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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

14 April - 18 June 1982

NEUTRON AND X-RAY DIFFRACTION STUDIES

(Transparencies)

J.E. ENDERBY

H.H. Wills Physics Lab.
University of Bristol
Royal Fort, Tyndall Avenue
Bristol BS8 1TL
U.K.

X-ray and Neutron Scattering

Concerned with STRUCTURE

& DYNAMICS

on a microscopic scale

STRUCTURE

$$g(r_{12}) = \frac{V^2 \int \cdots \int e^{(-\beta \Phi)}\, d\underset{\sim}{R_3} \cdots d\underset{\sim}{R_N}}{\int \cdots \int e^{(-\beta \Phi)}\, d\underset{\sim}{R_1} \cdots d\underset{\sim}{R_N}}$$

$$\beta = \frac{1}{k_B T}$$

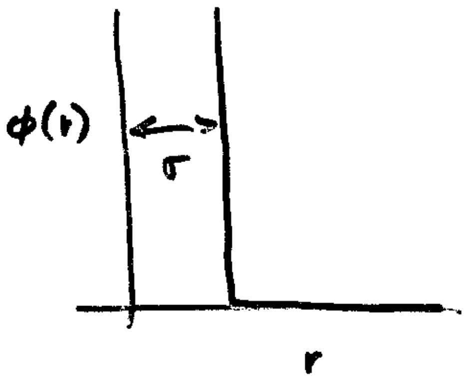
$$\Phi = \Phi(\underset{\sim}{R_1} \cdots \underset{\sim}{R_N})$$

$$r = r_{12} = |\underset{\sim}{R_1} - \underset{\sim}{R_2}|$$

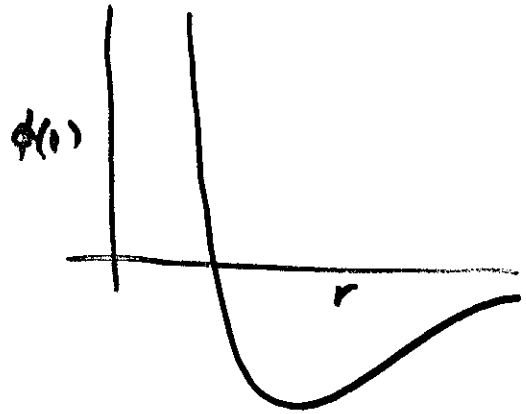
PAIR POTENTIALS

$$\Phi = \sum_{i<j} \phi(r_{ij})$$

Potentials



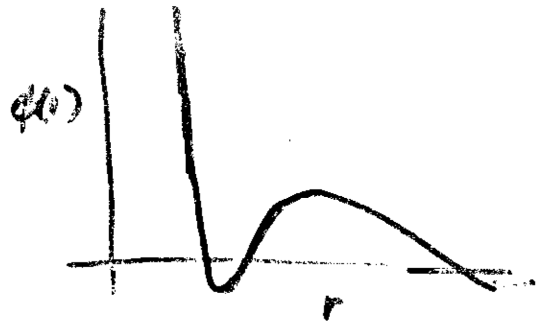
"HARD SPHERE"



"LENNARD - JONES"

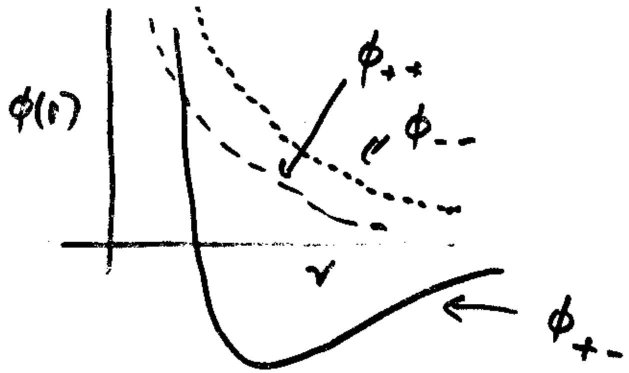
$$\phi(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

-3- Electrolyte Solutions



Metals
"EFFECTIVE POTENTIAL"

$$\boxed{\phi_{ij}(r) = A_{ij}(r) + \frac{z_i z_j e^2}{\varepsilon r}}$$

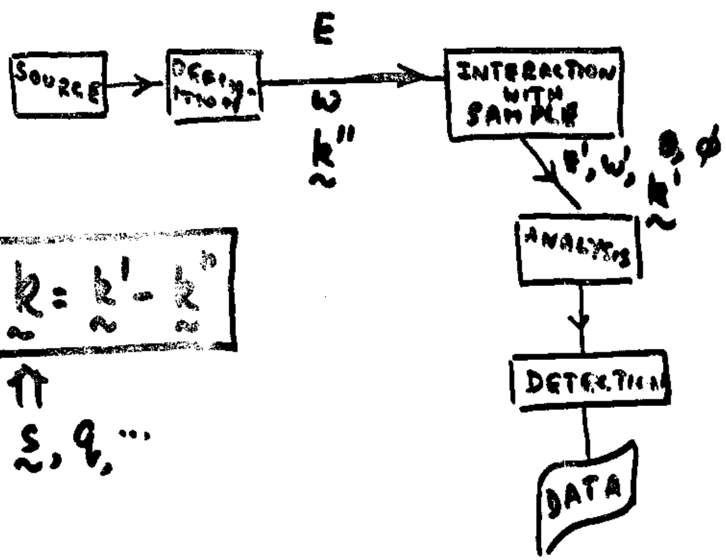


IONIC SYSTEMS

A_{11}	A_{22}	A_{12}	
0	0	0	D-H
∞ 0	∞ for $r \leq \sigma$ otherwise 0	∞ 0	Restricted
∞ σ_1 0	∞ for $r \leq$ σ_2 otherwise 0	∞ $(\sigma_1+\sigma_2)/2$ 0	Extended ~~Refined~~
$f_{11}(r)$	$f_{22}(r)$	$f_{12}(r)$	Refined

