Coulomb gas - jellium model

MUNI SCI Department of Condensed Matter Physics

- model specification

$$\hat{H} = \sum_{k\sigma} \varepsilon_{k\sigma} \hat{c}^+_{k\sigma} \hat{c}_{k\sigma} + \hat{H}_{e-e} + \hat{V}_{ext}$$

$\varepsilon_{k\sigma} = \frac{\hbar^2 k^2}{2m} - \mu$

$\hat{H}_{e-e}$: Coulomb interaction

$\hat{V}_{ext}$: interaction with the nuclei (approximate)

jellium model - approximate charge density of the nuclei by a homogeneous positive background (same density as the electron gas)

1) derivation of $\hat{V}_{ext}$

$$\hat{V}_{ext} = \int d^3\bar{r}\, \varphi(\bar{r})\, (-e)\, \hat{n}(\bar{r}) = \Omega \sum_q \varphi_{-q}\, (-e)\, \hat{n}_q$$

Fourier representation: $\varphi(\bar{r}) = \sum_q \varphi_q\, e^{i\bar{q}\cdot\bar{r}}$ and $\hat{n}_q = \frac{1}{\Omega} \sum_{k\sigma} \hat{c}^+_{k\sigma} \hat{c}_{k+q\,\sigma}$

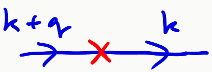
scalar potential satisfies Poisson equation $\nabla^2 \varphi = -\frac{\rho_{nucl}}{\varepsilon_0}$

in Fourier space $(iq)^2 \varphi_q = -\frac{1}{\varepsilon_0} \rho_{nucl,q} \longrightarrow \varphi_q = \frac{e n_0}{\varepsilon_0 q^2} \delta_{q,0}$

For homogeneous $\rho_{nucl} = e n_0$ we have $\rho_{nucl,q} = e n_0 \delta_{q,0}$

$$\hat{V}_{ext} = \sum_{qkG} \underbrace{-\frac{e^2 n_0}{\varepsilon_0 q^2} \delta_{q,0}}_{V^{ext}_{k,k+q}} \hat{c}^+_{kG} \hat{c}_{k+q,G}$$

$\to k = k+q$

represented by 

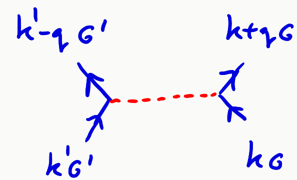
associated with $-V^{ext}_{k,k+q}$

Formally diverges but will be compensated by Hartree selfenergy of positive sign.

2) Coulomb interaction among electrons

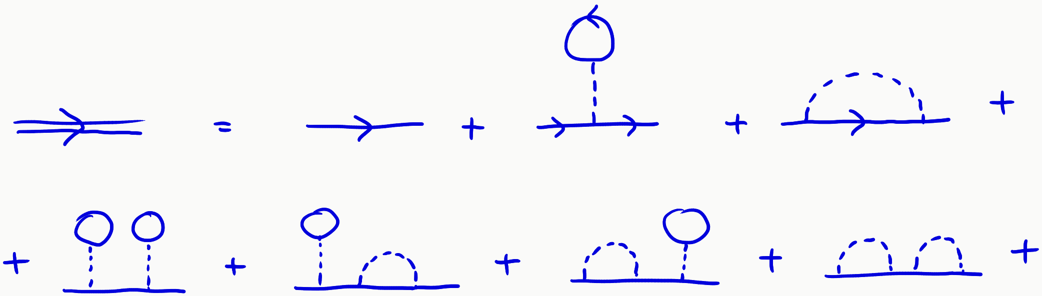
$$H_{e-e} = \frac{1}{2} \sum_{\substack{kk'q \\ GG'}} V_q \, \hat{c}^+_{k+qG} \hat{c}^+_{k'-qG'} \hat{c}_{k'G'} \hat{c}_{kG}$$

