Scattering Theory - Invariant

(Porod (1951))

$$Q = \int I(\underline{S})\, d\underline{S} = (1/(2\pi)^3) \int I(\underline{q})\, d\underline{q}$$

= total scattering over the whole of reciprocal space

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= total scattering over the whole of reciprocal space

$$Q = \Gamma_\rho(0) = \langle \rho^2 \rangle V$$

(see derivation in Roe, 1.5)

Pair distribution fcn

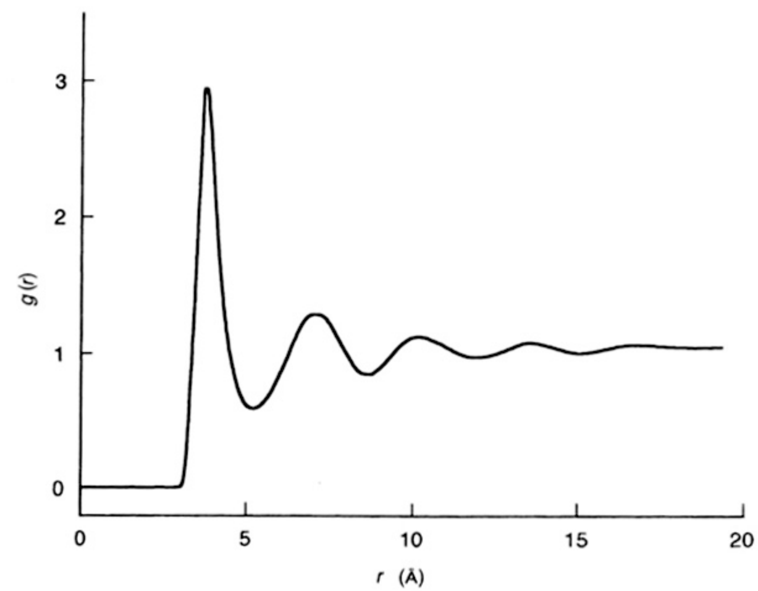
<u>Single atomic species</u> (Roe, Sect. 4.1)

Short range order

Atom environments vary - can only get an avg picture

Define PDF *g(r)* to describe structure

Can get PDF from scattering data



Pair distribution function of liquid argon at 84 K

Pair distribution fcn

Single atomic species (Roe, Sect. 4.1)

Short range order

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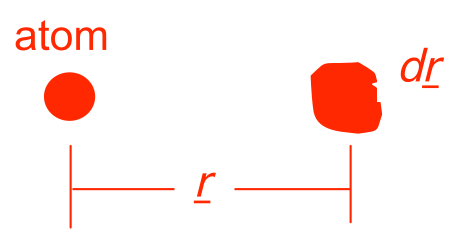
Define PDF $g(\underline{r})$ to describe structure



\# of atoms, on avg, in $d\underline{r} = n_2(\underline{r})\, d\underline{r}$, and

$$g(\underline{r}) = n_2(\underline{r}) / \langle n \rangle$$

where $\langle n \rangle$ = avg # density of atoms

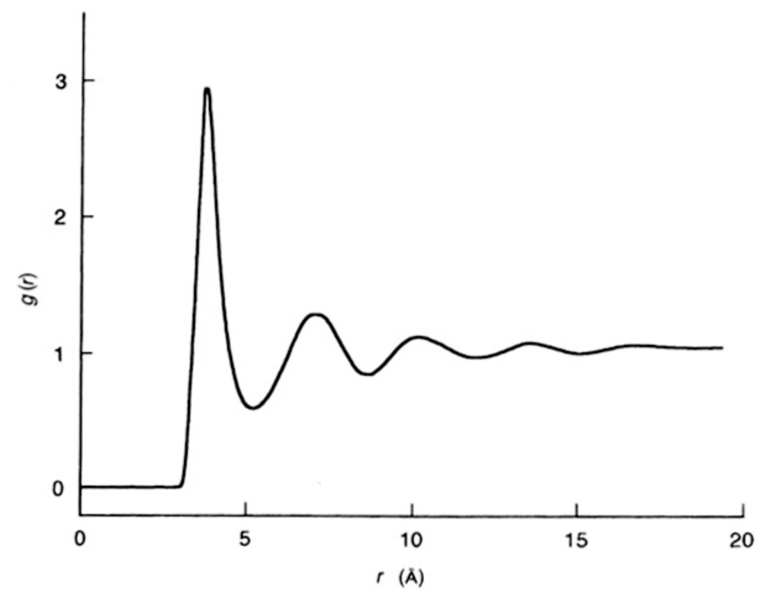
Pair distribution fcn

Single atomic species (Roe, Sect. 4.1)