Molten Salts : $\phi_{ij} = \frac{z_i z_j e^2}{r} + B_{ij}\exp(-\alpha_{ij} r) - \frac{C_{ij}}{r^6} - \frac{D_{ij}}{r^8}$

The Scattering Method



$$\boxed{\underset{\sim}{k} = \underset{\sim}{k}' - \underset{\sim}{k}''}$$

⇑

$\underset{\sim}{Q}$, $\underset{\sim}{s}$, q, ...

E = incident energy — E' = final energy

ω = .. equiv frequency — ω' = .. equiv freq

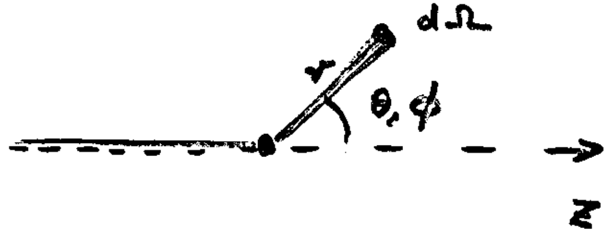
v = .. velocity — v' = final velocity

$\underset{\sim}{k}''$ .. wave vector — $\underset{\sim}{k}'$ = .. wave vector

λ = .. wavelength — λ' = .. wavelength

θ, φ — direction of scattered beam
(with respect to incident beam)

Scattering Cross-Sections



1) Partial Differential Cross-Section

written as:

$$\frac{d^2\sigma}{d\Omega\, dE'}$$

defined as:

(number of particles scattered per second into solid angle dΩ in the direction θ, φ with final energy between E' and E' + dE') / Φ dΩ dE'

Φ = incident particle flux

dimensions: area energy^{-1}.

ii) Differential scattering cross-section

written as:

$$\frac{d\sigma}{d\Omega}$$

defined as:

([illegible] of particles scattered per second into solid angle [illegible] θ, ϕ / Φ $d\Omega$ [illegible]

dimensions: area

iii) (Total) Scattering cross-section

written as:

$$\sigma_t$$

defined as:

(total number of particles scattered per second)/Φ

dimensions: area

Relationships

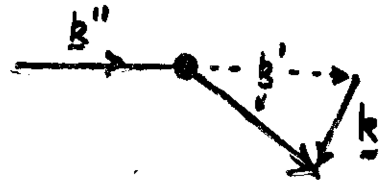
$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega\, dE'}\right) dE'$$

$$\sigma_t = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega$$

$$= 2\pi \int_0^\pi \left(\frac{d\sigma}{d\Omega}\right) \sin\theta\, d\theta$$

if axially symmetric

Formal Expressions for these cross-sections



$$|\underline{k}| = \frac{4\pi \sin\theta}{\lambda} \qquad |\underline{k}''| = |\underline{k}'|$$

In general, $|\underset{\sim}{k}''| \neq |\underset{\sim}{k}'|$

But consider the elastic case $|\underset{\sim}{k}''| = |\underset{\sim}{k}'|$

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Phi \, d\Omega} W_{k'' \to k'}$$

Fermi Golden Rule:

$$W_{k'' \to k'} = \frac{2\pi}{\hbar} \left| \int \psi_{k'}^{*} \hat{V} \psi_{k''} \, d\underset{\sim}{r} \right|^2 \rho_{k'}(E')$$

$$= \frac{2\pi}{\hbar} \frac{|\langle k' | \hat{V} | k'' \rangle|^2}{L^3} \rho_{k'}(E')$$

Now consider the inelastic case:

$|\underset{\sim}{k}''| \neq |\underset{\sim}{k}'|$

Target changes from $|\lambda\rangle$ to $|\lambda'\rangle$

Particle changes from $|k''\rangle$ to $|k'\rangle$

$$|\langle k'\lambda' | \hat{V} | k''\lambda \rangle|^2 \, \delta(E_\lambda - E_{\lambda'} + E - E')$$

This yields

$$\left(\frac{d^2\sigma}{d\Omega \, dE'}\right)_{\substack{k'' \to k' \\ \lambda \to \lambda'}}$$ but this

is not what is observed in an experiment

We must (a) sum over all final states λ' for given λ

and then (b) average over all initial states λ.

The resulting expression is therefore very complicated and we shall derive it only for the neutron case. In X-ray $E_{\lambda'} = E_\lambda$ (the "static" approximation) which will be discussed later.

[illegible]

- [illegible] ([illegible] in [illegible])
- no charge
- magnetic moment $\mu_n = -1.913\,\mu_N$

  $\mu_N = 5.051 \times 10^{-27}\ \mathrm{J\,T^{-1}}$
- spin $\frac{1}{2}$
- mass $1.675 \times 10^{-27}\ \mathrm{kg}$
- finite life (~ mins)
- may be polarised
- usually suffers low absorption
- scattered by the nucleus isotope sensitive

Neutron production

- lab sources

  $${}^{9}_{4}Be + {}^{4}_{2}He \rightarrow C^{12}_{6} + n$$
- reactors

  Fission reactors ~ [illegible]

  [illegible], energy $\boxed{[illegible]}$ [illegible] meV
- pulsed sources

  ([illegible])

  $4\ \mathrm{MeV}\ \bar{e} \dashrightarrow \square$

  [illegible] target

  $10^{13}\ n/s$

$\longrightarrow$ SNS at R.L.

