

# Chapter 3. Spatial structure of correlation functions.

## I. Introduction

### A. Motivation

$\varphi_{\text{stat}} \rightarrow N \sim 10^{23}$  particles

observables  $\begin{cases} A \rightarrow A(z) \\ B \rightarrow B(z) \end{cases}$   $\hat{n}(z)$ : particle density

$$\chi_{BA}(z, t; z', t') = \chi_{BA}(z - z', t - t'; 0, 0)$$

translation invariance spatial structure

interesting information!

### B. Important example: the compressibility

$$\text{in the exercise: } \hat{\chi}_{\text{pert}}(t) = \int d\mathbf{r} \hat{n}(\mathbf{r}) V^{\text{ext}}(\mathbf{r}, t) = \frac{1}{V} \sum_{\mathbf{q}} \hat{n}_{\mathbf{q}} V_{\mathbf{q}}^{\text{ext}}(t)$$

response: compressibility : response of  $\langle n_{\mathbf{q}}(t) \rangle$

$$x_{\mathbf{q}}(t) = -\frac{i}{\hbar \text{Vol}} \partial(t) \langle [n_{\mathbf{q}}(t), n_{-\mathbf{q}}] \rangle$$

$$\boxed{\tilde{x}(q, w)} = \frac{1}{V} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+q}}{tw + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q} + i0^+} \quad \text{structure factor Gas of free particles}$$

related correlation function:

$$\tilde{S}(q, w) \stackrel{\text{def}}{=} \frac{1}{\text{Vol}} \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \langle \hat{n}_{\mathbf{q}}(t) \hat{n}_{-\mathbf{q}} \rangle$$

FTD provides the relation:

$$\tilde{S}(q, w) = \frac{2t}{1 - e^{-\beta tw}} \quad \tilde{\xi}(q, w) = -\frac{2t}{1 - e^{-\beta tw}} \text{Im}[\tilde{x}(q, w)]$$

density fluctuations

Foring  $\langle [n_{\mathbf{q}}(t), n_{-\mathbf{q}}] \rangle$

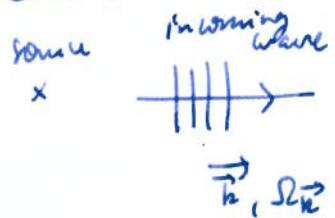
This is very useful! Although  $\tilde{S}(q, w)$  is not related to  $\langle [A, B] \rangle$ , it can thus be expressed very straightforwardly to one-body information:

$$\text{Gas of free particles: } \tilde{S}(q, w) = \frac{2\pi t}{1 - e^{-\beta tw}} \frac{1}{\text{Vol}} \sum_{\mathbf{k}} (f_{\mathbf{k}} - f_{\mathbf{k}+q}) \delta(tw + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q})$$

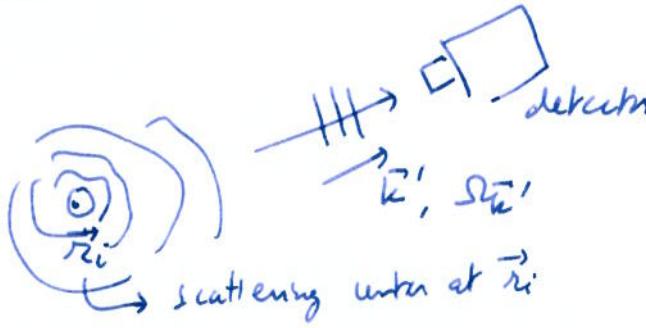
$$\begin{aligned} S(q, w) &\text{ obeys the detailed balance} \\ \tilde{S}(q, w) &= \tilde{S}(-q, -w) \\ \tilde{S}(-q, -w) &= S(q, w) \quad (\text{here } A \rightarrow n_{\mathbf{q}} \text{ and } A' \rightarrow n_{-\mathbf{q}}) \end{aligned}$$

### C. Brief review of several regimes for scattering

Consider static hinder:



photon, electron,  
neutron, ...



$$\text{elastic scattering: } \Omega_{\vec{k}} = \Omega_{\vec{k}'} \\ \| \vec{k} \| = \| \vec{k}' \|$$