$$V_q = \frac{1}{\Omega} \frac{e^2}{\varepsilon_0 q^2}$$



$-V_q$

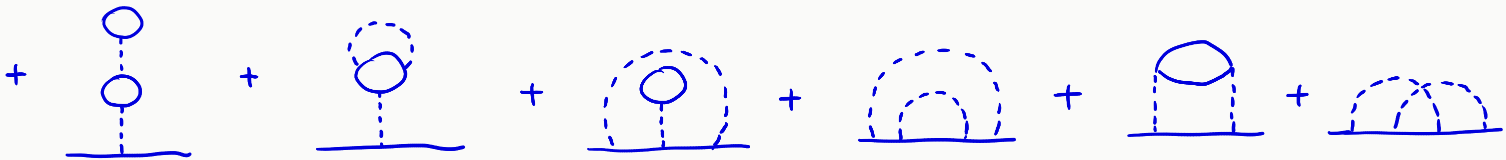
Ⓐ Selfenergy



0^{th} & 1^{st} order

2^{nd} order reducible

2^{nd} order irreducible



+ higher orders

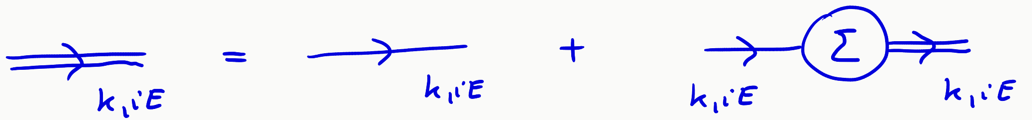
all the possible insertions

improper selfenergy :

only the irreducible insertions

proper selfenergy :

- Dyson's equation



(+ spin conservation)

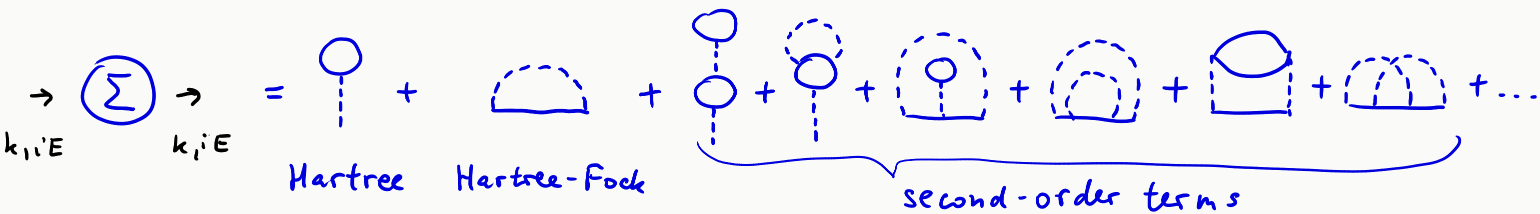
$$-\mathcal{G}(k, iE) \qquad -\mathcal{G}_0(k, iE) \qquad (-\mathcal{G}_0) \times (-\Sigma) \times (-\mathcal{G})$$ ← same arguments k, iE

$\rightarrow \quad \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}$ by dividing by $\mathcal{G}\mathcal{G}_0$ $\rightarrow \quad \mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$

electron propagator including selfenergy corrections

$$\mathcal{G}(k, iE) = \frac{1}{iE - \varepsilon_k - \Sigma(k, iE)}$$

(ε_k includes μ)



- Hartree selfenergy

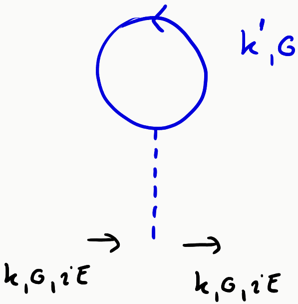


diagram translates to

$$(-1)\sum_{k'G'}\left(-V_{q=0}\right)\frac{1}{\beta}\sum_{iE'}-\mathcal{G}_0(k',iE')\; e^{-iE'\frac{0^-}{\hbar}}$$

to get $c^+_{k'}(\tau^+)\, c_{k'}(\tau)$ as in Coulomb int.

from $\langle T\{\hat{c}_{k'}(0^-)\,\hat{c}^+_{k'}(0)\}\rangle_0$

$$-\Sigma_H(k,iE) = (-1)\, V_{q=0}\sum_{k'G'}\underbrace{\frac{1}{\beta}\sum_{iE'}\frac{1}{iE'-\varepsilon_{k'}}\, e^{-iE0^-}}_{n_F(\varepsilon_{k'})} = (-1)\, V_{q=0}\, N$$

