

# Screening and plasmons in homogeneous electron liquid

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- 0) equilibrium quantum statistics
- 1) Kubo linear response theory
- 2) jellium model with non-interacting electrons
- 3) jellium model with interacting electrons

## 0 Equilibrium quantum statistics

### 0.1 Quantum-mechanical and statistical averaging

- basic statements of the quantum theory:
  - ▶ the pure state of a quantum-mechanical system is defined by a state vector  $|\Psi\rangle$  in the Hilbert space
  - ▶ a real physical observable is represented by a Hermitian operator  $A$
  - ▶ the quantum-mechanical average of the quantity (operator)  $A$  in the state  $|\Psi\rangle$  is given by

$$\bar{A}\{\Psi\} = \langle\Psi|A|\Psi\rangle, \quad (1)$$

where we assume the state vector normalized to unity,  
 $\langle\Psi|\Psi\rangle = 1$

- if the system can be prepared in several states  $|\Psi_j\rangle$  with probabilities  $p_j$  ( $j = 1, 2, \dots; p_j \geq 0, \sum_j p_j = 1$ ), the quantum-mechanical and statistical average is given by

$$\begin{aligned}\langle A \rangle &= \bar{A} = \sum_j p_j \langle \Psi_j | A | \Psi_j \rangle = \sum_j p_j \text{Tr}\{A | \Psi_j \rangle \langle \Psi_j | \} \\ &= \text{Tr} \left\{ A \left[ \sum_j p_j | \Psi_j \rangle \langle \Psi_j | \right] \right\} = \text{Tr}(A\rho),\end{aligned}\quad (2)$$

where  $\text{Tr}$  denotes the trace and where we introduced the density matrix (statistical operator)  $\rho$  given by

$$\rho = \sum_j | \Psi_j \rangle p_j \langle \Psi_j |, \quad (3)$$

which is a positive-definite Hermitian operator

- (two technical notes)
- ▶ within the Dirac formalism, a ket-vector  $|\phi\rangle$  and a bra-vector  $\langle\chi|$  define a linear operator  $|\phi\rangle\langle\chi|$ ; its action is given by  $|\psi\rangle \mapsto |\phi\rangle\langle\chi|\psi\rangle$ ; its trace equals the scalar product of both vectors:

$$\text{Tr}(|\phi\rangle\langle\chi|) = \langle\chi|\phi\rangle$$

- ▶ for any operators  $X$  and  $Y$ :  $\text{Tr}(XY) = \text{Tr}(YX)$

- the density matrix satisfies relations

$$\text{Tr}(\rho) = 1, \quad \text{Tr}(\rho^2) \leq 1, \quad (4)$$

where the former one is a direct consequence of  $\langle\Psi_j|\Psi_j\rangle = 1$  and  $\sum_j p_j = 1$ ; the equality sign in the latter relation is encountered only for pure states

## 0.2 Quantum canonical distribution

- the canonical distribution (Boltzmann statistics) for a system with Hamiltonian  $H$  and at temperature  $T$  is defined as

$$\rho(T) = \frac{1}{Z(T)} \exp(-\beta H), \quad (5)$$

where  $\beta = (k_B T)^{-1}$  and the partition function  $Z(T)$  is given by

$$Z(T) = \text{Tr}\{\exp(-\beta H)\} \quad (6)$$

- if the eigenvalues and normalized eigenvectors of  $H$  are denoted by  $E_n$  and  $|n\rangle$  ( $n = 1, 2, \dots$ ), we get for  $Z(T)$

$$Z(T) = \sum_n \exp(-\beta E_n), \quad (7)$$

for the density matrix  $\rho$  and its matrix elements  $\rho_{mn}$

$$\rho(T) = \sum_n |n\rangle w_n(T) \langle n|, \quad w_n(T) = \frac{\exp(-\beta E_n)}{Z(T)},$$
$$\rho_{mn}(T) = \langle m|\rho(T)|n\rangle = w_n(T) \delta_{mn}, \quad (8)$$

and for the general quantum-mechanical and statistical average (with matrix elements  $A_{mn} = \langle m|A|n\rangle$ )

$$\langle A \rangle(T) = \bar{A}(T) = \text{Tr}\{A\rho(T)\} = \sum_n w_n(T) \langle n|A|n\rangle$$
$$= \sum_n w_n(T) A_{nn} = \frac{1}{Z(T)} \sum_n \exp(-\beta E_n) A_{nn}, \quad (9)$$

which has the form of Eq. (2) [  $\bar{A} = \sum_j p_j \langle \Psi_j | A | \Psi_j \rangle$  ]

- (a technical note)

if we know all eigenvalues  $E_n$  ( $n = 1, 2, \dots$ ) and normalized eigenvectors  $|n\rangle$  of the Hamiltonian  $H$ , we can write its spectral representation

$$H = \sum_n E_n |n\rangle\langle n| = \sum_n |n\rangle E_n \langle n|;$$

this representation allows us to extend an arbitrary function  $f(x)$  of a real variable  $x$  to the same function of the operator  $H$ :

$$f(H) = \sum_n f(E_n) |n\rangle\langle n| = \sum_n |n\rangle f(E_n) \langle n|;$$

this definition can be used, e.g., for  $f(H) = \exp(-\beta H)$

• from the partition function  $Z(T)$ , other quantities [internal energy  $U(T)$ , free energy  $F(T)$ , entropy  $S(T)$ , heat capacity  $C(T)$ ] can be obtained in the same way as in the classical case; this leads, e.g., to expressions

$$U(T) = -\frac{\partial}{\partial\beta} \ln[Z(T)], \quad F(T) = -\frac{1}{\beta} \ln[Z(T)], \quad (10)$$

$$\begin{aligned} S(T) &= -\frac{\partial F(T)}{\partial T} = -k_B \operatorname{Tr}\{\rho(T) \ln[\rho(T)]\} \\ &= -k_B \sum_n w_n(T) \ln[w_n(T)], \end{aligned} \quad (11)$$

$$C(T) = \frac{\partial U(T)}{\partial T} = T \frac{\partial S(T)}{\partial T} = -T \frac{\partial^2 F(T)}{\partial T^2} \quad (12)$$

- the relations involving derivatives with respect to an external parameter  $\xi$  of the Hamiltonian  $H(\xi)$  require more effort in the quantum case, since the operators  $H(\xi)$  and  $\partial H(\xi)/\partial \xi$  do not commute in general. It can be proved that

$$\left\langle \frac{\partial H(\xi)}{\partial \xi} \right\rangle (T) = \frac{\partial F(T; \xi)}{\partial \xi}, \quad (13)$$

while in the special case of a linear  $\xi$ -dependence

$$H(\xi) = H_0 + \xi B, \quad \xi \rightarrow 0, \quad (14)$$

we get

$$\langle B \rangle_0(T) = \frac{\partial F(T; \xi = 0)}{\partial \xi}; \quad (15)$$

these relations coincide with their classical counterparts.

## 0.3 Quantum ideal gases

- systems of non-interacting particles: ideal gases;  
in the quantum case:
  - identical particles are indistinguishable
- two different classes (according to symmetry of wave-function  $\Psi$  with respect to permutation of two particles):
  - ▶ bosons –  $\Psi$  symmetric,  
integer spin (photons, phonons, magnons, ...)
  - ▶ fermions –  $\Psi$  antisymmetric (Pauli exclusion principle),  
half-integer spin (electrons, protons, neutrons, ...)
- many-particle systems in contact with surroundings:
  - ▶ varying energy  $\longrightarrow$  temperature  $T$
  - ▶ varying no. of particles  $\longrightarrow$  chemical potential  $\mu$

- for an ideal gas, its Hamiltonian  $\tilde{H}$  on the many-particle Hilbert space is determined by a one-particle Hamiltonian  $H$ ,

$$H = \sum_{\lambda=1}^{\mathcal{M}} |\lambda\rangle E_{\lambda} \langle\lambda|, \quad (16)$$

where  $|\lambda\rangle$  and  $E_{\lambda}$  ( $\lambda = 1, 2, \dots, \mathcal{M}$ ) are normalized eigenvectors and eigenvalues of  $H$

- the eigenstates of  $\tilde{H}$  (and the orthonormal basis in the many-particle Hilbert space) are given by

$$\mathcal{S} \{ |\lambda_1\rangle \otimes |\lambda_2\rangle \otimes \dots \otimes |\lambda_N\rangle \} = | \{n_{\lambda}\}_{\lambda=1}^{\mathcal{M}} \rangle, \quad (17)$$

where:  $N$  ( $N = 0, 1, 2, \dots$ ) – total number of particles,  
 $\mathcal{S}$  – (anti)symmetrization including normalization,  
 $n_{\lambda}$  – occupation numbers

$$\begin{aligned} \text{for bosons:} & \quad n_\lambda \in \{0, 1, 2, \dots\} \\ \text{for fermions:} & \quad n_\lambda \in \{0, 1\} \end{aligned} \quad (18)$$