#### Scattering amplitude (Born's)

$$| \text{initial} \rangle = | \vec{k} \rangle$$

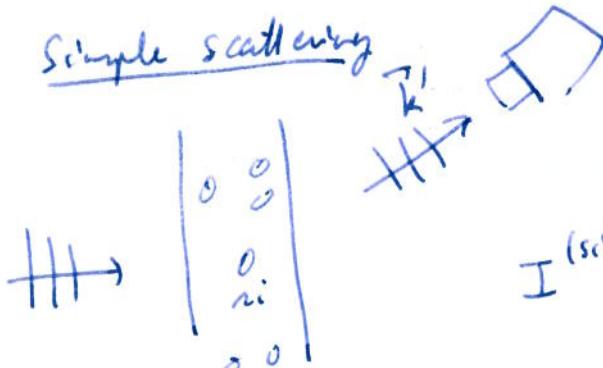
$$| \text{final} \rangle = | \vec{k}' \rangle$$

$$A_i(\vec{k} \rightarrow \vec{k}') \propto \langle \vec{k}' | \tilde{v}(\vec{R} - \vec{r}_i) | \vec{k} \rangle$$

scatt. potential      position of scattered particle  
scattering center

$$A_i(\vec{k} \rightarrow \vec{k}') \propto \tilde{v}(\vec{k}' - \vec{k}) e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}}$$

#### 1) Simple scattering

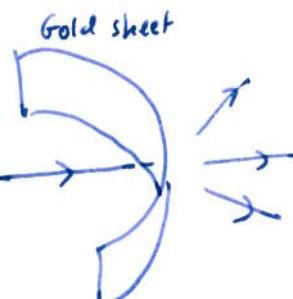


$$\boxed{\vec{q} = \vec{k}' - \vec{k}}$$

$$I^{(\text{simple})}(\vec{k}') \propto \text{sum of proba} \\ = \sum_i | A_i(\vec{k} \rightarrow \vec{k}') |^2 \\ \propto | \tilde{v}(\vec{q}) |^2$$

ex: Rutherford (1911)  
(Geiger & Marsden)

Radium  $\alpha$



$$| \tilde{v}_{\text{Coul}}(\vec{r}) |^2 \propto \frac{1}{r^4} \quad (\text{Coulomb scattering})$$

## 2) Bragg scattering

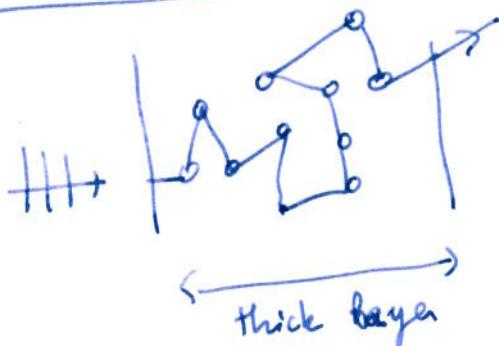
$$I^{(\text{Bragg})}(\vec{h}') \propto \left| \sum_i A_i (\vec{h} \rightarrow \vec{h}') \right|^2 \Rightarrow \boxed{\text{interference}}$$

$$I^{(\text{Bragg})}(\vec{h}') \propto \underbrace{|\tilde{v}(\vec{q})|^2}_{\text{form factor}} \times \underbrace{\left| \sum_{i,j} e^{-i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)} \right|^2}_{\text{structure factor}}$$

ex: X-ray spectroscopy  
→ crystals.

|| I will consider  
this regime

## 3) Multiple scattering - Incoherent

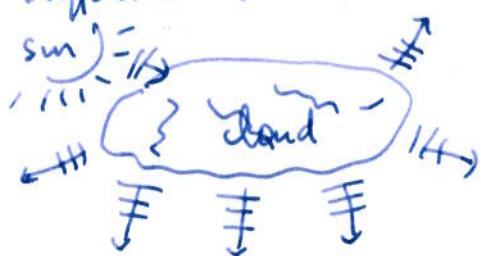


$$\epsilon = (\vec{r}_N, \vec{r}_{N-1}, \dots, \vec{r}_2, \vec{r}_1)$$

Amplitude depends on the sequence of scatt.-centers visited.

$$\stackrel{+}{I} \stackrel{(\text{mult.-scatt})}{=} \stackrel{+}{I} \stackrel{\text{incoherent}}{=} \sum_{\epsilon} |A_{\epsilon}|^2$$

ex: diffusion of light in a cloud.



## 4) Multiple scattering - coherent

$$I^{(\text{mult. coh.})} \propto \left| \sum_{\epsilon} A_{\epsilon} \right|^2 = \sum_{\epsilon} |A_{\epsilon}|^2 + \underbrace{\sum_{\epsilon \neq \epsilon'} A_{\epsilon} A_{\epsilon'}^*}_{\text{interf.}} \quad (\text{Anderson})$$

manifestation of localisation  
effects

ex: quantum correction to transport coeff. in a metal

## II. Static structure factor

scattering vector  $\rightarrow$  no dynamics.

