

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 Tr denotes the trace and where we introduced the density matrix (statistical operator) ρ 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 ρ and its matrix elements ρ_{mn}

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

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

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

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 ξ 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 ξ -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 Ψ with respect to permutation of two particles):
 - ▶ bosons – Ψ symmetric,
integer spin (photons, phonons, magnons, ...)
 - ▶ fermions – Ψ 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 μ

- 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_{λ} ($\lambda = 1, 2, \dots, \mathcal{M}$) 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_{λ} – occupation numbers

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

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

$$N_{\{n_\lambda\}} = \sum_{\lambda=1}^{\mathcal{M}} n_\lambda \tag{19}$$

and the corresponding eigenvalue of \tilde{H} is

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

- 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_λ^+) and annihilation (a_λ) 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

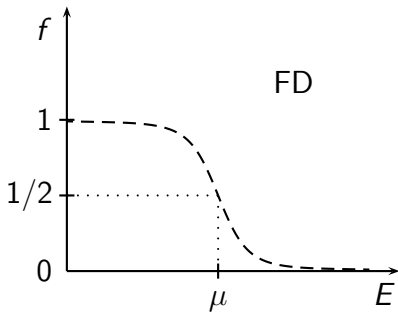
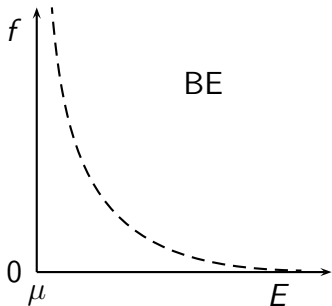
- in order to get the quantum-mechanical and statistical average of \tilde{A} , we need the statistical averages of the occupation numbers n_λ at a given temperature T and chemical potential μ
- the probability of a particular value $n_\lambda \propto \exp[\beta(\mu - E_\lambda)n_\lambda]$, which yields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

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

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 ρ_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 ρ_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 ρ_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 σ 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 δ -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 $x \rightarrow \pm\infty$;

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

- decomposition of the susceptibility in two terms:

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

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 δ -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:

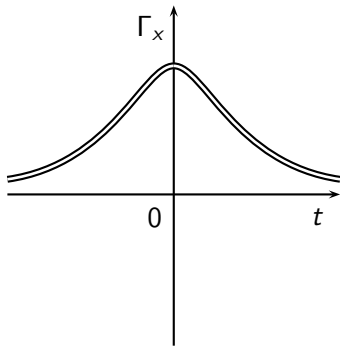
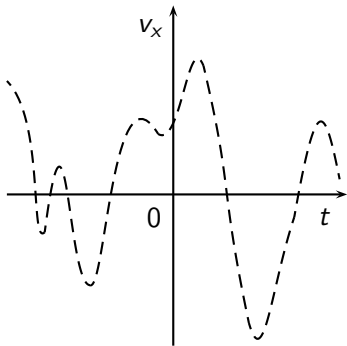
$$\begin{aligned} \int_{-\infty}^{\infty} \frac{1}{x - x_1 - i\eta_1} \frac{1}{x - x_2 + i\eta_2} dx &= \frac{2\pi i}{x_1 - x_2 + i(\eta_1 + \eta_2)} , \\ \int_{-\infty}^{\infty} \frac{1}{x - x_1 + i\eta_1} \frac{1}{x - x_2 + i\eta_2} dx &= 0 , \end{aligned}$$

where x_1, x_2 are real and η_1, η_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_λ, E_ν ; the equilibrium one-particle density matrix f is given in terms of average occupation numbers f_λ as

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

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

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

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

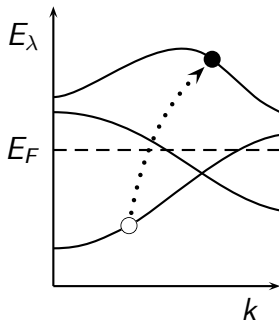
- ▶ the same formal structure as the general result, Eq. (43)
 - ▶ $|\lambda\rangle, |\nu\rangle$ and f_{λ}, f_{ν} instead of $|m\rangle, |n\rangle$ and w_m, w_n
 - ▶ Eq. (49) employs the one-particle Hilbert space
- the susceptibility $\chi_{AB}(\omega)$ consists of terms that exhibit singular behavior 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 $T = 0$)

\Rightarrow 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).