N: number of electrons

$$\Sigma_H(k,iE) = \frac{1}{\Omega}\left.\frac{e^2}{\varepsilon_0 q^2}\right|_{q=0} N = \left.\frac{n_0 e^2}{\varepsilon_0 q^2}\right|_{q=0}$$

$n_0 = \frac{N}{\Omega}$ is the electron density

Compensation of the positive background in $\hat{V}_{ext}$ ×

and Σ_H from averaged density of electrons

(at all levels in the diagrams exclude $V_{q=0}$)

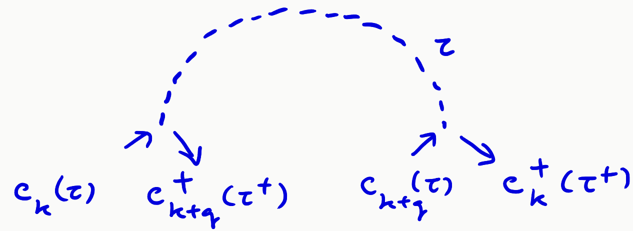
$$-\left.\frac{n_0 e^2}{\varepsilon_0 q^2}\right|_{q=0}$$

$$+\left.\frac{n_0 e^2}{\varepsilon_0 q^2}\right|_{q=0}$$

• Hartree-Fock selfenergy

Σ_{HF} = 

- spin determined by the outer lines
- infinitesimal factors:



translates to

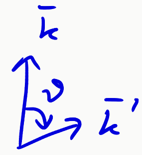
$$-\Sigma_{HF}(k,iE) = \sum_q \frac{1}{\beta}\sum_{i\nu}(-V_q)\left[-\mathcal{G}(k+q,iE+i\nu)\,e^{-(iE+i\nu)\frac{0^-}{\hbar}}\right] =$$

$$\Sigma_{HF}(k) = -\sum_q V_q\, n_F(\varepsilon_{k+q}) = -\sum_{k'} V_{k'-k}\, n_{k'} = -\underbrace{\frac{1}{\Omega}\sum_{k'}}_{\frac{1}{(2\pi)^3}\int d^3\bar{k}'} \frac{e^2}{\varepsilon_0|k'-k|^2}\, n_{k'}$$

evaluation at $T=0$

$$\Sigma_{HF}(k) = -\int_{k'<k_F}\frac{d^3\bar{k}'}{(2\pi)^3}\,\frac{e^2}{\varepsilon_0(\bar{k}-\bar{k}')^2}$$

in spherical coordinates with the axis pointing along $\bar{k}$



$$= -\frac{1}{(2\pi)^3} \int_0^{k_F} dk'\, k'^2 \int_0^{\pi} d\vartheta\, \sin\vartheta \int_0^{2\pi} d\varphi \; \frac{e^2}{\varepsilon_0} \, \frac{1}{k^2 + k'^2 - 2kk'\cos\vartheta}$$

$$= -\frac{e^2}{4\pi^2\varepsilon_0} \int_0^{k_F} dk'\, k'^2 \int_{-1}^{+1} d\xi \; \frac{1}{k^2 + k'^2 - 2kk'\xi} = \ldots = -\frac{e^2}{4\pi^2\varepsilon_0} k_F \left(1 + \frac{1-x^2}{2x} \ln\left|\frac{1+x}{1-x}\right|\right)$$

with $x = k/k_F$

This selfenergy has a log singularity in the derivative at $k = k_F$

$$\frac{\partial \Sigma_{HF}}{\partial k} = -\frac{e^2}{4\pi^2\varepsilon_0} \frac{d}{dx} \frac{1-x^2}{2x} \ln\left|\frac{1+x}{1-x}\right| \quad \sim \quad \text{contains non-compensated } \ln|1-x|$$

as a consequence, the density of states would vanish at $k = k_F$

$$\mathcal{G}(k, iE) = \frac{1}{iE - \varepsilon_k - \Sigma_{HF}(k)} \;\rightarrow\; \mathrm{DOS}(E) = \sum_k \delta\left(E - \varepsilon_k - \Sigma_{HF}(k)\right) \sim \iint \frac{dS}{\left|\nabla_k \left[\varepsilon_k + \Sigma_{HF}(k)\right]\right|}$$