$$S(q) \stackrel{\text{def}}{=} \frac{1}{\text{Vol}} \langle \hat{n}_q \hat{n}_{-q} \rangle = \frac{1}{\text{Vol}} \left\langle \sum_{i,j} e^{-iq(\vec{r}_i - \vec{r}_j)} \right\rangle$$

pair correlation fct.

$$n = \frac{N}{\text{Vol}}$$

$$g(r) \stackrel{\text{def}}{=} \frac{1}{n \cdot N} \left\langle \sum_{i,j} \delta(r - r_i + r_j) \right\rangle$$

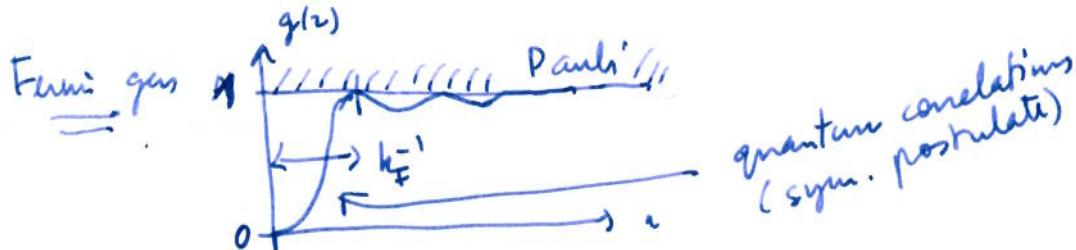
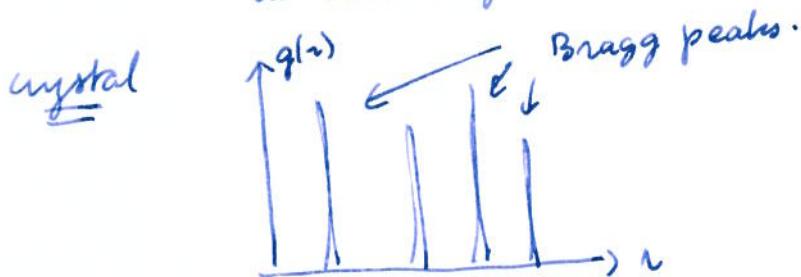
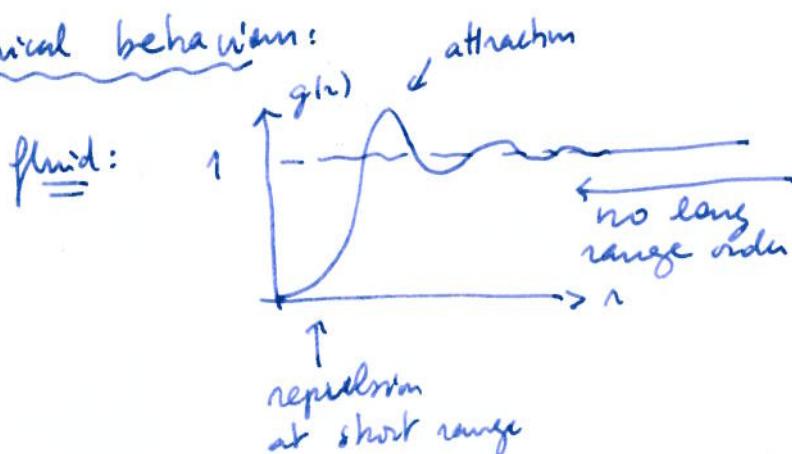
how distances are distributed.

$$\underline{\underline{z}}: \text{(trivial)} \prod_{i=1}^N P(r_i, \dots, r_N) = \prod_i \frac{dr_i}{\text{Vol}}$$

$$g(r) = \frac{1}{nN} \underbrace{\int \prod_i \frac{dr_i}{\text{Vol}} \sum_{i \neq j} \delta(r - r_i + r_j)}_{N(N-1)} = 1$$

$$\underbrace{\int \frac{dr_1 dr_2}{\text{Vol}^2} \delta(r - r_1 + r_2)}_{\frac{1}{\text{Vol}}}$$

typical behaviour:



Relation :

$$\tilde{g}(q) = \frac{1}{n \cdot N} \left\langle \sum_{i \neq j} e^{-iq(\gamma_i - \gamma_j)} \right\rangle$$

$$S(q) = \frac{1}{Vol} \left\langle \underbrace{\sum_{i,j} e^{-iq(\gamma_i - \gamma_j)}}_{N + \sum_{i \neq j} e^{-iq(\gamma_i - \gamma_j)}} \right\rangle = \frac{1}{Vol} [N + n \cdot n \tilde{g}(q)]$$
$$\boxed{S(q) = n + n^2 \tilde{g}(q)}$$

$$\downarrow F^{-1}$$
$$\left\langle u(\vec{r}) u(\vec{r}') \right\rangle = n \cdot \delta(\vec{r} - \vec{r}') + n^2 g(\vec{r} - \vec{r}')$$