- the total number of particles in a particular eigenstate, Eq. (17), is equal to

$$N_{\{n_\lambda\}} = \sum_{\lambda=1}^{\mathcal{M}} n_\lambda \quad (19)$$

and the corresponding eigenvalue of  $\tilde{H}$  is

$$\tilde{E}_{\{n_\lambda\}} = \sum_{\lambda=1}^{\mathcal{M}} n_\lambda E_\lambda \quad (20)$$

- let us consider a general one-particle operator  $A$ ,

$$A = \sum_{\lambda, \nu=1}^{\mathcal{M}} |\lambda\rangle A_{\lambda\nu} \langle \nu|, \quad A_{\lambda\nu} = \langle \lambda|A|\nu\rangle; \quad (21)$$

this operator leads naturally to its counterpart  $\tilde{A}$  acting on the many-particle states as follows:

$$\begin{aligned} & \tilde{A} \{ |\lambda_1\rangle \otimes |\lambda_2\rangle \otimes \dots \otimes |\lambda_N\rangle \} \\ &= (A|\lambda_1\rangle) \otimes |\lambda_2\rangle \otimes \dots \otimes |\lambda_N\rangle \\ &+ |\lambda_1\rangle \otimes (A|\lambda_2\rangle) \otimes \dots \otimes |\lambda_N\rangle \\ &+ \dots \\ &+ |\lambda_1\rangle \otimes |\lambda_2\rangle \otimes \dots \otimes (A|\lambda_N\rangle); \end{aligned} \quad (22)$$

examples of  $A/\tilde{A}$ : kinetic energy, magnetic moment, spin, ...

- (a comment on second quantization)  
in terms of creation ( $a_\lambda^+$ ) and annihilation ( $a_\lambda$ ) operators,  
the extended operators  $\tilde{H}$  and  $\tilde{A}$  can be written as

$$\tilde{H} = \sum_{\lambda=1}^{\mathcal{M}} E_\lambda a_\lambda^+ a_\lambda, \quad \tilde{A} = \sum_{\lambda, \nu=1}^{\mathcal{M}} A_{\lambda\nu} a_\lambda^+ a_\nu$$

- the quantum-mechanical averages of  $\tilde{A}$  in the eigenstates of  $\tilde{H}$  are given by

$$\langle \{n_\lambda\}_{\lambda=1}^{\mathcal{M}} | \tilde{A} | \{n_\lambda\}_{\lambda=1}^{\mathcal{M}} \rangle = \sum_{\lambda=1}^{\mathcal{M}} n_\lambda A_{\lambda\lambda} = \sum_{\lambda=1}^{\mathcal{M}} n_\lambda \langle \lambda | A | \lambda \rangle, \quad (23)$$

which has an obvious physical meaning

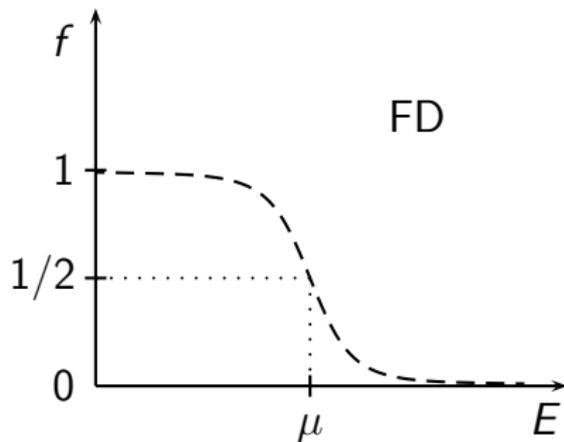
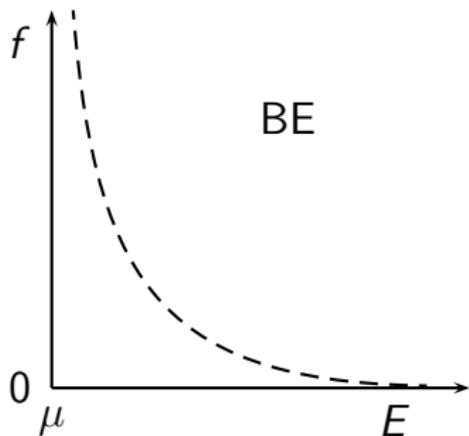
- in order to get the quantum-mechanical and statistical average of  $\tilde{A}$ , we need the statistical averages of the occupation numbers  $n_\lambda$  at a given temperature  $T$  and chemical potential  $\mu$
- the probability of a particular value  $n_\lambda \propto \exp[\beta(\mu - E_\lambda)n_\lambda]$ , which yields the average occupation number  $\langle n_\lambda \rangle$  as

$$\langle n_\lambda \rangle(T, \mu) = \frac{1}{\exp[\beta(E_\lambda - \mu)] \mp 1} \equiv f_\lambda(T, \mu). \quad (24)$$

This is the well-known Bose-Einstein or Fermi-Dirac distribution function (BE – upper sign, FD – lower sign).

- Bose-Einstein / Fermi-Dirac distribution functions

$$f(E; T, \mu) = \frac{1}{\exp[\beta(E - \mu)] \mp 1} \quad (25)$$



- the quantum-mechanical and statistical average of the observable  $\tilde{A}$  follows from Eq. (23) and Eq. (24):

$$\bar{A}(T, \mu) = \sum_{\lambda=1}^{\mathcal{M}} A_{\lambda\lambda} \langle n_{\lambda} \rangle(T, \mu) = \sum_{\lambda=1}^{\mathcal{M}} A_{\lambda\lambda} f_{\lambda}(T, \mu), \quad (26)$$

with an obvious physical meaning; this result can be recast as

$$\bar{A}(T, \mu) = \sum_{\lambda=1}^{\mathcal{M}} \langle \lambda | A | \lambda \rangle f_{\lambda}(T, \mu) = \text{Tr}\{A f(T, \mu)\}, \quad (27)$$

where the trace refers to the *one-particle Hilbert space* and where we introduced a one-particle density matrix

$$f(T, \mu) = \sum_{\lambda=1}^{\mathcal{M}} |\lambda\rangle f_{\lambda}(T, \mu) \langle \lambda| \quad (28)$$

# 1 Kubo linear response theory

## 1.0 Introduction

- ▶ the isothermic susceptibility refers to quasi-static perturbations (very slow changes of the Hamiltonian): the system remains in full thermodynamic equilibrium
- ▶ the Kubo theory describes an opposite limit: the perturbation and the response vary in time; full equilibrium only before the perturbation is switched on; the interaction system–surroundings is completely neglected during the process  $\implies$  'adiabatic' response
- ▶ despite this simplification, the Kubo theory proved very useful and successful for a wide class of problems
- ▶ here: basic properties of (non-)interacting electrons within a simple model and using a mean-field-like approximation

## 1.1 General formulation

- let us consider a time-independent Hamiltonian  $H_0$  of a quantum-mechanical system (in contact with surroundings) and let us add a small time-dependent perturbation

$$H_1(t) = B \exp(-i\omega t + \eta t) + B^+ \exp(i\omega t + \eta t), \quad (29)$$

where  $B$  is an operator and  $\eta \rightarrow 0^+$ , so that the total Hamiltonian

$$H(t) = H_0 + H_1(t) \quad (30)$$

coincides with  $H_0$  in very distant past ( $t \rightarrow -\infty$ )

- this setup corresponds to a slow (on a microscopic time scale) switching on the perturbation added to the original unperturbed time-independent Hamiltonian  $H_0$

- the equilibrium density matrix at temperature  $T$  [with  $\beta = 1/(k_B T)$ ] is

$$\rho_0 = \frac{1}{Z} \exp(-\beta H_0), \quad Z = \text{Tr}\{\exp(-\beta H_0)\}; \quad (31)$$

in the basis of eigenvectors  $|m\rangle$  of the Hamiltonian  $H_0$  with eigenvalues  $E_m$ , the matrix elements of  $\rho_0$  are given by

$$\langle m|\rho_0|n\rangle = \delta_{mn} w_m, \quad w_m = \frac{1}{Z} \exp(-\beta E_m), \quad (32)$$

the partition function is equal to  $Z = \sum_m \exp(-\beta E_m)$  and the operator  $\rho_0$  is explicitly given by

$$\rho_0 = \sum_m |m\rangle w_m \langle m| \quad (33)$$

- let us investigate the time evolution ( $\hbar = 1$ ) due to the total Hamiltonian  $H(t)$  of states  $|\Psi_m(t)\rangle$  and of the density matrix

$$\rho(t) = \sum_m |\Psi_m(t)\rangle w_m \langle \Psi_m(t)|, \quad (34)$$

which satisfy following initial conditions for  $t \rightarrow -\infty$ :

$$\exp(iE_m t) |\Psi_m(t)\rangle \rightarrow |m\rangle, \quad \rho(-\infty) = \rho_0 \quad (35)$$