"Spallation Neutron Source" 1984 +

$$\lambda = 6.283\left(\tfrac{1}{k}\right)$$

$$= 3.956 \tfrac{1}{v}$$

$$= 9.045/\sqrt{E}$$

$$= 30.81/\sqrt{T}$$

λ in Å, k in Å^{-1}, v in km s^{-1}

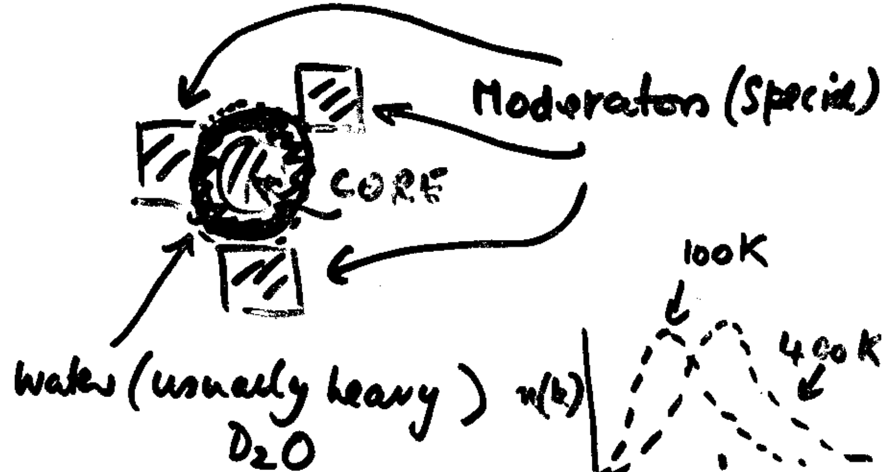
E in meV T in Kelvin

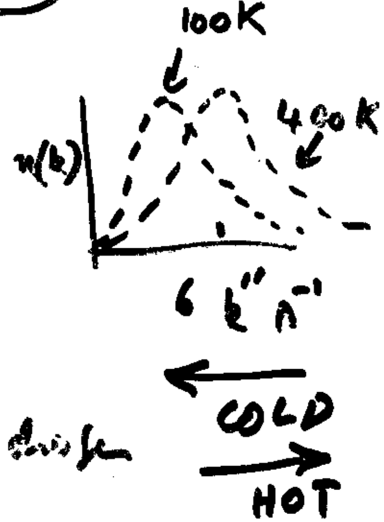
<u>Thus</u>

1 eV neutron is equivalent to:

$v = 1.383 \times 10^{4}$ m s^{-1}
$\lambda = 0.286$ Å
$k = 21.97$ Å^{-1}
$T = 1.16 \times 10^{4}$ K
$\omega = 1.52 \times 10^{15}$ rad s^{-1}

Moderation of initial neutrons
∴ essential





<u>Cold neutrons</u>

- volume of liquid hydrogen

<u>Hot neutrons</u>

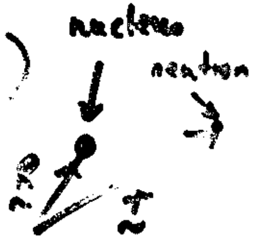
- a block of beryllium heated by γ-radiation

Cold :	0.1-10	1-120	30-3
Thermal :	5-100	60-1000	4-1
Hot :	100-500	1000-6000	1-0.4

Neutron Scattering from a single $\boxed{\text{nucleus}}$

neutron – nuclei interaction are strong (nuclear) short-ranged ($<< \lambda$). Scattering will be isotropic, S-like in character.

$$\hat{V}(r) = \frac{2\pi\hbar^2}{m} b \, \delta(\underline{r} - \underline{R})$$



Fermi pseudo-potential

scattering length

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} \frac{|\langle k'|V|k^\circ\rangle|^2 \rho_{k'}(E)}{L^3 \Phi \, d\Omega} \qquad (|\underline{k}'| = |\underline{k}^\circ|)$$

$$\rho_{k'} = \left(\frac{L}{2\pi}\right)^3 \frac{m k'}{\hbar^2} d\Omega$$

$$\Phi = \frac{\hbar k}{m L^3}$$

$\hbar k = m v$

$e^{-ik' r} \quad \delta \quad e^{-ik^\circ r}$

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle k'|\hat{V}|k^\circ\rangle|^2$$

$$\frac{d\sigma}{d\Omega} = |b|^2 \begin{cases} \text{SINGLE} \\ \text{BOUND} \\ \text{NUCLEUS} \end{cases}$$

Important properties of b

a) Unbound

$$b_{free} = \left(\frac{M}{m+M}\right) b$$

b) In general

$$b = b' + i b''$$

b'' associated with absorption

majority of cases $b'' = 0$

b indep. of E

c) b depends on isotope

e.g. ^{107}Ag $b = [illegible] \times 10^{-12}$ cm

^{109}Ag $b = [illegible] \times 10^{-12}$ cm

d) b depends on the spin state of the nucleus-neutron system [illegible]