Illustrations : cf. notes on the web

<http://www-lptms.u-psud.fr/~christophe-teixier/>

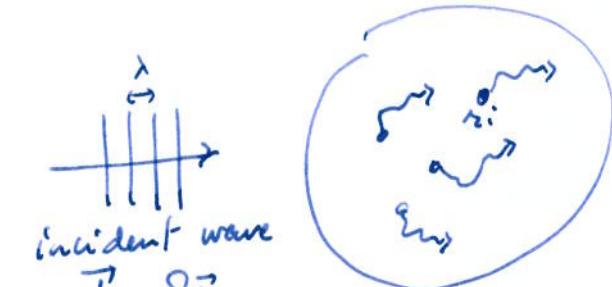
### III. Dynamical structure factor

#### A. Scattering experiment

I now consider the situation where the scattering centers have their own dynamics:

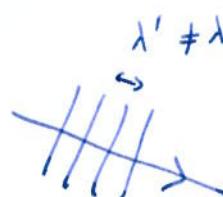
$$\text{matter} \left\{ \begin{array}{l} \text{position } \hat{r}_i \rightarrow \hat{r}_i(t) \\ \text{density } \hat{n}(r) \rightarrow \hat{n}(r, t) \end{array} \right.$$

$\Rightarrow$  implies that the wave can exchange energy with the matter

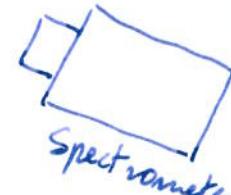


Incident wave  
 $k, \Delta k$

( $e^-$ , X-ray, neutrons...)



$k', \Delta k'$



Spectrometer  
detector ~~measures~~ selects  
the direction of  $k'$  but  
also  $\|k'\| \leftrightarrow \Delta k'$

Once again, the scattering experiment is assumed in the Bragg regime (single scattering + coherent)

Interaction:  $\hat{V} = \sum_i v(\hat{R} - \hat{r}_i)$  (drop  $\rightarrow$  in vectors)

incident particle (probe)      scattering centers: matter under study

more conveniently:  $\boxed{\hat{V} = \int d\mathbf{r} \underbrace{v(\hat{R}-\mathbf{r})}_{\text{wave}} \underbrace{\hat{n}(\mathbf{r})}_{\text{system}}}$

Transitions:  $|\Phi_i\rangle = \underbrace{|\mathbf{k}\rangle}_{\text{wave}} \otimes \underbrace{|\Psi_n\rangle}_{\text{system}}$ ,  $E_i = \omega_{\mathbf{k}} + E_n$

$\downarrow$   
 $|\Phi_f\rangle = |\mathbf{k}'\rangle \otimes |\Psi_m\rangle$ ,  $E_f = \omega_{\mathbf{k}'} + E_m$

## Matrix elements:

$$\begin{aligned}\langle \Psi_f | \hat{V} | \Psi_i \rangle &= \langle \vec{k}' | \otimes \Psi_m | \text{far } v(\vec{R}-\vec{r}) \hat{n}(r) | \vec{k} \rangle \otimes |\Psi_n\rangle \\ &= \text{far} \underbrace{\langle \vec{k}' | v(\vec{R}-\vec{r}) | \vec{k} \rangle}_{\int \frac{dR}{\text{Vol}} e^{-i(\vec{k}'-\vec{k}) \cdot \vec{R}}} \langle \Psi_m | \hat{n}(r) | \Psi_n \rangle \\ &\quad v(R-r) = \frac{1}{\text{Vol}} \tilde{v}(q) e^{-iq \cdot r} \\ &\quad \text{where } q = \vec{k}' - \vec{k}\end{aligned}$$

thus:  $\boxed{\langle \Psi_f | \hat{V} | \Psi_i \rangle = \frac{1}{\text{Vol}} \tilde{v}(q) \langle \Psi_m | \hat{n}_q | \Psi_n \rangle}$

Transfers: from the point of view of the wave, the scattering is inelastic

$$\left\{ \begin{array}{l} \vec{q} \stackrel{\text{def}}{=} \vec{k}' - \vec{k} \\ \omega \stackrel{\text{def}}{=} \Omega_{\vec{k}'} - \Omega_{\vec{k}} \end{array} \right.$$

Remark: at the microscopic level, the scattering may be a simple exchange of kinetic energy between the incoming particle and the particle of the matter

photon  $\rightarrow$  particle

but at a more macroscopic level, the incident particle is scattered by a medium with many degrees of freedom : this is why it may exchange energy with the matter, which is usually denoted as "inelastic scattering"

