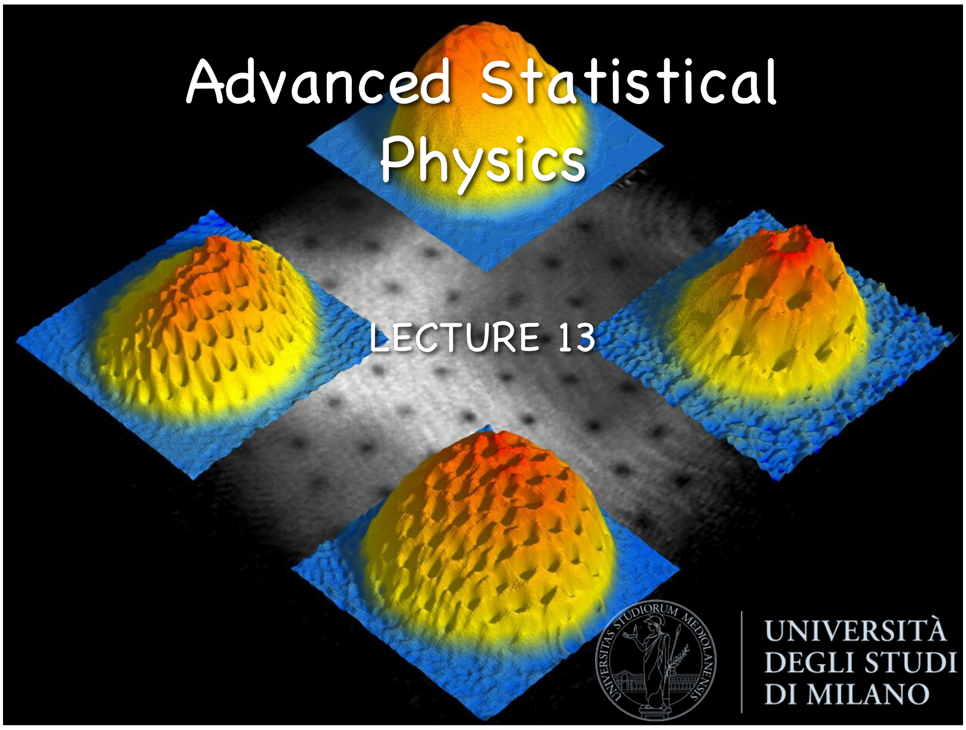


1

Outline

- Onsager's regression hypothesis
- Linear response
- Scattering
- Dynamic and static structure factors
- Density and distribution functions
- Structure factor: ideal Bose gas and WIBG

- Scope:
  - to study the connection among the response of a macroscopic system to a small perturbation and its equilibrium fluctuations, and thus to microscopic correlation functions
  - to investigate the connection among microscopic space-temporal correlations in macroscopic physical systems and scattering experiments
  - to investigate quantum interacting systems and to give a concrete example of dynamic structure factors

2

2

vogliamo studiare il comportamento di un sistema quando messo fuori equilibrio

Non-equilibrium statistical mechanics

- Up to this point, we have used statistical mechanics to describe time-independent equilibrium properties. One can be interested also in, eventually time-dependent, non-equilibrium properties
- An example of a non-equilibrium property is the rate at which a system absorbs energy when it is exposed to an external force. If this is done with one frequency -a monochromatic disturbance- this example is the absorption spectrum of a material. Another example of a non-equilibrium property is the relaxation rate by which a system reaches equilibrium from a prepared non-equilibrium state

- Our discussion of these properties will be confined to systems close to equilibrium: We often want to know how a system behaves when kicked in various fashions. Linear response theory is a broad, systematic method developed for equilibrium systems in the limit of gentle kicks

3

3

una perturbazione può dipendere dallo spazio e dal tempo → possiamo modellarla spazialm. e/o temporalmente

The regression hypothesis

- We can use statistical mechanics to calculate the response when a system is kicked by elastic stress, electric fields, magnetic fields, acoustic waves, light etc. . The space-time dependent linear response to the space-time dependent influence is described in each case by a susceptibility, χ.
- Moreover, a material in thermal equilibrium may be macroscopically homogeneous and static, but it moves on the microscale from thermal fluctuations. We measure how systems moves and evolve in space and time using correlation functions macroscopicamente in eq ma microscopic fluttuazioni → f. di correlazione
- When not far from equilibrium, the relaxation will be governed by a principle first enunciated in 1930 by Lars Onsager in his remarkable regression hypothesis:

  The relaxation of macroscopic non-equilibrium disturbances is governed by the same laws as the regression of spontaneous microscopic fluctuations in an equilibrium system

4

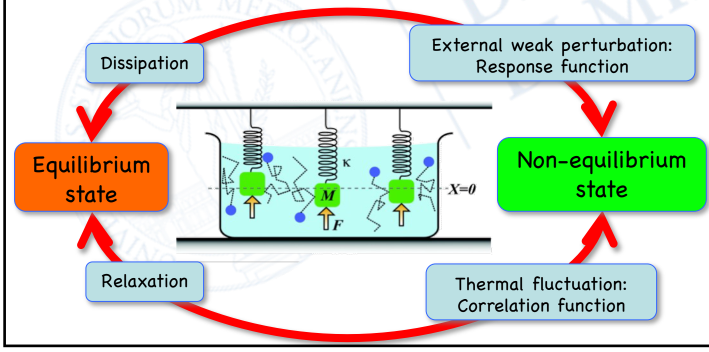
4

le fluttuazioni all'equilibrio sono collegate alle dissipazioni fuori dall' eq dall'ipotesi di regressione di Onsager

↳ Teo fluttuazione-dissipazione collega l'equilibrio e il non equilibrio

The fluctuation-dissipation connection

- This cryptic sounding principle is the cornerstone for nearly all modern work in time-dependent statistical and thermal physics. It earned Onsager the 1968 Nobel Prize in Chemistry.
- The regression hypothesis is an important consequence of the fluctuation-dissipation theorem (Callen and Welton, 1951): a relationship connecting relaxation and rates of absorption to the correlations between fluctuations that occur spontaneously at different times in equilibrium systems



Both ways are related through the Fluctuation-Dissipation theorem

5

5

Linear response regime: basic concepts

6

- Question: How do we measure the conductivity of a metal? Answer: we first introduce a weak electric field E, and then measure the electric current j. In general, j is a function of E, and then, provided that E is weak enough, we can make a Taylor expansion for this function:

$$j(E) = j(E=0) + j'(E=0)E + \frac{1}{2!} j''(E=0)E^2 + \cdots$$

- It is safe to assume that that when E=0 ⇒ j=0, so the first term in the equation above is zero. And therefore, the leading order term is the linear term of E (if E<<1). If we ignore all higher order terms beyond the leading order one, we get a linear relation between J and E

$$j(E) = j'(E=0)E = \sigma E$$

- Thus, as long as E is weak enough, j shall be proportional to E and the coefficient is the conductivity.
- Because j is a linear function of E at small E, the weak E limit is also known as the linear response regime
- The philosophy described above applies to many experimental techniques: typically, in an experiment we first introduce a small perturbation to the system and then we see how the system response to this perturbation

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Linear response (static uniform perturbation)

- We now consider a static and uniform small perturbation applied to a system; the Hamiltonian is modified as

$$\hat{H}(\lambda) = \hat{H} - \lambda \hat{A}$$

where λ characterizes the perturbation intensity

- Experiments indicates that in general if λ is small we obtain a linear response.

- The system response relative to an observable B is given by

si mostra ancora ricavabile così

$$\langle \hat{B} \rangle_\lambda = \frac{Tr\left(\hat{B}e^{-\beta(\hat{H}-\lambda\hat{A})}\right)}{Tr\left(e^{-\beta(\hat{H}-\lambda\hat{A})}\right)} = B_0 + \lambda\chi_{BA} + O(\lambda^2)$$

- χ_{BA} is the so called differential susceptibility:

$$\boxed{\chi_{BA} = \left.\frac{\partial \langle \hat{B} \rangle_\lambda}{\partial \lambda}\right|_{\lambda=0}}$$

We are interested in obtaining an expression for χ_{BA}

7

7

caso classico (quello quantistico non commutante è nei supplementari)

$[\hat{H},\hat{A}]=0$ case (for $[\hat{H},\hat{A}]\neq 0$ case: see supplementary material) :

- This case correspond also to the classical case; if λ is small

$$\langle \hat{B} \rangle_\lambda = \frac{Tr\left(\hat{B}e^{-\beta(\hat{H}-\lambda\hat{A})}\right)}{Tr\left(e^{-\beta(\hat{H}-\lambda\hat{A})}\right)} \approx \frac{Tr\left(\hat{B}e^{-\beta\hat{H}}(1+\beta\lambda\hat{A})\right)}{Tr\left(e^{-\beta\hat{H}}(1+\beta\lambda\hat{A})\right)} = \frac{Tr\left(\hat{B}e^{-\beta\hat{H}}\right) + \beta\lambda Tr\left(\hat{B}\hat{A}e^{-\beta\hat{H}}\right)}{Tr\left(e^{-\beta\hat{H}}\right) + \beta\lambda Tr\left(\hat{A}e^{-\beta\hat{H}}\right)}$$

$$= \frac{\langle \hat{B} \rangle + \beta\lambda\langle \hat{B}\hat{A} \rangle}{1+\beta\lambda\langle \hat{A} \rangle} \cong \left(\langle \hat{B} \rangle + \beta\lambda\langle \hat{B}\hat{A} \rangle\right)\left(1-\beta\lambda\langle \hat{A} \rangle\right) \cong \langle \hat{B} \rangle + \beta\lambda\left(\langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle\langle \hat{A} \rangle\right)$$

valori di aspettazione all'equilibrio

$$\Rightarrow \boxed{\chi_{BA} = \left.\frac{\partial \langle \hat{B} \rangle_\lambda}{\partial \lambda}\right|_{\lambda=0} \cong \beta\left(\langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle\langle \hat{A} \rangle\right) := \beta\langle \hat{B}\hat{A} \rangle_c} \; *$$

correlation function

- We can make some example:

Case (1): $\left(\hat{A} = \hat{B} = \hat{H}\right)$ this correspond to a variation of the temperature

$$\beta\left(\hat{H} - \lambda\hat{H}\right) = \frac{\hat{H}}{k_B T(1+\lambda)} + O(\lambda^2) \Rightarrow T_\lambda = (1+\lambda)T$$

$\hat{H}(1-\lambda)$

8

8

$1-\lambda \sim \frac{1}{1+\lambda}$

il calore specifico è dato dalle fluttuazioni di energia

- Moreover $\quad \dfrac{\partial\langle\hat{H}\rangle_\lambda}{\partial\lambda} = \dfrac{\partial T_\lambda}{\partial\lambda}\dfrac{\partial\langle\hat{H}\rangle_\lambda}{\partial T_\lambda} = T\dfrac{\partial\langle\hat{H}\rangle}{\partial T} = TC_V$
- Therefore

calore specifico

$$\chi_{HH} = TC_v = \beta\left(\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2\right) \quad\Rightarrow\quad C_V = \frac{\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2}{k_B T^2} = \frac{\langle\hat{H}^2\rangle_c}{k_B T^2}$$

- We now define a local energy-density operator: $\hat{H} = \int d\vec{r}\,\hat{\varepsilon}(\vec{r})$

$$\hat{\varepsilon}(\vec{r}) = \frac{1}{2}\sum_i\left[\delta(\vec{r}-\hat{\vec{r}}_i)\frac{\hat{\vec{p}}_i^{\,2}}{2m} + \frac{\hat{\vec{p}}_i^{\,2}}{2m}\delta(\vec{r}-\hat{\vec{r}}_i)\right] + \frac{1}{2}\sum_{i\neq j} v(\hat{\vec{r}}_i-\hat{\vec{r}}_j)\,\delta\left(\vec{r}-\tfrac{\hat{\vec{r}}_i+\hat{\vec{r}}_j}{2}\right)$$

- We obtain:

$$\langle\hat{H}^2\rangle_c = \left\langle\int d\vec{r}\int d\vec{r}\,'\,\hat{\varepsilon}(\vec{r})\,\hat{\varepsilon}(\vec{r}\,')\right\rangle_c = \int d\vec{r}\int d\vec{r}\,'\left\langle\hat{\varepsilon}(\vec{r})\hat{\varepsilon}(\vec{r}\,')\right\rangle_c = V\int d\vec{r}\left\langle\hat{\varepsilon}(\vec{r})\hat{\varepsilon}(0)\right\rangle_c$$

- This lead us to

$$\boxed{C_V = \frac{\langle\hat{H}^2\rangle_c}{k_B T^2} = \frac{V}{k_B T^2}\int d\vec{r}\left\langle\hat{\varepsilon}(\vec{r})\hat{\varepsilon}(0)\right\rangle_c}$$

forma microscopica

Response function

Spontaneous fluctuation

correlation function

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Case (2): we now take λ to be a magnetic field variation δh, and $\hat{A}$ the magnetization operator ; if also the operator B=M we have that $\langle B\rangle$ is the induced magnetization in the system and χ_{MM} the magnetic susceptibility

- We assume $\left[\hat{H},\hat{M}\right] = 0 \quad\Rightarrow$ the magnetization is a constant of motion

$$\chi_{MM} = \frac{\partial M}{\partial h} = \frac{\langle\hat{M}^2\rangle_c}{k_B T} = \frac{\langle\hat{M}^2\rangle - \langle\hat{M}\rangle^2}{k_B T}$$

- Magnetization can be written as an integral over a local magnetization operator

$$\hat{M} = \int d\vec{r}\,\hat{m}(\vec{r})$$

- It follows that $\quad \langle\hat{M}^2\rangle_c = \int d\vec{r}\int d\vec{r}\,'\left\langle\hat{m}(\vec{r})\hat{m}(\vec{r}\,')\right\rangle_c = V\int d\vec{r}\left\langle\hat{m}(\vec{r})\hat{m}(0)\right\rangle_c$