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 $\delta \varrho(\mathbf{r}, t)$
- the most general form of the linear response is given by

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

- 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 ($\mathbf{r} \rightarrow \mathbf{q}$, $t \rightarrow \omega$):

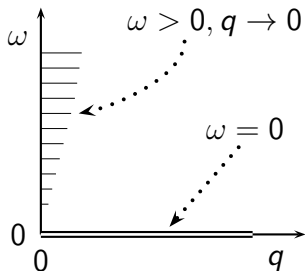
$$\delta \tilde{\varrho}(\mathbf{q}, \omega) = \tilde{\chi}_0(\mathbf{q}, \omega) \delta \tilde{V}(\mathbf{q}, \omega), \quad (53)$$

where $\delta\tilde{\varrho}(\mathbf{q}, \omega) = \int \int \exp(-i\mathbf{q} \cdot \mathbf{r} + i\omega t) \delta\varrho(\mathbf{r}, t) d^3\mathbf{r} dt$
 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):

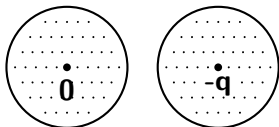
We identify $|\lambda\rangle, |\nu\rangle$ with $|\mathbf{k}\rangle, |\mathbf{k}'\rangle$. The ω -component of the local perturbing potential $\delta V(\mathbf{r}, t)$ leads to the matrix elements $B_{\nu\lambda} \equiv (2\pi)^{-3} \delta \tilde{V}(\mathbf{k}' - \mathbf{k}, \omega)$. The Fourier transformed 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

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

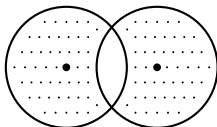
which coincides with Eq. (53) and Eq. (54).

- (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

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

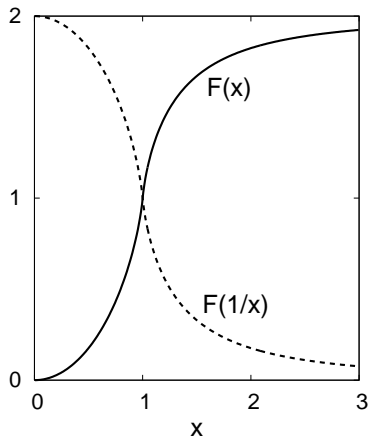
which shows that the static susceptibility is real. We get:

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

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 ($|\mathbf{r}| \equiv r$)

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

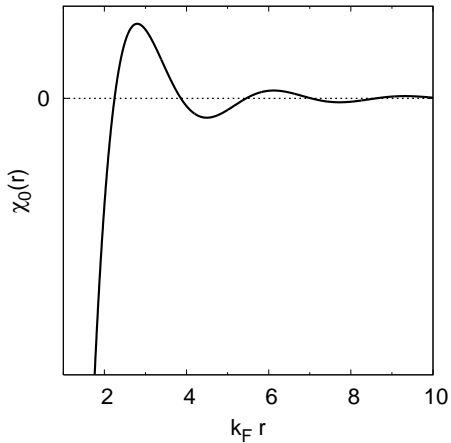
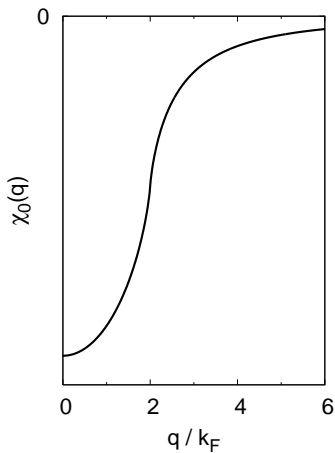
- the most important features of these functions are:
 - ▶ infinite derivative of $\tilde{\chi}_0(\mathbf{q}, 0)$ at $q = 2k_F$ ('touching Fermi spheres')
 - ▶ oscillatory behavior of $\chi_0(\mathbf{r}, 0)$ for $r \rightarrow \infty$ with a period π/k_F and an amplitude decaying as r^{-3} (Friedel oscillations)

Static non-interacting susceptibility of the jellium model:

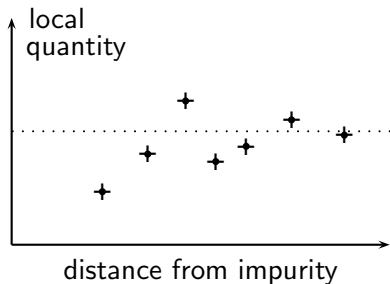
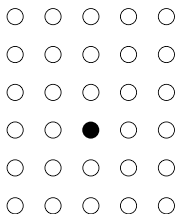
$$\tilde{\chi}_0(q, 0)$$