## Fermi Golden Rule

Differential scattering cross section  
initial state

$$E_f - E_i = \Delta \vec{k}' - \Delta \vec{k} + E_m - E_i$$

$$\frac{d\sigma}{d\Omega_{\vec{k}'}} \propto \sum_{\substack{\text{f such} \\ \text{that } \vec{k}' \text{ is} \\ \text{fixed}}} \left| \underbrace{\langle \Psi_f | \hat{V} | \Psi_i \rangle}_{\frac{1}{\text{Vol}} \tilde{v}(q) (\hat{n}_q)_{mn}} \right|^2 \delta(E_f - E_i)$$

$\Downarrow$

$\vec{k}$  and  $\vec{k}'$  are fixed  $\Rightarrow \vec{q}$  and  $\omega$  are fixed

i.e.  $\sum_{\substack{\text{f with } \vec{k}' \text{ fixed}}} \rightarrow \sum_m$  only

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detected intensity:

$$I_{inelastic}(\vec{k}') = \sum_n P_n \frac{d\sigma^{(q_n)}}{d\omega_{k'}} \propto \sum_{n,m} P_n |\tilde{v}(q) (\hat{n}_q)_{nm}|^2 \delta(\omega - \omega_{nm}) \\ = |\tilde{v}(q)|^2 \sum_{n,m} P_n |(\hat{n}_q)_{nm}|^2 \delta(\omega - \omega_{nm})$$

$$\Rightarrow I_{inelastic}(\vec{k}') \propto \underbrace{|\tilde{v}(q)|^2}_{\text{form factor}} \underbrace{\tilde{S}(-\vec{q}, -\omega)}_{\text{structure factor}} \quad (*)$$

where  $\tilde{S}(\vec{q}, \omega) = \frac{1}{\text{Vol}} \int dt e^{i\omega t} \langle \hat{n}_q(t) \hat{n}_{-\vec{q}} \rangle$

is the dynamical structure factor

Remark: arguments are negative  $\tilde{S}(-\vec{q}, -\omega)$  because  $\vec{q}$  and  $\omega$  measure the transfer from the point of view of the scattered wave.  $\omega = \omega_{in} - \omega_{out} \Rightarrow$  energy gained by the incoming particle.  $\Rightarrow$  lost by the matter etc.

remember that  $\tilde{S}(\vec{q}, \omega)$  for  $\omega > 0$   
is related to absorption process for the matter.

Relation with the static structure factor:

$$\tilde{S}(\vec{q}, \omega) = \int dt e^{i\omega t} \frac{1}{\text{Vol}} \langle \hat{n}_q(t) \hat{n}_{-\vec{q}} \rangle$$

↓

$$\int d\omega \tilde{S}(\vec{q}, \omega) \rightarrow \langle \hat{n}_q \hat{n}_{-\vec{q}} \rangle$$

$$\boxed{\int \frac{d\omega}{2\pi} \tilde{S}(\vec{q}, \omega) = S(\vec{q})}$$

remove the spectrometer on the detector and measure  
the total intensity.

## B. Relation to the microscopic dynamics:

### Example of the charged Fermi liquid

We discuss an important example: charged Fermi gas at  $T=0$  ( $\epsilon_F \gg T$ ) in a first step and the Fermi liquid in a second step.

Starting point is the  $T=0$  structure factor:  $\xrightarrow{\text{Fermi gas}} \text{free particles: } \epsilon_k$

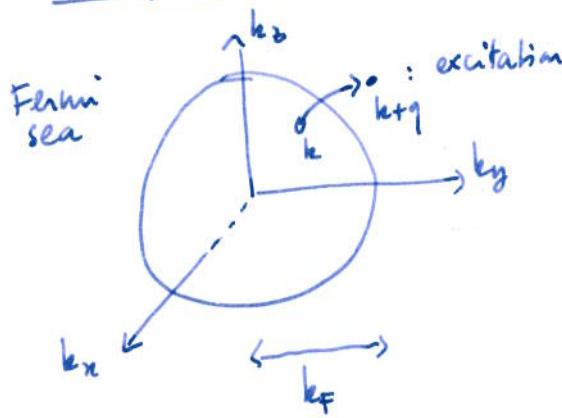
$$\tilde{S}(q, \omega) = \frac{2\pi\hbar}{1 - e^{-\beta\hbar\omega}} \frac{1}{\text{Vol}} \sum_{\mathbf{k}} (f_{\mathbf{k}} - f_{\mathbf{k}+q}) \delta(\hbar\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q})$$