- And therefore

$$\boxed{\Rightarrow \chi_{MM} = \frac{\langle\hat{M}^2\rangle - \langle\hat{M}\rangle^2}{k_B T} = \frac{V}{k_B T}\int d\vec{r}\left\langle\hat{m}(\vec{r})\hat{m}(0)\right\rangle_c}$$

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Response function

Spontaneous fluctuation

correlation function

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Linear response (time dependent perturbation)

- The most important approach to the experimental and theoretical studies of the properties of many body systems can be traced back to the measure or calculation of the response of the system (induced electrical charge polarization and current, magnetization, thermal current etc.) to an externally applied space and time-dependent perturbation (electric and magnetic fields, temperature gradients, etc.)
- In this case, linear response is characterized by a dynamic susceptibility which depends both from the wave vector **k** and the frequency $\nu=\omega/2\pi$; as we shall see $\chi(\mathbf{k},\omega)$ is expressed in terms of space and time-dependent correlation functions
- In fact, there is a very direct relation between the dynamic susceptibility and the spontaneous fluctuations spectrum of physical observables, called the fluctuation dissipation theorem (see supplementary material)
- Let us apply now an external time-dependent perturbation which couples to the system through a local observable $\hat{a}(\mathbf{r})$

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- The time dependent Hamiltonian becomes

$$\hat{H}(t) = \hat{H}_0 - \int d\vec{r}\, \lambda(\vec{r},t)\hat{a}(\vec{r}) = \hat{H}_0 + \hat{H}_1(t)$$

- The function $\lambda(\mathbf{r},t)$ is a given function of time, describing the strength of a classical external field acting on the system.
- The action of such an external field will drive the system out of equilibrium, and the density matrix will be the solution of the equation of motion, the Von Neumann equation

$$i\hbar\frac{d\hat{\rho}(t)}{dt} = \left[\hat{H}(t),\hat{\rho}(t)\right]$$

- In order fix it uniquely, we have to supplement this equation with an appropriate initial condition. We shall assume the perturbation to vanish in the "far past", i.e.:

$$\lim_{t\to-\infty} \lambda(\vec{r},t) = 0 \qquad \forall \vec{r}$$

- an that, again in the "far past", the system is in its thermodynamic equilibrium state. This will fix the initial condition as:

$$\lim_{t\to-\infty} \hat{\rho}(t) = \hat{\rho}_0 = e^{-\beta\hat{H}_0}\Big/Tr(e^{-\beta\hat{H}_0})$$

condizioni iniziale

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Come fa Molinari

Adiabatic switching on

- The function $\lambda(\mathbf{r},t)$ extends in time for an infinite interval (from $t=-\infty$ to some finite time), and on such a long time interval, no matter how weak the coupling between the system and the external probe is, the deviation of the system from the equilibrium may not be regarded as small.

- If this is the case, non-linear effects can become important, and our linear approach can break down.

- One way out of this problem, is to assume that the coupling between the system and the external probe is switched on very slowly with respect to the typical time scales of the system, in such a way that no real transitions in the system are induced and the ground state (or the density matrix at finite temperatures) follows "adiabatically" the perturbation.

- This is usually incorporated into the formalism by replacing $\lambda(\mathbf{r},t)$ by: $[\lambda(\mathbf{r},t)\exp(\delta t)]$, with δ a positive small quantity, and considering only linear response, and then letting $\delta \to 0^+$ at the end of the calculations.

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The Kubo formula

- (see supp. material for the details of the derivation)
- For a time dependent perturbation which couple to the system through a local observable $\hat{a}(r)$, at linear order, the response measured in the local variation of the observable B is:

$$\left\langle \hat{B}(\vec{r},t)\right\rangle - \left\langle \hat{B}\right\rangle_0 = \int_{-\infty}^{+\infty} dt' \int d\vec{r}' \, \tfrac{i}{\hbar}\theta(t-t')\left\langle\left[\hat{B}_H(\vec{r},t),\hat{a}_H(\vec{r}',t')\right]\right\rangle_0 \lambda(\vec{r}',t')$$

where $\hat{O}_H(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t}$

Thus the generalized dynamic susceptibility is:

$$\Rightarrow \quad \boxed{\chi_{BA}(\vec{r},\vec{r}',t-t') = -\frac{i}{\hbar}\theta(t-t')\left\langle\left[\hat{B}_H(\vec{r},t),\hat{a}_H(\vec{r}',t')\right]\right\rangle_0}$$

- This is the Kubo formula which shows that, at linear order, the variation of any measurable quantity is obtained through the linear response function (dynamic susceptibility) which is only related to averages on the unperturbed system

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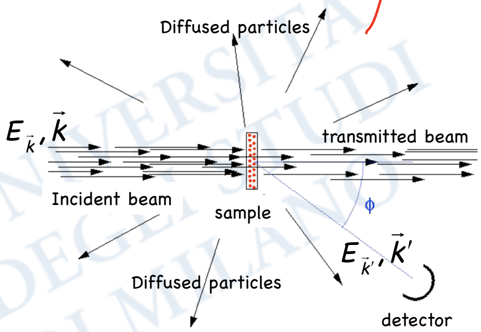
quindi risposta lineare solo nel condizione interazione molto debole

↳ campione praticamente trasparente

↳ così da avere un solo urto per particella scatterata e poter valutare l'energia assorbita dal materiale come ΔE della particella del fascio

Scattering experiments

- In a typical scattering (diffusion) experiment a beam of "particles" (photons, neutrons, electrons,…) with linear momentum $\hbar\mathbf{k}$ and energy $E_\mathbf{k}$ is radiated over a sample.



- The scattering experiments analyses how these "particles" are diffused, i.e. one counts how many "particles" of the incident beam come out with linear momentum $\hbar\mathbf{k}'$ and energy $E_{\mathbf{k}'}$

Exchanged momentum: $\hbar\mathbf{q} = \hbar(\mathbf{k}-\mathbf{k}')$

Exchanged energy: $\hbar\omega = E_\mathbf{k} - E_{\mathbf{k}'}$

- Hypothesis: the "particles" of the incident beam interact weakly with the sample

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1^{st} Born approximation

- This means that most of the "probe-particles" do not exchange energy or momentum with the sample, thus they are found in the transmitted beam
- In such case we can treat the interaction term among "particles" and the sample at first order of perturbative theory, which is called 1^{st} Born approximation
- The 1^{st} Born approximation, in practice, assumes that the field inside the scattering volume is constant and equal to the incident field, and ensures that each particle in the beam is involved in at most one scattering event
- This is the case of thermal neutrons ($E_k \approx k_BT$) , and of photons (visible light and X-rays) scattered by a transparent sample, i.e. matter which is not reflecting like a metal for visible light and that does not present absorption for the considered photon frequency
- To be concrete we will discuss an incident beam of non-relativistic massive particles, i.e. the ("thermal") neutron scattering case

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Neutron scattering

- Since neutrons are neutral, their interaction with the nuclei is short-ranged; in contrast to electrons, they penetrate deep into the solid.
- Furthermore, due to their magnetic moment and the associated dipole interaction with magnetic moments of the solid, neutrons can also be used to investigate magnetic properties like magnetic order in the system or dynamical properties: spin waves
- Therefore, the usefulness of neutron scattering originates from the comparatively simple and weak interaction of the neutrons with condensed matter and the well adapted "mechanical properties" ($\lambda_{DB}\approx$inter-atomic distance for "thermal" energies) of the neutron beams to the microscopic and energetic structure of matter
- The weakness of the interaction renders the system in the ground state for elastic scattering or in a well defined excited state for inelastic scattering

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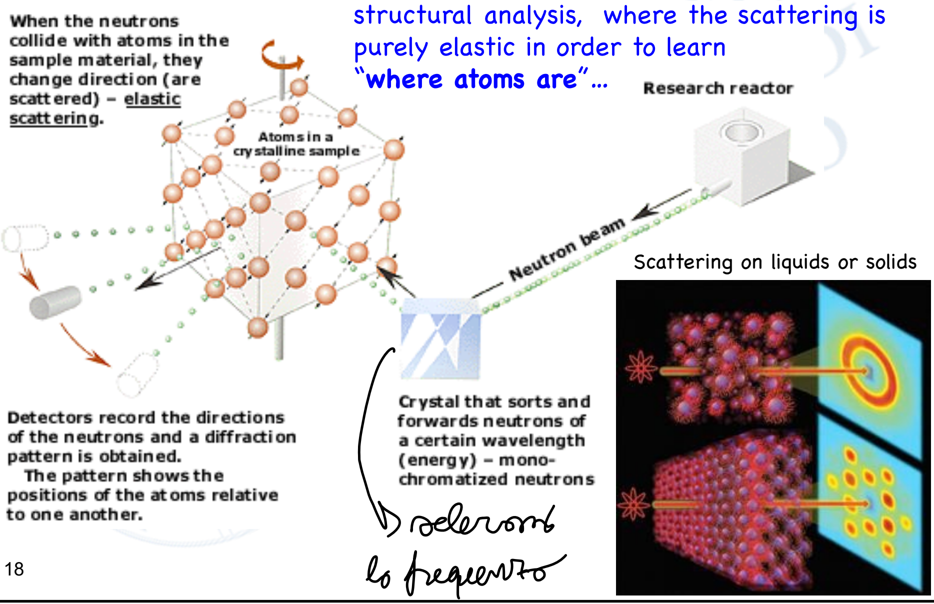
Elastic scattering: where atoms are?

Thus, neutron scattering can be used in structural analysis, where the scattering is purely elastic in order to learn "**where atoms are**"…



seleziono la frequenza

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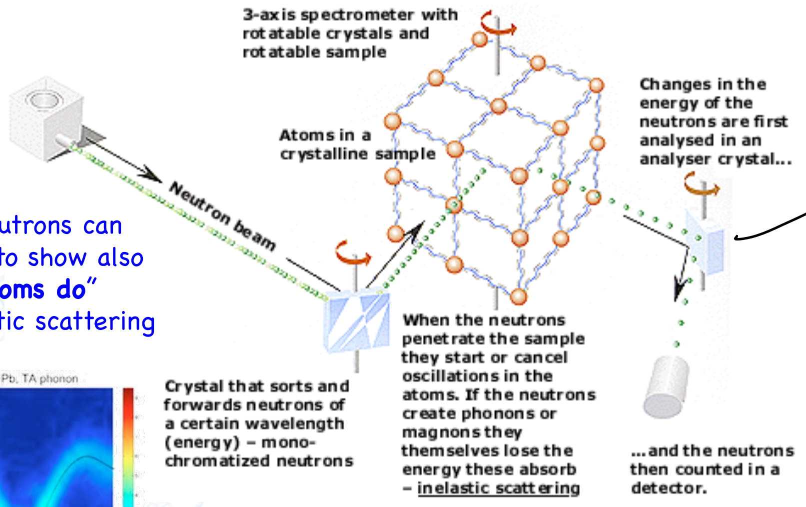
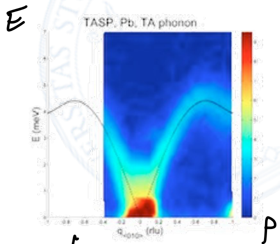
conteggio non dipendente dall'energia ⇒ solo distribuzione spaziale del campione

Inelastic scattering: what atoms do?



selezione anche l'energia uscente

... but neutrons can be used to show also "**what atoms do**" by inelastic scattering



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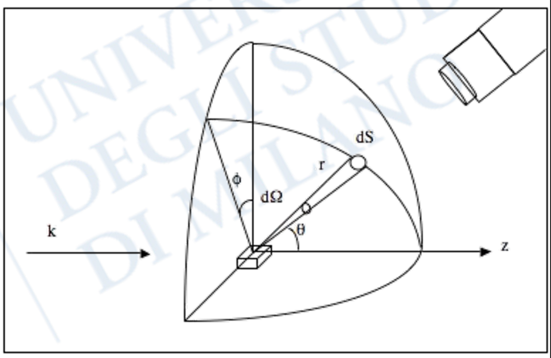
→ mi dà la legge di dispersione degli stati eccitati E(k) del cristallo

Scattering cross sections

- Consider a beam of thermal (i.e. cooled down [moderated] to thermal energy 2-100 meV [30 <T< 1100 K]) neutrons, all with the same energy E (monochromatic beam) incident on a target



- Suppose we set up a neutron counter and measure the number of neutrons scattered in a given direction as function of their energy E'.
- The distance of the counter from the target is assumed to be large compared with to the dimensions of the counter and the target, so that the small angle $d\Omega$ subtended by the counter at the target is well defined. Let the directions of the scattered neutron be θ and ϕ

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- The partial differential cross section is defined as:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{\text{(number of neutrons scattered per second into a small solid angle } d\Omega \text{ in the direction } \theta \text{ and } \phi \text{ with final energy between } E' \text{ and } E'+dE')}{(\Phi \, d\Omega \, dE')}$$

where Φ is the flux of the incident neutrons, i.e. the number through unit area per second

- Suppose we do not analyse the energy of the scattered neutrons, but simply count all the neutrons scattered into a solid angle $d\Omega$ in the direction θ and ϕ . The cross section corresponding to these measurements, known as the differential cross section, is defined by

solo direzione spaziale

$$\frac{d\sigma}{d\Omega} = \frac{\text{(number of neutrons scattered per second into } d\Omega \text{ in the direction } \theta, \phi)}{(\Phi \, d\Omega)}$$

- The total scattering cross section is defined by the equation

$$\sigma_{tot} = \frac{\text{(total number of neutrons scattered per second)}}{(\Phi)}$$

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- From their definitions the three cross-sections are related by the following equations

$$\frac{d\sigma}{d\Omega} = \int_0^\infty dE' \left(\frac{d^2\sigma}{d\Omega dE'} \right) \quad ; \quad \sigma_{tot} = \int d\Omega \left(\frac{d\sigma}{d\Omega} \right)$$