- physically, this procedure corresponds to a complete neglect of the interaction between the studied system and its surroundings during the switching on the perturbation  $H_1(t)$  (this interaction is responsible for bringing the system into thermodynamic equilibrium at temperature  $T$  for  $t = -\infty$ )

$\implies$  'adiabatic' (mechanical) response

- the Schrödinger equation ( $\hbar = 1$ ) for the states  $|\Psi_m(t)\rangle$ ,

$$i \frac{\partial}{\partial t} |\Psi_m(t)\rangle = H(t) |\Psi_m(t)\rangle,$$

leads to the Liouville (von Neumann) equation for the density matrix  $\rho(t)$ ,

$$i \frac{\partial}{\partial t} \rho(t) = [H(t), \rho(t)], \quad (36)$$

where  $[A, B] = AB - BA$  denotes the commutator

- let us write the total density matrix in a form

$$\rho(t) = \rho_0 + \rho_1(t), \quad \rho_1(-\infty) = 0, \quad (37)$$

where  $\rho_1(t)$  is considered as an infinitesimally small correction to  $\rho_0$  due to the perturbation  $H_1(t)$

- this yields (with keeping only linear terms)

$$i \frac{\partial}{\partial t} \rho_1(t) = [H_0 + H_1(t), \rho_0 + \rho_1(t)] \approx [H_0, \rho_1(t)] + [H_1(t), \rho_0]$$

and finally a differential equation for the  $\rho_1(t)$ ,

$$\begin{aligned} i \frac{\partial}{\partial t} \rho_1(t) + [\rho_1(t), H_0] &= [H_1(t), \rho_0] \\ &= [B, \rho_0] \exp(-i\omega t + \eta t) + [B^+, \rho_0] \exp(i\omega t + \eta t). \end{aligned} \quad (38)$$

The latter can be solved by using an Ansatz

$$\rho_1(t) = \sigma \exp(-i\omega t + \eta t) + \sigma^+ \exp(i\omega t + \eta t), \quad (39)$$

where  $\sigma$  is a time-independent operator (matrix).  
Substitution of this Ansatz into Eq. (38) leads to

$$i(-i\omega + \eta)\sigma + [\sigma, H_0] = [B, \rho_0] \quad (40)$$

and to an equivalent (Hermitian conjugate) relation.

- the solution of Eq. (40),

$$(\omega + i\eta)\sigma + [\sigma, H_0] = [B, \rho_0],$$

can be done in the basis of the eigenstates of  $H_0$   
(with  $\langle n|\sigma|m\rangle = \sigma_{nm}$ ,  $\langle n|B|m\rangle = B_{nm}$ ). One obtains:

$$(\omega + i\eta)\sigma_{nm} + \sigma_{nm}(E_m - E_n) = B_{nm}(w_m - w_n),$$

which provides the final result in a form

$$\sigma_{nm} = B_{nm} \frac{w_m - w_n}{\omega + i\eta + E_m - E_n}. \quad (41)$$

## 1.2 Generalized susceptibility and Kramers-Krönig relations

- a physical quantity of the system, given by the statistical average of a Hermitian operator  $A$ , depends on time as

$$\begin{aligned}\bar{A}(t) &= \text{Tr}\{A\rho(t)\} = \bar{A}_0 + \bar{A}_1(t), \\ \bar{A}_0 &= \text{Tr}\{A\rho_0\}, \quad \bar{A}_1(t) = \text{Tr}\{A\rho_1(t)\},\end{aligned}$$

where the (infinitesimally small) time-dependent term is

$$\begin{aligned}\bar{A}_1(t) &= \text{Tr}\{A\sigma\} \exp(-i\omega t + \eta t) + \text{c.c.} \\ &= \sum_{mn} A_{mn} \sigma_{nm} \exp(-i\omega t + \eta t) + \text{c.c.} \\ &\equiv \chi_{AB}(\omega) \exp(-i\omega t + \eta t) + \text{c.c.},\end{aligned}\tag{42}$$

where c.c. denotes a complex conjugate term

- the quantity  $\chi_{AB}(\omega)$  is the generalized (Kubo) susceptibility that is explicitly given by

$$\chi_{AB}(\omega) = \sum_{nm} A_{mn} B_{nm} \frac{W_m - W_n}{\omega + i\eta + E_m - E_n}. \quad (43)$$

The limit  $\eta \rightarrow 0^+$  is implicitly assumed in Eq. (43).

- the susceptibility  $\chi_{AB}(\omega)$  is a complex number; its magnitude describes the strength of the response while its phase refers to the phase shift between the periodic perturbation  $H_1(t)$  and the induced response  $\bar{A}_1(t)$
- the susceptibility  $\chi_{AB}(\omega)$  consists of terms that exhibit singular behavior for frequencies  $\omega = E_n - E_m$ , i.e., for frequencies corresponding to excitation energies of the system

• an example: a system at  $T = 0$  with a non-degenerate ground state  $(|0\rangle, E_0)$

$\implies w_0 = 1$  (ground state),

$w_n = 0$  for  $n = 1, 2, \dots$  (excited states),

which yields:

$$\chi_{AB}(\omega) = \sum_{n=1}^{+\infty} \left( \frac{A_{0n}B_{n0}}{\omega + i\eta + E_0 - E_n} - \frac{A_{n0}B_{0n}}{\omega + i\eta + E_n - E_0} \right)$$

$\implies$  poles at the excitation energies  $\omega = E_n - E_0$  ( $n \geq 1$ ):

¶ a pole in the susceptibility  $\longleftrightarrow$  an excited state

¶ weights of the singular terms: selection rules for  $A_{0n}, B_{0n}$

- the limit  $\eta \rightarrow 0^+$  in  $\chi_{AB}(\omega)$  can be performed using the relation

$$\lim_{\eta \rightarrow 0^+} \frac{1}{x \pm i\eta} = \wp \frac{1}{x} \mp i\pi\delta(x), \quad (44)$$

where  $x$  is a real variable,  $\wp$  denotes the principal value, and  $\delta(x)$  is the Dirac  $\delta$ -function; this relation means

$$\begin{aligned} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{\varphi(x)}{x + i\eta} dx &= \lim_{\eta \rightarrow 0^+} \left( \int_{-\infty}^{-\eta} + \int_{\eta}^{+\infty} \right) \frac{\varphi(x)}{x} dx \\ &\quad - i\pi\varphi(0) \end{aligned}$$

for smooth functions  $\varphi(x)$  rapidly decaying for  $x \rightarrow \pm\infty$  ;

$$\implies \wp \int_b^a x^{-1} dx = \ln |a/b| \quad \text{for } b < 0 < a$$

- decomposition of the susceptibility in two terms:

$$\begin{aligned}
 \chi_{AB}(\omega) &= \lim_{\eta \rightarrow 0^+} \sum_{nm} A_{mn} B_{nm} \frac{\omega_m - \omega_n}{\omega + i\eta + E_m - E_n} \\
 &\equiv \chi_{AB}^{(1)}(\omega) + i\chi_{AB}^{(2)}(\omega), \\
 \chi_{AB}^{(1)}(\omega) &= \sum_{nm} A_{mn} B_{nm} (\omega_m - \omega_n) \wp \frac{1}{\omega + E_m - E_n}, \\
 \chi_{AB}^{(2)}(\omega) &= -\pi \sum_{nm} A_{mn} B_{nm} (\omega_m - \omega_n) \delta(\omega + E_m - E_n),
 \end{aligned} \tag{45}$$

where  $\chi_{AB}^{(1)}(\omega)$  – dispersive part,

$\chi_{AB}^{(2)}(\omega)$  – absorptive part

- notes on the absorptive part:

- ▶ for  $B = A = A^+$ , we get:

$$\chi_{AA}^{(2)}(\omega) \sim \sum_{nm} |A_{mn}|^2 (w_m - w_n) \delta(\omega + E_m - E_n)$$

- ▶  $\chi_{AA}^{(2)}(\omega)$  coincides with the imaginary part of  $\chi_{AA}(\omega)$
- ▶ close relation to the Fermi golden rule: probability (per unit time) of transitions between two eigenstates  $|m\rangle$  and  $|n\rangle$  of  $H_0$  is  $\sim |A_{mn}|^2 \delta(\omega + E_m - E_n)$
- ▶ the rate of energy dissipation/absorption by the system due to the time-dependent perturbation is  $\sim \omega \chi_{AA}^{(2)}(\omega)$
- ▶ analogy with classical electric circuits:  
the Joule's heat is due to resistivity  $R$  – the real part of the impedance  $\mathcal{Z}(\omega) = R + i[L\omega - (C\omega)^{-1}]$