$I + \frac{1}{2}$ $\quad$ $I - \frac{1}{2}$

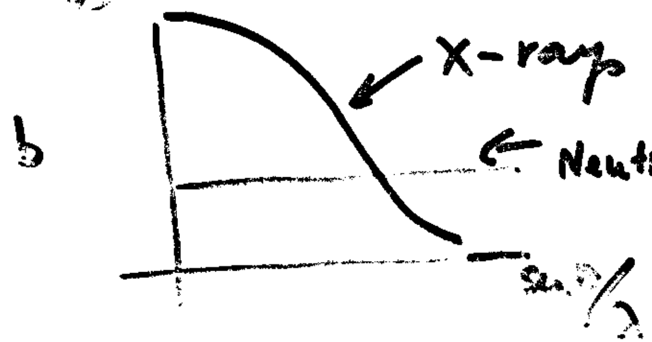
b_+ $\quad$ b_-

e.g. proton ^1H

$b^+ = 1.04 \times 10^{-12}$ cm

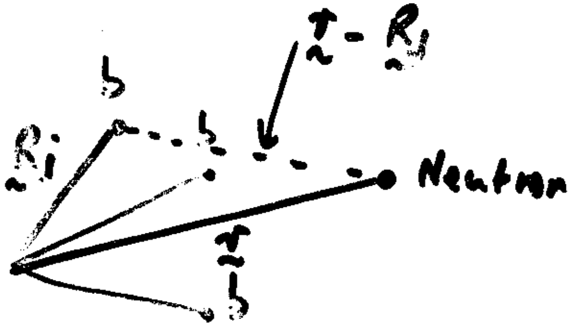
$b^- = -4.74 \times 10^{-12}$ cm

In general (aside from magnetic scattering) b does not depend on θ



An array of nuclei

- bound, identical, spinless



$$\hat{V}(\mathbf{r}) = \frac{2\pi\hbar^2}{m} b \sum_j \delta(\mathbf{r} - \mathbf{R}_j)$$

$$\langle \mathbf{k}' | \hat{V} | \mathbf{k}^0 \rangle = \frac{2\pi\hbar^2}{m} b \sum_j \int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, \delta(\mathbf{r} - \mathbf{R}_j)$$

$$e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= \frac{2\pi\hbar^2}{m} b \sum_j \int d(\mathbf{r} - \mathbf{R}_j)\, \delta(\mathbf{r} - \mathbf{R}_j)\, e^{i\mathbf{k}\cdot(\mathbf{r} - \mathbf{R}_j)}\, e^{i\mathbf{k}\cdot\mathbf{R}_j}$$

Note

$$\int \delta(\mathbf{r}) \exp(i\,\mathbf{k}\cdot\mathbf{r})\, d\mathbf{r} = 1$$

$$\langle \mathbf{k}' | \hat{V} | \mathbf{k}^0 \rangle = \frac{2\pi\hbar^2}{m} b \sum e^{i\mathbf{k}\cdot\mathbf{R}_j}$$

$$\frac{d\sigma}{d\Omega} = b^2 \left| \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} \right|^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{obs} = b^2 \left\langle \left| \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} \right|^2 \right\rangle$$

$$S(\mathbf{k}) = \frac{1}{Nb^2}\left(\frac{d\sigma}{d\Omega}\right)_{obs} = \frac{1}{N}\left\langle \left| \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} \right|^2 \right\rangle = \frac{1}{N}\left\langle \sum_i \sum_j e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \right\rangle$$

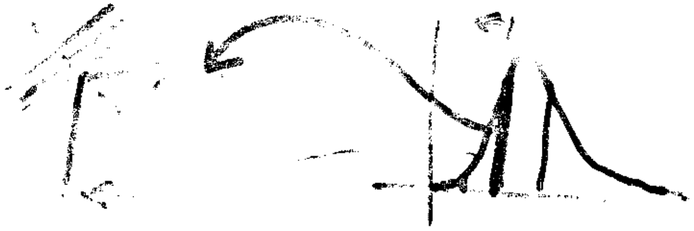
"Structure factor"

For crystals

$e^{i k \cdot 2\pi}$ = 0 unless [illegible]

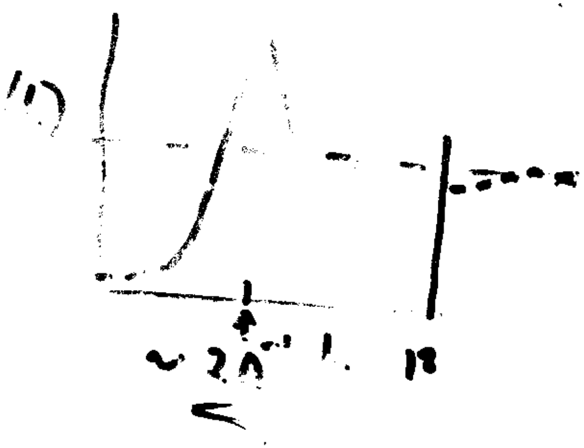
[illegible]

λ, λ/2



This is used to produce a monochromatic beam.

For liquids and amorphous [illegible]



$$g(r) = 1 + \frac{1}{2\pi^2 \rho r}\int_0^\infty dk\, k \sin kr\,[S(k)-1]$$

$\frac{4\pi}{\lambda}$

Note in practice ⇒ [illegible]

[illegible].