- The dimensions of the total cross-section is [area], and more precisely is an area rescaled with the ratio of two pure numbers: the number of scattered neutrons divided by the number of incoming neutrons, i.e. the percentage of the scattered neutrons; it is a sort of measure of the "surface" able to deviate the beam. The definition of cross-sections apply to any kind of scattering

- The nuclear forces which cause the scattering have a range of about 10^{-14} to 10^{-15} m; the wavelength of thermal neutrons is of the order of 10^{-10} m, and is thus much larger than this range. In these circumstances the scattering, analysed in terms of partial waves, comes entirely from s waves (l=0)

- In fact, if waves of any kind are scattered by an object small compared to the wavelength of the waves, then the scattered wave is spherically symmetric

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The dynamic structure factor

- One can show that (See supplementary material; it is essentially an application of the time-dependent perturbation theory and the Fermi's golden rule):

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{N}\frac{k'}{k}\frac{a^2}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{i\omega t}\sum_{\lambda} p_{\lambda}\left\langle \lambda \left| \sum_j e^{-i\vec{q}\cdot\vec{R}_j(t)} \sum_j e^{i\vec{q}\cdot\vec{R}_j} \right| \lambda \right\rangle = \frac{k'}{k}\frac{a^2}{\hbar} S(\vec{q},\omega)$$

where we have introduced the dynamic structure factor defined as

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle \sum_j e^{-i\vec{q}\cdot\vec{R}_j(t)} \sum_j e^{i\vec{q}\cdot\vec{R}_j} \right\rangle = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}_{\vec{q}}^{+}(0)\right\rangle$$ è FT di $D^{T}(k,\omega)$ di Molti-Corpi

- In the definition of the dynamic structure factor, which has been assumed proportional to the partial differential cross section and is therefore directly measured in an inelastic scattering experiment, we have also introduced the operator $\rho_{\mathbf{q}}$ (in the coordinate representation) defined as

$$\hat{\rho}_{\vec{q}}(t) \equiv \sum_j e^{-i\vec{q}\cdot\vec{r}_j(t)} = \hat{\rho}_{-\vec{q}}^{+}(t)$$ $\rho(k,\tau)$

Structure factors and density fluctuations

- It is very easy to see that $\rho_{\mathbf{q}}$, which is generally called the density fluctuation operator, is the Fourier transform of the number density operator:

$$\hat{\rho}(\vec{r},t) = \sum_j \delta(\vec{r}-\vec{r}_j(t)) \quad \Rightarrow \quad \hat{\rho}_{\vec{q}}(t) = \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}}\hat{\rho}(\vec{r},t) = \sum_j e^{-i\vec{q}\cdot\vec{r}_j(t)}$$

- For isotropic systems, in second quantization, such operator can be expressed as

onda piana

$$\hat{\rho}_{\vec{q}}^{+} = \hat{\rho}_{-\vec{q}} = \int d\vec{r} e^{i\vec{q}\cdot\vec{r}}\hat{\Psi}^{+}(\vec{r})\hat{\Psi}(\vec{r}) = \sum_{\vec{k}',\vec{k}} a_{\vec{k}'}^{+}a_{\vec{k}}\int d\vec{r} e^{i\vec{q}\cdot\vec{r}}\left\langle \vec{r} \middle| \vec{k}\right\rangle\left\langle \vec{k}' \middle| \vec{r}\right\rangle = \sum_{\vec{k}',\vec{k}} a_{\vec{k}'}^{+}a_{\vec{k}}\int d\vec{r} e^{i(\vec{q}+\vec{k}-\vec{k}')\cdot\vec{r}}$$

$$\Rightarrow \quad \hat{\rho}_{\vec{q}}^{+} = \sum_{\vec{k}} a_{\vec{k}+\vec{q}}^{+}a_{\vec{k}}$$

this form naturally leads to an interpretation of $\rho_{\mathbf{q}}^{+}$ in terms of linear combinations of terms which represent the action of destroying an atom of momentum $\hbar\mathbf{k}$ and creating one with momentum $\hbar(\mathbf{k}+\mathbf{q})$, i.e. a linear superposition of particle-hole excitations

- It is easy to see that, in an isotropic system, the dynamical structure factor corresponds to a Fourier transform of the density-density correlation function:

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t}\left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}^{+}_{\vec{q}}(0)\right\rangle =$$

$$= \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t}\int d\vec{r}\, d\vec{r}' e^{i\vec{q}\cdot(\vec{r}'-\vec{r})}\left\langle \hat{\rho}(\vec{r},t)\hat{\rho}(\vec{r}',0)\right\rangle =$$

$$= \frac{V}{2\pi N}\int_{-\infty}^{\infty} dt\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}+i\omega t}\boxed{\left\langle \hat{\rho}(\vec{r},t)\hat{\rho}(\vec{r}+\vec{R},0)\right\rangle}$$

related to the probability to find a particle in **r+R** at t=0 and a particle in **r** at t>0

- Generally S(**q**,ω) as function of ω, at fixed **q** shows non-zero values in correspondence of the excitation energies of the elementary excitations in the system ⇒ one can extract the excitation spectrum (energy-momentum dispersion relation)

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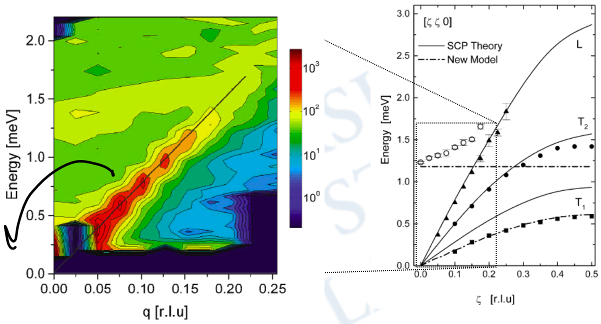
- We give her two examples:

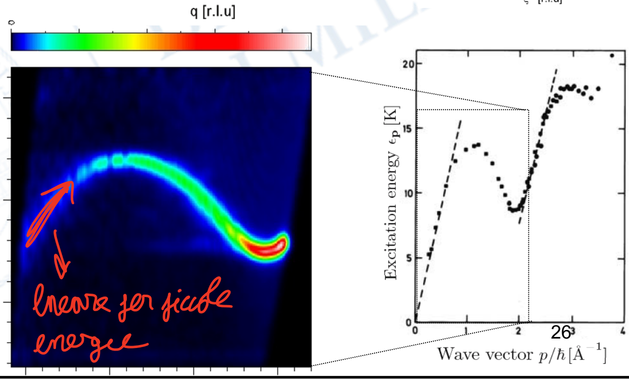
Inelastic scattering: S(**q**,ω) in solids (phonons)

parte lineare dei fononi



Inelastic scattering: S(**q**,ω) in He-II

elio II superfluido



lineare per piccole energie

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Fluctuation dissipation theorem

- The response in density of a system to a space and time-dependent density fluctuation is characterized by a dynamic susceptibility $\chi(\mathbf{k},\omega)$ which depends both from the wave vector **k** and the frequency $\nu=\omega/2\pi$.
- $\chi(\mathbf{k},\omega)$ is the space-temporal Fourier transform of the susceptibility $\chi_{AB}(\mathbf{r},\mathbf{r}',t-t')$ obtained with the choice: $\hat{B}(\vec{r}) = \hat{\rho}(\vec{r});\ \hat{A}(\vec{r}') = \hat{\rho}(\vec{r}')$
- The relation between this dynamic susceptibility and the spectrum of density fluctuations, i.e. the dynamic structure factor, is one of the passible cases of the so called fluctuation dissipation theorem (see supplementary material)
- The relationship is proved to be:

χ'' è la parte immaginaria

$$\boxed{\chi''(\vec{k},\omega) = \frac{1-e^{-\beta\hbar\omega}}{2\hbar} S(\vec{k},\omega) \underset{\hbar\to 0}{\to} \frac{\beta\omega}{2} S(\vec{k},\omega)}$$

where we have shown also the classical limit ($\hbar\to 0$).

- The dynamic structure factor of a neutron scattering experiment is thus connected with the imaginary part (i.e. the dissipative part) of the density-density response function

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The static structure factor

- The differential scattering cross-section is connected with a scattering experiment in which one registers all events related to a momentum transfer equal to $\hbar\mathbf{q}$ but independently on any particular energy transfer
- It is obtained by integrating with respect to the energy the partial differential scattering cross-section:

integro su tutte le ω

$$\frac{d\sigma}{d\Omega} = \int dE \frac{d^2\sigma}{d\Omega dE} = \hbar \int_{-\infty}^{\infty} d\omega \frac{k'}{k}\frac{a^2}{\hbar} S(\vec{q},\omega) = \frac{k'}{k} a^2 \int_{-\infty}^{\infty} d\omega\, S(\vec{q},\omega) = \frac{k'}{k} a^2 S(\vec{q})$$

it then proportional to the function $S(\mathbf{q})$ which is called static structure factor

- This function is also easily obtained in a scattering experiment and it is very important because give information on the static structure of the system:

$$S(\vec{q}) = \int_{-\infty}^{\infty} d\omega\, S(\vec{q},\omega) = \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi N} \int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}^{+}_{\vec{q}}(0)\right\rangle = \ldots$$

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The n-particle densities

- Thus

$$S(\vec{q}) = \frac{1}{N}\int_{-\infty}^{\infty} dt\, \delta(t) \left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}^{+}_{\vec{q}}(0)\right\rangle = \frac{1}{N}\left\langle \hat{\rho}_{\vec{q}}\hat{\rho}^{+}_{\vec{q}}\right\rangle$$

misuro come sono distribuite allo stesso istante

- S(**q**) , in an isotropic system, corresponds to the spatial Fourier transform of the static density-density correlation function …

isotropo

$$S(\vec{q}) = \frac{1}{N}\left\langle \hat{\rho}_{\vec{q}}\hat{\rho}^{+}_{\vec{q}}\right\rangle = \frac{1}{N}\int d\vec{r}\, d\vec{r}' e^{i\vec{q}\cdot(\vec{r}'-\vec{r})}\left\langle \hat{\rho}(\vec{r})\hat{\rho}(\vec{r}')\right\rangle =$$

$$= \frac{V}{N}\int d\vec{R}\, e^{i\vec{q}\cdot\vec{R}}\left\langle \hat{\rho}(\vec{r})\hat{\rho}(\vec{r}+\vec{R})\right\rangle$$

which is related to the probability to find a particle in **r** and one in **r+R**

- We can define the n-particles density function as

probabilità che n particelle su N si distribuiscano in un certo modo

$$\rho_N^{(n)}(\vec{r}_1,\cdots,\vec{r}_n) \equiv \frac{N!}{(N-n)!}\int d\vec{r}_{n+1}\cdots d\vec{r}_N\, p(\vec{r}_1,\cdots,\vec{r}_N) =$$

media sulle N-m restanti

$$= \frac{N!}{(N-n)!}\int d\vec{r}_{n+1}\cdots d\vec{r}_N\, \rho_N(\vec{r}_1,\cdots,\vec{r}_N;\vec{r}_1,\cdots,\vec{r}_N)$$

N-particles diagonal density matrix

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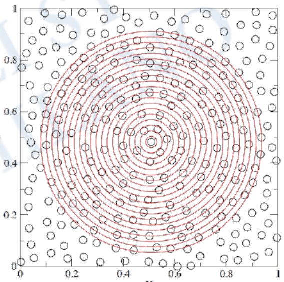
The n-particle distributions

- For example $\rho^{(1)}$ is the usual local density

- It is a measure of the probability to find n particles in ($\mathbf{r}_1 \ldots \mathbf{r}_n$) averaged over the position of the other N-n particles in the system

For example with $\rho^{(2)}$ one measures the probability to find a couple of particles in ($\mathbf{r}_1$ $\mathbf{r}_2$) , so, given a particle in $\mathbf{r}_1$, to this probability will contribute particles at distance $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$



- Now define the n-particles distribution function as

distribuzione non densità

è quella di simulazione

$$g_N^{(n)}(\vec{r}_1,\cdots,\vec{r}_n) = \frac{\rho_N^{(n)}(\vec{r}_1,\cdots,\vec{r}_n)}{\prod_i^n \rho_N^{(1)}(\vec{r}_i)}$$

usi normalizzata

it gives information on the density function in a system normalized with the one of a system characterized by a random (ideal gas) distribution

- In an isotropic and homogeneous system there is a direct relation between S(**q**) and the radial (2-particles) distribution function:

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- In fact, we obtain

$$S(\vec{q}) = \frac{1}{N}\left\langle \sum_j e^{-i\vec{q}\cdot\vec{r}_j} \sum_l e^{i\vec{q}\cdot\vec{r}_l} \right\rangle = 1 + \frac{1}{N}\left\langle \sum_{j\neq l} e^{-i\vec{q}\cdot(\vec{r}_j-\vec{r}_l)} \right\rangle = \dots$$

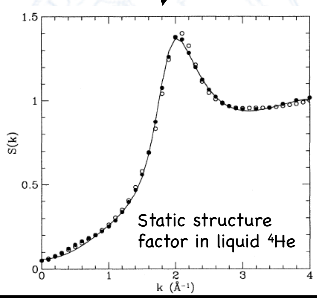
$$= 1 + \frac{1}{N}\left\langle \sum_{j\neq l} \int d\vec{r}\, d\vec{r}' e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \delta(\vec{r}-\vec{r}_j)\,\delta(\vec{r}'-\vec{r}_l) \right\rangle = 1 + \frac{1}{N}\int d\vec{r}\, d\vec{r}' e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \rho^{(2)}(\vec{r},\vec{r}') =$$