- each of both parts of the susceptibility can be expressed by means of the other part using the Kramers-Krönig relations:

$$\begin{aligned}\chi_{AB}^{(1)}(\omega) &= -\frac{1}{\pi} \wp \int_{-\infty}^{\infty} \frac{1}{\omega - \zeta} \chi_{AB}^{(2)}(\zeta) d\zeta, \\ \chi_{AB}^{(2)}(\omega) &= \frac{1}{\pi} \wp \int_{-\infty}^{\infty} \frac{1}{\omega - \zeta} \chi_{AB}^{(1)}(\zeta) d\zeta, \quad (46)\end{aligned}$$

provided that the integrals on the r.h.s. converge

- these relations reflect the causality between a general time-dependent perturbation and the resulting response:

$$\bar{A}(t) = \int_{-\infty}^t \mathcal{F}[t, t', A, H_0, H_1(t')] dt'$$

(integration only over  $t' \leq t$ )

- (proof of the Kramers-Krönig relations)

The first of Eq. (46) can be proved using Eq. (45) and the well-known property of the  $\delta$ -function, namely

$$\int_{-\infty}^{\infty} g(x) \delta(x - x_1) dx = g(x_1) ,$$

while the second of Eq. (46) can be obtained from an identity

$$\int_{-\infty}^{\infty} \wp \frac{1}{x - x_1} \wp \frac{1}{x - x_2} dx = \pi^2 \delta(x_1 - x_2) .$$

The latter follows from Eq. (44) and from integrals:

$$\int_{-\infty}^{\infty} \frac{1}{x - x_1 - i\eta_1} \frac{1}{x - x_2 + i\eta_2} dx = \frac{2\pi i}{x_1 - x_2 + i(\eta_1 + \eta_2)} ,$$

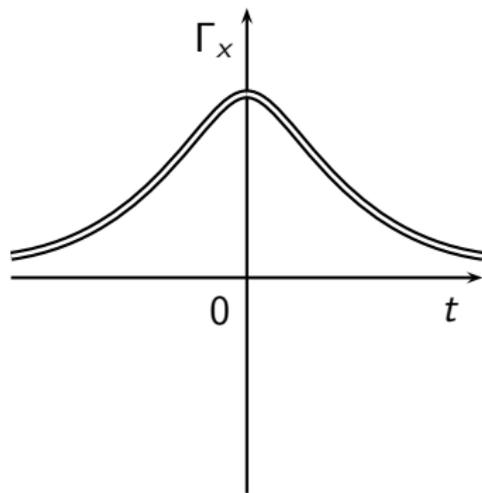
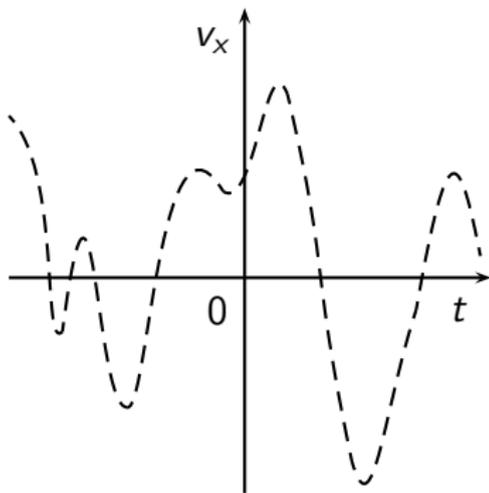
$$\int_{-\infty}^{\infty} \frac{1}{x - x_1 + i\eta_1} \frac{1}{x - x_2 + i\eta_2} dx = 0 ,$$

where  $x_1, x_2$  are real and  $\eta_1, \eta_2$  are positive.

## 1.3 Fluctuation-dissipation theorem

- a relation between the Kubo susceptibility and the correlation of time-dependent fluctuations in the unperturbed system
- in classical statistics – autocorrelation of particle velocity  $v_x$ :

$$\langle v_x \rangle = 0 \quad \text{vs.} \quad \Gamma_x(t) \equiv \langle v_x(t)v_x(0) \rangle \neq 0$$



- for a quantum system with an unperturbed Hamiltonian  $H_0$  and for a Hermitian operator  $A$ , we introduce (Heisenberg picture)

$$A(t) = \exp(iH_0 t) A \exp(-iH_0 t)$$

and define the corresponding autocorrelation function as

$$\Gamma_A(t) = \frac{1}{2} \langle A(t)A + AA(t) \rangle = \frac{1}{2} \text{Tr}\{\rho_0[A(t)A + AA(t)]\}, \quad (47)$$

where  $\rho_0 = Z^{-1} \exp(-\beta H_0)$ ,  $Z = \text{Tr}\{\exp(-\beta H_0)\}$

- for the Fourier transformation of  $\Gamma_A(t)$ , defined by

$$\tilde{\Gamma}_A(\omega) = \int_{-\infty}^{+\infty} \exp(i\omega t) \Gamma_A(t) dt ,$$

one can prove the fluctuation-dissipation theorem:

$$\tilde{\Gamma}_A(\omega) = -\coth\left(\frac{\beta\omega}{2}\right) \chi_{AA}^{(2)}(\omega) \quad (48)$$

- proof of Eq. (48): In the basis of eigenvectors of  $H_0$ , we get

$$\tilde{\Gamma}_A(\omega) = \pi \sum_{nm} |A_{mn}|^2 (w_m + w_n) \delta(\omega + E_m - E_n) ,$$

where we employed the identity  $\int_{-\infty}^{+\infty} \exp(i\Omega t) dt = 2\pi\delta(\Omega)$ .

According to Eq. (45) we have

$$\chi_{AA}^{(2)}(\omega) = -\pi \sum_{nm} |A_{mn}|^2 (w_m - w_n) \delta(\omega + E_m - E_n) .$$

With the use of the identity

$$w_m \delta(\omega + E_m - E_n) = \exp(\beta\omega) w_n \delta(\omega + E_m - E_n) ,$$

we get relations

$$\tilde{\Gamma}_A(\omega) = \pi [1 + \exp(\beta\omega)] \sum_{nm} |A_{mn}|^2 w_n \delta(\omega + E_m - E_n) ,$$

$$\chi_{AA}^{(2)}(\omega) = \pi [1 - \exp(\beta\omega)] \sum_{nm} |A_{mn}|^2 w_n \delta(\omega + E_m - E_n) ,$$

from which the validity of Eq. (48) can easily be seen.

- relation to classical electric circuits:

the macroscopic measurement of the impedance

$\mathcal{Z}(\omega) = R + i[L\omega - (C\omega)^{-1}]$  at temperature  $T$  provides an information about the microscopic equilibrium thermal noise, the so-called Johnson-Nyquist noise due to the current and voltage fluctuations (present in circuits without an external source)

## 1.4 Non-interacting many-particle systems

- the linear response theory for non-interacting many-particle systems with  $A$  and  $B$  being one-particle operators can be formulated entirely in terms of the one-particle Hamiltonian  $H(t) = H_0 + H_1(t)$

- eigenvectors and eigenvalues of  $H_0$ :  $|\lambda\rangle, |\nu\rangle$  and  $E_\lambda, E_\nu$ ; the equilibrium one-particle density matrix  $f$  is given in terms of average occupation numbers  $f_\lambda$  as

$$f = \sum_{\lambda} |\lambda\rangle f_{\lambda} \langle\lambda|, \quad f_{\lambda} = \frac{1}{\exp[\beta(E_{\lambda} - \mu)] \pm 1},$$

where  $\mu$  is the chemical potential of the particles and (+/-) refers to fermions/bosons

- the resulting generalized non-interacting Kubo susceptibility is given by

$$\chi_{AB}(\omega) = \sum_{\lambda\nu} A_{\lambda\nu} B_{\nu\lambda} \frac{f_{\lambda} - f_{\nu}}{\omega + i\eta + E_{\lambda} - E_{\nu}} \quad (49)$$

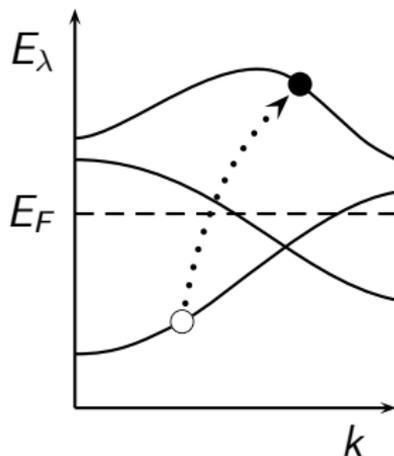
- ▶ the same formal structure as the general result, Eq. (43)
  - ▶  $|\lambda\rangle, |\nu\rangle$  and  $f_{\lambda}, f_{\nu}$  instead of  $|m\rangle, |n\rangle$  and  $w_m, w_n$
  - ▶ Eq. (49) employs the one-particle Hilbert space
- the susceptibility  $\chi_{AB}(\omega)$  consists of terms that exhibit singular behavior for frequencies  $\omega = E_{\nu} - E_{\lambda}$ , i.e., for frequencies given by excitation energies of the one-particle Hamiltonian. These frequencies correspond to the so-called pair excitations of the non-interacting many-particle system.