$\downarrow T \rightarrow 0$   
 $\beta \rightarrow \infty$

$$\tilde{S}(q, \omega) = \frac{2\pi}{\text{Vol}} \sum_{\mathbf{k}} (f_{\mathbf{k}} - f_{\mathbf{k}+q}) \delta(\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q}) \quad \text{for } \omega > 0$$

$(\tilde{S}(q, \omega) = 0 \text{ for } \omega < 0)$

### 1. The particle-hole continuum



$\epsilon_{\mathbf{k}+q} - \epsilon_{\mathbf{k}}$  is the energy of an elementary excitation

$|k\rangle \rightarrow |k+q\rangle$

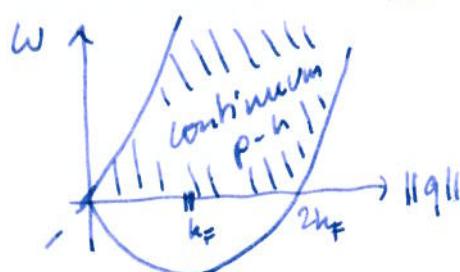
which creates a particle-hole excitation here.

Remark: for a given  $\omega_q = \epsilon_{\mathbf{k}+q} - \epsilon_{\mathbf{k}}$  and  $q$  several  $\mathbf{k}$  are possible.

$\approx$  free electron  $\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}$

$$\omega_q = \left( \frac{\hbar k}{2m} \right)^2 - \frac{\hbar^2}{2m} = \frac{\vec{q}^2}{2m} + \vec{v}_F \cdot \vec{q} \quad \text{where } \vec{v}_F = \frac{\hbar}{m}$$

fixed

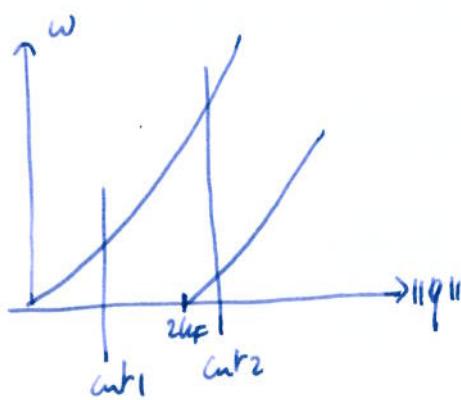


$$\frac{\vec{q}^2}{2m} \pm v_F \vec{q} \parallel$$

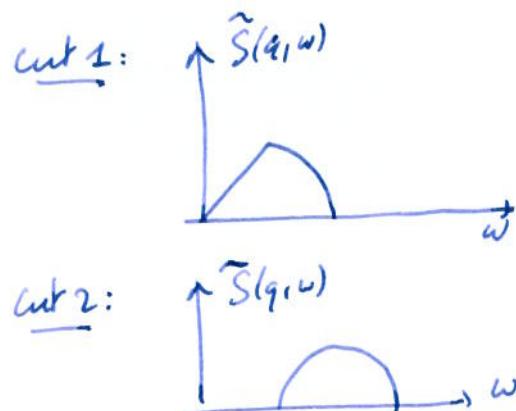
$$E[-v_F \vec{q} \parallel, v_F \vec{q} \parallel]$$

i.e. in the dashed region, there exist  $k$  such that  
 $\omega = E_{\text{ext}} + q - E_k \Rightarrow \tilde{S}(\vec{q}, \omega) \neq 0$  in this area

shape?



calculation shows (g. notes  
on the web)



this smooth structure  
in the dynamical structure factor  
is characteristic of the p-h continuum

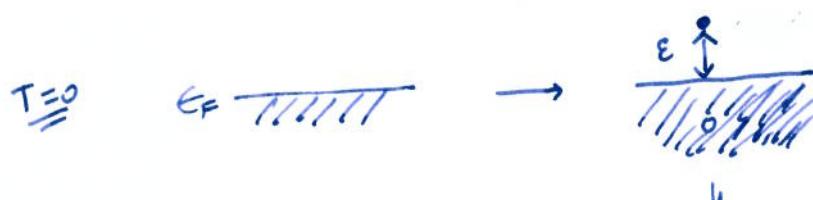
related to elementary excitations  
"localised" in momentum space