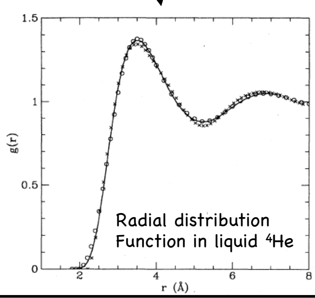
$$= 1 + \rho \int d(\vec{r}-\vec{r}') e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} g^{(2)}(\vec{r}-\vec{r}') = 1 + \rho\int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} g(\vec{r})$$

Uniform system

$g^2 = \frac{\rho^2}{\rho}$ per sistema uniforme

$$\boxed{S(\vec{q}) = 1 + \rho\int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} g(\vec{r})}$$





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→ è un microscopio: se misuro $S(q)$ trovo la distribuzione $g(r)$

Dynamic structure factor

- We now are going to obtain (equivalent) new expressions (→ in 2° quantizz.) for the dynamic and static structure factor (canonical ensemble):

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt\, e^{i\omega t} \left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}^+_{\vec{q}}(0) \right\rangle = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt\, e^{i\omega t} \sum_n \frac{e^{-\beta E_n}}{Z} \left\langle n \middle| \hat{\rho}_{\vec{q}}(t)\hat{\rho}^+_{\vec{q}}(0) \middle| n \right\rangle =$$

(→ media termica canonica)

$$= \int_{-\infty}^{\infty} \frac{dt}{2\pi N} e^{i\omega t} \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \left\langle n \middle| e^{\frac{i}{\hbar}\hat{H}t} \hat{\rho}_{\vec{q}} e^{-\frac{i}{\hbar}\hat{H}t} \middle| m \right\rangle \left\langle m \middle| \hat{\rho}^+_{\vec{q}} \middle| n \right\rangle =$$

↳ introduco una completezza

$$= \frac{\hbar}{N}\sum_{n,m} \frac{e^{-\beta E_n}}{Z} \left\langle n \middle| \hat{\rho}_{\vec{q}} \middle| m \right\rangle \left\langle m \middle| \hat{\rho}^+_{\vec{q}} \middle| n \right\rangle \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{\frac{i}{\hbar}[\hbar\omega-(E_m-E_n)]t} =$$

→ creazione energia → per eccitare

stato energia

↳ creazione buca particella

$$\Rightarrow \boxed{S(\vec{q},\omega) = \frac{\hbar}{N}\sum_{m,n} \frac{e^{-\beta E_n}}{Z} \left|\left\langle m \middle| \hat{\rho}^+_{\vec{q}} \middle| n \right\rangle\right|^2 \delta[\hbar\omega - (E_m - E_n)]}$$

- when T=0 K , S(**q**,ω) becomes

↓ quindi sono per forza nel g.s. $n \equiv 0$

$$\boxed{S(\vec{q},\omega) = \frac{\hbar}{N}\sum_m \left|\left\langle m \middle| \hat{\rho}^+_{\vec{q}} \middle| 0 \right\rangle\right|^2 \delta[\hbar\omega - (E_m - E_0)]}$$

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mi conto le fluttuazioni soggette a possibili eccitazioni

Static structure factor

- The static structure factor:

$$S(\vec q)=\int_{-\infty}^{\infty} d\omega\, S(\vec q,\omega)=\frac{\hbar}{N}\int_{-\infty}^{\infty}d\omega\sum_{m,n}\frac{e^{-\beta E_n}}{Z}\left|\left\langle m\left|\hat\rho^+_{\vec q}\right|n\right\rangle\right|^2\delta\left[\hbar\omega-(E_m-E_n)\right]=$$

$$=\boxed{\frac{1}{N}\sum_{m,n}\frac{e^{-\beta E_n}}{Z}\left|\left\langle m\left|\hat\rho^+_{\vec q}\right|n\right\rangle\right|^2}=\frac{1}{N}\sum_{m,n}\frac{e^{-\beta E_n}}{Z}\left\langle n\left|\hat\rho_{\vec q}\right|m\right\rangle\left\langle m\left|\hat\rho^+_{\vec q}\right|n\right\rangle=$$

$$=\frac{1}{N}\sum_{n}\frac{e^{-\beta E_n}}{Z}\left\langle n\left|\hat\rho_{\vec q}\hat\rho^+_{\vec q}\right|n\right\rangle=\frac{1}{N}\mathrm{Tr}\left(\hat\rho\,\hat\rho_{\vec q}\hat\rho^+_{\vec q}\right)=\frac{1}{N}\left\langle\hat\rho_{\vec q}\hat\rho^+_{\vec q}\right\rangle$$

- when T=0 K , S(**q**) becomes

$$\boxed{S(\vec q)=\frac{1}{N}\sum_m\left|\langle m|\hat\rho^+_{\vec q}|0\rangle\right|^2}=\frac{1}{N}\langle 0|\hat\rho_{\vec q}\hat\rho^+_{\vec q}|0\rangle$$

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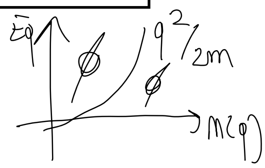
→ mi aspetto



Structure factors: ideal Bose gas

- In the ideal Bose gas, the structure factors can be computed analytically (even thought one should recognize that this model in inadequate for describing the dynamics of a real gas at small **q**)

$$\frac{N}{\hbar}S(\vec q,\omega)=\sum_{m,n}\frac{e^{-\beta E_n}}{Z}\left|\left\langle m\left|\hat\rho^+_{\vec q}\right|n\right\rangle\right|^2\delta\left[\hbar\omega-(E_m-E_n)\right]=$$

- by writing the density fluctuation operator in second quantization, it is easy to see that the matrix elements in S(q,ω) vanishes unless (E_m-E_n) is equal to the difference between single-(free)-particle energies:

$$\left(\hat\rho^+_{\vec q}=\sum_{\vec p}a^+_{\vec p+\vec q}a_{\vec p}\quad ;\quad \hat\rho_{\vec q}=\hat\rho^+_{-\vec q}=\sum_{\vec p}a^+_{\vec p-\vec q}a_{\vec p}=\sum_{\vec p}a^+_{\vec p}a_{\vec p+\vec q}\right)$$

$$=\sum_{\vec p,\vec p'}\sum_{m,n}p_n\left\langle n\left|a^+_{\vec p}a_{\vec p+\vec q}\right|m\right\rangle\left\langle m\left|a^+_{\vec p'+\vec q}a_{\vec p'}\right|n\right\rangle\delta\left[\hbar\omega-(E_m-E_n)\right]=$$

δ_{mm}

Due to the delta, matrix elements ≠0 only if **p'**=**p**

$$\left(E_m-E_n=\frac{\hbar^2(\vec p+\vec q)^2}{2m}-\frac{\hbar^2p^2}{2m}\right)$$

$$=\sum_{\vec p}\sum_{n}p_n\left\langle n\left|a^+_{\vec p}a_{\vec p+\vec q}a^+_{\vec p+\vec q}a_{\vec p}\right|n\right\rangle\delta\left[\hbar\omega-\left(\frac{\hbar^2q^2}{2m}+\frac{\hbar^2\vec p\cdot\vec q}{m}\right)\right]=\cdots$$

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usando le c.c R

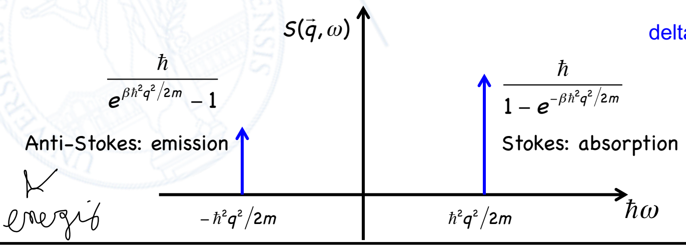
$$\cdots = \sum_{\vec p}\sum_n p_n \left\langle n \middle| \hat n_{\vec p}(1+\hat n_{\vec p+\vec q}) \middle| n\right\rangle \delta\left[\hbar\omega - \left(\frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 \vec p\cdot\vec q}{m}\right)\right] =$$

$$= \sum_{\vec p} n_{\vec p}(1+n_{\vec p+\vec q})\ \delta\left[\hbar\omega - \left(\frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 \vec p\cdot\vec q}{m}\right)\right]$$

Average occupation numbers

- at $T \ll T_C$ contribute only the terms p=0 or p=-q : $\Rightarrow$ ricordo $n(p) = \begin{cases} 1 & p=0 \\ 0 & p\neq 0 \end{cases}$

$$\boxed{S(\vec q,\omega) = \frac{\hbar}{1-e^{-\beta\hbar\omega}}\left[\delta\left(\hbar\omega - \frac{\hbar^2 q^2}{2m}\right) - \delta\left(\hbar\omega + \frac{\hbar^2 q^2}{2m}\right)\right]}$$



delta-like contributions:
Infinite lifetime!

assorbe energia

cede energia

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- The static structure factor for $T \ll T_c$ turns out to be

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$$S(\vec q) = \int_{-\infty}^{\infty} d\omega\, \frac{\hbar}{1-e^{-\beta\hbar\omega}}\left[\delta\left(\hbar\omega - \frac{\hbar^2 q^2}{2m}\right) - \delta\left(\hbar\omega + \frac{\hbar^2 q^2}{2m}\right)\right] =$$

$$= \frac{1}{1-e^{-\beta\hbar^2q^2/2m}} - \frac{1}{1-e^{\beta\hbar^2q^2/2m}} = \frac{e^{-\beta\hbar^2q^2/2m} - e^{\beta\hbar^2q^2/2m}}{2-e^{-\beta\hbar^2q^2/2m} - e^{\beta\hbar^2q^2/2m}} =$$

$$= \frac{-(e^{\beta\hbar^2q^2/4m}+e^{\beta\hbar^2q^2/4m})(e^{\beta\hbar^2q^2/4m}-e^{-\beta\hbar^2q^2/4m})}{-(e^{\beta\hbar^2q^2/4m}-e^{-\beta\hbar^2q^2/4m})(e^{\beta\hbar^2q^2/4m}-e^{-\beta\hbar^2q^2/4m})} = \coth\left(\frac{\hbar^2q^2}{4mk_BT}\right)$$

S(**q**) approaches 1 when q is larger than the inverse of the thermal wavelength λ_T

- For $q<1/\lambda_T$ S(q) exhibits the divergent behaviour

$$S(\vec q) = \coth\left(\frac{\hbar^2q^2}{4mk_BT}\right) \underset{q\to 0}{\approx} \frac{4mk_BT}{\hbar^2q^2}$$

reflecting the infinite compressibility of the ideal gas in presence of BEC

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Structure factors: WIBG

- Consider now the weakly interacting Bose gas; Bogoliubov theory assumes $T \ll T_c$ (small thermal depletion of the condensate) and the diluteness condition: $na^3 \ll 1$ ($a \equiv$ scattering length)

- The evaluation of the matrix elements of the density fluctuation operator is simplified by the fact that (thanks to the Bogoliubov transformation) the Hamiltonian takes a diagonal form; the eigenstates of H are consequently classified in terms of the occupation numbers of the quasiparticle excitations, the ground state corresponding to the vacuum of quasiparticles

- Strategy: write the density fluctuation operator in terms of the creation and annihilation operators of quasi-particles.

Bogoliubov accuracy

$$\hat{\rho}_{\vec{q}} = \hat{\rho}^{+}_{-\vec{q}} = \sum_{\vec{p}'} a^{+}_{\vec{p}-\vec{q}} a_{\vec{p}} \cong \boxed{a^{+}_{0} a_{\vec{q}} + a^{+}_{-\vec{q}} a_{0} \cong \sqrt{N}(a_{\vec{q}} + a^{+}_{-\vec{q}})} =$$

$$= \sqrt{N}\left[(u_q b_{\vec{q}} + v_q b^{+}_{-\vec{q}}) + (u_q b^{+}_{-\vec{q}} + v_q b_{\vec{q}})\right] = \boxed{\sqrt{N}(u_q + v_q)(b^{+}_{-\vec{q}} + b_{\vec{q}})}$$

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- The dynamical structure factor takes the form:

$$\left[(u_q + v_q)^2 = \frac{\hbar^2 q^2}{2m\varepsilon_q}\right]$$

$$S(\vec{q},\omega) = \frac{\hbar}{N} N(u_q + v_q)^2 \sum_{m,n} p_n \left|\left\langle m \left| b^{+}_{\vec{q}} + b_{-\vec{q}} \right| n \right\rangle\right|^2 \delta\left[\hbar\omega - \left(E_m - E_n\right)\right] =$$

$$\begin{cases} |m\rangle = b^{+}_{\vec{q}}|n\rangle \Rightarrow (E_m - E_n) = \varepsilon_q \\ |m\rangle = b_{-\vec{q}}|n\rangle \Rightarrow (E_m - E_n) = -\varepsilon_q \end{cases}$$

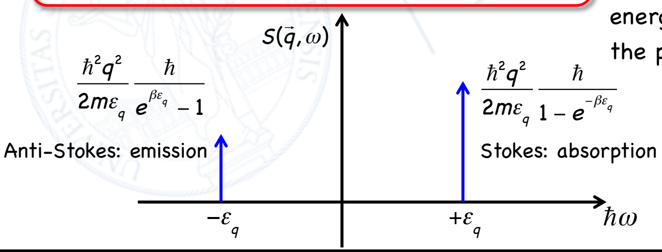
$$= \hbar \frac{\hbar^2 q^2}{2m\varepsilon_q} \sum_{m,n} p_n \left\langle n \left| b_{\vec{q}} + b^{+}_{-\vec{q}} \right| m \right\rangle \left\langle m \left| b^{+}_{\vec{q}} + b_{-\vec{q}} \right| n \right\rangle \delta\left[\hbar\omega - \left(E_m - E_n\right)\right] =$$

$$= \hbar \frac{\hbar^2 q^2}{2m\varepsilon_q} \left[\sum_n p_n \left\langle n \left| b_{\vec{q}} b^{+}_{\vec{q}} \right| n \right\rangle \delta(\hbar\omega - \varepsilon_q) + \sum_n p_n \left\langle n \left| b^{+}_{-\vec{q}} b_{-\vec{q}} \right| n \right\rangle \delta(\hbar\omega + \varepsilon_q)\right] =$$

$$= \hbar \frac{\hbar^2 q^2}{2m\varepsilon_q} \left[\left(1 + \left\langle b^{+}_{\vec{q}} b_{\vec{q}} \right\rangle\right) \delta(\hbar\omega - \varepsilon_q) + \left\langle b^{+}_{-\vec{q}} b_{-\vec{q}} \right\rangle \delta(\hbar\omega + \varepsilon_q)\right] =$$

$$\Rightarrow \boxed{S(\vec{q},\omega) = \hbar \frac{\hbar^2 q^2}{2m\varepsilon_q} \frac{1}{1 - e^{-\beta\hbar\omega}} \left[\delta(\hbar\omega - \varepsilon_q) - \delta(\hbar\omega + \varepsilon_q)\right]}$$

With respect to the IG the free particle energy is replaced by the Bogoliubov energy and the strength of the peaks is renormalized



delta-like contributions:
Infinite lifetime!