Real systems

— nuclei not necessarily identical even for chemically pure systems (spin, isotopes)

— nuclei not bound, also at T = 0 (zero point motion)

[illegible]

[illegible]

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right) = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} b_j b_{j'} \int_{-\infty}^{\infty} dt\, e^{-i\omega t}\langle \exp\{-i\underset{\sim}{k}\cdot\hat{R}_{j'}(0)\}\exp\{i\underset{\sim}{k}\cdot\hat{R}_j(t)\}\rangle$$

$\omega = \frac{E-E'}{\hbar}$ $\quad$ $\hat{R}_j(t)$ is an operator

$\exp(iHt/\hbar)\,\hat{R}_j\,\exp(-iHt/\hbar)$

operator

and $\langle \hat{A} \rangle$

means $\sum_\lambda p_\lambda \langle\lambda|\hat{A}|\lambda\rangle$

p_λ is the probability that the scattering system is in the λ^{th} state

$$p_\lambda = \frac{1}{Z}\exp(-E_\lambda\beta)$$

$$Z = \sum_\lambda \exp(-E_\lambda\beta)$$

$$\sum_\lambda p_\lambda = 1$$

Note $\hat{R}_j(t)$ and $\hat{R}_{j'}(0)$ do not commute except at $t=0$

Some Consequences

b varies from nucleus to nucleus. Let c_i be the fraction of nuclei with scattering length b_i

$$\bar{b} = \sum c_i b_i \qquad \overline{b^2} = \sum c_i b_i^2$$

The distribution of isotopes (and spins) is random

Then $b_j\, b_{j'}$ can be replaced by $\overline{b_j b_{j'}}$

$$\overline{b_j b_{j'}} = (\bar{b})^2 \qquad j' \neq j$$

$$\overline{b_j b_{j'}} = \overline{b^2} \qquad j' = j$$

So:

$$\frac{d^2\sigma}{d\Omega\, dE'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\left[(\bar{b})^2 \sum_{j \neq j'} f_{j'j} + \overline{b^2} \sum_j f_{jj}\right]$$

$$= \frac{k'}{k}\frac{1}{2\pi\hbar}\left[(\bar{b})^2 \sum_{j,j'} f_{jj'} + \left(\overline{b^2} - (\bar{b})^2\right)\sum_j f_{jj}\right]$$

$$= \frac{k'}{k}\frac{1}{2\pi\hbar}\left[\frac{\sigma_{coh}}{4\pi}\sum_{j,j'} f_{jj'} + \frac{\sigma_{inc}}{4\pi}\sum_j f_{jj}\right]$$

$$\frac{d\sigma}{d\Omega} = b^2$$

$$\sigma = 4\pi b^2$$

$$\sigma_{coh} = 4\pi\,(\bar{b})^2$$

$$\sigma_{inc} = 4\pi\left[\overline{b^2} - (\bar{b})^2\right]$$

Returning to the elastic case, but this time with b_i

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{coh} + \left(\frac{d\sigma}{d\Omega}\right)_{inc}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = |\bar{b}|^2 \left\langle \left| \sum e^{i\underset{\sim}{k}\cdot\underset{\sim}{R}_l} \right|^2 \right\rangle$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{inc} = N\left[\,\overline{b^2} - (\bar{b})^2\right]$$

$$\equiv N\,\overline{|b - \bar{b}|^2}$$

<u>Coherent</u> : relative position and motion of two particles

<u>Incoherent</u> : motion of a single particle

Values of $\bar{b}$ and $\overline{b^2}$

<u>ISOTOPIC INCOHERENCE</u>

Silver	b $\times 10^{-12}$	c
^{107}Ag	0.83	0.513
^{109}Ag	0.43	0.487

$$\bar{b} = 0.513 \times 0.83 + 0.487 \times 0.43$$
$$= 0.63 \times 10^{-12}\,\text{cm}$$

barn

$$\sigma_{coh} = 4\pi(\bar{b})^2 \sim 5 \times 10^{-24}\,\text{cm}^2 = 5\,\text{b}$$

$$\overline{b^2} = 0.513 \times (0.83)^2 + 0.487 \times (0.43)^2$$
$$= 0.40 \times 10^{-24}\,\text{cm}^2$$

$$\sigma_{inc} = 4\pi\left[\overline{b^2} - (\bar{b})^2\right] \sim 0.5\,\text{b}$$

<u>SPIN Incoherence</u>

nuclear spin = I

neutron spin = $1/2$

$I + 1/2$ $\qquad$ $I - 1/2$

$2(I + 1/2) + 1$ states for b_+

$2(I - 1/2) + 1$ " " b_-

$c_+ = \frac{I+1}{2I+1} \quad c_- = \frac{I}{2I+1}$

$\bar{b} = \left(\frac{I+1}{2I+1}\right) b_+ + \left(\frac{I}{2I+1}\right) b_-$

$\overline{b^2} = \frac{(I+1)(b_+)^2}{2I+1} + \frac{I(b_-)^2}{2I+1}$

Eg hydrogen ^1H $I = 1/2$

$b^+ = 1.04 \times 10^{-12}$ cm

$b^- = -4.74 \times 10^{-12}$ cm

$\bar{b} = -0.375 \times 10^{-12}$ cm

$\overline{b^2} = 6.49 \times 10^{-24}$ cm^2

$\boxed{\sigma_{inc} = 80\ b}$ $\sigma_{coh} = 1.8\ b$

Outline proof for master equation (full details in Squires "Introduction to Thermal Neutron Scattering")