Short range order

$g(\underline{r})$ = radial distribution fcn

when material is amorphous (isotropic)



Pair distribution function of liquid argon at 84 K

Pair distribution fcn

Single atomic species

$$I(\underline{q}) = |A(\underline{q})|^2 = \left(b\sum_{j=1}^{N} exp(i\underline{q}\bullet\underline{r}_j)\right)\left(b\sum_{k=1}^{N} exp(-i\underline{q}\bullet\underline{r}_k)\right)$$

$$= N b^2 + b^2 \sum_{j=1}\sum_{j\neq k}^{N} exp(-i\underline{q}\bullet\underline{r}_{jk}) \qquad \underline{r}_{jk} = \underline{r}_j - \underline{r}_k$$

$$= N b^2 + N b^2 \int_V n_2(\underline{r})\, exp(-i\underline{q}\bullet\underline{r}_k)\, d\underline{r}$$

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$$= N b^2 + N b^2 \int [n_2(\underline{r}) - \langle n \rangle] exp(-i\underline{q} \bullet \underline{r}_k)\, d\underline{r} + N b^2 \int \langle n \rangle exp(-i\underline{q} \bullet \underline{r}_k)\, d\underline{r}$$

$$= N b^2 + N b^2 \langle n \rangle \int [g(r) - 1] exp(-iq\, r_k)\, dr + N b^2 \langle n \rangle\, \delta(q)$$

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$$= N b^2 + N b^2 \langle n \rangle \int [g(r) - 1] exp(-iqr) \, dr + N b^2 \langle n \rangle \, \delta(q)$$

unobservable - ignore

Define interference fcn $= i(q) = (I(q) - N b^2)/ N b^2$

Pair distribution fcn

Single atomic species

$$= N\, b^2 + N\, b^2 \langle n \rangle \int_V [g(r) - 1]\exp(-iqr)\, dr + N\, b^2 \langle n \rangle\, \delta(q)$$

unobservable - ignore

Define interference fcn $= i(q) = (I(q) - N\, b^2)/\, N\, b^2$

Then

$$i(q) = \langle n \rangle \int_V [g(r) - 1]\exp(-iqr)\, dr$$

And get $g(r) - 1$ from inverse Fourier transform of $i(q)$

$$[g(r) - 1] = 1/\langle n \rangle \int_V i(q) \exp(iqr)\, dq$$

Pair distribution fcn

Simple polymer (Cs & Hs)

Need $g_{CC}(r)$, $g_{HH}(r)$, & $g_{CH}(r)$

$$g_{CH}(r) = n_{CH}(r) / \langle n_H \rangle$$

$\langle n_H \rangle$ = avg # density of H atoms

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$\langle n_H \rangle$ = avg # density of H atoms

$$g_{CH}(r) = g_{HC}(r)$$

Pair distribution fcn

Simple polymer

$$I(q) = \sum_{\alpha=1}^{m} N_\alpha\, b_\alpha^{\,2} + \sum_{\alpha=1}^{m} N_\alpha\, b_\alpha \sum_{\beta=1}^{m} b_\beta \int_V n_{\alpha\beta}(r)\, \exp(-iqr)\, dr$$

m different types of atoms (for C & H, *m=2*)
α, β (= 1....m) denote atom types
N_α = # of α atoms

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N_α = # of α atoms

$N_\alpha = N\, x_\alpha$; $\langle n_\alpha \rangle = \langle n \rangle\, x_\alpha$; x_α = # fraction of α atoms

Then

$$I(q) = N \sum_{\alpha=1}^{m} x_\alpha\, b_\alpha^2 + N \langle n \rangle \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} x_\alpha\, x_\beta\, b_\alpha\, b_\beta \int_V [g_{\alpha\beta}(r) - 1]\, \exp(-iqr)\, dr$$

Pair distribution fcn

Simple polymer

$$I(q) = N\sum_{\alpha=1}^{m} x_\alpha\, b_\alpha^2 + N\,\langle n\rangle \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} x_\alpha\, x_\beta\, b_\alpha\, b_\beta \int_V [g_{\alpha\beta}(r) - 1]\, \exp(-iqr)\, dr$$

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$$i(q) = \int_V [g(r) - 1] \exp(-iqr)\, dr$$

If:

$$w_\alpha = x_\alpha b_\alpha / \sum_{\alpha=1}^{m} x_\alpha b_\alpha$$

then:

$$\int_V g(r) \exp(-iqr)\, dr = \sum_{\alpha=1}^{m}\sum_{\beta=1}^{m} w_\alpha w_\beta \int_V g_{\alpha\beta}(r) \exp(-iqr)\, dr$$

Pair distribution fcn

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Can get *g(r),* but not separate $g_{\alpha\beta}$. Need additional data sets.