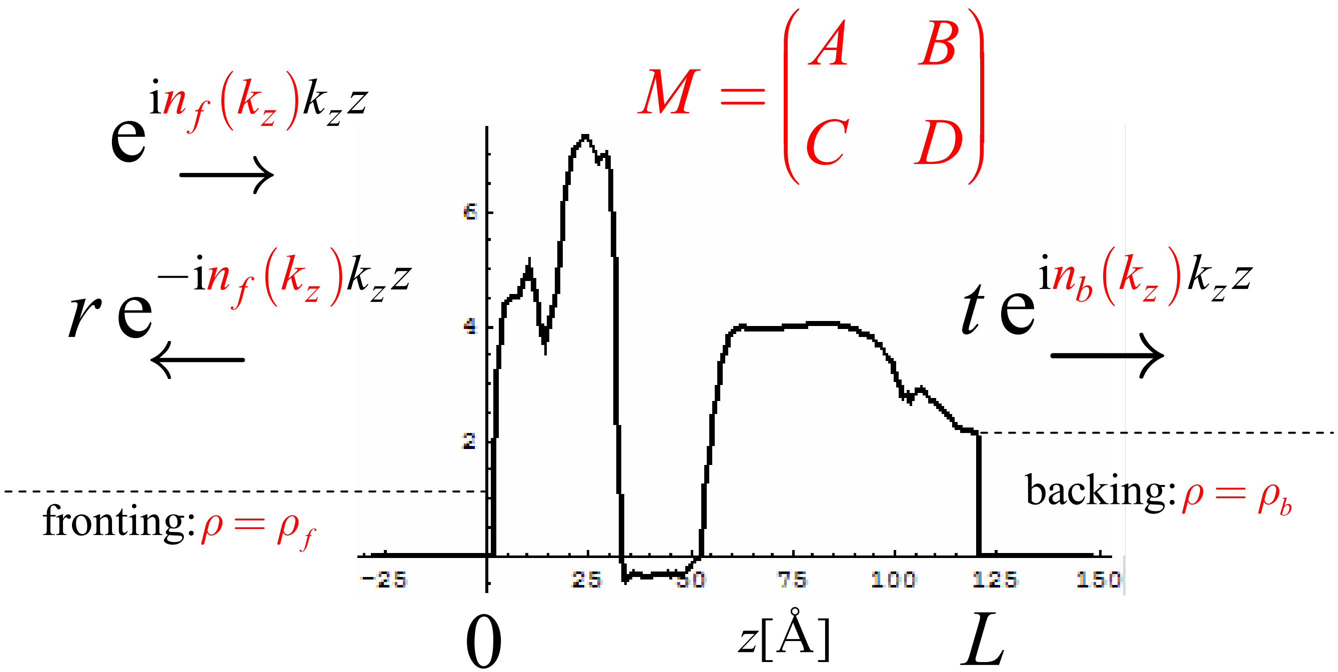
Good for $\mathrm{N} \geq Q_{\max} L$



$$M_j = \begin{pmatrix} \cos\left[\xi_j\left(k_z\right)\right] & \sin\left[\xi_j\left(k_z\right)\right] / n_j\left(k_z\right) \\ -n_j\left(k_z\right)\sin\left[\xi_j\left(k_z\right)_n\right] & \cos\left[\xi_j\left(k_z\right)\right] \end{pmatrix}$$

$$\xi_j\left(k_z\right) = n_j\left(k_z\right) k_z d_n, \quad n_j(k_z) = \sqrt{1 - \frac{4\pi\rho_j}{k_z^2}}$$

Surrounded film

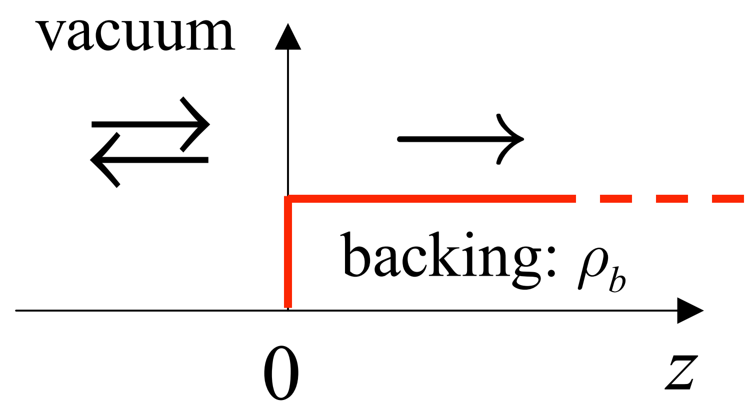


$$\alpha \to \alpha^{fb},\ \beta \to \beta^{fb},\ \gamma \to \gamma^{fb}$$

$$\boxed{r = -\frac{\alpha^{fb} - \beta^{fb} + 2\mathrm{i}\gamma^{fb}}{\alpha^{fb} + \beta^{fb}}}$$

