

Structure of liquids - module of the course "structure of matter"

Struttura della materia Modulo "Struttura dei liquidi"

<http://www.nano.cnr.it/>

Suggested text books:

N.H. March and M.P. Tosi
Atomic Dynamics in Liquids
(first ~3 chapters)

D. L. Goodstein – States of matter, chapter 4 (part)

M. Born and K. Huang
Dynamical Theory of Cristal Lattices

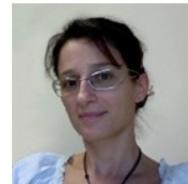
Ashcroft-Mermin,
Solid state physics



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PISA NEST

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Info

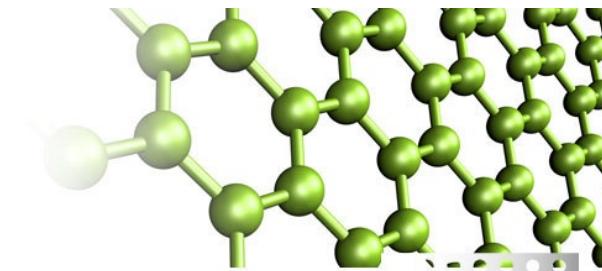
- Pubs in ResearcherID
- Pubs in GoogleScholar
- Pubs in Scopus
- Full publications list
- Conferences and Seminars
- Curriculum Vitae

Address

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Running projects

Graphene Flagship
2013-2019
GRAFLEX MSCA-IF action, 2015-2017
Flexoelectricity in naturally corrugated graphene: a DFT study
ISCRRA-B, 2015-2016



21.01.2016 Python for Computational Science, Modena 25-27/01/2016
A course about Python for Computational Science, held by CINECA developers, will take place in Moden...

21.01.2016 CECAM Workshop
Announcement of workshop: "Ultra-fast phenomena in quantum physics: a challenge for theory & ex..."

23.12.2015 Nest Colloquia 2016
In 2016, following the great success of Colloquia 2015, one researcher a month in Pisa NEST will pre...

search

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Structure of liquids – module of the course “structure of matter”

Preliminaries: states of matter

What are the states of matter?

Solid



Liquid



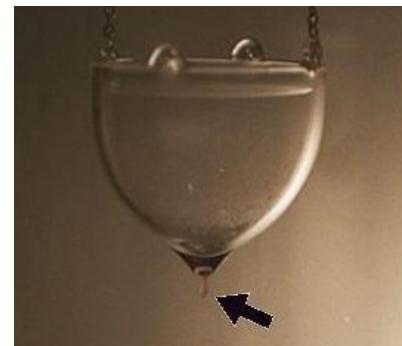
Gas



Crystal



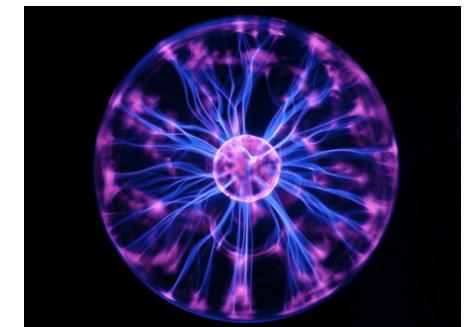
Superfluid



Glass



Plasma



Structure of liquids - module of the course "structure of matter"

Preliminaries: states of matter

Which are the properties of different states?

	crystal	glass	liquid	gas	superfluid	Plasma
Primary school definition	It has its shape and volume		It has its shape	It expands at will	Very cold	Very hot
compressibility	very small	very small	small	large	Infinite ?	vanishing
rigidity, stiffness	Very large	Less large	Null or very small	null	null	null
symmetry, structure	periodic	disordered	uniform, isotropic	uniform, isotropic	uniform, isotropic	uniform, isotropic, charged
viscosity	infinite	very large	large	small	null	Non-linear
Sound velocity (longitudinal)	very large	large	Less large	small	Ideally null, in reality large	Coupled to EM
Other "sounds"	transverse	transverse	None or viscoelastic	none	rotons, surface waves (third sound)...	Plasmons, ...

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Preliminaries: states of matter

This part of the course is about understanding these properties and relating them to the microscopic structure, with a special focus on liquids

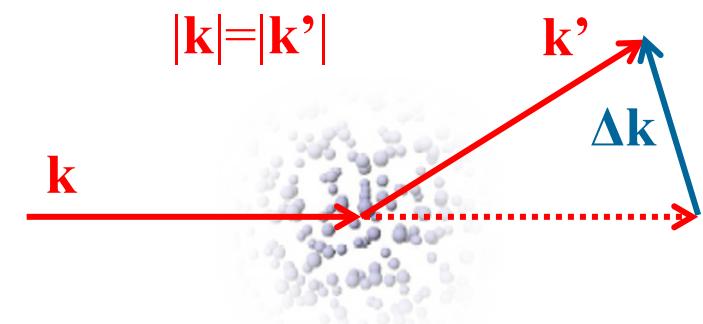
Lesson 1: Elastic scattering

- ✓ Elastic scattering and space Fourier transforms
- ✓ Definition of structure determinants
 - ❖ Two particles density probability
 - ❖ Pair distribution function
 - ❖ Static structure function
- ✓ Phenomenology:
 - ❖ Diffraction from crystalline systems
 - ❖ Diffraction from polycrystalline, amorphous and liquid systems

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Elastic scattering (diffusion):

interaction of a probe with matter **without exchange of energy**. The momentum of the probe can change, not its energy

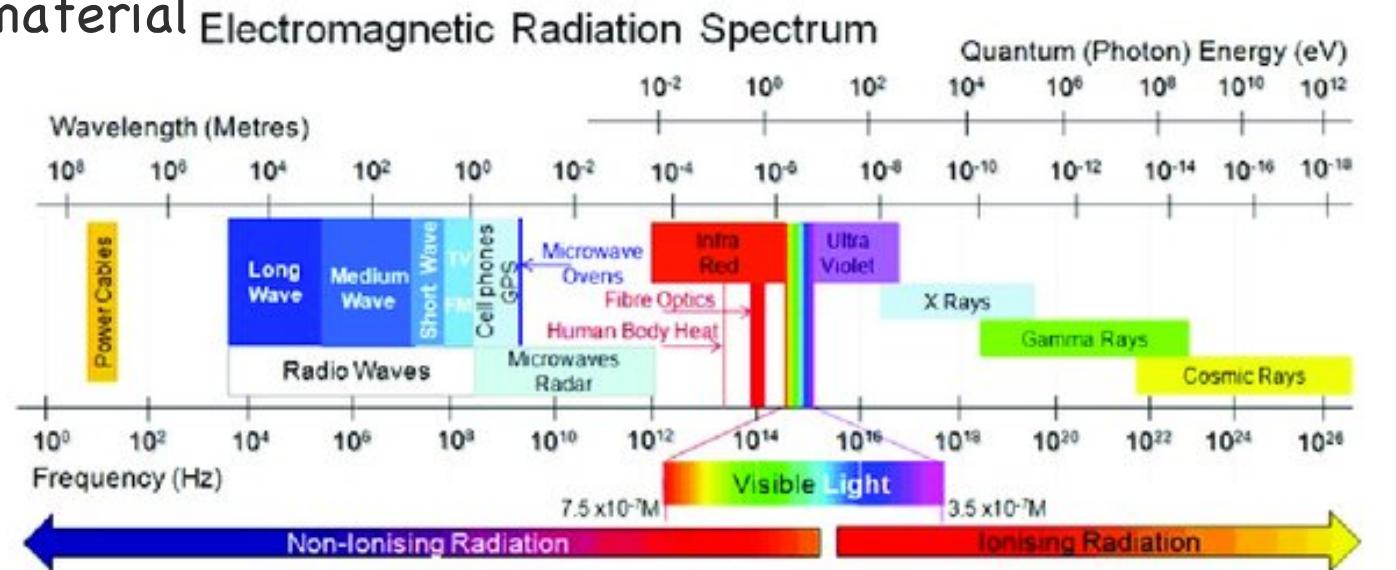


EM radiation interaction with matter:

In general, EM interacts accelerating charges (electrons). It can be adsorbed, elastically or inelastically diffused, promote electrons, or even ionize matter. The prevalence of one or another phenomenon depends on the wavelength and on the material

$$E[\text{eV}] \sim 1240/\lambda[\text{nm}]$$

IR, microwaves: The frequency is resonant with vibrations and phonons, and can therefore be absorbed (**IR absorption**) and/or inelastically scattered (**Brillouin and Raman Scattering**)

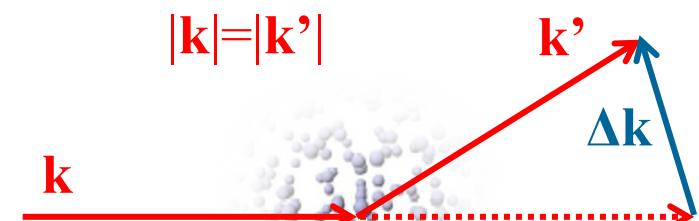


Visible/UV: The frequency is resonant with electronic excitation energies (**UV/Vis absorption**). For hard UV the system can be ionized (**photoelectric effect**)

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Elastic scattering (diffusion):

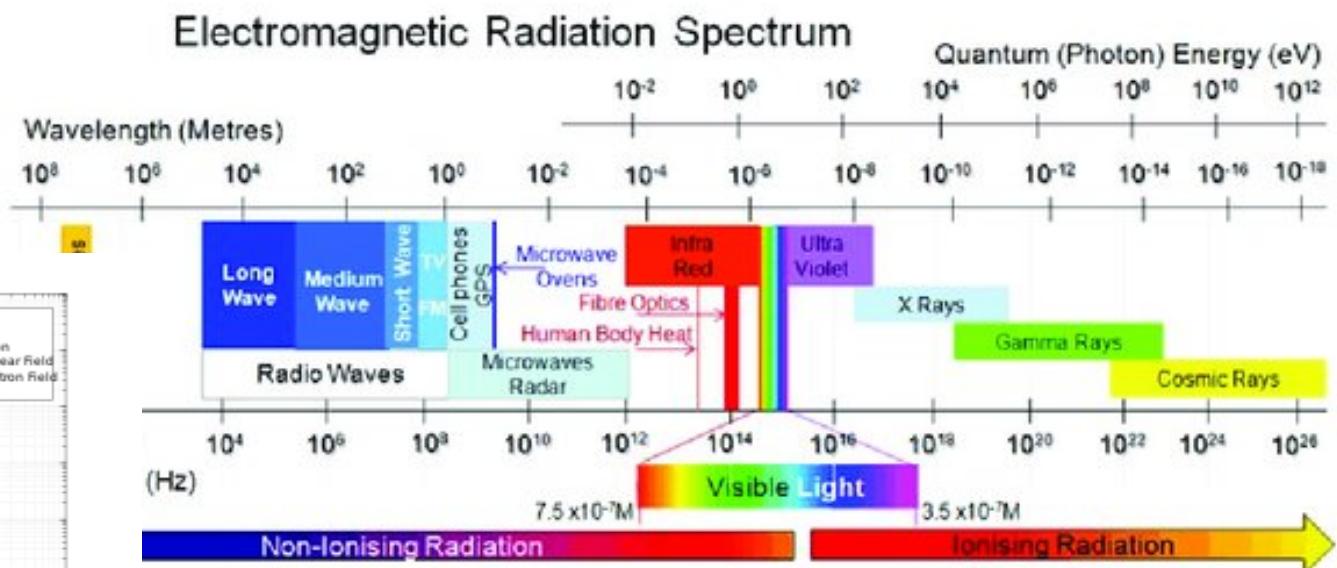
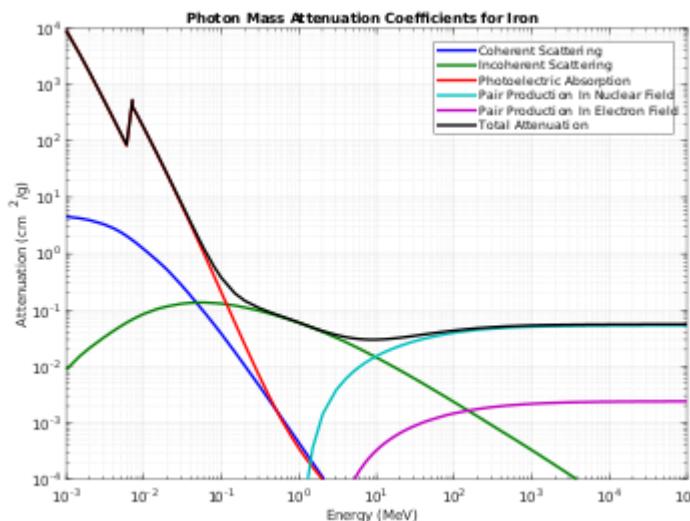
interaction of a probe with matter **without exchange of energy**. The momentum of the probe can change, not its energy.



Xray: wavelengths comparable with the inter-atomic distances

At large energies, elastic diffusion competes with ionization and photon-electron scattering (**Compton**). However in the mild X-ray region, the **elastic diffusion** (**Rayleigh and Thomson**) generally prevails over ionization

$$E[\text{eV}] \sim 1240/\lambda[\text{nm}]$$

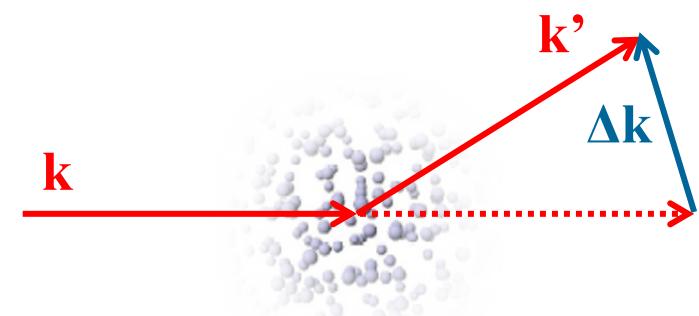


With wavelengths 1-10 Å **Xray** are elastically scattered by electron clouds around atoms

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Elastic scattering (diffusion):

interaction of a probe with matter **without exchange of energy**. The momentum of the probe can change, not its energy.



