Scattering (continued)

Note Title 30/01/2012

$$\frac{d^2\sigma}{d\Omega} \propto |U(\vec{q})|^2 S(\vec{q})$$

$|U(\vec{q})|^2$: depends on probing particle

$\frac{1}{N}$ or $\frac{1}{V}$

$$S(\vec{q}) = \frac{1}{N}\left\langle \sum_{\alpha,\alpha'} e^{i\vec{q}\cdot(\vec{x}_\alpha - \vec{x}_{\alpha'})} \right\rangle$$: Structure factor

: F.T. of correlation fn. $C_{nn}(\vec{x}_1, \vec{x}_2) = \langle n(\vec{x}_1)\, n(\vec{x}_2)\rangle$

$$S(\vec{q}) = \frac{1}{V}\int e^{-i\vec{q}\cdot(\vec{x}_1 - \vec{x}_2)} C_{nn}(\vec{x}_1, \vec{x}_2)\, d\vec{x}_1 d\vec{x}_2 \quad \checkmark$$

Ursell function.

$$\begin{aligned} S_{nn}(\vec{x}_1, \vec{x}_2) &\equiv \langle \delta n(\vec{x}_1)\, \delta n(\vec{x}_2)\rangle \\ &= \left\langle \left(n(\vec{x}_1) - \langle n(\vec{x}_1)\rangle\right)\left(n(\vec{x}_2) - \langle n(\vec{x}_2)\rangle\right)\right\rangle \\ &= \langle n(\vec{x}_1)\, n(\vec{x}_2)\rangle - \langle n(\vec{x})\rangle^2 \\ &= C_{nn}(\vec{x}_1, \vec{x}_2) - \langle n(\vec{x})\rangle^2 \quad \checkmark \end{aligned}$$

Useful b/c $S_{nn} \to 0$ as $|\vec{x}_1 - \vec{x}_2| \to \infty$

$$S_{nn}(\vec{q}) = \frac{1}{V}\int d\vec{x}_1 d\vec{x}_2\, e^{-i\vec{q}\cdot(\vec{x}_1 - \vec{x}_2)} S_{nn}(\vec{x}_1, \vec{x}_2) \quad \checkmark$$

$$S(\vec{q}) = S_{nn}(\vec{q}) + \frac{1}{V}\left| \int d\vec{x}\, e^{-i\vec{q}\cdot\vec{x}} \langle n(\vec{x})\rangle \right|^2$$

For liquid: $\langle n(\vec{x}) \rangle = \langle n \rangle$ constant

$$S(\vec{q}) = \underbrace{S_{nn}(\vec{q})}_{\text{scattering}} + \langle n \rangle^2 (2\pi)^3 \delta(\vec{q})$$

For solid: (crystal). $\langle n(\vec{x}) \rangle$ is a periodic fn of $\vec{x}$

$$\langle n(\vec{x}) \rangle = \sum_{\vec{G}} \langle n_{\vec{G}} \rangle e^{i \vec{G} \cdot \vec{x}} \quad ; \text{ Fourier expansion}$$

Fourier transform of $\langle n(\vec{x}) \rangle$ is not zero @ only $\vec{G}$ (reciprocal lattice vector)

$$S(\vec{q}) = S_{nn}(\vec{q}) + \sum_{\vec{G}} |\langle n_{\vec{G}} \rangle|^2 (2\pi)^3 \delta(\vec{q} - \vec{G})$$

$S_{nn}(\vec{q})$: fluctuation diffuse scattering ← static disorder

$\sum_{\vec{G}} |\langle n_{\vec{G}} \rangle|^2 (2\pi)^3 \delta(\vec{q} - \vec{G})$: elastic (diffraction) part → Bragg peaks

Analogously consider time

If we define time-dep. Ursell fn. as

$$S_{nn}(\vec{x}_1, \vec{x}_2, t, t') = \langle \delta n(\vec{x}_1, t) \, \delta n(\vec{x}_2, t') \rangle$$

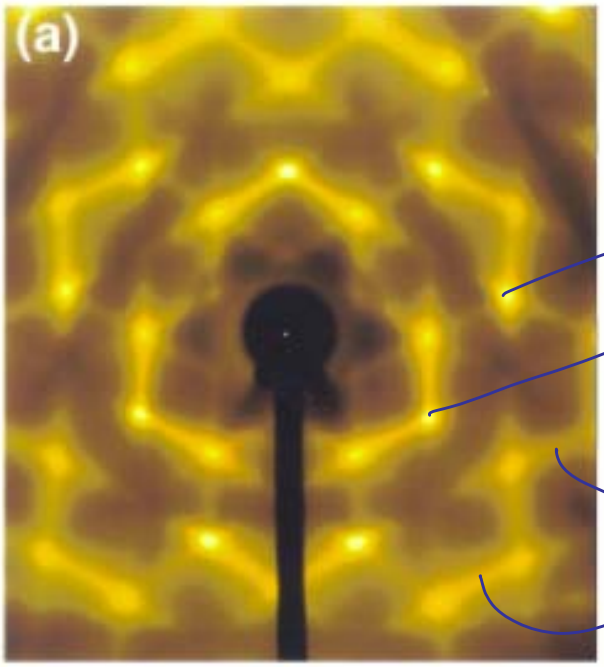
Dynamic Structure factor becomes

$$\Rightarrow S(\vec{q}, \omega) = \underbrace{S_{nn}(\vec{q}, \omega)}_{\text{time-dep. fluctuations}} + \underbrace{\sum |\langle n_{\vec{G}} \rangle|^2 (2\pi)^3 \delta(\vec{q} - \vec{G}) \, \delta(\omega)}_{\text{Static (time-indep.) order}}$$

$\Rightarrow$ usual diffraction

(quantum / thermal fluctuations)

Example of thermal fluctuations



Holt et. al. (PRL 83, 3317)
X-ray data for Si(111)

These spots are Bragg peaks ($\int(\vec{q}-\vec{G})$ terms)

These correspond to thermal diffuse scattering

U(q) part (theory)

Probes	Light	X-ray	Neutron	Electron
Interaction	Relatively weak	Weak	Very weak	Strong
Primary Interaction	Charge	Charge	Spin Nucleus	Charge
Other interactions	Spin (SO)	Spin (SO)		Spin (Exchange)
Probing depth	Medium (~μm)	Medium (~μm)	Long (~cm)	Short (~nm)
Index of refraction	1~2	N~1-δ		
Multiple scattering	Y	N	N	Y

U(q) part (expt)

Probes	Light	X-ray	Neutron	Electron
Wavelength	500nm	~1 Å	~1 Å	0.01~0.1 Å
Q($2\pi/\lambda$)	~10^{-3} $Å^{-1}$	~6 $Å^{-1}$	~6 $Å^{-1}$	~60 $Å^{-1}$
Diffraction	n/a	Y	Y	Y
Scattering	Y	Y	Y	N
Energy	1~2 eV	~10 keV	~30 meV	1~100 keV
Spectroscopy	Very good	OK (IXS)	Very good	OK (EELS)
Source	Bright (laser)	Bright (synchrotron, XFEL)	Dim	Does not matter
Focusing (sample size)	Good	Good	Bad	Good