- for a many-fermion system at  $T = 0$ :

$$f_{\lambda} = 1 \text{ for } E_{\lambda} < E_F, \quad f_{\lambda} = 0 \text{ for } E_{\lambda} > E_F,$$

where  $E_F$  – the Fermi energy ( $E_F = \mu$  for  $T = 0$ )

$\implies$  the  $\chi_{AB}(\omega)$  consists of terms connecting an occupied state with an unoccupied state (particle-hole excitations)



- ▶ this scheme explains various electronic properties of solids (optical conductivities, el. and magn. susceptibilities, ...)

## 2 Response of homogeneous electron gas

### 2.1 Jellium model

- atomic nuclei of a solid are replaced by a positively charged classical homogeneous background on which electrons move
- we consider non-interacting electrons in a constant potential. The unperturbed one-particle Hamiltonian is ( $\hbar = 1$ ):

$$H_0 = -\frac{\Delta}{2m}, \quad (50)$$

where  $m$  is the electron mass;

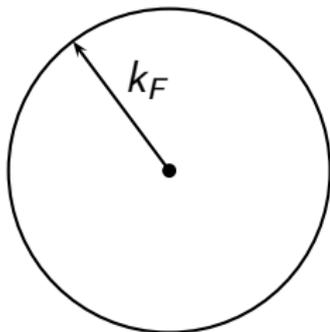
its eigenvectors are labelled by the reciprocal-space vector  $\mathbf{k}$ :

$$|\lambda\rangle \dots |\mathbf{k}\rangle, \quad \langle \mathbf{r}|\lambda\rangle \dots \frac{\exp(i\mathbf{k} \cdot \mathbf{r})}{\sqrt{(2\pi)^3}}, \quad E_\lambda \dots E_{\mathbf{k}} = \frac{k^2}{2m}$$

(electron spin ignored – sometimes a factor of 2 added).

- the jellium model is specified by a single parameter – the homogeneous density  $\rho$  (no. of electrons per unit volume); for  $T = 0$ , the occupied states are for  $|\mathbf{k}| \equiv k \leq k_F$ , where  $k_F$  – the Fermi-sphere radius, related to  $E_F$  and  $\rho$ :

$$E_F = \frac{k_F^2}{2m}, \quad k_F = \sqrt[3]{3\pi^2\rho} \quad (51)$$



- values of  $k_F$  for simple metals (Li, K, Mg, Ca, Al, ...):

$$0.4 \leq k_F a_0 \leq 1$$

$[a_0 = 1/(me'^2)$  – Bohr radius ( $\hbar = 1$ )  
and  $e'^2 \equiv e^2/(4\pi\epsilon_0)]$

## 2.2 Non-interacting susceptibility of jellium

- as the perturbation, we consider an infinitesimal time- and space-dependent local potential  $\delta V(\mathbf{r}', t')$  which leads to infinitesimal changes of the electron density  $\delta \rho(\mathbf{r}, t)$
- the most general form of the linear response is given by

$$\delta \rho(\mathbf{r}, t) = \int \int_{-\infty}^t \chi_0(\mathbf{r}, \mathbf{r}', t, t') \delta V(\mathbf{r}', t') d^3\mathbf{r}' dt' \quad (52)$$

- the unperturbed state of jellium is homogeneous in space and time  $\implies \chi_0(\mathbf{r}, \mathbf{r}', t, t') = \chi_0(\mathbf{r} - \mathbf{r}', t - t')$  and Eq. (52) can be simplified by the Fourier transformation ( $\mathbf{r} \rightarrow \mathbf{q}$ ,  $t \rightarrow \omega$ ):

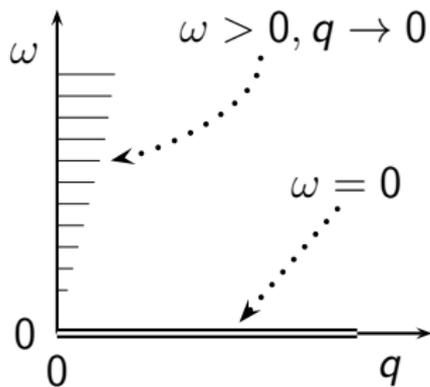
$$\delta \tilde{\rho}(\mathbf{q}, \omega) = \tilde{\chi}_0(\mathbf{q}, \omega) \delta \tilde{V}(\mathbf{q}, \omega), \quad (53)$$

where  $\delta\tilde{\varrho}(\mathbf{q}, \omega) = \iint \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t) \delta\varrho(\mathbf{r}, t) d^3\mathbf{r} dt$   
 and similarly for  $\delta\tilde{V}(\mathbf{q}, \omega)$  and  $\tilde{\chi}_0(\mathbf{q}, \omega)$ , and where

$$\tilde{\chi}_0(\mathbf{q}, \omega) = \frac{2}{(2\pi)^3} \int \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\omega + i\eta + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} d^3\mathbf{k} \quad (54)$$

denotes the non-interacting (bare, unrenormalized) susceptibility of the homogeneous electron gas

- a closed analytic formula for  $\tilde{\chi}_0(\mathbf{q}, \omega) = \tilde{\chi}_0(q, \omega)$  exists ( here  $q \equiv |\mathbf{q}|$  )  
 (Lindhard function –  
 – not too transparent)



- proof of Eq. (54):

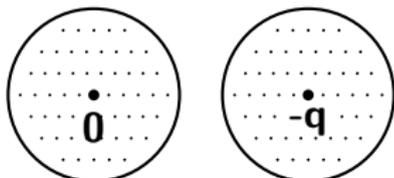
We identify  $|\lambda\rangle, |\nu\rangle$  with  $|\mathbf{k}\rangle, |\mathbf{k}'\rangle$ . The  $\omega$ -component of the local perturbing potential  $\delta V(\mathbf{r}, t)$  leads to the matrix elements  $B_{\nu\lambda} \equiv (2\pi)^{-3} \delta\tilde{V}(\mathbf{k}' - \mathbf{k}, \omega)$ . The Fourier transformed electron density corresponds to the local operator  $\exp(-i\mathbf{q} \cdot \mathbf{r})\delta(\mathbf{r} - \mathbf{r}')$  and its matrix elements are  $A_{\lambda\nu} \equiv 2\delta(\mathbf{k}' - \mathbf{k} - \mathbf{q})$ , where the factor of 2 accounts for the electron spin and where we used the identity  $\int \exp(i\mathbf{Q} \cdot \mathbf{r})d^3\mathbf{r} = (2\pi)^3\delta(\mathbf{Q})$ . The quantity  $\delta\tilde{\rho}(\mathbf{q}, \omega)$  can be identified with  $\chi_{AB}(\omega)$ , Eq. (49), and it is explicitly given by

$$\begin{aligned} \delta\tilde{\rho}(\mathbf{q}, \omega) &= 2(2\pi)^{-3} \iint \delta(\mathbf{k}' - \mathbf{k} - \mathbf{q}) \delta\tilde{V}(\mathbf{k}' - \mathbf{k}, \omega) \\ &\quad \times \frac{f_{\mathbf{k}} - f_{\mathbf{k}'}}{\omega + i\eta + E_{\mathbf{k}} - E_{\mathbf{k}'}} d^3\mathbf{k} d^3\mathbf{k}' \\ &= 2(2\pi)^{-3} \delta\tilde{V}(\mathbf{q}, \omega) \int \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{\omega + i\eta + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} d^3\mathbf{k}, \end{aligned}$$

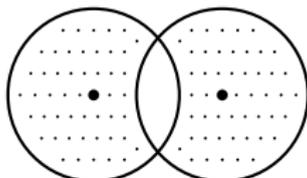
which coincides with Eq. (53) and Eq. (54).

- (a technical note on the  $\mathbf{k}$ -integration)
- ¶ original integration region for  $\tilde{\chi}_0(\mathbf{q}, \omega)$  – two Fermi spheres

for  $q > 2k_F$



for  $q < 2k_F$



¶ with substitution  $\mathbf{k} \rightarrow -\mathbf{k} - \mathbf{q}$  ( $f_{\mathbf{k}} \leftrightarrow f_{\mathbf{k}+\mathbf{q}}$ ,  $E_{\mathbf{k}} \leftrightarrow E_{\mathbf{k}+\mathbf{q}}$ )  
we obtain

$$\tilde{\chi}_0(\mathbf{q}, \omega) = \frac{2}{(2\pi)^3} \int \left( \frac{1}{\omega + i\eta + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} + \frac{1}{-\omega - i\eta + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} \right) f_{\mathbf{k}} d^3\mathbf{k} \quad (55)$$

(integration over a single Fermi sphere)

## 2.3 Properties of non-interacting susceptibility

- in the static limit ( $\omega = 0$ ), Eq. (55) and Eq. (44) yield

$$\tilde{\chi}_0(\mathbf{q}, 0) = \frac{4}{(2\pi)^3} \wp \int \frac{f_{\mathbf{k}}}{E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} d^3\mathbf{k},$$