Xray are elastically scattered by electron clouds around atoms

Neutrons

- ✓ “see” both neutral and charged particles, in any motion state
- ✓ can produce elastic scattering (or also inelastic, from which one can extract other kind of information)
- ✓ have a “contact like” interaction with nuclei, locating the position of atoms, instead of a less defined “cloud”
- ✓ neutrons with wavelengths 1-10Å are “thermal” (10-100 meV)

Would be preferable with respect to Xrays, but are more difficult to produce and handle

Electrons

- ✓ Combine problems of both X-ray and Neutrons...
- ✓ Little penetrating within matter

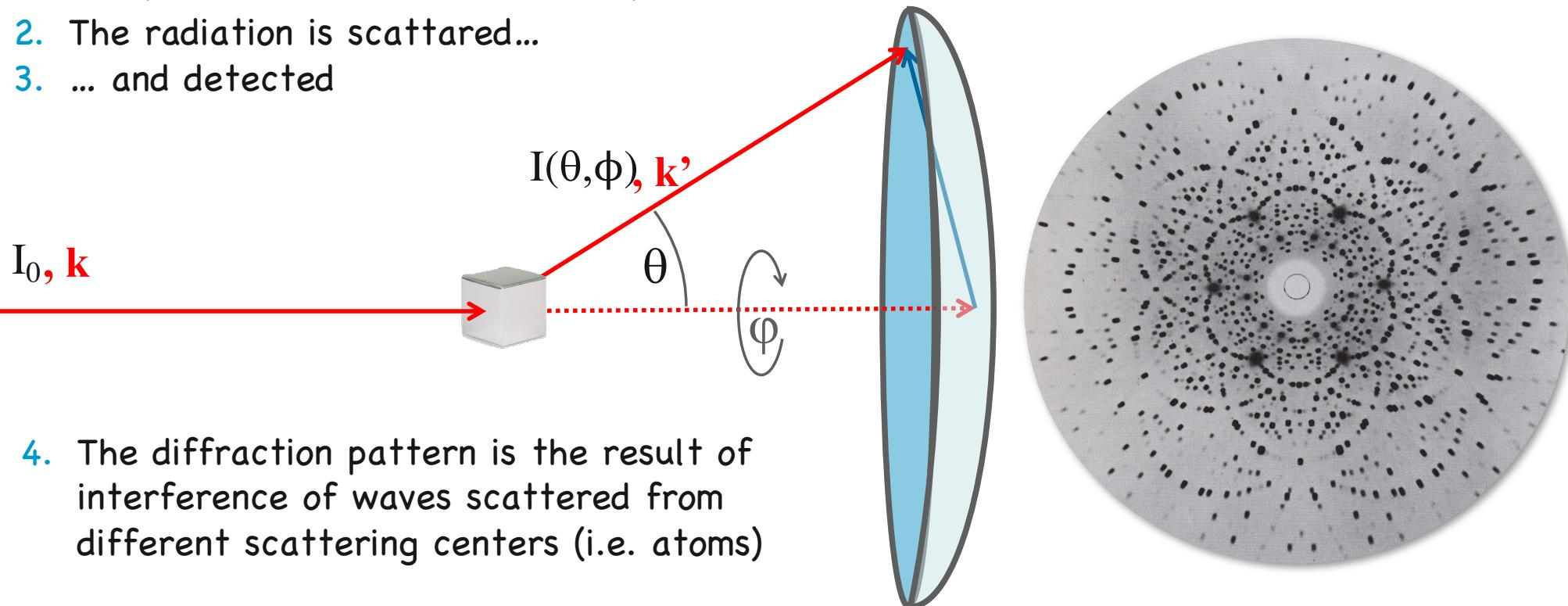
Not very much used

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Elastic scattering (diffusion):

interaction of a probe with matter **without exchange of energy**. The momentum of the probe can change, not its energy.

1. The probe radiation hits the sample
2. The radiation is scattered...
3. ... and detected



4. The diffraction pattern is the result of interference of waves scattered from different scattering centers (i.e. atoms)

- ⇒ The wavelength of the probe must be of the same order of magnitude of inter-atomic distance
- ⇒ In general, the resolution of the technique is determined by the diffraction limit (~wavelength of the probe).

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Elastic scattering (diffusion):

interaction of a probe with matter **without exchange of energy**. The momentum of the probe can change, not its energy.

1. In-coming probe wave (e.g. EM field): $I_0 \sim |\phi_0(r)|^2$

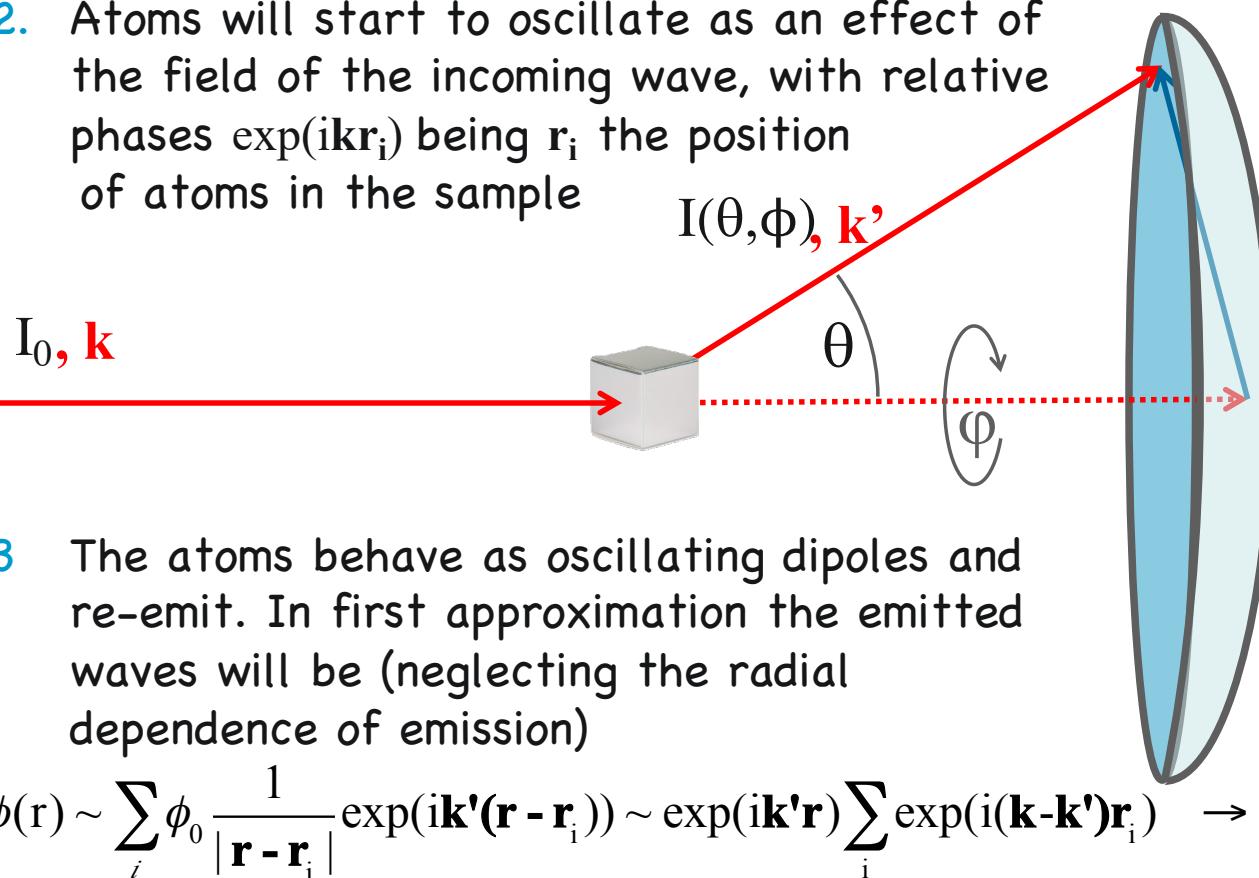
$$\phi_0(r) \sim \exp(i\mathbf{k}r)$$

$$\Delta\mathbf{k} = 2|\mathbf{k}| \sin(\theta/2)$$

2. Atoms will start to oscillate as an effect of the field of the incoming wave, with relative phases $\exp(i\mathbf{k}\mathbf{r}_i)$ being \mathbf{r}_i the position of atoms in the sample