### Effect of interaction

gas  $\rightarrow$  liquid

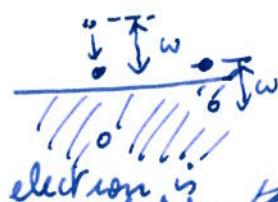
Fermi liquid theory  $\rightarrow$ 

- $\exists$  a Fermi surface
- low energy excitations to the elementary excitations are similar to the gas excitation of the gas ( $\pm qe$  and spin  $1/2$ )
- $\Rightarrow p/h$  (charge)



$$e^- \rightarrow e^- + (e^+ + \bar{e}) \rightarrow \dots$$

coupling to a continuum



concept of quasi-electron is meaningful for  $\Sigma \gg 0$

$$\frac{1}{T_{\text{ee}}} \propto \frac{\epsilon^2}{\epsilon_F} \ll \epsilon$$

## Multipair excitations

$$\tilde{S}(q, \omega) = \frac{1}{\text{Vol}} \sum_{n,m} P_n \underbrace{|(nq)_{nm}|^2}_{\langle \Psi_n | \hat{n}_q | \Psi_m \rangle} \delta(\omega + \omega_{nm})$$

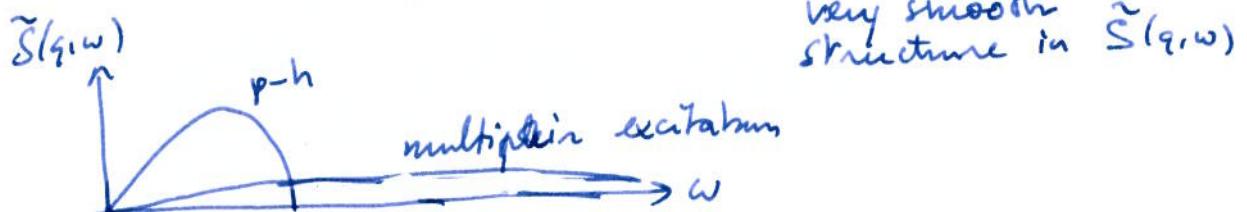
$$\hat{n}_q = \sum_k \hat{c}_k^\dagger \hat{c}_{k+q}$$

gas  $\Rightarrow$   $|\Psi_n\rangle, |\Psi_m\rangle \rightarrow$  excited states  
 (no int.)  $\hat{c}_k^\dagger \hat{c}_{k+q} |\Psi_n\rangle = |\Psi_n + \text{one p-h}\rangle$   
 fermion      gas

liquid:  $\hat{c}_k^\dagger \hat{c}_{k+q} |\Psi_n\rangle$   
 fermion      liquid  $\Rightarrow$  eigenstate  
 of the many body pb.

$$= (\dots) |\Psi_n + \text{one p-h}\rangle + (\dots) |\Psi_n + \text{two p-h}\rangle + \dots$$

then  $\omega = \underbrace{\omega_{q_1} + \omega_{q_2} + \dots + \omega_{q_n}}_{n \text{ p-h excitations}} \Rightarrow$  very soft constraint  
 $\Downarrow$

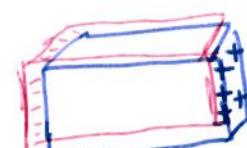


## Plasma modes

interaction  $\rightarrow$  collective modes



is a  $(+)\text{background}$   
 and electrons moving  
 $\rightarrow$  electrically neutral



Coulomb interaction acts as a spring force  
 + ~~opposite~~ - in order to  
 restore electron neutrality  
 $\Downarrow$

Screening

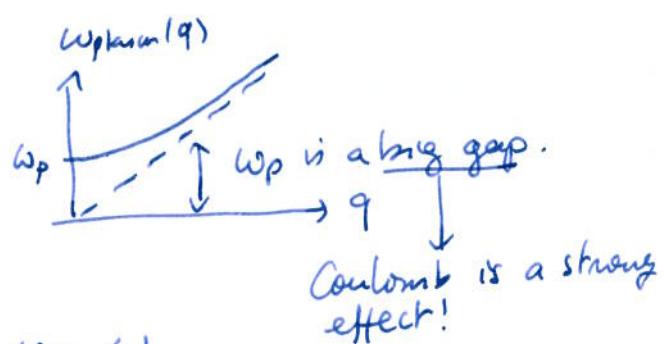
dimensional analysis:  $\frac{e^2}{\text{Coulomb}} \cdot \frac{m}{\text{mass}} \cdot \frac{n}{\text{(motion of electrons)}} \rightarrow \text{electron density}$

$$e^2 = \frac{q^2}{4\pi\epsilon_0}$$

$$\Rightarrow \boxed{\omega_p = \sqrt{4\pi \frac{ne^2}{m}}} \text{ is the } \underline{\text{plasma frequency}}$$

collective motion of the electrons: oscillations at frequency  $\omega_p$ .

rather a dispersion relation



Collective motion (oscillation) a  $\omega = \omega_{\text{plas.}}(q)$

$$\rightarrow \chi(q, \omega) \sim \frac{1}{\omega_p(q)^2 - (\omega + i\delta)^2}$$