1) k' $\propto$ final density of states

k'' $\propto$ incident flux

hence $\left(k'/k''\right)$ factor

2) Integral representation of δ function

$$\delta(E_\lambda - E_{\lambda'} + E - E') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{-i\omega t} \times \exp\{i(E_{\lambda'} - E_\lambda)t/\hbar\}$$

where

$\hbar\omega = E - E'$

3 Operator Properties

$$\hat{H}|\lambda\rangle = E|\lambda\rangle$$

$$\hat{H}^n|\lambda\rangle = E^n|\lambda\rangle$$

$$\exp(-i\hat{H}t/\hbar)|\lambda\rangle = \exp(-iEt/\hbar)|\lambda\rangle$$

$$\left[e^{-x} = 1 - x + \tfrac{1}{2}x^2 \ldots \right]$$

4. Closure (sum over λ')

$$\sum_{\lambda'} \langle\lambda|\hat{A}|\lambda'\rangle\langle\lambda'|\hat{B}|\lambda\rangle = \langle\lambda|\hat{A}\hat{B}|\lambda\rangle$$

5 Average over λ

$$\langle\hat{A}\rangle = \sum P_\lambda \langle\lambda|\hat{A}|\lambda\rangle$$

Structure + Dynamics of Liquids

Let us define

$$I(\underset{\sim}{k}, t) = \frac{1}{N}\sum_{j,j'} \langle \exp\{-i\underset{\sim}{k}\cdot\hat{\underset{\sim}{R}}_{j'}(0)\} \times \exp\{i\underset{\sim}{k}\cdot\hat{\underset{\sim}{R}}_j(t)\}\rangle$$

The Scattering law is then

$$S(\underset{\sim}{k}, \omega) = \frac{1}{2\pi\hbar}\int I(\underset{\sim}{k}, t)\exp(-i\omega t)\,dt$$

The Van Hove Correlation function is then

$$G(\underset{\sim}{r}, t) = \frac{1}{(2\pi)^3}\int I(\underset{\sim}{k}, t)\exp(-i\underset{\sim}{k}\cdot\underset{\sim}{r})\,d\underset{\sim}{k}$$

$S(\underset{\sim}{k}, \omega)$ is related to $G(r, t)$

+ vice versa

eg $G(\underset{\sim}{r}, t) = \left(\frac{\hbar}{2\pi}\right)^3 \iint S(\underset{\sim}{k}, \omega) \times \exp\{-i(\underset{\sim}{k}\cdot\underset{\sim}{r} - \omega t)\} d\underset{\sim}{k}\, d\omega$

But $S(\underset{\sim}{k}, \omega)$ is also related to $\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh}$ through

$$\underline{\underline{\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh}}} = \underline{\underline{\frac{\sigma_{coh}}{4\pi}\frac{k'}{k''} N S(\underset{\sim}{k}, \omega)}}$$

Introduce I_s ("self") $j = j'$

$$G_s(\underset{\sim}{r}, t) = \frac{1}{(2\pi)^3}\int I_s(\underset{\sim}{k}, t) e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} dk$$

$$= \frac{\hbar^3}{2\pi} \iint S_i(\underset{\sim}{k}, \omega) \cdots dk\, d\omega$$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\underline{inc}} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k''} N\, \underline{\underline{S_i}}(\underset{\sim}{k}, \omega)$$

Because of the operator character of $\hat{R}_j(t)$, there is no probabilistic interpret^n of $G(r, t)$ but if we ignore this ("the classical approximation")

$G(\underset{\sim}{r}, t)$ is the probability that, given a particle at the origin at time $t=0$, any particle (including the original one) is in the volume $d\underset{\sim}{r}$ at position $\underset{\sim}{r}$ at time t

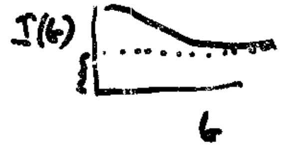
$G_s(\underset{\sim}{r}, t)$ ..... given a particle at the origin at time $t=0$, the $\boxed{\text{SAME}}$ particle is in the volume $d\underset{\sim}{r}$ at position r at time t

$\left(\frac{d\dot{\sigma}}{d\Omega dE'}\right)_{inc} \Rightarrow$ diffusive motion of particles

$$G(r,0) = \delta(r) + \rho\, g(r)$$

$$G_s(r,0) = \delta(r)$$

Elastic scattering is directly related to $I(k,\infty)$ or $G(r,\infty)$



Let $I(t) = I(\infty) + I_1(t)$

(for some chosen k)

$$S(\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\left[I(\infty) + I_1(t)\right]\exp(-i\omega t)\,dt$$

$$\omega = \frac{\Delta E}{\hbar} \quad = \frac{1}{\hbar}\delta(\omega)\, I(\infty) + \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} I_1(t) \sim dt$$

0 unless $\omega = 0$

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{\substack{coh\\ elas}} = \frac{\sigma_{coh}}{4\pi}\frac{N}{\hbar}\,\underline{\underline{\delta(\omega)}}\, I(k,\infty)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh\, \boxed{elas}} = \frac{\sigma_{coh}}{4\pi} N I(k,\infty)$$

It follows that in a <u>liquid</u> there is $\boxed{\text{no}}$ elastic scattering

$G(r,0) =$

$$G(r,\infty) \longrightarrow \rho \quad \text{a const}$$

$G(r,\infty) = g(r)$

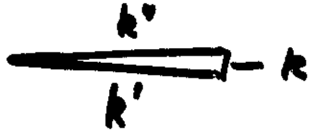
$$I(k,\infty) = \int G(r,\infty)\exp(i\,\underset{\sim}{k}\cdot\underset{\sim}{r})\,d\underset{\sim}{r}$$

$$= \delta(\underset{\sim}{k})$$

which is zero unless $\underset{\sim}{k} = 0$,

but this corresponds to no scattering

$\underset{\sim}{k} = \underline{k}' - \underset{\sim}{k}'$



To find $S(k) \rightleftarrows g(r)$

$$\underline{S(k)} = \int S(k,\omega)\, d\omega$$

$\Downarrow$

$g(r)$

"The zeroth energy moment of $S(k,\omega)$"