$$I(\theta, \phi), \mathbf{k}'$$

$$I_0, \mathbf{k}$$

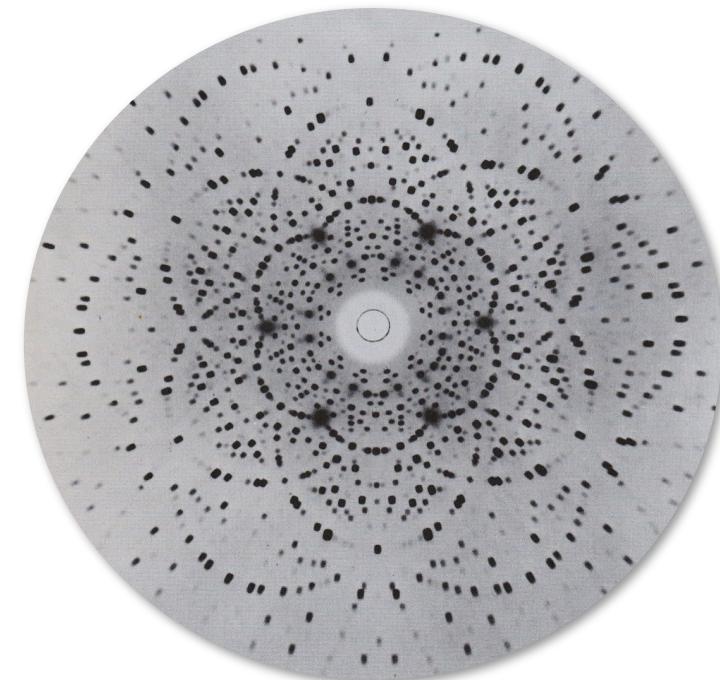
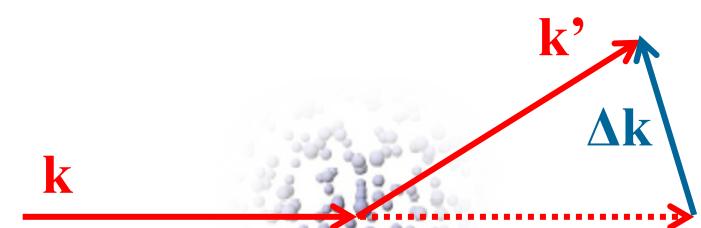


3. The atoms behave as oscillating dipoles and re-emit. In first approximation the emitted waves will be (neglecting the radial dependence of emission)

$$\phi(r) \sim \sum_i \phi_0 \frac{1}{|\mathbf{r} - \mathbf{r}_i|} \exp(i\mathbf{k}'(\mathbf{r} - \mathbf{r}_i)) \sim \exp(i\mathbf{k}'\mathbf{r}) \sum_i \exp(i(\mathbf{k} - \mathbf{k}')\mathbf{r}_i)$$

$$\rightarrow I \sim I_0 \left\langle \left| \sum_i \exp(i(\mathbf{k} - \mathbf{k}')\mathbf{r}_i) \right|^2 \right\rangle$$

This term generates interference, and depends on the atom relative position!
⇒ from the scattering one can extract information on the internal structure of the sample

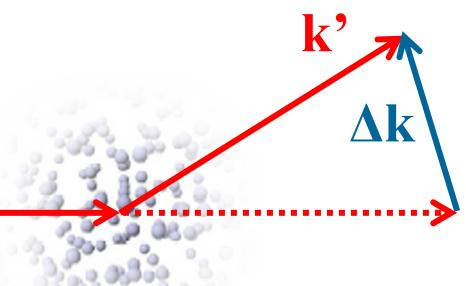


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Elastic scattering

Let's analyze the scattering function

$$\frac{I(\Delta\mathbf{k})}{I_0} = \frac{I(k, \theta, \varphi)}{I_0} \sim \left\langle \left| \sum_i \exp(i(\mathbf{k}-\mathbf{k}')\mathbf{r}_i) \right|^2 \right\rangle = \left\langle \sum_{i,j} \exp(-i\Delta\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)) \right\rangle$$



$$\Delta\mathbf{k} = 2|\mathbf{k}| \sin(\theta/2)$$

For $\Delta\mathbf{k}=0$ (forward scattering) one has $I/I_0=N^2$. This term is always present and do not bring information about the structure. Therefore it is usually subtracted. Note that however, this depends on N^2 (N =number of particles), i.e. behaves as terms bringing constructive interference (i.e. coherent), and at variance with what expected for incoherent terms, scaling as N . Therefore the considered function is usually

$$\frac{I(\Delta\mathbf{k})}{NI_0} - N\delta_{\mathbf{k},\mathbf{k}'} = S(\mathbf{q}) = \frac{1}{N} \left\langle \sum_{i,j} \exp(-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)) \right\rangle - N\delta_{\mathbf{q},\mathbf{0}} \quad \mathbf{q} = \Delta\mathbf{k}$$

$S(\mathbf{q})$ is named the **static structure factor**. Note that

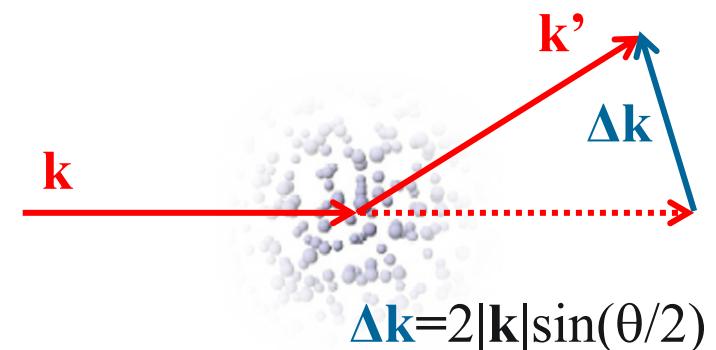
- ✓ For $\mathbf{q}=0$ $S(\mathbf{q})$ is null by definition. But because this is an effect of a Dirac delta subtraction, it is not guaranteed that its behavior for vanishingly small \mathbf{q} is continuous. I.e.: $S(\mathbf{q} \rightarrow \mathbf{0}) = \text{const}$ **usually different from 0** (though usually small)
- ✓ For large \mathbf{q} , the exponential oscillates fast for $i \neq j$ and the $i=j$ terms prevails having null oscillation. This gives $S(\mathbf{q} \rightarrow \infty) = 1$
- ✓ If the system is composed of different atomic species, these might have different scattering power, therefore the expression under sum must be weighted by $f_i f_j$, i.e. by the "atomic form factors".