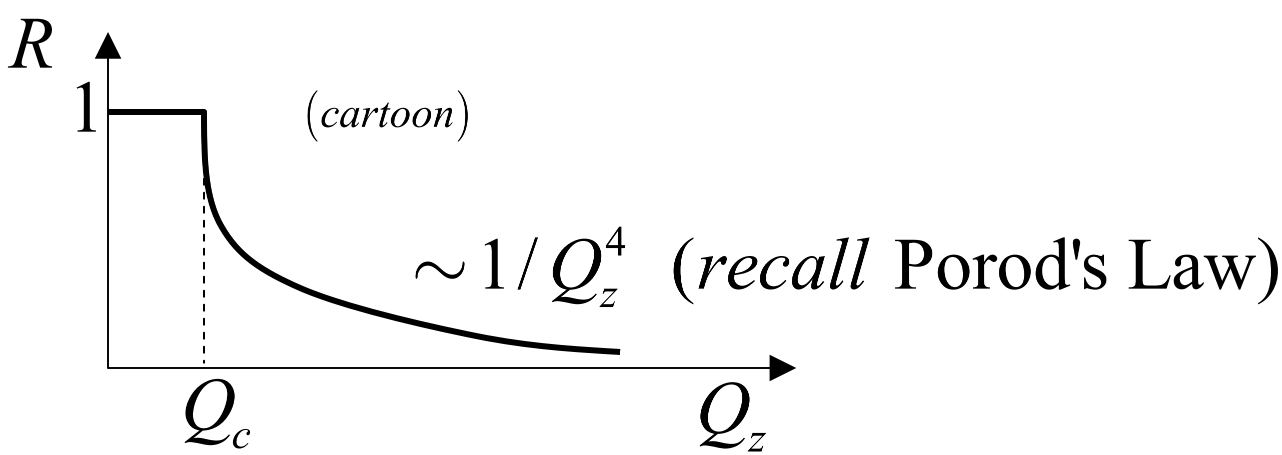
Two prototypes

1) Fresnel Problem: backing only



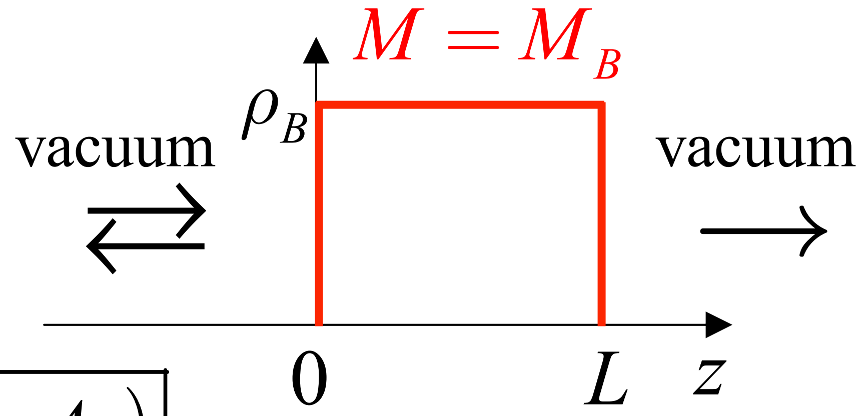
$$\boxed{r(Q_z) = \frac{1 - n_\mathrm{b}(Q_z/2)}{1 + n_\mathrm{b}(Q_z/2)}} \qquad n_\mathrm{b}(k_z) = \sqrt{1 - \frac{16\pi\rho_\mathrm{b}}{Q_z^2}}$$

$$n_\mathrm{b}(Q_z/2) = {\color{red}\mathrm{i}}\left|n_\mathrm{b}(Q_z/2)\right| \text{ for } Q_z \le \sqrt{16\pi\rho_\mathrm{b}} = Q_c$$



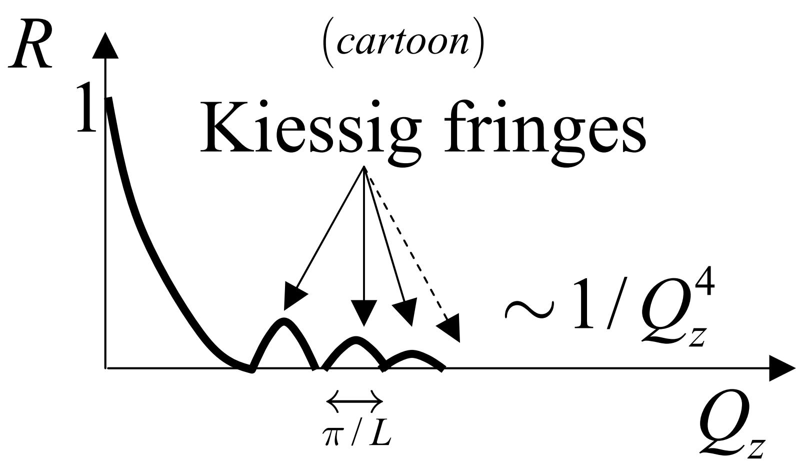
Two prototypes

2) Free barrier



$$\boxed{r(Q_z) = \frac{B_B + C_B + \mathrm{i}(D_B - A_B)}{B_B - C_B + \mathrm{i}(D_B + A_B)}}$$

$$n_B(Q_z/2) = \sqrt{1 - 16\pi\rho_B / Q_z^2}$$



$\boxed{\text{Enjoy the rest of the course!}}$