– corrected when higher-order terms in $\Sigma(k, iE)$ are included

- selection of higher-order terms

1) density-dependence estimate

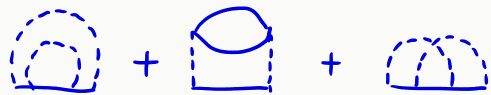
- by pulling out powers of k_F e.g. $\int d\bar{k}^{3} \to k_F^3 \times$ dimensionless , $G_0 = \frac{1}{iE - \varepsilon_k} \sim k_F^{-2} \ldots$

- for the contribution with n interaction lines

$$\Sigma^{(n)}(k, iE) \sim k_F^{-(n-2)} \sim r_s^{n-2}$$ high-density limit is $r_s \to 0$

2) degree of divergence

relevant second-order contributions to the self energy



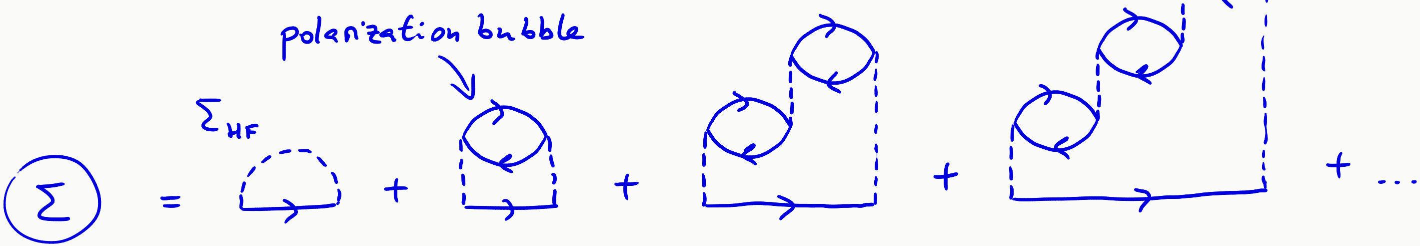
$V_q V_{q'}$ $\quad$ V_q^2 $\quad$ $V_q V_{q'}$

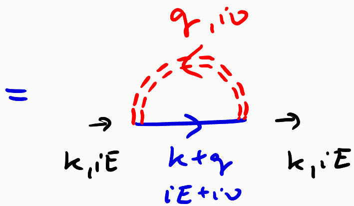
$\int dq \frac{1}{q^4}$ in the middle one diverges

$\rightarrow$ include only diagrams with the strongest divergence

- max. number of Coulomb lines with the same q

- RPA (random phase approximation) for the selfenergy





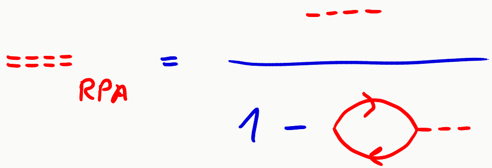
effective Coulomb interaction
(contains the screening effects)

with the renormalized Coulomb interaction within RPA

translated to

$$-V_{RPA}(q, i\nu) \qquad -V_q \qquad (-V_q)(\Omega\,\Pi_0)(-V_q) \qquad (-V_q)(\Omega\,\Pi_0)(-V_q)(\Omega\,\Pi_0)(-V_q)$$

Summation of the series



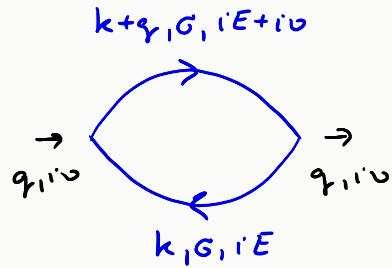
$$-V_{RPA} = \frac{-V_q}{1 - \Omega \Pi_0 (-V_q)}$$

explicitly

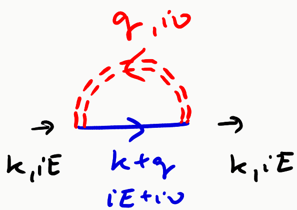
$$V_{RPA}(q, i\nu) = \frac{V_q}{\varepsilon_{RPA}(q, i\nu)} \qquad \varepsilon_{RPA}(q, i\nu) = 1 + \frac{e^2}{\varepsilon_0 q^2} \Pi_0(q, i\nu)$$

with

$$\Pi_0(q, i\nu) = -\frac{1}{\Omega} \sum_{k\sigma} \frac{1}{\beta} \sum_{iE} \mathcal{G}_0(k+q, iE+i\nu)\, \mathcal{G}_0(k, iE)$$