Structure of liquids – module of the course “structure of matter”

Elastic scattering

What is the relation of structure function (defined in the “reciprocal space”) to the “real space” structure?

$$\frac{I(\Delta k)}{NI_0} - N\delta_{k,k'} = S(\mathbf{q}) = \frac{1}{N} \left\langle \sum_{i,j} \exp(-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)) \right\rangle - N\delta_{\mathbf{q},0}$$



$$\mathbf{q} = \Delta \mathbf{k}$$

$$\Delta \mathbf{k} = 2|\mathbf{k}| \sin(\theta/2)$$

Let's define two “real space” structure functions

1-particle density

$$\rho(\mathbf{r}) = \left\langle \sum_i \delta(\mathbf{r}_i - \mathbf{r}) \right\rangle \quad \int \rho(\mathbf{r}) d\mathbf{r} = N$$

2-particles density

$$\begin{aligned} \rho_2(\mathbf{r}, \mathbf{r}') &= \left\langle \sum_{i,j} \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_j - \mathbf{r}') \right\rangle = \\ &= \left\langle \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_j - \mathbf{r}') \right\rangle + \left\langle \sum_i \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_i - \mathbf{r}') \right\rangle = \bar{\rho}_2(\mathbf{r}, \mathbf{r}') + \left\langle \sum_i \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_i - \mathbf{r}') \right\rangle \\ \int \rho_2(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' &= N^2 \quad \int \bar{\rho}_2(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' = N^2 - N \end{aligned}$$

- ✓ Particle density: to obtain mass density, multiply by m. $\rho(\mathbf{r})$ is proportional to the probability of finding a particle at \mathbf{r}

- ✓ Classical definition and $\langle \rangle$ is the statistical average
- ✓ In quantum case, wavefunctions or field operators must be used

- ✓ Probability of finding a particle at \mathbf{r} and one at \mathbf{r}'
- ✓ Please note the double definition: the first include self-particle probability, and is rather unphysical, but sometimes mathematically useful; the second is physically acceptable in all cases. In the thermodynamic limit they coincide

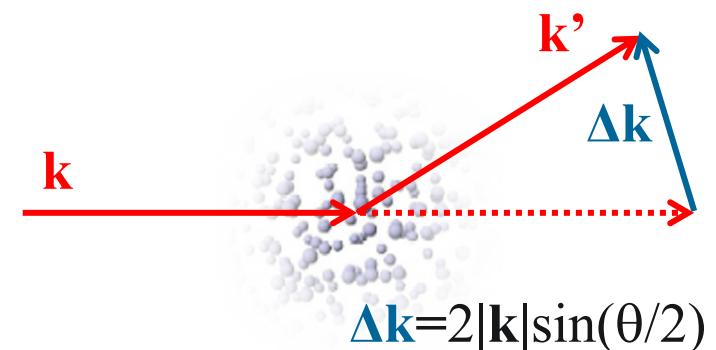
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$\mathbf{q} = \Delta \mathbf{k}$



$$\Delta \mathbf{k} = 2|\mathbf{k}| \sin(\theta/2)$$

Now let's Fourier transform:

$$\int \exp(i\mathbf{k}\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} = \left\langle \sum_i \int \exp(i\mathbf{k}\mathbf{r}) \delta(\mathbf{r}_i - \mathbf{r}) d\mathbf{r} \right\rangle = \left\langle \sum_i \exp(i\mathbf{k}\mathbf{r}_i) \right\rangle$$

1-particles density

First we make a variable change $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$

2-particles density

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \left\langle \sum_{i,j} \delta(\mathbf{r}_i - \mathbf{r}_1) \delta(\mathbf{r}_j - \mathbf{r}_2) \right\rangle = \left\langle \sum_{i,j} \delta(\mathbf{r} - (\mathbf{r}_i - \mathbf{r}_j)) \delta(\mathbf{R} - (\mathbf{r}_j + \mathbf{r}_i)/2) \right\rangle = \hat{\rho}_2(\mathbf{r}, \mathbf{R}) = \hat{\rho}_2(\mathbf{r}_1 - \mathbf{r}_2, (\mathbf{r}_1 + \mathbf{r}_2)/2)$$

We then Fourier transform with respect to \mathbf{r} and \mathbf{R} :

$$\left\langle \sum_{i,j} \int \delta(\mathbf{r} - (\mathbf{r}_i - \mathbf{r}_j)) \exp(-i\mathbf{q}\mathbf{r}) d\mathbf{r} \int \delta(\mathbf{R} - (\mathbf{r}_j + \mathbf{r}_i)/2) \exp(-i\mathbf{Q}\mathbf{R}) d\mathbf{R} \right\rangle = \left\langle \sum_{i,j} \begin{array}{|c|c|} \hline \exp(-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)) & \exp(-i\mathbf{Q}((\mathbf{r}_j + \mathbf{r}_i)/2)) \\ \hline \sim S(\mathbf{q}) & \sim FT[\rho(\mathbf{r})] \\ \hline \end{array} \right\rangle = \hat{S}(\mathbf{q}, \mathbf{Q})$$

Exact relation: $S(\mathbf{q}) = \hat{S}(\mathbf{q}, \mathbf{Q}=0)$

$$S(\mathbf{q}) = \frac{1}{N} \iint d\mathbf{r} d\mathbf{R} \exp(-i\mathbf{q}\mathbf{r}) \rho_2(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) - N\delta_{\mathbf{q},0} = \frac{1}{N} \iint d\mathbf{r}_1 d\mathbf{r}_2 \exp(-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)) \rho_2(\mathbf{r}_1, \mathbf{r}_2) - N\delta_{\mathbf{q},0}$$

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Elastic scattering

$$S(\mathbf{q}) = \frac{1}{N} \iint d\mathbf{r}_1 d\mathbf{r}_2 \exp(-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)) \rho_2(\mathbf{r}_1, \mathbf{r}_2) - N\delta_{\mathbf{q},0}$$

Therefore in general, elastic scattering is related to the **FT of the correlation part of the two particle density**, averaging out the global single particle density fluctuations ("out of diagonal" part of the ρ_2)

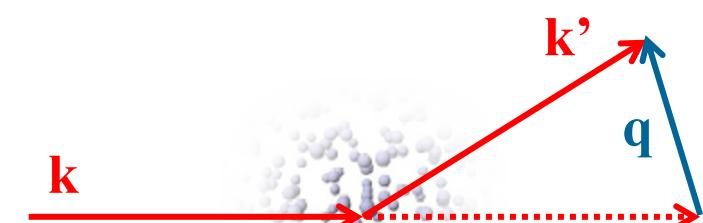
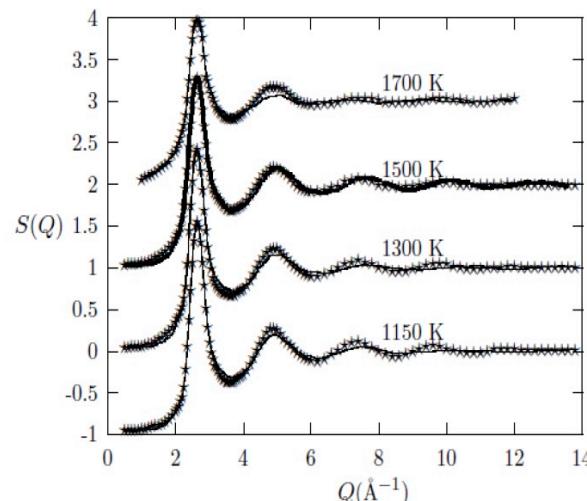
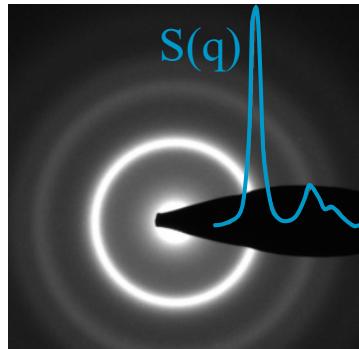
Special cases: liquids