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- The static structure factor is also easily evaluated and takes the nontrivial form (calculation is identical to the ideal Bose case with ε_q in place of $\hbar^2 q^2/2m$)

$$S(\vec{q}) = \frac{\hbar^2 q^2}{2m\varepsilon_q}\int_{-\infty}^{\infty} d\omega \frac{\hbar}{1-e^{-\beta\hbar\omega}}\left[\delta\left(\hbar\omega-\varepsilon_q\right)-\delta\left(\hbar\omega+\varepsilon_q\right)\right] = \frac{\hbar^2 q^2}{2m\varepsilon_q}\coth\left(\frac{\varepsilon_q}{2k_B T}\right)$$

which generalize the ideal Bose gas result and at low temperatures reduces to

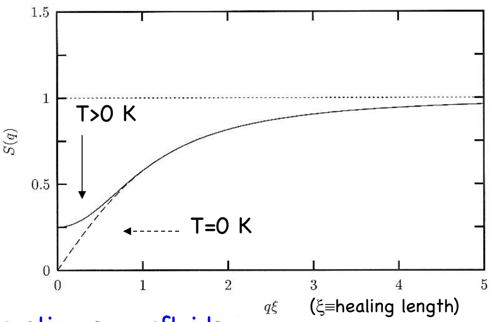
$$S(\vec{q}) = \frac{\hbar^2 q^2}{2m\varepsilon_q}\coth\left(\frac{\varepsilon_q}{2k_B T}\right) \xrightarrow[T\to 0]{} \frac{\hbar^2 q^2}{2m\varepsilon_q}$$

- Notice that at T=0 K the static structure factor at small q vanishes like

$$S(\vec{q}) \xrightarrow[T\to 0]{} \frac{\hbar^2 q^2}{2m\varepsilon_q} \underset{q\to 0}{\approx} \frac{\hbar^2 q^2}{2mc\hbar q} = \frac{\hbar q}{2mc}$$

where c is the sound velocity.

This behaviour is not peculiar to the dilute Bose gas, but holds in general for interacting superfluids



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- The T=0 result for the static structure factor for the WIBG :

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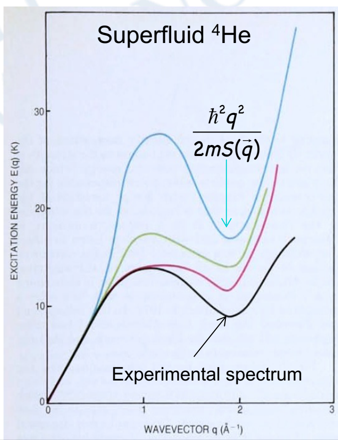
$$S_{T=0}(\vec{q}) = \frac{\hbar^2 q^2}{2m\varepsilon_q}$$

It connects the static structure factor with the elementary excitation spectrum ε_q

- One can invert this result to try to obtain an expression for the energy-momentum dispersion relation:

$$\varepsilon_q = \frac{\hbar^2 q^2}{2mS(\vec{q})}$$



- This approximate expression for ε_q is known as the "Feynman approximation" (Feynman, 1954); it is very useful (exact!) when the spectrum consists of a single elementary excitation with infinite lifetime

- Using the experimental S(q) , measured via neutron scattering, in superfluid ^{4}He one finds in ε_q the appearance of a local minimum which qualitatively reproduces the one effectively present in the experimental data

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Lecture 13: Suggested books

- L. Peliti, "Appunti di meccanica statistica", Bollati Boringhieri
- G.F. Mazenko, "Non equilibirum statistical mechanics", Wiley
- R. K. Pathria, "Statistical mechanics", II ed., Oxford
- S.W. Lovesey "Theory of Neutron Scattering from Condensed Matter", Clarendon Press, Oxford (1986)
- L. Pitaevskii, S. Stringari "Bose Einstein Condensation", Clarendon Press, Oxford

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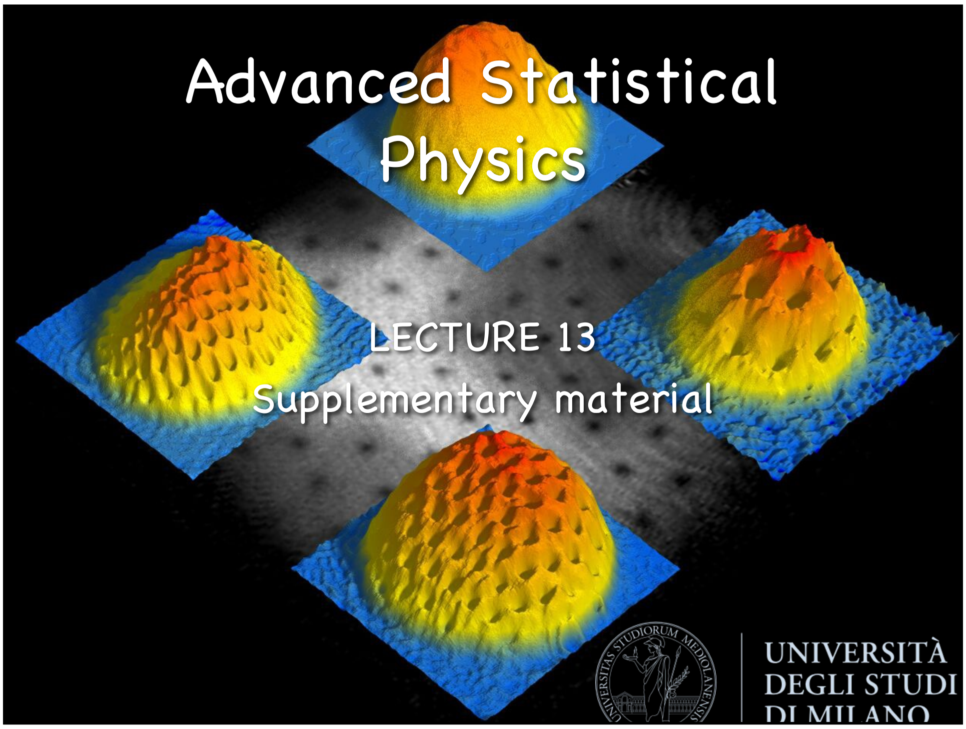

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Outline Supplementary information

- Linear response: static & uniform perturbation [Ĥ,Â]≠0 case
- Linear response: local perturbation
- Linear response: time dependent perturbation
- Causality ⇔ Kramers-Kronig relations
- Fluctuation dissipation theorem
- Scattering, time dependent perturbation & Fermi's golden rule

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Linear response (static uniform perturbation)

Static uniform perturbation, [Ĥ,Â]≠0 case:

- We define $\hat{U}(\beta) = e^{\beta\hat{H}}e^{-\beta(\hat{H}-\lambda\hat{A})} \quad \left(\hat{U}(\beta=0) \equiv identity\right)$

and we compute the derivatives with respect to β. We obtain

$$\frac{\partial \hat{U}(\beta)}{\partial \beta} = \hat{H}e^{\beta\hat{H}}e^{-\beta(\hat{H}-\lambda\hat{A})} + e^{\beta\hat{H}}\left(-\hat{H}+\lambda\hat{A}\right)e^{-\beta(\hat{H}-\lambda\hat{A})} = e^{\beta\hat{H}}\lambda\hat{A}e^{-\beta(\hat{H}-\lambda\hat{A})}$$

$$= e^{\beta\hat{H}}\lambda\hat{A}\,e^{-\beta\hat{H}}e^{\beta\hat{H}}e^{-\beta(\hat{H}-\lambda\hat{A})} = e^{\beta\hat{H}}\lambda\hat{A}\,e^{-\beta\hat{H}}\,\hat{U}(\beta)$$

- Remember that the operator Â evolved at time t is $\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}\,e^{-\frac{i}{\hbar}\hat{H}t}$
- We can consider therefore the imaginary time evolved t=-iβħ

$$\hat{A}(\beta) = e^{\beta\hat{H}}\hat{A}\,e^{-\beta\hat{H}}$$

- The previous equation turns out to be

$$\frac{\partial \hat{U}(\beta)}{\partial \beta} = \lambda\hat{A}(\beta)\,\hat{U}(\beta) \quad \Rightarrow \quad \hat{U}(\beta) = 1 + \lambda\int_0^\beta d\tau\,\hat{A}(\tau) + O(\lambda^2)$$

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- We can use this result to compute $\langle \hat{B} \rangle_\lambda$
- We obtain

$$\langle \hat{B} \rangle_\lambda = \frac{Tr\left(\hat{B}e^{-\beta(\hat{H}-\lambda\hat{A})}\right)}{Tr\left(e^{-\beta(\hat{H}-\lambda\hat{A})}\right)} = \frac{Tr\left(\hat{B}e^{-\beta\hat{H}}\hat{U}(\beta)\right)}{Tr\left(e^{-\beta\hat{H}}\hat{U}(\beta)\right)} \cong \frac{Tr\left(\hat{B}e^{-\beta\hat{H}}\left[1+\lambda\int_0^\beta d\tau\,\hat{A}(\tau)\right]\right)}{Tr\left(e^{-\beta\hat{H}}\left[1+\lambda\int_0^\beta d\tau\,\hat{A}(\tau)\right]\right)}$$

- And thus

$$\Rightarrow \boxed{\chi_{BA} = \left.\frac{\partial\langle \hat{B} \rangle_\lambda}{\partial\lambda}\right|_{\lambda=0} \cong \int_0^\beta d\tau\left[\langle \hat{A}(\tau)\hat{B}\rangle - \langle \hat{A}(\tau)\rangle\langle \hat{B}\rangle\right]}$$

- To obtain this result we have redone the previous steps and we have used the following property

$$Tr(\hat{A}\hat{B}\hat{C}) = Tr(\hat{C}\hat{A}\hat{B}) = Tr(\hat{B}\hat{C}\hat{A})$$

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Linear response (local perturbation)

- In fact, quite often the perturbation depends on the position in the system, i.e. it assumes different values for different positions. For example an electric field **E**(**r**)
- In these cases one can have also a parameter which depends on the position in the system: λ(**r**)
- The perturbed Hamiltonian becomes $\hat{H}(\lambda) = \hat{H} - \int d\vec{r}\,\lambda(\vec{r})\hat{a}(\vec{r})$
- Previous case is recovered taking λ(**r**)=const. and $\hat{A} = \int d\vec{r}\,\hat{a}(\vec{r})$
- λ(**r**) can be broken up in a Fourier series (integral); therefore we can assume a (single Fourier component) periodic perturbation of the kind

$$\lambda(\vec{r}) = \lambda_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

- and later on we will sum up all the effects; we can do this because we are in linear response regime

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- Therefore we have $$\hat{H}(\lambda_{\vec{k}}) = \hat{H} - \lambda_{\vec{k}}\int d\vec{r}\, e^{i\vec{k}\cdot\vec{r}}\hat{a}(\vec{r}) = \hat{H} - \lambda_{\vec{k}}\hat{A}_{\vec{k}}$$
- We consider the particular case:
$$\hat{B}_{-\vec{k}} = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\hat{a}(\vec{r}) = \hat{A}_{-\vec{k}}$$
- Which allow us to measure the response of â to the perturbation. It can be proved that this is the only Fourier component which responds to the perturbation if the unperturbed system is translationally invariant; we thus assume translational invariance.
- Moreover we consider the $[\hat{H},\hat{A}_k]=0$ case:
- where $$\left\langle \hat{A}_{-\vec{k}} \right\rangle = \frac{\lambda_k}{V}\chi_{a,a}(\vec{k}) = \frac{\lambda_k}{V}\beta\left\langle \hat{A}_{-\vec{k}}\hat{A}_{\vec{k}} \right\rangle_c$$

$$\chi_{a,a}(\vec{k}) = \beta\left\langle \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\hat{a}(\vec{r})\int d\vec{r}'\, e^{i\vec{k}\cdot\vec{r}'}\hat{a}(\vec{r}')\right\rangle_c = \beta\int d\vec{r}\int d\vec{r}'\, e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')}\left\langle \hat{a}(\vec{r})\hat{a}(\vec{r}')\right\rangle_c =$$

$$= \beta V\int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\left\langle \hat{a}(\vec{r})\hat{a}(0)\right\rangle_c = \beta V\int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} G_{a,a}(\vec{r}) = \beta V\tilde{G}_{a,a}(\vec{k})$$

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- It follows that the response function to a spatially periodic perturbation is proportional to the Fourier component of the correlation function of the corresponding quantity $$\chi_{a,a}(\vec{k}) = \beta V\tilde{G}_{a,a}(\vec{k})$$

(when $[\hat{H},\hat{A}_k]\neq 0$ this relation is modified)

