Scattering Theory - Correlation

(Read Roe, section 1.5)

Normalized amplitude for multiple atom types:

$$A(\underline{q}) = \sum_j b_j \exp(-i\underline{q} \bullet \underline{r})$$

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Normalized amplitude for an electron density distribution

$$A(\underline{q}) = \int_V \rho(\underline{r}) \exp(-i\underline{q} \bullet \underline{r})\, d\underline{r}$$

$$\rho(\underline{r}) = b_e\, n(\underline{r}) \qquad \text{(no polarization factor)}$$

Scattering Theory - Correlation

$$I(\underline{q}) = \left| A(\underline{q}) \right|^2 = \left| \int_V \rho(\underline{r}) \exp(-i\underline{q} \cdot \underline{r})\, d\underline{r} \right|^2$$

$$= A^*(\underline{q})\, A(\underline{q})$$

Scattering Theory - Correlation

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$$= A^*(\underline{q})\, A(\underline{q}) = \left[\int \rho(\underline{u}') \exp(i\underline{q} \bullet \underline{u}')\, d\underline{u}' \right] \left[\int \rho(\underline{u}) \exp(-i\underline{q} \bullet \underline{u})\, d\underline{u} \right]$$

Scattering Theory - Correlation

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Let $\underline{u}' = \underline{u} + \underline{r}$ After some algebra:

$$I(\underline{q}) = \int \left[\int \rho(\underline{u}+\underline{r})\, \rho(\underline{u})\, d\underline{u} \right] \exp(-i\underline{q} \bullet \underline{r})\, d\underline{r}$$

$$= \int \Gamma_\rho \exp(-i\underline{q} \bullet \underline{r})\, d\underline{r}$$

Scattering Theory - Correlation

$$\Gamma_p(\underline{r}) = \int \rho(\underline{u}+\underline{r})\, \rho(\underline{u})\, d\underline{u}$$

$\Gamma_p(\underline{r})$ is known as:

autocorrelation function

correlation function

pair correlation function

fold of ρ into itself

self-convolution function

pair distribution function

radial distribution function

Patterson function

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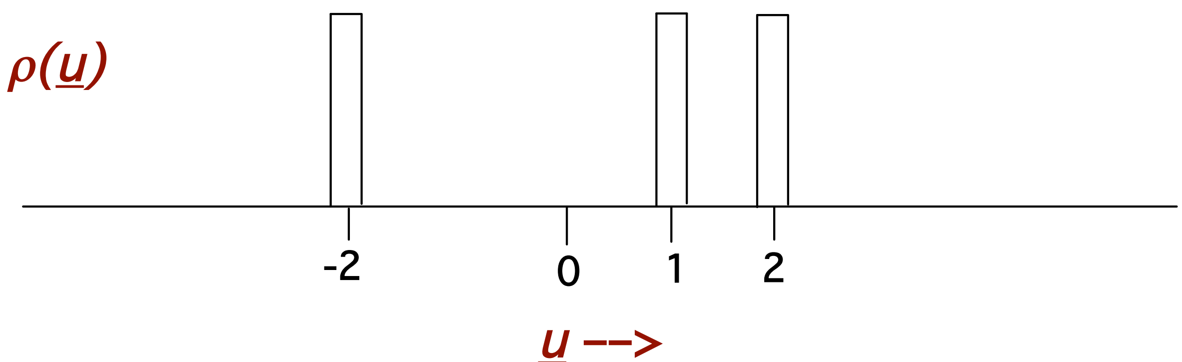
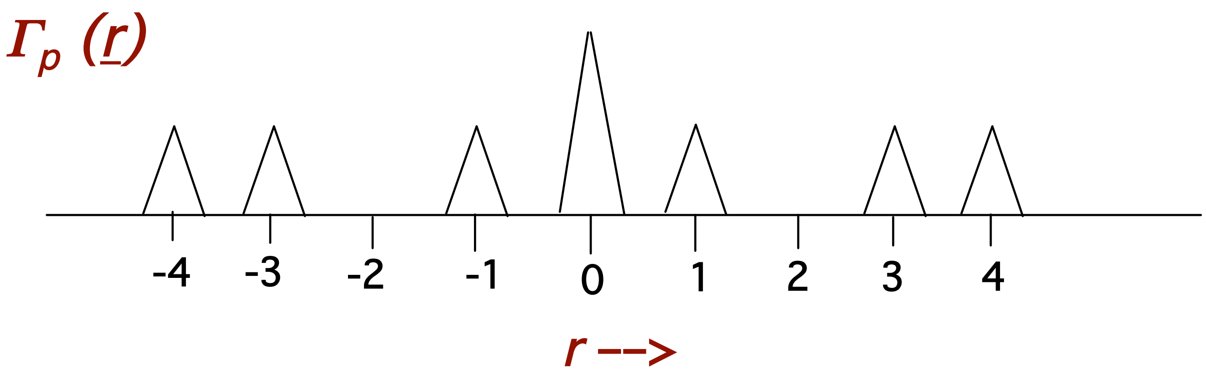
But, whatever it's called, it represents correlation betwn $\rho(\underline{u}')$ and $\rho(\underline{u})$ on avg.

Scattering Theory - Correlation

$$\Gamma_p(\underline{r}) = \int \rho(\underline{u}+\underline{r})\,\rho(\underline{u})\,d\underline{u}$$

Simple example:





Scattering Theory - Correlation

$$\Gamma_p(\underline{r}) = \int \rho(\underline{u}+\underline{r})\,\rho(\underline{u})\,d\underline{u}$$

More:

If we know $A(\underline{S})$, then

$$\rho(\underline{r}) = \int A(\underline{S})\ \exp(-2\pi i\,\underline{S} \bullet \underline{r}_k)\,d\underline{S}$$

Scattering Theory - Correlation

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Scattering Theory - Correlation

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Note:

Since $A(\underline{S})$ is complex, can only get $\rho(\underline{r})$ from $A(\underline{S})$ & $\Gamma(\underline{r})$ from $I(\underline{S})$ & inverses.....nothing else

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This means must model in some way to get $\rho(\underline{r})$ from
$I(\underline{S})$ or $\Gamma(\underline{r})$

Saxs uses $\Gamma(\underline{r})$