Liquids are **uniform and isotropic** systems, therefore $\rho(\mathbf{r}) = \rho = \frac{V}{N}$

ρ_2 depends only on the particle distance $r = |\mathbf{r}_1 - \mathbf{r}_2|$

$$S(q) = \frac{\rho}{V} \int [g(r) + V\delta(r)] e^{-iqr} d\mathbf{r} - N\delta_{0,q} = 1 + \rho \int_0^\infty [g(r) - 1] \frac{\sin(qr)}{qr} 4\pi r^2 dr$$

$$S(q) - 1 = \text{FT}[g(r) - 1]$$



$$q = 2|\mathbf{k}| \sin(\theta/2)$$

$$\rho_2(\mathbf{r}_1, \mathbf{r}_2) = \rho^2 [g(r) + V\delta(r)]$$

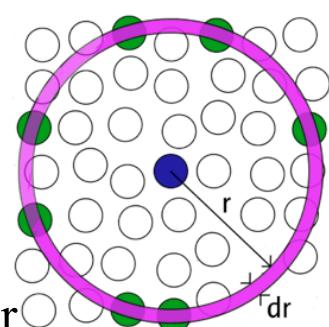
Different particles contribution

Same particles contribution

Pair correlation function

Number of particles in the spherical shell at distance r

a given one: $dN = \rho 4\pi r^2 g(r) dr$

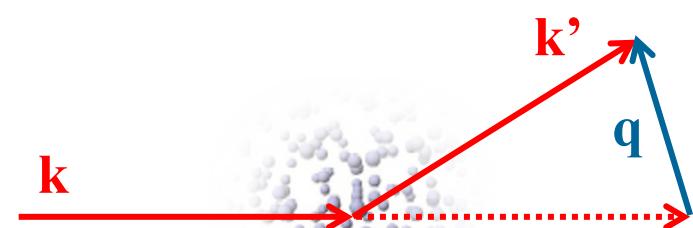


$S(q)$ tends to 1 for large q by construction: in that region, pair correlation contribution from different particles is vanishingly small

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$$S(\mathbf{q}) = \frac{1}{N} \iint d\mathbf{r}_1 d\mathbf{r}_2 \exp(-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)) \rho_2(\mathbf{r}_1, \mathbf{r}_2) - N\delta_{\mathbf{q},0}$$



Special cases: liquids

$$S(q) = \frac{\rho}{V} \int [g(r) + V\delta(r)] e^{-iqr} d\mathbf{r} - N\delta_{0,\mathbf{q}} = 1 + \rho \int_0^\infty [g(r) - 1] \frac{\sin(qr)}{qr} 4\pi r^2 dr$$

Disordered systems (glasses, amorphous)

What changes in glasses with respect to liquids?

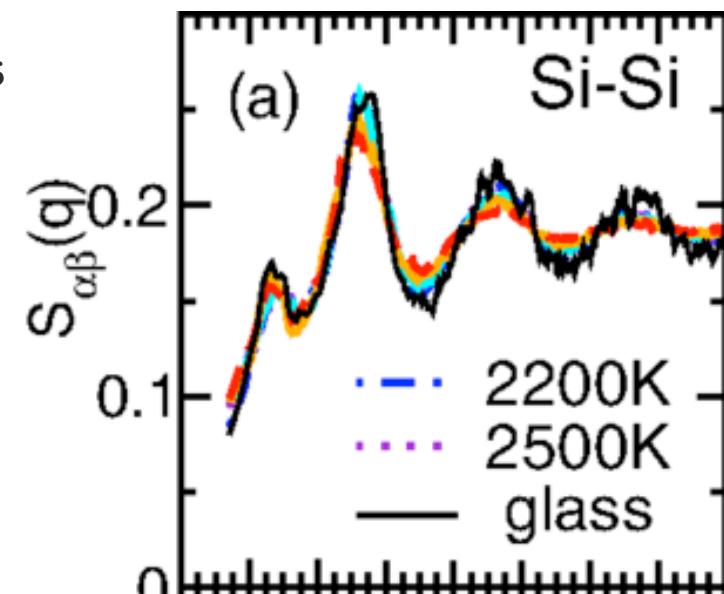
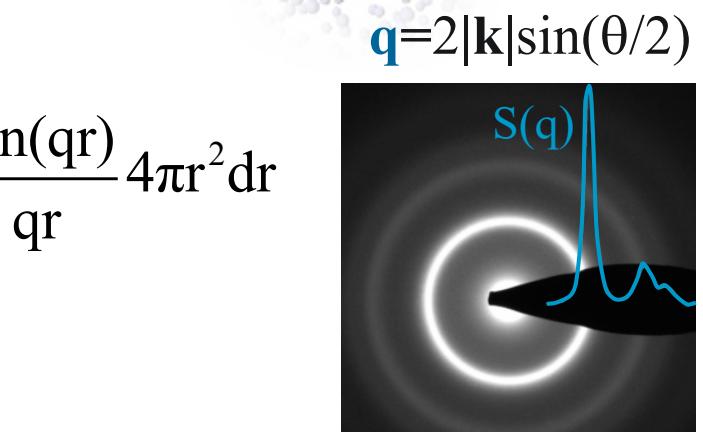
From the point of view of “static” structure factor...

basically nothing

$S(q)$ is very similar, only little more noisy in glasses across transition

This is because the scattering process takes a series of “snapshots” of the system (inter particle correlations at the same times), therefore it sees a disordered system in both cases.

Average is taken over positions (double integral) and over different subsequent snapshots (ensemble) and is little more efficient in liquids where atoms move between snapshots



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$$S(\mathbf{q}) = \frac{1}{N} \iint d\mathbf{r}_1 d\mathbf{r}_2 \exp(-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)) \rho_2(\mathbf{r}_1, \mathbf{r}_2) - N\delta_{\mathbf{q},0}$$

Special cases: liquids

Disordered systems (glasses, amorphous)

$$S(q) = \frac{\rho}{V} \int [g(r) + V\delta(r)] e^{-iqr} d\mathbf{r} - N\delta_{0,q} = 1 + \rho \int_0^\infty [g(r) - 1] \frac{\sin(qr)}{qr} 4\pi r^2 dr$$

Crystals

$$\rho(\mathbf{r}) = \sum_i f(\mathbf{r} - \mathbf{R}_i) \quad \text{periodic and usually localized on sites}$$

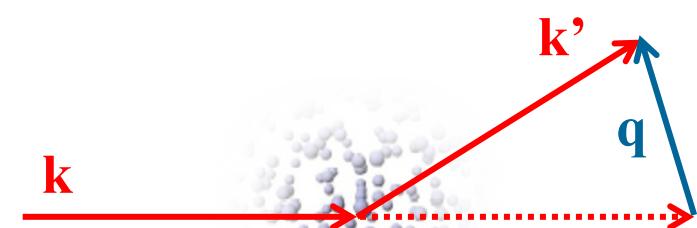
$$\bar{\rho}_2(\mathbf{r}_1, \mathbf{r}_2) \approx \rho(\mathbf{r}_1)\rho(\mathbf{r}_2) - \delta(\mathbf{r}_1 - \mathbf{r}_2)\rho(\mathbf{r}_1)$$