In the $\boxed{\text{static approx}}$ we assume that the constant k path is the same as the constant θ path

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

$S(\underline{k}) = \int S(\underline{k},\omega)\,d\omega$

For X-rays this is excellent. The reason is that for most condensed systems the characteristic relaxation time $\sim 10^{-13} - 10^{-12}$ s (t_0)

Time for incident radiation to pass from one particle to the next is

$$\sim \frac{a}{c} \sim 10^{-18}\,\text{s}\ (t_1) \qquad t_1/t_0$$

$t_1 << t_0$ "Rigid"

For neutrons, not so good

$$t_1 \sim \frac{a}{v} \sim 10^{-13}\,\text{s}$$

short λ

Thus $S(k) = S^{SA}(k) + P(k)$

$P(k)$ are "Placzek Corrections" derived from $\int \omega^n S(k,\omega)\,d\omega$ and are unreliable for $\left(\frac{m}{M}\right) \gtrsim 1/5$

Protons (water) are especially difficult

Summary

If coherent + incoherent can be separated,

Coherent ≡ structure + collective motion

Incoherent ≡ single particle dynamics

$$\int \frac{d^2\sigma}{d\Omega\, dE'}\, dE' \equiv S(k) \text{ for X-rays}$$

$S(k) + P(k)$ for neutrons

Neutron Diffraction

Sources: Reactors now, pulsed Sources in future

ILL GRENOBLE
BROOKHAVEN
HIFAR OAK RIDGE

Typical Fluxes 10^{16} - 10^{19} thermal neutrons /cm² sec.

[illegible] WNR SNS

Monochromator

[illegible], using the [illegible]

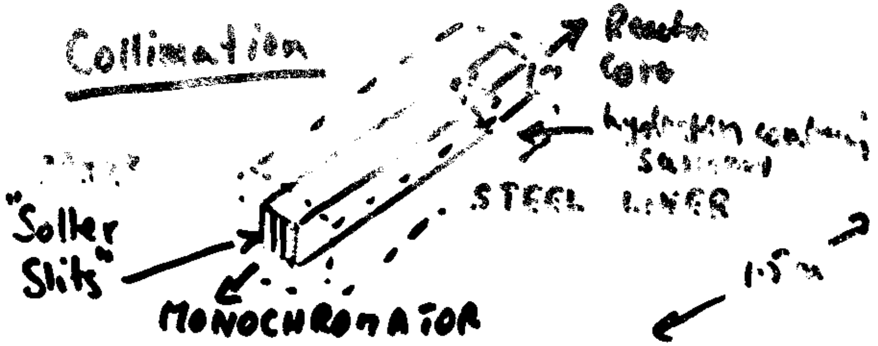
Condition [illegible] $= n(\lambda)$

Note: reflectivity versus resolution

$\frac{\delta\lambda}{\lambda} \sim \cot\theta\, d\theta \to 0$ for $\theta \to \pi/2$

"Back scattering"

Collimation



Detection

Enriched BF_3 counters or ^3He

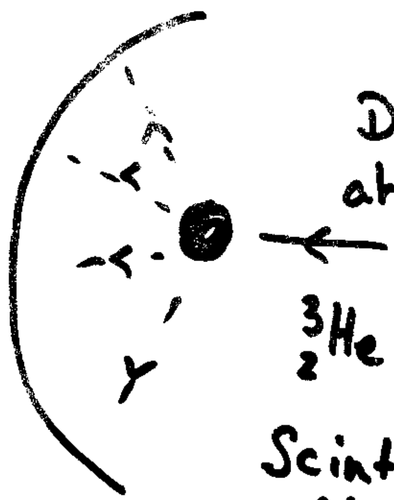
$$^{10}_{5}B + {}^{1}_{0}n \to {}^{7}_{3}Li + {}^{4}_{2}He + 2.8\,MeV$$

Path length [illegible] $\cong 10^{-3}$ [illegible]

$$^{3}_{2}He + {}^{1}_{0}n \to {}^{1}_{1}H + {}^{3}_{1}H + 0.76\,MeV$$

Higher efficiency at low λ

Position Sensitive Detection



Data collected at many angles

^3_2He banks or

Scintillators (^6Li loaded glass)

HIFAR

Interaction with Sample

V, Ti–Zr alloy have $\bar{b} = 0$

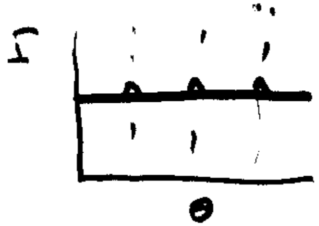
Total Absorption ~ 10% as a rule
(i.e. true absorption
+ Scattering)

$$I(\theta) = \alpha(\theta)\left[S(k) + \delta(\theta)\right]$$

Observed

Calibration parameter

$\alpha(\theta)$	$\delta(\theta)$
Geometry	Multiple Scattering
Absorption (Sample)	Sample: inelastic scattering
(Can)	Can: scattering
	Placzek correction