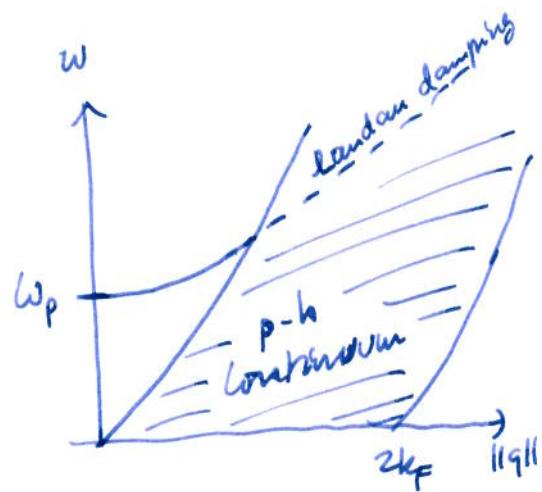
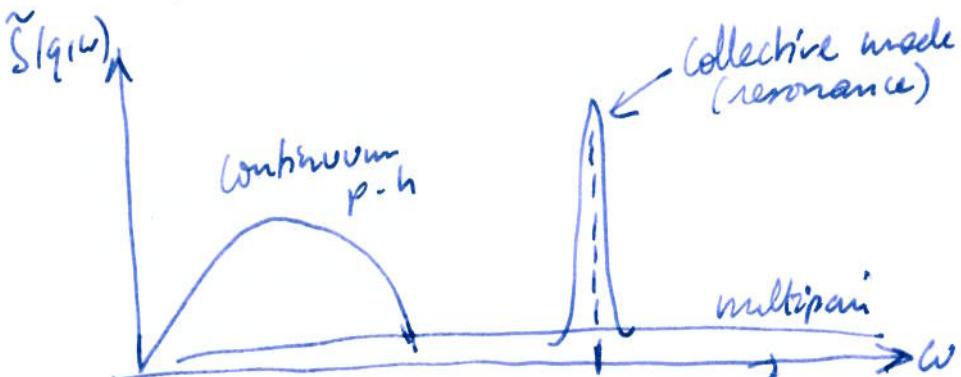
$\tilde{S}(q, \omega)$

structure for the harm. oscill.

$\omega_{\text{peak}}(q)$

lifetime of the plasmon mode

Conclusion: the several structures expected are



## Plasma oscillation.

$$1) \quad \phi = \phi^{\text{ext}} + \phi^{\text{ind}}$$

$$2) \quad \phi^{\text{ind}} = -\chi_0 \phi \quad (\text{response})$$

self consistent (not  $\phi^{\text{ext}}$ )

$$3) \quad \Delta\phi + 4\pi\rho = 0 \quad (\cos) \quad (\text{Poisson} \Rightarrow \text{Coulomb force})$$

Q:  $\chi_0 = ?$       P.F.D.       $-\vec{\omega} \times \vec{\mathbf{E}_w} = \frac{e}{m} \vec{\mathbf{v}_{\text{perp}}} \times \vec{\mathbf{E}_w}$   
 $e^-$  perp      electric field

$$\text{Polarisation} \quad P_w = n e \vec{\mathbf{v}_w} = -\frac{n e^2}{m \omega^2} \vec{\mathbf{E}_w}$$

$$\text{find} = -\nabla P \Rightarrow \underline{\underline{\text{find}}} = -iq \underline{\underline{P_w}} = +\frac{ine^2q}{m\omega^2} \underline{\underline{\mathbf{E}_w}} = +\frac{ne^2q^2}{m\omega^2} \underline{\underline{\phi_w}}$$

(condition 2:  $\underline{\underline{\chi_0}} = \frac{ne^2q^2}{m\omega^2}$ )

$$\underline{\underline{\mathbf{E}}} = -\nabla \underline{\underline{\phi}}$$

$$\underline{\underline{\mathbf{E}_w}} = -iq\underline{\underline{\phi_w}}$$

## Oscillation

$$\underbrace{\Delta\phi + 4\pi\rho}_{\text{Poisson}} \rightarrow -\underbrace{q^2 \phi_w}_{(\text{i.e. Coulomb Force})} + 4\pi \rho = 0$$

$$-\frac{m\omega^2}{ne^2} \underbrace{\text{find}}_{\rho - \rho_{\text{ext}}} \downarrow$$

$$-\frac{m\omega^2}{ne^2} (\rho - \rho_{\text{ext}}) + 4\pi \rho = 0$$

$$\left( \frac{d^2}{dt^2} + 4\pi \frac{ne^2}{m} \right) \rho = \frac{d^2 \rho_{\text{ext}}}{dt^2}$$

$$\boxed{\omega_p = \sqrt{\frac{4\pi ne^2}{m}}}$$

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