2-particle correlations dominated by crystal symmetry

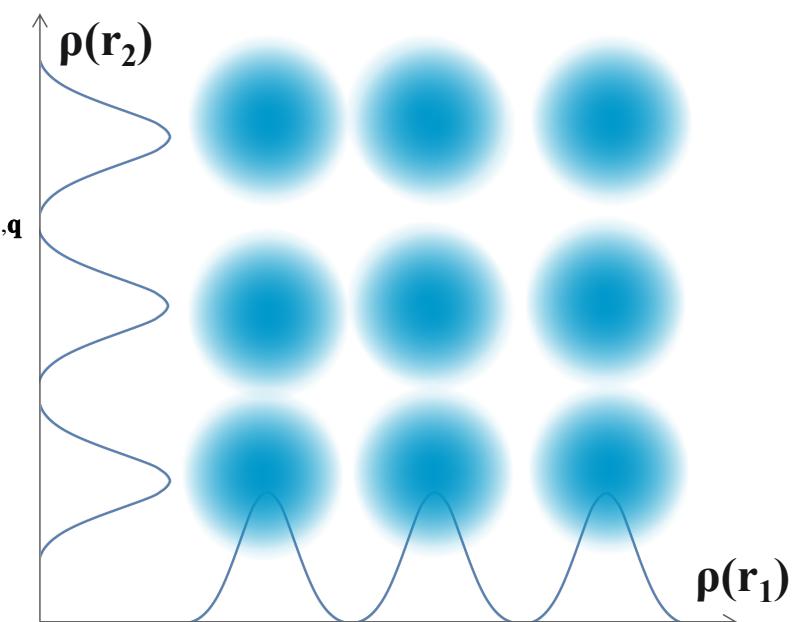
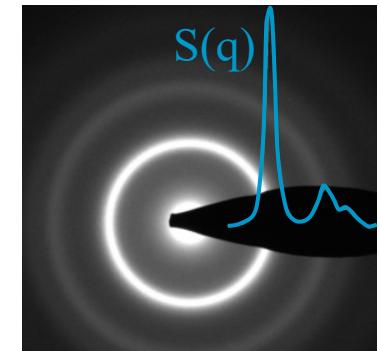
$$S(\mathbf{q}) = 1 + \frac{1}{N} \int \rho(\mathbf{r}')\rho(\mathbf{r}) e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} d\mathbf{r} d\mathbf{r}' - \frac{1}{N} \int \delta(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}) e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} d\mathbf{r} d\mathbf{r}' - N\delta_{0,q}$$

$$S(\mathbf{q}) + N\delta_{0,q} = \frac{1}{N} \left| \int \rho(\mathbf{r}) e^{i\mathbf{q}(\mathbf{r})} d\mathbf{r} \right|^2 = |FT[\rho(\mathbf{r})]|^2$$

What is the relationship of this formula to the Bragg's law "constructive interference occurs when $2d \sin(\theta) = n\lambda$ " (d =crystal planes distance)?



$$q = 2|\mathbf{k}| \sin(\theta/2)$$



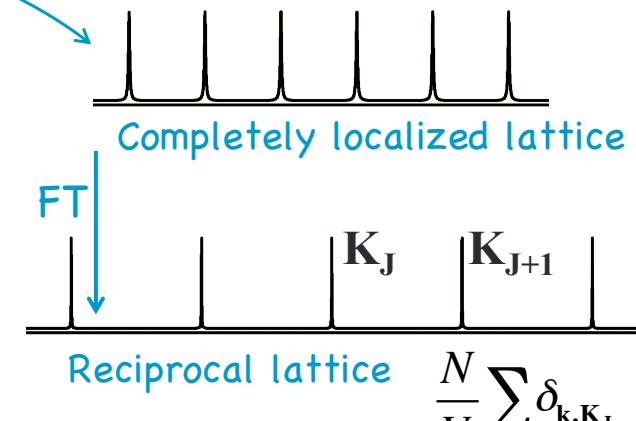
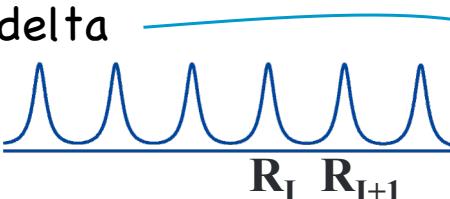
Structure of liquids - module of the course "structure of matter"

Digression: all measurement techniques making use of the interference phenomenon practically operate a Fourier Transform (FT). This is true for interferometry (both in time and space domains), in which usually frequency or wavelength is varied to obtain a time or space domain spectral analysis, but also for diffraction. For elastic scattering the wavelength is usually not varied (though it could be done), but the diffusion wave number q is the difference between two non-collinear vectors, therefore it varies also in modulus, and can span the reciprocal spectral space, even if wavelength is not varied.

Space FT of a crystal density

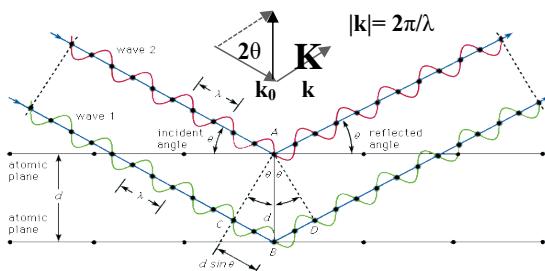
- ✓ A crystal particle density can be described as the sum of a given function $f(\mathbf{r})$ centered over the sites of a lattice. Let's assume for the moment a (unrealistic) case of fully localized particles: then f is a Dirac delta

$$\rho(\mathbf{r}) = \sum_I f(\mathbf{r} - \mathbf{R}_I) \rightarrow \sum_I \delta(\mathbf{r} - \mathbf{R}_I)$$



$$FT[\rho(\mathbf{r})] = \frac{1}{V} \int \sum_I \delta(\mathbf{r} - \mathbf{R}_I) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} = \frac{1}{V} \sum_I e^{i\mathbf{k}\mathbf{R}_I} = \frac{N}{V} \sum_J \delta_{\mathbf{k}, \mathbf{K}_J}$$

The last equality can be easily proven using $e^{-i\mathbf{R}\mathbf{K}}=1$ with $\{\mathbf{K}\}$ the reciprocal lattice of $\{\mathbf{R}\}$ and it is equivalent to the statement of constructive interference only for \mathbf{k} belonging to the reciprocal lattice

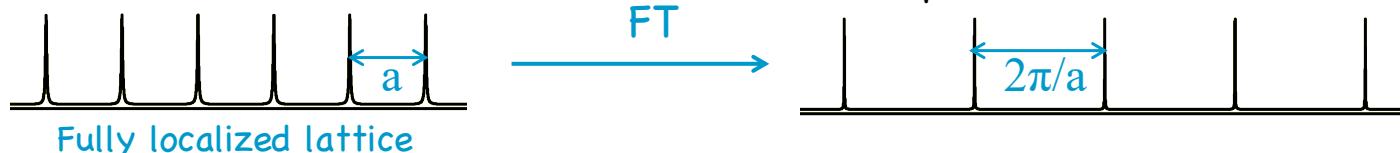


It can be easily shown that the Bragg's condition, when applied to any possible set of crystal planes, is equivalent to $e^{-i\mathbf{R}\mathbf{K}}=1$ (Beware of $\theta/2 \rightarrow \theta$ in Bragg's angles definition)

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✓ The FT of a periodic sum of Dirac deltas is a sum of Kronecker deltas on the reciprocal lattice sites \mathbf{K}

⇒ The diffraction pattern of a **fully localized lattice** is a set of **equal bright spots**