$\boxed{\int_0^{k_{max}} S(k)}$

1. Use V as a calibrant
2. Use cylindrical samples, absorption isotropic for weak absorption
3. Use thin samples ~10% attenuation

4. Use V or Ti–Zr cells if possible. Otherwise fused silica
5. Use shortest λ possible a) to minimise Placzek b) to maximise k_{max} [Hot Source]

$S(k)$ has [illegible]

can use for further calibration

1) $S(k) \rightarrow 1$ for large k

2) $S(0) \rightarrow \rho k_B T \chi_T$ for $k=0$

3) $S(k)$ obeys a sum rule

$$g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^\infty dk\,(S(k)-1)\,k \sin kr$$

$$g(0) = 0$$

$$\therefore 0 = 1 + \frac{1}{2\pi^2 \rho} \int dk\,(S(k)-1)\,k^2$$

$$\text{i.e.} \int dk\,(S(k)-1)\,k^2 = -2\pi^2 \rho$$

$S(k)$ now accurate to a few % absolutely, 1% relatively

X-ray diffraction

Sources

Laboratory: X-ray generator, 60kV or less, Ag or Mo shortest wavelengths

Rotating anode, 150kV

W K_α line a possibility.

Synchrotron: DESY, DARESBURY......

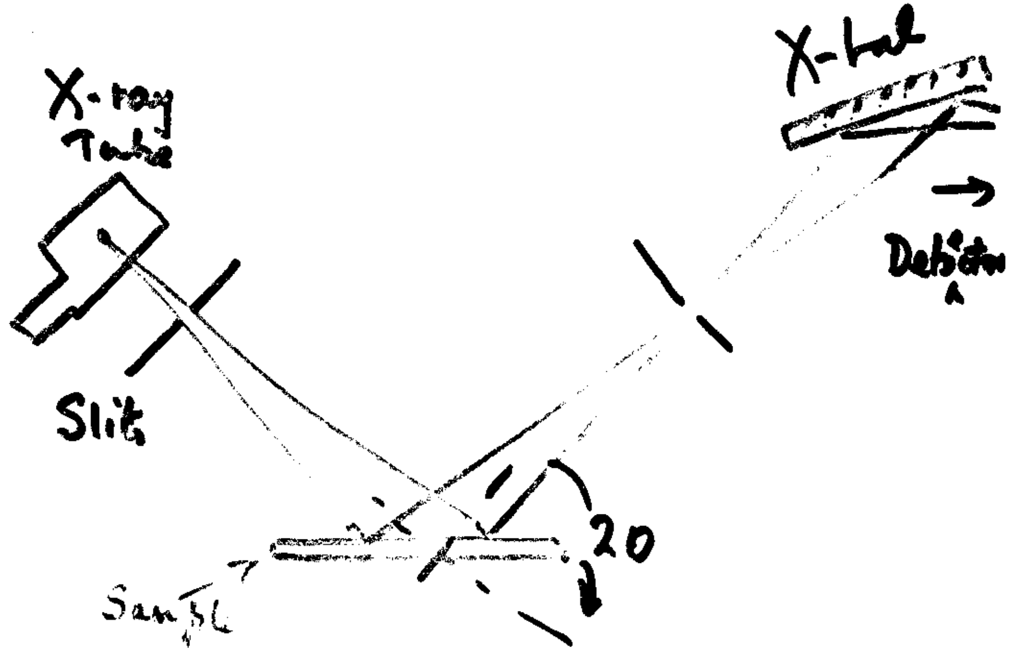
Monochromator

Placed either in the incident or scattered beam (usual case)

Graphite used for laboratory sources, Silicon for synchrotrons

Detection

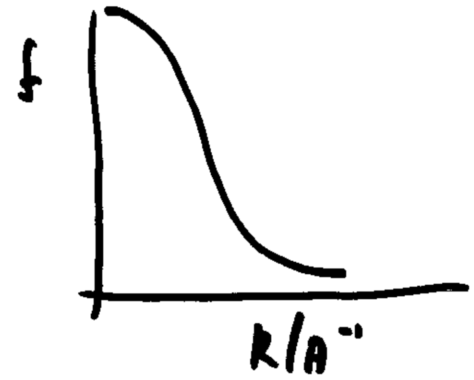
		$\delta E/E$
	Scintillation	~30%
	Proportional	~15%
Li/Si	Solid State	~2%



$\alpha(k)$	$\delta(k)$
Geometry	$\boxed{\text{Compton Scattering}}$
Polarisation	Multiple Scattering
[illegible]	

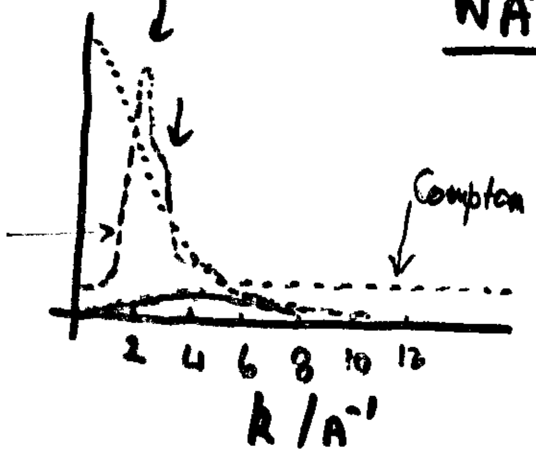
No V-calibration Equivalent.

Compton Scattering a problem for light elements



$$S(k) = \frac{I}{Nf^2}$$

WATER



See Neutron Vol 1: Water, a Comprehensive Treatise p311