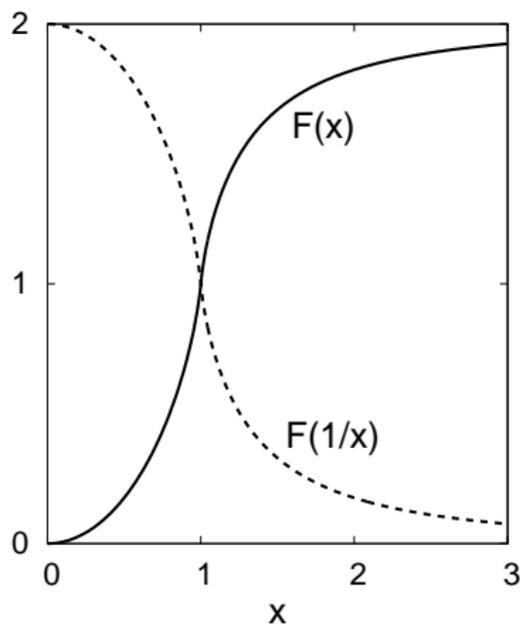
which shows that the static susceptibility is real. We get:

$$\begin{aligned}\tilde{\chi}_0(\mathbf{q}, 0) &= \frac{8\pi}{(2\pi)^3} \wp \int_0^{k_F} k^2 dk \int_0^\pi \sin\theta d\theta \frac{-2m}{2kq \cos\theta + q^2} \\ &= -\frac{2m}{\pi^2} \wp \int_0^{k_F} k^2 dk \int_{-1}^1 du \frac{1}{2kqu + q^2} \\ &= -\frac{m}{\pi^2 q} \int_0^{k_F} k dk \ln \left| \frac{2k + q}{-2k + q} \right| \\ &= -\frac{mq}{4\pi^2} \int_0^{2k_F/q} y \ln \left| \frac{y + 1}{y - 1} \right| dy,\end{aligned}$$

where we substituted  $\cos\theta = u$  and  $k = qy/2$ .

- let us introduce a special function  $F(x)$  defined for  $x > 0$  as

$$F(x) = \frac{1}{x} \int_0^x y \ln \left| \frac{y+1}{y-1} \right| dy = 1 + \frac{x^2 - 1}{2x} \ln \left| \frac{x+1}{x-1} \right| \quad (56)$$



its properties:

- ▶ for  $x \rightarrow 0$ :  $F(x) \approx 2x^2/3$
- ▶ for  $x \rightarrow +\infty$ :  
 $F(x) \approx 2 - 2/(3x^2)$
- ▶  $F(1) = 1$  and  $F'(1) = +\infty$   
(infinite derivative)
- ▶ for all  $x$ :  $F(x) + F(x^{-1}) = 2$

- the resulting static non-interacting susceptibility in the reciprocal space is

$$\tilde{\chi}_0(\mathbf{q}, 0) = -\frac{mk_F}{2\pi^2} F\left(\frac{2k_F}{q}\right), \quad (57)$$

and its real-space counterpart is ( $|\mathbf{r}| \equiv r$ )

$$\begin{aligned} \chi_0(\mathbf{r}, 0) &= (2\pi)^{-3} \int \exp(i\mathbf{q} \cdot \mathbf{r}) \tilde{\chi}_0(\mathbf{q}, 0) d^3\mathbf{q} \\ &= \frac{m}{(2\pi)^3} \frac{(2k_F r) \cos(2k_F r) - \sin(2k_F r)}{r^4} \end{aligned} \quad (58)$$

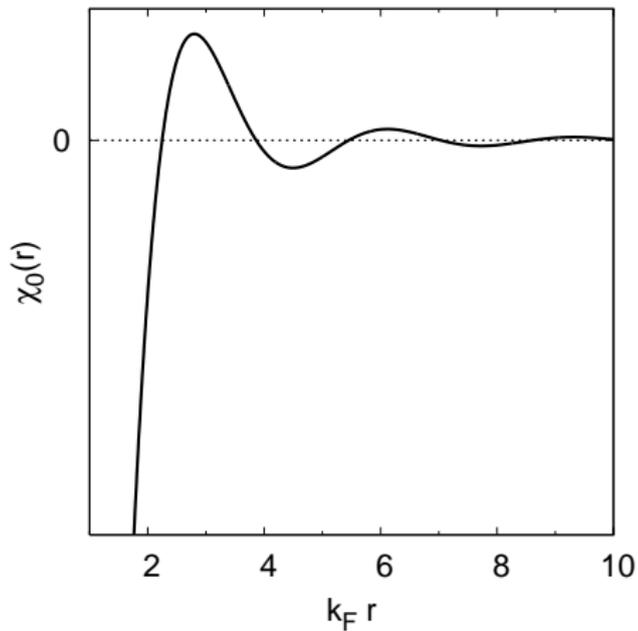
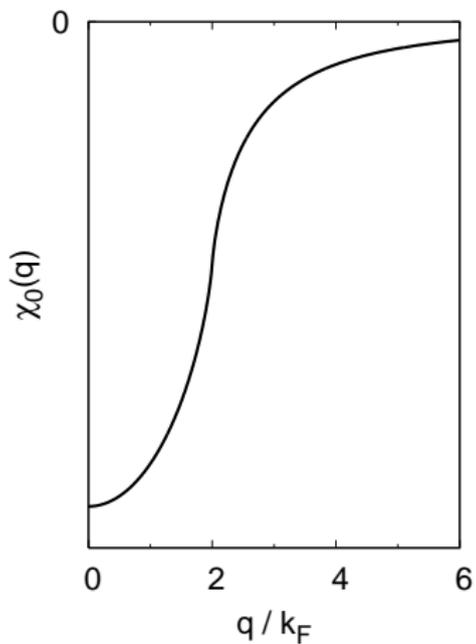
- the most important features of these functions are:
  - ▶ infinite derivative of  $\tilde{\chi}_0(\mathbf{q}, 0)$  at  $q = 2k_F$  ('touching Fermi spheres')
  - ▶ oscillatory behavior of  $\chi_0(\mathbf{r}, 0)$  for  $r \rightarrow \infty$  with a period  $\pi/k_F$  and an amplitude decaying as  $r^{-3}$  (Friedel oscillations)

Static non-interacting susceptibility of the jellium model:

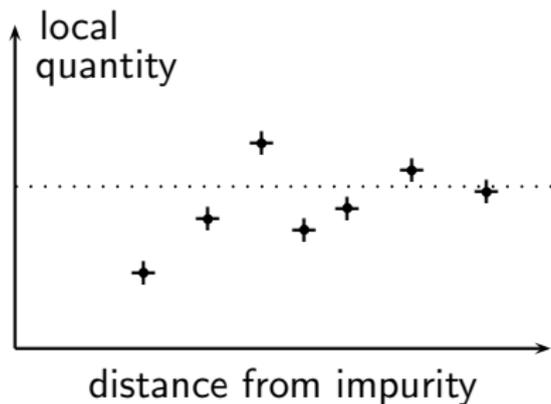
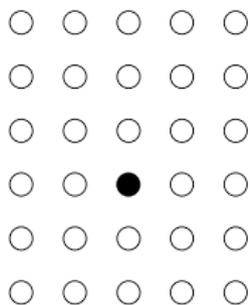
$$\tilde{\chi}_0(q, 0)$$

and

$$\chi_0(r, 0)$$



- experimental verification of the Friedel oscillations:
  - ▶ variations of local quantities induced by defects:  
non-monotonic dependence on distance from the defect
  - ▶ in magnetism: the RKKY interaction between localized magnetic moments mediated by the conduction electrons



- for  $\omega > 0$ , the imaginary part of  $\tilde{\chi}_0(\mathbf{q}, \omega)$  is according to Eq. (55) and Eq. (44) given by

$$\sim \int [\delta(\omega + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}) - \delta(\omega - E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}})] f_{\mathbf{k}} d^3\mathbf{k},$$