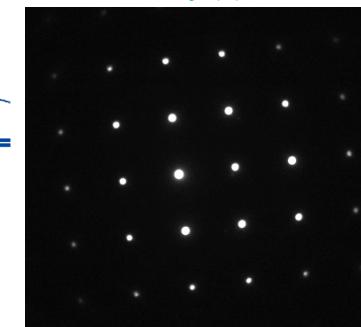
$$\rho(\mathbf{r}) = \sum_I \delta(\mathbf{r} - \mathbf{R}_I) \xrightarrow{FT} \frac{N}{V} \sum_J \delta_{\mathbf{k}, \mathbf{K}_J}$$

✓ In reality, electrons form a delocalized cloud around atoms, described by the **atomic form factor $f(r)$**

⇒ The diffraction pattern of a **monoatomic lattice** is a set of **spots with decreasing intensity**

$$\rho(\mathbf{r}) = \sum_I f(\mathbf{r} - \mathbf{R}_I) \xrightarrow{FT} \frac{N}{V} \sum_J \bar{f}(k) \delta_{\mathbf{k}, \mathbf{K}_J} \quad \bar{f}(k) = FT[f(r)]$$

The larger the $f(r)$, the narrower the $\bar{f}(k)$ i.e. the fastest the space brightness decay



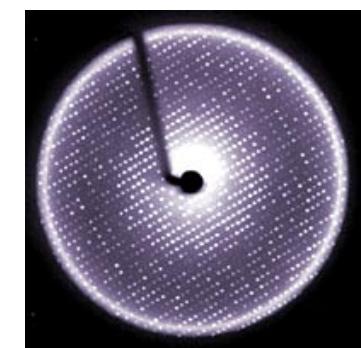
✓ If the crystal is polyatomic, the atomic structure factor sum with phases

⇒ The diffraction pattern

of a **polyatomic lattice** is modulated (**different brightness**)

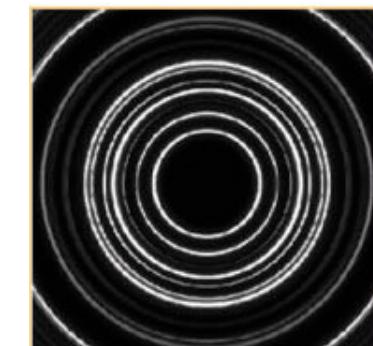
$$\rho(\mathbf{r}) = \sum_I \sum_i f_i(\mathbf{r} - \mathbf{r}_i - \mathbf{R}_I) \xrightarrow{FT} \frac{N}{V} \sum_J \sum_i \bar{f}_i(k) e^{i \mathbf{k} \cdot \mathbf{r}_i} \delta_{\mathbf{k}, \mathbf{K}_J}$$

Because the unit cells in real space is larger for polyatomic systems, the reciprocal lattice vectors (and the spots in diffraction pattern) have a smaller separation, but still reflect the global crystal symmetry



✓ The above setup assumes a well defined orientation of the crystalline planes with respect to the incident beam. If crystalline planes are randomly oriented, the pattern is rotationally averaged over the φ angle defining the rotation of the crystal planes with respect to the incident beam axis.

⇒ The diffraction pattern of a **polycrystalline lattice (or powder)** is a set of **circles with modulated intensity**. The circles satisfy the Bragg condition $2d \sin \theta = n \lambda$



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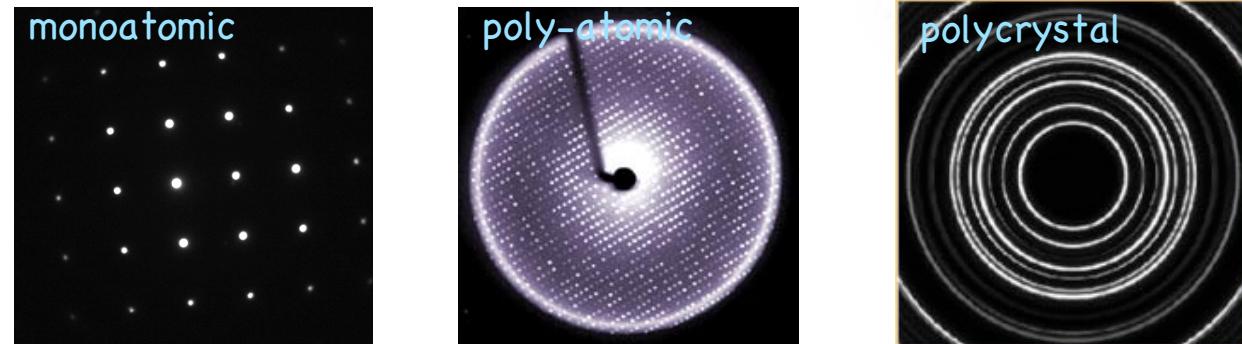
In summary: elastic scattering operate space Fourier transform of the (same time) particle space correlation function.

$$S(\mathbf{q}) = \frac{1}{N} \iint d\mathbf{r}_1 d\mathbf{r}_2 \exp(-i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)) \rho_2(\mathbf{r}_1, \mathbf{r}_2) - N\delta_{\mathbf{q},0}$$



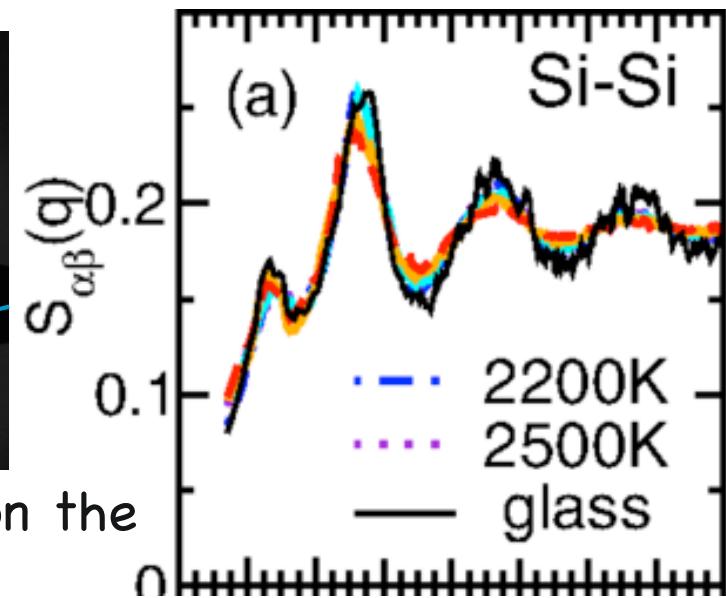
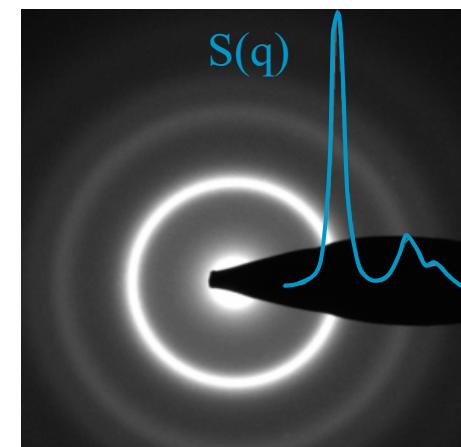
Crystals

$$S(\mathbf{q}) + N\delta_{0,\mathbf{q}} \approx |FT[\rho(\mathbf{r})]|^2$$



Fluids, glasses

$$S(q) = 1 + \rho \int [g(r) - 1] e^{-iqr} d\mathbf{r}$$



Therefore: elastic scattering gives information on the internal (atomic) structure of a system

Next: How do I use and interpret this information?