- We now return to a generic perturbation $\lambda(\mathbf{r})$ and measure the physical response in a certain position $\langle\hat{a}(\mathbf{r})\rangle$ (i.e. sum up all the effects of each single periodic perturbation)

$$\hat{A}_{-\vec{k}} = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\hat{a}(\vec{r}) \quad \Rightarrow \quad \hat{a}(\vec{r}) = \int \tfrac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\hat{A}_{-\vec{k}}$$

$$\left\langle \hat{a}(\vec{r})\right\rangle = \int \tfrac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\left\langle \hat{A}_{-\vec{k}}\right\rangle = \int \tfrac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\frac{\lambda_k}{V}\chi_{a,a}(\vec{k}) = \int \tfrac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\lambda_k\beta\,\tilde{G}_{a,a}(\vec{k}) =$$

$$= \int \tfrac{d\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}}\lambda_k\beta\int d\vec{r}'\, e^{-i\vec{k}\cdot\vec{r}'}G_{a,a}(\vec{r}') = \beta\int d\vec{r}'\,\lambda(\vec{r}-\vec{r}')\,G_{a,a}(\vec{r}') = \beta\int d\vec{r}''\,\lambda(\vec{r}'')\,G_{a,a}(\vec{r}-\vec{r}'')$$

- Thus the response in r depends from the values of $\lambda(r)$ in an interval around r , the range of the correlation function G determines the extension of the non-locality

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- A particular case consists in perturbation described by an external potential which acts on the particles:

$$-\lambda\hat{A} = \sum_i \phi(\hat{\vec{r}}_i) = \int d\vec{r}\phi(\vec{r})\hat{\rho}(\vec{r})$$

- where the local density operator $\hat{\rho}(\vec{r}) = \sum_i \delta(\vec{r} - \hat{\vec{r}}_i)$

- has Fourier components, $\hat{\rho}_{\vec{k}} = \sum_i e^{-i\vec{k}\cdot\hat{\vec{r}}_i}$, which represent the density fluctuation operator

- In this case we have $\boxed{-\lambda(\vec{r}) = \phi(\vec{r}) \quad a(\vec{r}) = \hat{\rho}(\vec{r})}$

$$\Rightarrow \quad \hat{A}_{-\vec{k}} = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\hat{a}(\vec{r}) = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\hat{\rho}(\vec{r}) = \hat{\rho}_{\vec{k}}$$

$$\Rightarrow \quad G_{\rho,\rho}(\vec{r}) = \left\langle \hat{a}(\vec{r})\hat{a}(0)\right\rangle_c = \left\langle \hat{\rho}(\vec{r})\hat{\rho}(0)\right\rangle_c$$

$$\tilde{G}_{\rho,\rho}(\vec{k}) = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} \left\langle \hat{\rho}(\vec{r})\hat{\rho}(0)\right\rangle_c = \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} \left\langle \hat{\rho}(\vec{r})\hat{\rho}(0)\right\rangle - \rho^2 \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} =$$

$$= \rho S(\vec{k}) - \rho^2 \int d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} = \rho S(\vec{k}) - \rho^2 (2\pi)^3 \delta(\vec{k})$$

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- Which implies $\chi_{\rho,\rho}(\vec{k}) = \beta N\left[S(\vec{k}) - \rho(2\pi)^3\delta(\vec{k})\right]$

- where S(**k**) is the static structure factor that we introduced in the scattering theory

- Conclusion: a scattering measurements and a local linear response give equivalent information, the local density correlation function, if the perturbation couples with matter as "radiation" does

- This does not means that these two experimental probes are able to explore the same range of wave vectors

- Previous connection among the susceptibility and the static structure factor is valid in the classical case, where all "operators" commute

- We have given examples only for operator A=B, but for example one can consider a thermal flux connected to an electric field etc. etc.

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Dissipation

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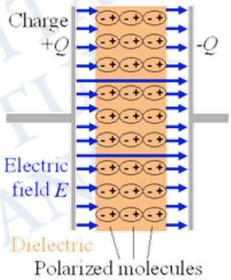
- The "electric susceptibility" χ_e of a dielectric material is a measure of how easily it polarizes in response to an electric field. It is defined as the constant of proportionality relating an electric field **E** to the induced dielectric polarization **P**



$$\vec{P} = \chi_e \vec{E}$$

- When **E** is constant there is no dissipation; if we apply an alternate field $\mathbf{E}=\mathbf{E}_0\cos(\omega t)$ the polarization is no more in phase with the field due to dynamic effects in the sample: dissipation sets in!
- Thus, the AC susceptibility measurement yields two quantities its magnitude and a phase shift. Alternatively, one can think of the susceptibility as having an in-phase, or real, component and an out-of-phase, or imaginary (dissipative):

$$\chi_e = \chi_e' + i\chi_e''$$

$$\chi_e' = \chi_e \cos\phi \qquad \chi_e = \sqrt{\chi_e'^2 + \chi_e''^2}$$

$$\chi_e'' = \chi_e \sin\phi \qquad \phi = \arctan(\chi''/\chi')$$

- another example is the refractive index in a (quasi)-transparent medium.
- What is the origin of dissipation? Is there a relation among χ' and χ''?

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Linear response (time dependent perturbation)

- It is convenient to work in the interaction representation/picture (or Dirac picture) which is an intermediate representation between the Schrödinger picture and the Heisenberg picture. Whereas in the other two pictures either the state vector or the operators carry time dependence, in the interaction picture both carry part of the time dependence of observables
- The interaction picture is useful because it enable to construct the solution to the many body problem as the solution to a simpler solvable problem plus some unknown (interaction) part.
- To switch into the interaction picture, as in the present discussion, one should recognize the Schrödinger picture Hamiltonian as divided into two parts,

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

- typically be chosen so that $\hat{H}_0$ is well understood and exactly solvable, while $\hat{H}_1$ contains some harder-to-analyse perturbation to this system. If $\hat{H}$ has explicit time-dependence, as in the present case, it will usually be advantageous to include the explicitly time-dependent terms with $\hat{H}_1$, leaving $\hat{H}_0$ time-independent.

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- A state vector in the interaction picture is defined as $\left|\psi_I\right\rangle_t = e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_S\right\rangle_t$

  where $\left|\psi_S\right\rangle_t$ is the same state vector as in the Schrödinger

- An operator in the interaction picture is defined as

$$\hat{O}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}_S(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

- This also define the density operator in the interaction picture:

$$\hat{\rho}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

  which satisfies the following equation of motion

$$i\hbar\frac{d\hat{\rho}_I(t)}{dt} = -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t} + i\hbar e^{\frac{i}{\hbar}\hat{H}_0 t}\frac{d\hat{\rho}(t)}{dt}e^{-\frac{i}{\hbar}\hat{H}_0 t} + e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0 =$$

$$= -\left[\hat{H}_0, \hat{\rho}_I(t)\right] + e^{\frac{i}{\hbar}\hat{H}_0 t}\left[\hat{H}_0 + \hat{H}_1, \hat{\rho}(t)\right]e^{-\frac{i}{\hbar}\hat{H}_0 t} =$$

$$= \cancel{-\left[\hat{H}_0, \hat{\rho}_I(t)\right]} + \cancel{\left[\hat{H}_0, \hat{\rho}_I(t)\right]} + e^{\frac{i}{\hbar}\hat{H}_0 t}\left(\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t}e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}(t) - \hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t}e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{\rho}(t)\right)e^{-\frac{i}{\hbar}\hat{H}_0 t} =$$

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- We obtain: $$\boxed{i\hbar\frac{d\hat{\rho}_I(t)}{dt} = \left[\hat{H}_1^I(t), \hat{\rho}_I(t)\right]}$$

- In our case $\hat{H}_1^I(t) = -\int d\vec{r}\,\lambda(\vec{r},t)e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{a}(\vec{r})e^{-\frac{i}{\hbar}\hat{H}_0 t} = -\int d\vec{r}\,\lambda(\vec{r},t)\hat{a}_H(\vec{r},t)$

being $\hat{a}_H(\mathbf{r},t)$ the "unperturbed" evolution of $\hat{a}(\mathbf{r})$ in the Heisenberg picture

- We solve the equation of motion for $\hat{\rho}_I(t)$ perturbatively in λ, i.e.

$$\hat{\rho}_I(t) = \sum_{n=0}^{\infty}\hat{\rho}_{I,n}(t) \qquad \hat{\rho}_I(t=-\infty) = \hat{\rho}_0$$

  where the n^{th}-term contains n-powers of the perturbation.

  We will limit our analysis to the linear response, hence we just need the first order term which satisfies:

$$i\hbar\frac{d\hat{\rho}_{I,1}(t)}{dt} = \left[\hat{H}_1^I(t), \hat{\rho}_{I,0}(t)\right]$$

- With solution:

$$\hat{\rho}_{I,1}(t) = -\frac{i}{\hbar}\int_{-\infty}^{t}dt'\left[\hat{H}_1^I(t'), \hat{\rho}_{I,0}(t')\right] = -\frac{i}{\hbar}\int_{-\infty}^{t}dt'\left[\hat{H}_1^I(t'), \hat{\rho}_0\right]$$

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- Now, at linear order,

$$\left\langle \hat{B}(t) \right\rangle = Tr\left[\hat{\rho}_I(t)\hat{B}_I(t)\right] \cong Tr\left[\hat{\rho}_0\hat{B}_I(t)\right] + Tr\left[\hat{\rho}_{I,1}(t)\hat{B}_I(t)\right] =$$

$$= Tr\left[\hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t}\right] + Tr\left[\hat{\rho}_{I,1}(t)e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t}\right] =$$

$$= Tr\left[\hat{\rho}_0\hat{B}\right] - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, Tr\left\{\left[\hat{H}_1^I(t'), \hat{\rho}_0\right] e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t}\right\} =$$

$$= \left\langle \hat{B} \right\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, Tr\left\{e^{\frac{i}{\hbar}\hat{H}_0 t'}\hat{H}_1(t')e^{-\frac{i}{\hbar}\hat{H}_0 t'}\hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t} - \hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0 t'}\hat{H}_1(t')e^{-\frac{i}{\hbar}\hat{H}_0 t'}e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t}\right\} =$$

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$$= \left\langle \hat{B} \right\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, Tr\left\{\hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{H}_1(t') - \hat{\rho}_0\hat{H}_1(t')e^{\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\right\} =$$

$$= \left\langle \hat{B} \right\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, Tr\left\{\hat{\rho}_0\left[\hat{B}_H(t-t'), \hat{H}_1(t')\right]\right\} =$$

$$\Rightarrow \boxed{\left\langle \hat{B}(t) \right\rangle = \left\langle \hat{B} \right\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \left\langle \left[\hat{B}_H(t-t'), \hat{H}_1(t')\right] \right\rangle_0}$$

To obtain this result we have used:

$$Tr\left[\hat{A}\hat{B}\hat{C}\right] = Tr\left[\hat{B}\hat{C}\hat{A}\right] = Tr\left[\hat{C}\hat{A}\hat{B}\right]$$

$$\left[\hat{\rho}_0, \hat{H}_0\right] = 0 = \left[\hat{\rho}_0, e^{\pm\frac{i}{\hbar}\hat{H}_0 t}\right]$$

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- Remember also that $\hat{H}_1(t) = -\int d\vec{r}'\, \lambda(\vec{r}',t)\hat{a}(\vec{r}')$
- It follows: $\boxed{\left\langle \hat{B}(t) \right\rangle - \left\langle \hat{B} \right\rangle_0 =}$

$$= \tfrac{i}{\hbar}\int_{-\infty}^{t} dt' \int d\vec{r}'\, Tr\left\{ \hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{a}(\vec{r}') - \hat{\rho}_0\hat{a}(\vec{r}')e^{\frac{i}{\hbar}\hat{H}_0(t-t')}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0(t-t')} \right\} \lambda(\vec{r}',t') =$$

$$= \tfrac{i}{\hbar}\int_{-\infty}^{t} dt' \int d\vec{r}'\, Tr\left\{ \hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t} e^{\frac{i}{\hbar}\hat{H}_0 t'}\hat{a}(\vec{r}')e^{-\frac{i}{\hbar}\hat{H}_0 t'} - \hat{\rho}_0 e^{\frac{i}{\hbar}\hat{H}_0 t'}\hat{a}(\vec{r}')e^{-\frac{i}{\hbar}\hat{H}_0 t'} e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{B}e^{-\frac{i}{\hbar}\hat{H}_0 t} \right\} \lambda(\vec{r}',t') =$$

$$= \tfrac{i}{\hbar}\int_{-\infty}^{t} dt' \int d\vec{r}'\, Tr\left\{ \hat{\rho}_0 \left[\hat{B}_H(t), \hat{a}_H(r',t') \right] \right\} \lambda(\vec{r}',t') =$$

$$\boxed{= \tfrac{i}{\hbar}\int_{-\infty}^{t} dt' \int d\vec{r}'\, \left\langle \left[\hat{B}_H(t), \hat{a}_H(\vec{r}',t') \right] \right\rangle_0 \lambda(\vec{r}',t')}$$

Again, we have used:

$$Tr\left[\hat{A}\hat{B}\hat{C}\right] = Tr\left[\hat{B}\hat{C}\hat{A}\right] = Tr\left[\hat{C}\hat{A}\hat{B}\right] \qquad \left[\hat{\rho}_0, \hat{H}_0\right] = 0 = \left[\hat{\rho}_0, e^{\pm\frac{i}{\hbar}\hat{H}_0 t}\right]$$

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- Therefore, at linear order, we have found that:

$$\left\langle \hat{B}(t) \right\rangle - \left\langle \hat{B} \right\rangle_0 = -\tfrac{i}{\hbar}\int_{-\infty}^{t} dt' \left\langle \left[\hat{B}_H(t-t'), \hat{H}_1(t') \right] \right\rangle_0$$

where $\hat{O}_H(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{O}e^{-\frac{i}{\hbar}\hat{H}_0 t}$

- … and that:

$$\left\langle \hat{B}(t) \right\rangle - \left\langle \hat{B} \right\rangle_0 = -\tfrac{i}{\hbar}\int_{-\infty}^{+\infty} dt'\, \theta(t-t') \left\langle \left[\hat{B}_H(t-t'), \hat{H}_1(t') \right] \right\rangle_0 =$$

$$\cdots = \int_{-\infty}^{+\infty} dt' \int d\vec{r}'\, \tfrac{i}{\hbar}\theta(t-t') \left\langle \left[\hat{B}_H(\vec{r},t), \hat{a}_H(\vec{r}',t') \right] \right\rangle_0 \lambda(\vec{r}',t')$$

$$\Rightarrow \boxed{\chi_{BA}(\vec{r},\vec{r}',t-t') = -\frac{i}{\hbar}\theta(t-t') \left\langle \left[\hat{B}_H(\vec{r},t), \hat{a}_H(\vec{r}',t') \right] \right\rangle_0}$$

- This is the Kubo formula which shows that, at linear order, the variation of any measurable quantity is obtained through the linear response function (dynamic susceptibility) which is only related to averages on the unperturbed system

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Causality

- The fact that, as a consequence of the adiabatic switching, the response function (dynamic susceptibility) vanishes for (t < t') is of course an expression of causality: the physical response at a given time depends only on the action of the external perturbation that the system has received at all earlier times.