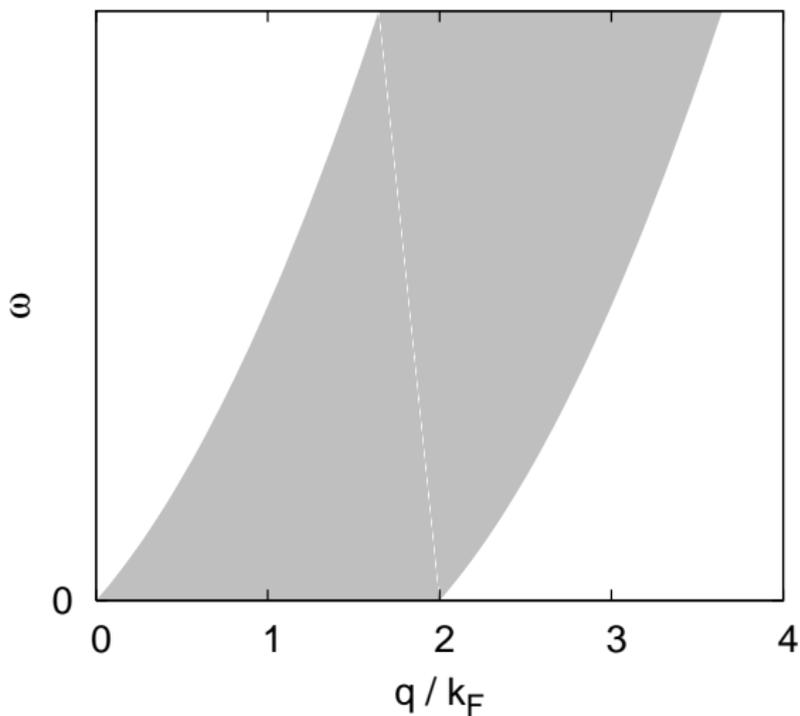
which (for a given vector  $\mathbf{q}$  and at  $T = 0$ ) is non-zero only for frequencies satisfying

$$\frac{q^2}{2m} - \frac{k_F q}{m} < \omega < \frac{q^2}{2m} + \frac{k_F q}{m}, \quad (59)$$

which defines a region between two parabolas

- perturbations with  $\delta\tilde{V}(\mathbf{q}, \omega) \neq 0$  for  $(q, \omega)$  inside this region are accompanied by energy dissipation

Spectrum of particle-hole excitations of the jellium model  
[region of non-zero imaginary part of  $\tilde{\chi}_0(q, \omega)$ ]



## 3 Response of homogeneous electron liquid

### 3.1 Hartree approximation and interacting susceptibility

- a complete inclusion of the electron-electron interaction in the response properties requires the general formalism of sections 1.1 and 1.2 (intractable exactly)
- a mean-field-like alternative is the Hartree approximation: the original relation  $\delta\rho = \chi_0 * \delta V$  is employed, but with replacement of the local perturbing potential  $\delta V(\mathbf{r}, t)$  by an effective total potential  $\delta V_{tot}(\mathbf{r}, t)$  given by

$$\delta V(\mathbf{r}, t) \rightarrow \delta V_{tot}(\mathbf{r}, t) = \delta V_{ext}(\mathbf{r}, t) + \delta V_H(\mathbf{r}, t), \quad (60)$$

where:  $\delta V_{ext}$  – the external (applied) potential,  
 $\delta V_H$  – the Hartree term due to the induced density change  $\delta\rho$  (classical electrostatics):

$$\delta V_H(\mathbf{r}, t) = e'^2 \int \frac{\delta \rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}', \quad e'^2 \equiv \frac{e^2}{4\pi\epsilon_0}. \quad (61)$$

The Hartree term – analogy to the Weiss molecular field.

- this leads to relations between the Fourier transforms:

$$\begin{aligned} \delta \tilde{\rho}(\mathbf{q}, \omega) &= \tilde{\chi}_0(\mathbf{q}, \omega) \delta \tilde{V}_{tot}(\mathbf{q}, \omega), \\ \delta \tilde{V}_{tot}(\mathbf{q}, \omega) &= \delta \tilde{V}_{ext}(\mathbf{q}, \omega) + \delta \tilde{V}_H(\mathbf{q}, \omega), \\ \delta \tilde{V}_H(\mathbf{q}, \omega) &= \tilde{U}(\mathbf{q}) \delta \tilde{\rho}(\mathbf{q}, \omega), \end{aligned} \quad (62)$$

where

$$\tilde{U}(\mathbf{q}) = \int \exp(-i\mathbf{q} \cdot \mathbf{r}) \frac{e'^2}{r} d^3 \mathbf{r} = \frac{4\pi e'^2}{q^2} \quad (63)$$

is the Fourier transformation of the Coulomb interaction  
 $(r \equiv |\mathbf{r}|, \quad q \equiv |\mathbf{q}|)$

- Eqs. (62) yield a closed linear relation for the induced density change:

$$\delta\tilde{\rho}(\mathbf{q}, \omega) = \tilde{\chi}_0(\mathbf{q}, \omega) \left[ \delta\tilde{V}_{\text{ext}}(\mathbf{q}, \omega) + \tilde{U}(\mathbf{q}) \delta\tilde{\rho}(\mathbf{q}, \omega) \right],$$

which leads to the final expression

$$\delta\tilde{\rho}(\mathbf{q}, \omega) = \tilde{\chi}(\mathbf{q}, \omega) \delta\tilde{V}_{\text{ext}}(\mathbf{q}, \omega), \quad (64)$$

where

$$\tilde{\chi}(\mathbf{q}, \omega) = \frac{\tilde{\chi}_0(\mathbf{q}, \omega)}{1 - \tilde{U}(\mathbf{q}) \tilde{\chi}_0(\mathbf{q}, \omega)} \quad (65)$$

is the interacting (full, renormalized) susceptibility

- Eq. (65) bears a general form of a renormalization of the non-interacting susceptibility due to the interaction

- analogy with the susceptibility of a ferromagnet in the mean-field approximation for the classical Ising model:

$$\bar{s} = \tanh[\beta(b + \mathcal{J}\bar{s})]$$

- ▶ the susceptibility of a single isolated spin ( $\mathcal{J} = 0$ ) is (the Curie law)

$$\chi_0(T) = \beta = \frac{1}{k_B T}$$

- ▶ the high-temperature susceptibility of the ferromagnet (the Curie-Weiss law) can be written as

$$\chi(T) = \frac{1}{k_B T - \mathcal{J}} = \frac{\chi_0(T)}{1 - \mathcal{J}\chi_0(T)}$$

## 3.2 Relation to dielectric constant

- the external perturbing potential  $\delta V_{\text{ext}}(\mathbf{r}, t)$  is usually created by means of the density  $\delta \rho_{\text{ext}}(\mathbf{r}, t)$  of a classical external charge, so that

$$\delta V_{\text{ext}}(\mathbf{r}, t) = e'^2 \int \frac{\delta \rho_{\text{ext}}(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}',$$

$$\delta \tilde{V}_{\text{ext}}(\mathbf{q}, \omega) = \tilde{U}(\mathbf{q}) \delta \tilde{\rho}_{\text{ext}}(\mathbf{q}, \omega),$$

which yields [according to Eq. (64) and Eq. (65)] the induced electron density in terms of the external density as

$$\delta \tilde{\rho}(\mathbf{q}, \omega) = \frac{\tilde{U}(\mathbf{q}) \tilde{\chi}_0(\mathbf{q}, \omega)}{1 - \tilde{U}(\mathbf{q}) \tilde{\chi}_0(\mathbf{q}, \omega)} \delta \tilde{\rho}_{\text{ext}}(\mathbf{q}, \omega) \quad (66)$$

- the change of the total (induced and external) density

$$\delta\rho_{tot}(\mathbf{r}, t) = \delta\rho(\mathbf{r}, t) + \delta\rho_{ext}(\mathbf{r}, t)$$

due to the external density is

$$\delta\tilde{\rho}_{tot}(\mathbf{q}, \omega) = \frac{1}{1 - \tilde{U}(\mathbf{q})\tilde{\chi}_0(\mathbf{q}, \omega)} \delta\tilde{\rho}_{ext}(\mathbf{q}, \omega) \quad (67)$$

- in a homogeneous and isotropic medium, the electric field intensity ( $\mathbf{E}$ ) / induction ( $\mathbf{D}$ ) is generated by the total ( $\delta\rho_{tot}$ ) / external ( $\delta\rho_{ext}$ ) density of electric charge:

$$\epsilon_0 \mathbf{E} = \epsilon_r^{-1} \mathbf{D} \quad \Longrightarrow \quad 1 - \tilde{U}(\mathbf{q})\tilde{\chi}_0(\mathbf{q}, \omega) \equiv \tilde{\epsilon}_r(\mathbf{q}, \omega), \quad (68)$$

which defines the relative permittivity (dielectric constant) of the electron liquid in a random-phase approximation (RPA) or in a self-consistent-field (SCF) method

### 3.3 Static screening of external charge

- the electron density induced by a static ( $\omega = 0$ ) external charge density is given by

$$\delta\tilde{\rho}(\mathbf{q}, 0) = -\tilde{K}(\mathbf{q}) \delta\tilde{\rho}_{\text{ext}}(\mathbf{q}, 0), \quad (69)$$

where the quantity  $\tilde{K}(\mathbf{q})$  describes a screening cloud of electrons around the perturbing classical external charge. It is given according to Eq. (66) by

$$\begin{aligned} \tilde{K}(\mathbf{q}) &= -\frac{\tilde{U}(\mathbf{q}) \tilde{\chi}_0(\mathbf{q}, 0)}{1 - \tilde{U}(\mathbf{q}) \tilde{\chi}_0(\mathbf{q}, 0)} \\ &= \frac{1}{1 - \tilde{U}^{-1}(\mathbf{q}) \tilde{\chi}_0^{-1}(\mathbf{q}, 0)}. \end{aligned} \quad (70)$$