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

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

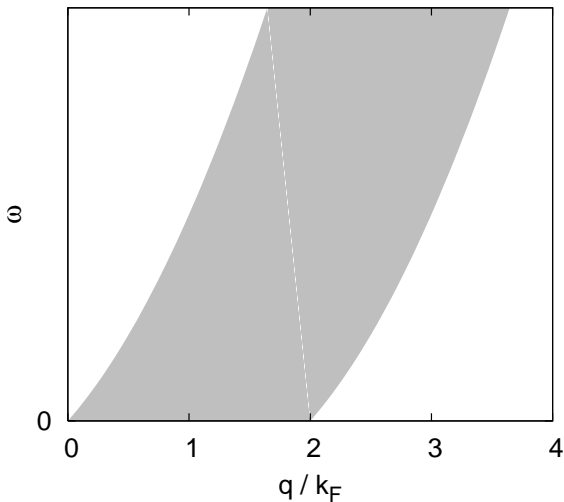
which (for a given vector \mathbf{q} and at $T = 0$) is non-zero only for frequencies satisfying

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

which defines a region between two parabolas

- perturbations with $\delta\tilde{V}(\mathbf{q}, \omega) \neq 0$ for (q, ω) 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: δV_{ext} – the external (applied) potential,
 δV_H – the Hartree term due to the induced density change $\delta\rho$ (classical electrostatics):

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

The Hartree term – analogy to the Weiss molecular field.

- this leads to relations between the Fourier transforms:

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

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:

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

which leads to the final expression

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

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 $\delta \varrho_{\text{ext}}(\mathbf{r}, t)$ of a classical external charge, so that

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

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

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

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

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

$$\delta \varrho_{tot}(\mathbf{r}, t) = \delta \varrho(\mathbf{r}, t) + \delta \varrho_{ext}(\mathbf{r}, t)$$

due to the external density is

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

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

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

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

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

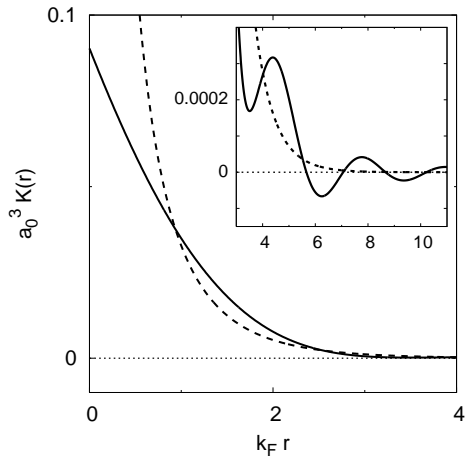
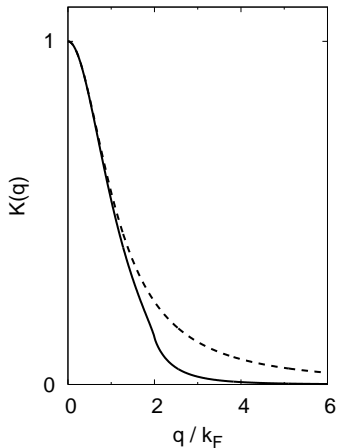
where $\tilde{K}_{TF}(\mathbf{q})$ – Thomas-Fermi screening kernel in reciprocal space and λ_{TF} – Thomas-Fermi screening length ($\simeq a_0$)

- 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 $k_F a_0 = 1$

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



- 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 $k_F - \varrho$ relation, Eq. (51), was used

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

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

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

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

where ω_{pl} denotes the classical plasma frequency

¶ a pole in the susceptibility \longleftrightarrow an excited state

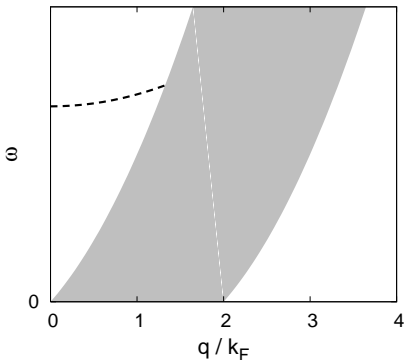
- the pole in the susceptibility points to a collective excitation of the homogeneous electron liquid – the plasmon

- 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 ϱ)
- ▶ fixed charge-compensating homogeneous background
- ▶ the restoring force proportional to the displacement
 \implies harmonic vibrations