- We can define $$\chi''_{BA}(\vec{r},\vec{r}',t-t') = -\frac{1}{2\hbar}\left\langle\left[\hat{B}_H(\vec{r},t),\hat{a}_H(\vec{r}',t')\right]\right\rangle_0$$

$$\Rightarrow \quad \chi_{BA}(\vec{r},\vec{r}',t-t') = 2i\,\theta(t-t')\,\chi''_{BA}(\vec{r},\vec{r}',t-t')$$

- If B and A are Hermitian operators $\chi''_{BA}(r,r',t-t')$ is imaginary, in fact

$$\left\langle\left[\hat{B},\hat{A}\right]\right\rangle = \left\langle\hat{B}\hat{A}-\hat{A}\hat{B}\right\rangle = \left\langle\hat{B}\hat{A}\right\rangle - \left\langle\hat{A}\hat{B}\right\rangle = \left\langle\hat{B}\hat{A}\right\rangle - \left\langle(\hat{B}\hat{A})^{+}\right\rangle = \left\langle\hat{B}\hat{A}\right\rangle - \left\langle\hat{B}\hat{A}\right\rangle^{*} = 2i\,\mathrm{Im}\left\langle\hat{B}\hat{A}\right\rangle$$

- We introduce also the Fourier transforms (dependence on r, r' is made implicit)

$$\chi_{BA}(\omega) = \int_{-\infty}^{+\infty} d\omega\, e^{i\omega t}\chi_{BA}(t) \qquad \chi_{BA}(t) = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\chi_{BA}(\omega)$$

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- Given the Fourier representation of the step function

$$\theta(t) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}e^{-i\omega' t}\frac{i}{\omega'+i\varepsilon^{+}}$$

- We find

$$\chi_{BA}(\omega) = 2i\int_{-\infty}^{+\infty} d\omega\, e^{i\omega t}\theta(t)\chi''_{BA}(t) =$$

$$= -\int_{-\infty}^{+\infty} d\omega\, e^{i\omega t}\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}e^{-i\omega' t}\frac{1}{\omega'+i\varepsilon^{+}}\int_{-\infty}^{+\infty}\frac{d\omega''}{\pi}e^{-i\omega'' t}\chi''_{BA}(\omega'') =$$

$$= -\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{1}{\omega'+i\varepsilon^{+}}\int_{-\infty}^{+\infty}\frac{d\omega''}{\pi}\chi''_{BA}(\omega'')\,2\pi\,\delta(\omega-\omega'-\omega'')$$

$$\Rightarrow \quad \chi_{BA}(\omega) = -\int_{-\infty}^{+\infty}\frac{d\omega''}{\pi}\frac{\chi''_{BA}(\omega'')}{\omega-\omega''+i\varepsilon^{+}}$$

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- If we use the relations $\dfrac{1}{\omega \pm i\varepsilon^+} = P\left(\dfrac{1}{\omega}\right) \mp i\pi\delta(\omega)$

- We obtain $\chi_{BA}(\omega) = P\int_{-\infty}^{+\infty} \frac{d\omega''}{\pi} \dfrac{\chi''_{BA}(\omega'')}{\omega'' - \omega} + i\chi''_{BA}(\omega'')$

- This yields the following decomposition $\boxed{\chi_{BA}(\omega) = \chi'_{BA}(\omega) + i\chi''_{BA}(\omega)}$

  with
  $$\chi'_{BA}(\omega) = P\int_{-\infty}^{+\infty} \frac{d\omega''}{\pi} \frac{\chi''_{BA}(\omega'')}{\omega'' - \omega}$$

- In the typical case, when A and B are Hermitian, we know that $\chi''_{BA}(r,r',t-t')$ is imaginary. Usually, observables corresponding to operators A and B have definite signature ($\varepsilon=\pm1$) under time reversal. Assuming $\varepsilon_A=\varepsilon_B=1$, one can prove (see Mazenko)

$$\chi''_{BA}(\vec{r},\vec{r}',t-t') = -\chi''_{BA}(\vec{r},\vec{r}',t'-t) \quad \Rightarrow \quad \mathrm{Im}\,\chi''_{BA}(\omega) = 0$$

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Kramers-Krönig relations ≡ causality

- Thus, the previous relation

$$\chi_{BA}(\omega) = \chi'_{BA}(\omega) + i\chi''_{BA}(\omega)$$

- corresponds always (given A & B Hermitian) to a decomposition of the response function in a real and imaginary (dissipative) part.

- Which is the dissipative part depends on the signature under time reversal of A and B

- The relations
$$\boxed{\begin{aligned}\chi'_{BA}(\omega) &= P\int_{-\infty}^{+\infty} \frac{d\omega''}{\pi} \frac{\chi''_{BA}(\omega'')}{\omega'' - \omega} \\ \chi''_{BA}(\omega) &= P\int_{-\infty}^{+\infty} \frac{d\omega''}{\pi} \frac{\chi'_{BA}(\omega'')}{\omega - \omega''}\end{aligned}}$$
(we proved the 1st)

- say that the real and the imaginary part of the response function (dynamic susceptibility) are not independent, they are known as the Kramers-Krönig relations; their physical origin is the causality of the response function

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Fluctuation dissipation theorem

- Consider the correlation function

$$\boxed{S_{BA}(t-t') := -\left\langle \hat{B}_H(t)\hat{A}_H(t')\right\rangle_0} = -\frac{1}{Q} Tr\left[e^{-\beta\hat{H}_0}\hat{B}_H(t)\hat{A}_H(t')\right] =$$

$$= -\frac{1}{Q} Tr\left[e^{-\beta\hat{H}_0}\hat{B}_H(t)e^{\beta\hat{H}_0}e^{-\beta\hat{H}_0}\hat{A}_H(t')\right] = -\frac{1}{Q} Tr\left[\hat{B}_H(t+i\beta\hbar)e^{-\beta\hat{H}_0}\hat{A}_H(t')\right] =$$

$$= -\frac{1}{Q} Tr\left[e^{-\beta\hat{H}_0}\hat{A}_H(t')\hat{B}_H(t+i\beta\hbar)\right] = S_{AB}(t'-t-i\beta\hbar)$$

- In terms of the Fourier transform we obtain

$$\boxed{S_{BA}(\omega)} = \int d(t-t')\, e^{i\omega(t-t')} \int \frac{d\varpi}{2\pi}\, e^{-i\varpi(t'-t-i\beta\hbar)} S_{AB}(\varpi) =$$

$$= \int \frac{d\varpi}{2\pi}\, e^{-\beta\hbar\varpi} S_{AB}(\varpi)\, 2\pi\delta(\omega+\varpi) = \boxed{e^{\beta\hbar\omega} S_{AB}(-\omega)}$$

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- We can now use this result in treating the linear response function:

$$\chi''_{BA}(t-t') = -\frac{1}{2\hbar}\left\langle\left[\hat{B}_H(t), \hat{A}_H(t')\right]\right\rangle_0 = \frac{1}{2\hbar}\left\langle S_{BA}(t-t') - S_{AB}(t'-t)\right\rangle_0$$

and

$$\boxed{\chi''_{BA}(\omega)} = \frac{1}{2\hbar}\left\langle S_{BA}(\omega) - S_{AB}(-\omega)\right\rangle_0 = \boxed{\frac{1-e^{-\beta\hbar\omega}}{2\hbar} S_{BA}(\omega)}$$

- The relationship connecting the correlation function and the response function is the fluctuation-dissipation theorem. In the classical limit, where $\hbar \to 0$, the fluctuation-dissipation theorem becomes

$$\boxed{\chi''_{BA}(\omega) = \lim_{\hbar\to 0}\frac{1-e^{-\beta\hbar\omega}}{2\hbar} S_{BA}(\omega) = \frac{\beta\omega}{2} S_{BA}(\omega)}$$

- If we now return to our example of the fluid, we easily obtain, choosing

$$\hat{B}(\vec{r}) = \hat{\rho}(\vec{r});\ \hat{A}(\vec{r}') = \hat{\rho}(\vec{r}') \qquad \Rightarrow \qquad S(\vec{k},\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''(\vec{k},\omega)$$

- Thus the dynamic structure factor of a neutron scattering experiment is connected with the imaginary part of the density-density response function

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Scattering by a generic system

- Suppose now that the neutron beam is incident on a scattering system in a state characterized by an index λ . Denote with $\psi_{\mathbf{k}}$ the wave-function of the neutron and χ_λ that of the scattering system.
- Suppose the neutron interacts with the system via a potential U, and is scattered so that its final wave-vector is **k'** ; the final state of the scattering system is λ'.
- Consider the differential scattering cross section $(d\sigma/d\Omega)_{\lambda\to\lambda'}$ representing the sum of all processes in which the state of the scattering system changes from λ to λ', and the state of the neutron changes from **k** to **k'**:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi d\Omega}\sum_{\vec{k}'(\in d\Omega)} W_{\vec{k}\lambda\to\vec{k}'\lambda'}$$

where W is the number of transition per second from state $|\mathbf{k}\,\lambda\rangle$ to state $|\mathbf{k}'\lambda'\rangle$; we have to find a form for this quantity

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Fermi's golden rule

- Assume the system is described by a Hamiltonian, H, of the form

$$\hat{H}(t) = \hat{H}_0 + \hat{U}(t)$$

- Where H_0 is the unperturbed Hamiltonian, for which the eigenfunctions are known, and U is the time-dependent perturbation. The eigenfunctions of the unperturbed Hamiltonian being $|\lambda\rangle$
- The basic strategy is to express the solution as a sum over the eigenstates of H_0 with time-dependent coefficients:

$$|\psi\rangle_t = \sum_\lambda a_\lambda(t)|\lambda\rangle e^{-\frac{i}{\hbar}E_\lambda t}$$

- Next, substitute $|\psi\rangle_t$ into the Schrodinger equation for H and use the orthogonality conditions to obtain:

$$\hat{H}|\psi\rangle_t = i\hbar\frac{\partial}{\partial t}|\psi\rangle_t \quad \Rightarrow \quad i\hbar\frac{\partial a_{\lambda'}(t)}{\partial t} = \sum_\lambda a_\lambda(t)\langle\lambda'|\hat{U}(t)|\lambda\rangle e^{-\frac{i}{\hbar}(E_\lambda - E_{\lambda'})t}$$

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- Where $\langle \lambda' | \hat{U}(t) | \lambda \rangle$ is often called transition amplitude. The difficulty in solving this equation arises from the fact that the coefficients are expressed in terms of themselves: $i\hbar \frac{\partial a_{\lambda'}(t)}{\partial t} = \sum_{\lambda} a_{\lambda}(t) \langle \lambda' | \hat{U}(t) | \lambda \rangle e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t}$
- In the context of scattering, this equations is generally solved approximately by a "perturbation expansion". The $(p+1)^{th}$-order approximation is found from the p^{th}-order solution by:

$$i\hbar \frac{\partial a_{\lambda'}^{(p+1)}(t)}{\partial t} \approx \sum_{\lambda} a_{\lambda}^{(p)}(t) \langle \lambda' | \hat{U}(t) | \lambda \rangle e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t}$$

- A 0^{th}-order approximation would correspond to

$$\partial a_{\lambda'}^{(0)}(t) / \partial t = 0$$

- Which implies that the coefficients are constant and no transition occur
- As a 1^{th}-order approximation we make some assumptions:

1. The system is initially in a specific state $|\lambda\rangle$, i.e. $a_{\lambda'}(t=0)=\delta_{\lambda\lambda'}\ \forall\lambda'$
2. The perturbation is very weak and applied for a short period of time

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- With this in mind, we obtain $i\hbar \frac{\partial a_{\lambda'}^{(1)}(t)}{\partial t} = \langle \lambda' | \hat{U}(t) | \lambda \rangle e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t'}$
- Which can be integrated to give:

$$i\hbar a_{\lambda'}^{(1)}(t) = \int_{-\infty}^{t} dt' \langle \lambda' | \hat{U}(t') | \lambda \rangle e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t'}$$

- By assuming (1) and (2) we deprived the system of any capability of reaching the final state by alternate routes, i.e. only direct transitions from state $|\lambda\rangle$ to $|\lambda'\rangle$ are possible.
- Next it is assumed that:

3. the perturbation "turns on" at $t_0=0$ and is constant over the interval $0 \le t' < t$. We obtain

$$i\hbar a_{\lambda'}^{(1)}(t) = \langle \lambda' | \hat{U} | \lambda \rangle \int_{0}^{t} dt' e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t'} = \langle \lambda' | \hat{U} | \lambda \rangle \frac{e^{-\frac{i}{\hbar}(E_{\lambda}-E_{\lambda'})t} - 1}{-i(E_{\lambda} - E_{\lambda'})/\hbar} =$$

$$= \langle \lambda' | \hat{U} | \lambda \rangle e^{-\frac{i}{2\hbar}(E_{\lambda}-E_{\lambda'})t} \frac{e^{-\frac{i}{2\hbar}(E_{\lambda}-E_{\lambda'})t} - e^{\frac{i}{2\hbar}(E_{\lambda}-E_{\lambda'})t}}{-i(E_{\lambda} - E_{\lambda'})/\hbar} = \langle \lambda' | \hat{U} | \lambda \rangle e^{-\frac{i}{2\hbar}(E_{\lambda}-E_{\lambda'})t} \frac{\sin\left[(E_{\lambda} - E_{\lambda'})t/2\hbar\right]}{(E_{\lambda} - E_{\lambda'})/2\hbar}$$

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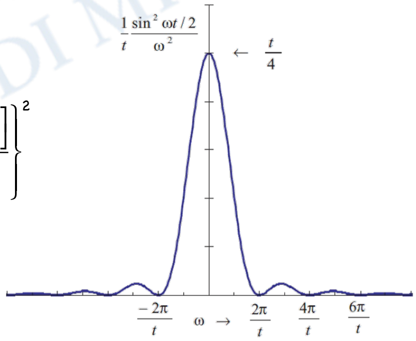
- The application of the perturbation changes the state of the system from the initial state $|\lambda\rangle$ to a final state $|\lambda'\rangle$, both of which are eigenstates of the unperturbed Hamiltonian H_0 . The probability at time t that the system undergoes a transition from state $|\lambda\rangle$ to a state $|\lambda'\rangle$ is:

$$\left|a_{\lambda'}(t)\right|^2 = \frac{1}{\hbar^2}\left|\left\langle\lambda'\left|\hat{U}\right|\lambda\right\rangle\right|^2 \left\{\frac{\sin\left[(E_\lambda - E_{\lambda'})t/2\hbar\right]}{(E_\lambda - E_{\lambda'})/2\hbar}\right\}^2$$

- The number of transition per second from state $|\mathbf{k}\ \lambda\rangle$ to state $|\mathbf{k}'\lambda'\rangle$ is thus (making again explicit the whole system neutron+target)

$$W_{\vec{k}\lambda\to\vec{k}'\lambda'} = \frac{1}{t}\left|a_{\lambda'}(t)\right|^2 =$$

$$\frac{4}{\hbar^2}\left|\left\langle\vec{k}'\lambda'\left|\hat{U}\right|\vec{k}\lambda\right\rangle\right|^2 \frac{1}{t}\left\{\frac{\sin\left[(E_\lambda - E_{\lambda'})t/2\hbar\right]}{(E_\lambda - E_{\lambda'})/\hbar}\right\}^2$$



- Note that the function in figure is strongly peaked near $\omega=(E_{\lambda'}-E_\lambda)/\hbar$

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- Therefore the states to which transitions can occur must have $E_{\lambda'}\simeq E_\lambda$ forcing energy conservation

- In general, there will be some number of states dn within an interval of energies around $E_{\lambda'}$

$$dn = \rho_{\vec{k}'}\, dE_{\lambda'}$$

where $\rho_{\vec{k}'} = \dfrac{dn}{dE_{\lambda'}}$ is the density of states per unit energy interval near $E_{\lambda'}$

- The physically meaningful quantity is the total transition rate (total number of transition per second) to state near the state $|\mathbf{k}\ \lambda\rangle$

$$W_{\vec{k}\lambda\to\vec{k}'\lambda'} = \int dE_{\lambda'}\rho_{\vec{k}'}\frac{4}{\hbar^2}\left|\left\langle\vec{k}'\lambda'\left|\hat{U}\right|\vec{k}\lambda\right\rangle\right|^2 \frac{1}{t}\left\{\frac{\sin\left[(E_\lambda - E_{\lambda'})t/2\hbar\right]}{(E_\lambda - E_{\lambda'})/\hbar}\right\}^2 =$$

$$\cong \frac{4}{\hbar}\left|\left\langle\vec{k}'\lambda'\left|\hat{U}\right|\vec{k}\lambda\right\rangle\right|^2 \rho_{\vec{k}'}\int_{-\infty}^{\infty} d\omega\,\frac{1}{t}\frac{\sin^2(\omega t/2)}{\omega^2} = \frac{2\pi}{\hbar}\left|\left\langle\vec{k}'\lambda'\left|\hat{U}\right|\vec{k}\lambda\right\rangle\right|^2 \rho_{\vec{k}'}$$

- This is the Fermi's Golden rule, and this is the expression for W we were looking for

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Scattering cross sections

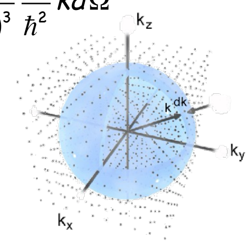
Thanks to the Fermi's golden rule we can write:

$$\sum_{\vec{k}'(\in d\Omega)} W_{\vec{k}\lambda\to\vec{k}'\lambda'} = \frac{2\pi}{\hbar}\rho_{\vec{k}'}\left|\left\langle\vec{k}'\lambda'\middle|U\middle|\vec{k}\lambda\right\rangle\right|^2 = \frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{m}{\hbar^2}k'd\Omega\left|\left\langle\vec{k}'\lambda'\middle|U\middle|\vec{k}\lambda\right\rangle\right|^2$$

where $\rho_{k'}$ is the number of momentum states in $d\Omega$ per unit energy range, i.e. the number of wave-vector points in the volume $k'^2dk'd\Omega$:

$$\rho_{\vec{k}} = \frac{1}{V_u}\frac{k^2dk\,d\Omega}{dE} = \frac{V}{(2\pi)^3}\frac{k^2dk\,d\Omega}{\hbar^2k\,dk\,/\,m} = \frac{V}{(2\pi)^3}\frac{m}{\hbar^2}kd\Omega$$

(V_u=lattice's unit-cell volume)



- We now consider the wave-function of the incoming neutron $\psi_{\mathbf{k}}$ as a plane wave of the form

$$\psi_{\vec{k}} = \frac{1}{\sqrt{V}}\exp(i\vec{k}\cdot\vec{r})$$

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- The flux of the incident neutrons is the product of their density and velocity:

$$\Phi = \frac{dN}{dSdt} = \frac{d(V\rho_{inc})}{dSdt} = \frac{\rho_{inc}\cancel{dS}\,dx}{\cancel{dS}\,dt} = \left|\psi_{\vec{k}}\right|^2 v = \frac{1}{V}\frac{\hbar}{m}k$$

- We thus obtain

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi d\Omega}\sum_{\vec{k}'(\in d\Omega)} W_{\vec{k}\lambda\to\vec{k}'\lambda'} = \frac{k'}{k}\left(\frac{mV}{2\pi\hbar^2}\right)^2\left|\left\langle\vec{k}'\lambda'\middle|U\middle|\vec{k}\lambda\right\rangle\right|^2$$

- If E and E′ are the initial and final energies of the neutron, and E_λ and $E_{\lambda'}$ are the initial and final energies of the scattering system then $\Rightarrow$ $E+E_\lambda=E'+E_{\lambda'}$ i.e. in mathematical terms the energy distribution of the scattered neutrons is a delta-function; so the expression for the partial differential cross-section is

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{mV}{2\pi\hbar^2}\right)^2\left|\left\langle\vec{k}'\lambda'\middle|U\middle|\vec{k}\lambda\right\rangle\right|^2\delta(E_\lambda - E_{\lambda'} + E - E')$$

- We now consider the potential of the neutron due to the j-th nucleus of the form $u(\mathbf{r}-\mathbf{R}_j)$; so the potential for the whole scattering system is $U=\Sigma_j\, u(\mathbf{r}-\mathbf{R}_j)$

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The Fermi pseudo-potential

- The first step in evaluating the matrix element in the partial differential cross section is to integrate with respect to the neutron coordinate:

$$\langle \vec{k}'\lambda' | U | \vec{k}\lambda \rangle = \frac{1}{V}\int d\vec{r} \langle \lambda' | e^{-i\vec{k}'\cdot\vec{r}} \sum_j u(\vec{r}-\vec{R}_j)\, e^{i\vec{k}\cdot\vec{r}} | \lambda \rangle =$$

$\vec{r}' = \vec{r} - \vec{R}_j$

$$= \frac{1}{V}\langle \lambda' | \sum_j e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j} \int d\vec{r}'\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'} u(\vec{r}') | \lambda \rangle = \frac{u(\vec{q})}{V} \langle \lambda' | \sum_j e^{i\vec{q}\cdot\vec{R}_j} | \lambda \rangle$$

where **q**=**k**-**k**′ and where u(**q**) is

$$u(\vec{q}) = \int d\vec{r}'\, u(\vec{r}')e^{i\vec{q}\cdot\vec{r}'}$$

- The next step is to insert a specific function for u . To find a suitable mathematical function we make a digression and calculate $d\sigma/d\Omega$ for a single fixed nucleus using the present formalism: there is only one term in the sum and since the nucleus is fixed at the origin $R_1=0$ and $\lambda=\lambda'$.

- Thus $$\langle \vec{k}'\lambda' | U | \vec{k}\lambda \rangle = \frac{u(\vec{q})}{V}\langle \lambda | \lambda \rangle = \frac{1}{V}\int d\vec{r}\, u(\vec{r})e^{i\vec{q}\cdot\vec{r}}$$

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- Inserting this result together with |**k**|=|**k**′| gives

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{k'}{k}\left(\frac{mV}{2\pi\hbar^2}\right)^2 \left|\langle \vec{k}'\lambda' | U | \vec{k}\lambda \rangle\right|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int d\vec{r}\, u(\vec{r})e^{i\vec{q}\cdot\vec{r}}\right|^2$$

- Now we know that u(**r**) is short range and we approximate it with u(**r**)=gδ(**r**) where g is a real constant
- Therefore we obtain $$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int d\vec{r}\, g\delta(\vec{r})e^{i\vec{q}\cdot\vec{r}}\right|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 g^2 = a^2$$

Where [a] is the scattering length ($\sigma_{tot}=4\pi a^2$) and we can write

$$u(\vec{r}) = \frac{2\pi\hbar^2}{m} a\,\delta(\vec{r})$$

- This potential, known as the Fermi pseudo-potential, is the one we shall adopt; the positive sign in the last equation implies a positive scattering length for a repulsive potential

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- If the nucleus is free (not bound) the scattering must be treated in the center of mass system.
- The result is the same as if the nucleus were fixed, but the mass m of the neutron must be replaced with the reduced mass of the nucleus-neutron system; in the "extreme" case (target and probe are the same kind of particle):

$$u(\vec{r}) = \frac{2\pi\hbar^2}{\mu} a\,\delta(\vec{r}) \rightarrow \frac{4\pi\hbar^2}{m} a\,\delta(\vec{r})$$

- We return now to the expression for the cross-section for a general scattering system in which we define $\hbar\omega = E - E'$:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\lambda\to\lambda'} = \frac{k'}{k} a^2 \left|\left\langle \lambda' \middle| \sum_j e^{-i\vec{q}\cdot\vec{R}_j} \middle| \lambda \right\rangle\right|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

- We can express the delta-function for energy as an integral with respect to time

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

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The dynamic structure factor

- Let also H be the Hamiltonian of the scattering system. The states λ and λ′ are eigenfunction of H with eigenvalues E_λ and $E_{\lambda'}$; thus we obtain

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\frac{a^2}{2\pi\hbar}\int_{-\infty}^{\infty} dt \left\langle \lambda \middle| \sum_j e^{\frac{i}{\hbar}\hat{H}t} e^{-i\vec{q}\cdot\vec{R}_j} e^{-\frac{i}{\hbar}\hat{H}t} \middle| \lambda' \right\rangle \left\langle \lambda' \middle| \sum_j e^{i\vec{q}\cdot\vec{R}_j} \middle| \lambda \right\rangle e^{i\omega t}$$

- In actual experiment we do not measure the cross-section for a process in which the scattering system goes from a specific state λ to another λ′ but the partial differential cross section which is obtained from the previous one by summing over all final states λ′ keeping the initial state λ fixed and then averaging over all λ
- By using the closure relation $\Sigma_{\lambda'}|\lambda'\rangle\langle\lambda'|=1$ and by moving from an average on "pure" states to a quantum statistical mechanic average (dividing by 1/N) we obtain the partial differential cross section per target atom

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- Which is:

$$\frac{d^2\sigma}{d\Omega dE'} = \sum_{\lambda\lambda'} p_\lambda \left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\lambda\to\lambda'} =$$

$$= \frac{1}{N}\frac{k'}{k}\frac{a^2}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{i\omega t} \sum_\lambda p_\lambda \left\langle \lambda \middle| \sum_j e^{-i\vec{q}\cdot\vec{R}_j(t)} \sum_j e^{i\vec{q}\cdot\vec{R}_j} \middle| \lambda \right\rangle = \frac{k'}{k}\frac{a^2}{\hbar} S(\vec{q},\omega)$$

where we have introduced the dynamic structure factor defined as

$$S(\vec{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \sum_j e^{-i\vec{q}\cdot\vec{R}_j(t)} \sum_j e^{i\vec{q}\cdot\vec{R}_j} \right\rangle = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt e^{i\omega t} \left\langle \hat{\rho}_{\vec{q}}(t)\hat{\rho}^{+}_{\vec{q}}(0)\right\rangle$$

- In the definition of the dynamic structure factor, which has been assumed proportional to the partial differential cross section and is therefore directly measured in an inelastic scattering experiment, we have also introduced the operator $\rho_{\mathbf{q}}$ (in the coordinate representation) defined as

$$\hat{\rho}_{\vec{q}}(t) \equiv \sum_j e^{-i\vec{q}\cdot\vec{r}_j(t)} = \hat{\rho}^{+}_{-\vec{q}}(t)$$

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