- for small values of  $q$  ( $q \ll 2k_F$ ), one can employ Eq. (57) and Eq. (63) to approximate Eq. (70) by

$$\begin{aligned} \tilde{K}(\mathbf{q}) &\approx \left( 1 + \frac{q^2}{4\pi e'^2} \frac{\pi^2}{mk_F} \right)^{-1} = \frac{1}{1 + \lambda_{TF}^2 q^2} \\ &\equiv \tilde{K}_{TF}(\mathbf{q}), \quad \lambda_{TF} = \sqrt{\frac{\pi a_0}{4k_F}}, \end{aligned} \quad (71)$$

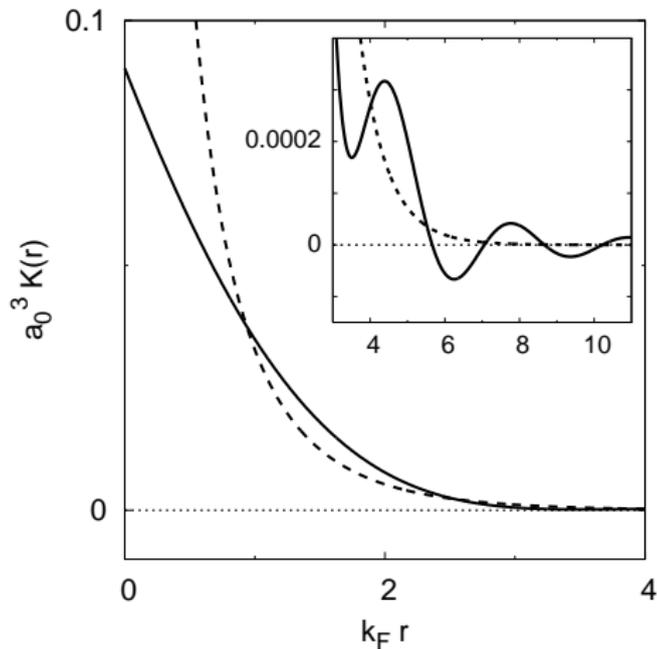
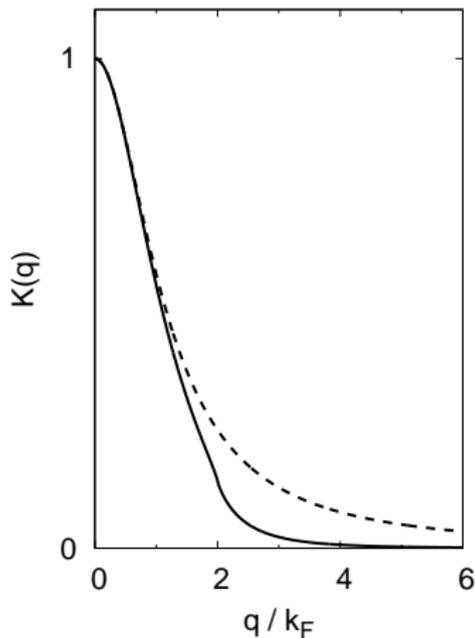
where  $\tilde{K}_{TF}(\mathbf{q})$  – Thomas-Fermi screening kernel in reciprocal space and  $\lambda_{TF}$  – Thomas-Fermi screening length ( $\simeq a_0$ )

- the Thomas-Fermi screening kernel is applicable to static external charge densities with very slow spatial variations; its real-space representation is (screened Coulomb potential)

$$K_{TF}(\mathbf{r}) = (4\pi\lambda_{TF}^2 r)^{-1} \exp(-r/\lambda_{TF}) \quad (72)$$

The SCF (full lines) and Thomas-Fermi (dashed lines) screening kernels for the jellium model with  $k_F a_0 = 1$

$\tilde{K}(q), \tilde{K}_{TF}(q)$  and  $K(r), K_{TF}(r)$



- properties of the full (RPA, SCF) screening kernel  $\tilde{K}(\mathbf{q})$ , Eq. (70), and of its real-space counterpart  $K(\mathbf{r})$ :
  - ▶ for  $q \ll 2k_F$ , the full screening  $\tilde{K}(\mathbf{q})$  can be replaced by the Thomas-Fermi screening  $\tilde{K}_{TF}(\mathbf{q})$
  - ▶ it holds  $\tilde{K}(\mathbf{0}) = 1$  and  $\int K(\mathbf{r})d^3\mathbf{r} = 1 \implies$  an external charge is fully screened by the induced electron cloud (similarly to the Thomas-Fermi screening)
  - ▶ the divergence of  $\partial\tilde{\chi}_0(\mathbf{q}, 0)/\partial q$  for  $q = 2k_F$  leads to a divergence of  $\partial\tilde{K}(\mathbf{q})/\partial q \implies K(\mathbf{r})$  also contains the Friedel-like oscillations for  $r \rightarrow \infty$  (in contrast to the Thomas-Fermi screening)
  - ▶ for  $q \rightarrow \infty$ , the asymptotics of the full screening is  $\tilde{K}(\mathbf{q}) \sim q^{-4} \implies K(\mathbf{r})$  remains finite for  $r \rightarrow 0$  [in contrast to the divergence of  $K_{TF}(\mathbf{r})$  for  $r \rightarrow 0$ ]

### 3.4 Dynamical response and plasmons

- let us investigate the response functions at  $T = 0$  for  $|\mathbf{q}| = q \rightarrow 0$  and  $\omega > 0$  (strictly for  $k_F q + \frac{1}{2}q^2 \ll m\omega$ )
- the non-interacting susceptibility, Eq. (55), can be written [using  $(\omega + h)^{-1} \approx \omega^{-1} - \omega^{-2}h$  for  $|h| \ll \omega$ ] as

$$\begin{aligned}\tilde{\chi}_0(\mathbf{q}, \omega) &= \frac{2}{(2\pi)^3} \int \left( \frac{1}{\omega + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} \right. \\ &\quad \left. + \frac{1}{-\omega + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} \right) f_{\mathbf{k}} d^3\mathbf{k} \\ &\approx \frac{2}{(2\pi)^3} \omega^{-2} \int 2(E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}}) f_{\mathbf{k}} d^3\mathbf{k} \\ &= \frac{q^2}{m\omega^2} \frac{k_F^3}{3\pi^2} = \frac{\rho q^2}{m\omega^2},\end{aligned}\tag{73}$$

where the  $k_F - \rho$  relation, Eq. (51), was used

- the SCF-permittivity, Eq. (68), can be written as

$$\tilde{\epsilon}_r(\mathbf{q}, \omega) = 1 - \frac{4\pi e'^2}{q^2} \frac{\rho q^2}{m\omega^2} = 1 - \frac{e^2 \rho}{\epsilon_0 m} \frac{1}{\omega^2}; \quad (74)$$

the zero of  $\tilde{\epsilon}_r(\mathbf{q}, \omega)$  (and the corresponding pole of the interacting susceptibility) occurs at a frequency

$$\omega = \sqrt{\frac{e^2 \rho}{\epsilon_0 m}} \equiv \omega_{pl}, \quad (75)$$

where  $\omega_{pl}$  denotes the classical plasma frequency

¶ a pole in the susceptibility  $\longleftrightarrow$  an excited state

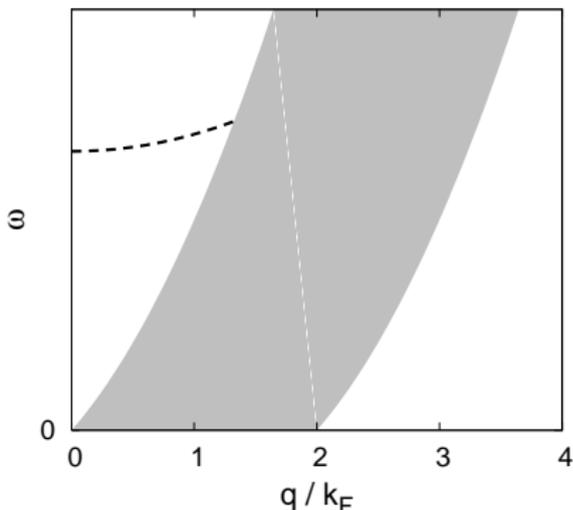
- the pole in the susceptibility points to a collective excitation of the homogeneous electron liquid – the plasmon

- more accurate treatment

$$\implies \omega(q)$$

(plasmon dispersion law)

- the plasmon mode for bigger values of  $q$  merges into the continuum of the particle-hole excitations



- the plasmon energy:  $\hbar\omega_{pl} \approx (k_F a_0)^{3/2} \times 18 \text{ eV}$   
 $\implies$  activation by elevated temperatures is inefficient,  
interaction with high-energy particles is needed

- a simple derivation of the classical plasma frequency:

- ▶ electrons (mass  $m$ , charge  $e$ , uniform density  $\rho$ )
- ▶ fixed charge-compensating homogeneous background
- ▶ the restoring force proportional to the displacement  
 $\implies$  harmonic vibrations