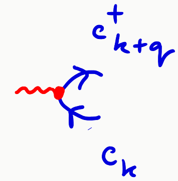
selfenergy



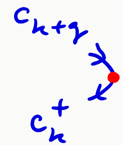
$$\Sigma(k, iE) = -\sum_q \frac{1}{\beta} \sum_{i\nu} \frac{V_q}{\varepsilon_{RPA}(q, i\nu)}\, \mathcal{G}_0(k+q, iE+i\nu)$$

(B) RPA susceptibility & plasmons

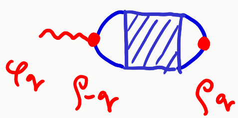
interaction with external field $\int \varphi(\bar{r})\,\rho(\bar{r}) \to \sum_q \varphi_q\, \hat{\rho}_{-q}$



measurement of charge density $\hat{\rho}_q = (-e)\,\frac{1}{\Omega} \sum_{k\sigma} \hat{c}^+_{k\sigma}\,\hat{c}_{k+q\,\sigma}$



charge susceptibility - thermal version $\sim \langle T\{\rho_q(\tau)\,\rho_{-q}(0)\}\rangle$



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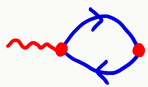
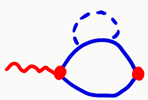


\+ ← 0^{th} order

Lindhard function

1^{st} order contributions



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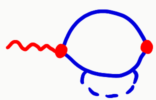

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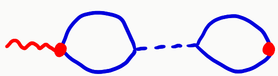

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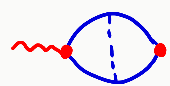


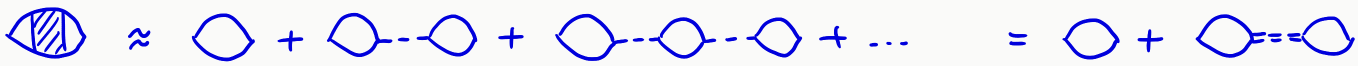
\+ higher-order terms

renormalization of G

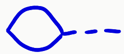
included in RPA

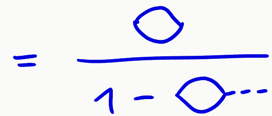
"vertex correction"

- in RPA approximation



$$\chi_{RPA}(q,i\nu) = \frac{\chi_0(q,i\nu)}{1 - \text{[bubble]}} = \frac{\chi_0(q,i\nu)}{\varepsilon_{RPA}(q,i\nu)}$$





using the Lindhard Function

dimensionless

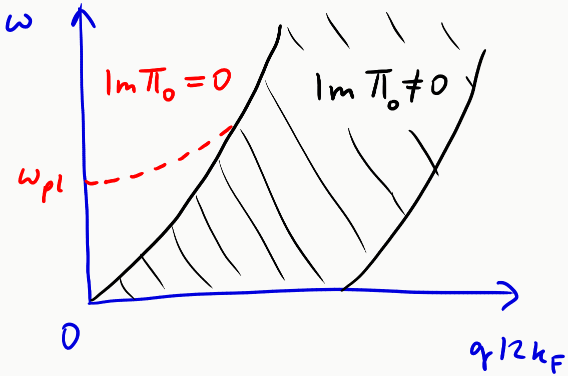
$$\varepsilon_{RPA}(q,\omega) = 1 + \frac{e^2}{\varepsilon_0 q^2}\frac{m k_F}{2\pi^2\hbar^2}\tilde{\Pi}_0(q,\omega)$$

spectral density of the effective interaction

$$B(q,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left[\frac{1}{\varepsilon_{RPA}(q,\omega)} - 1\right] \qquad V_{eff}(q,i\nu) = V_q\left[1 + \int_{-\infty}^{\infty} d\omega\,\frac{B(q,\omega)}{i\nu - \omega}\right]$$

this quantity fulfills the conditions for KK relations

- plasmons



contributions to $B(q,\omega)$:

1) particle-hole continuum where $\mathrm{Im}\,\Pi_0 \neq 0$

2) plasmon contribution where $\varepsilon_{RPA} = 0$

dispersion given by $\varepsilon_{RPA}(q, \omega_{pe}(q)) = 0$

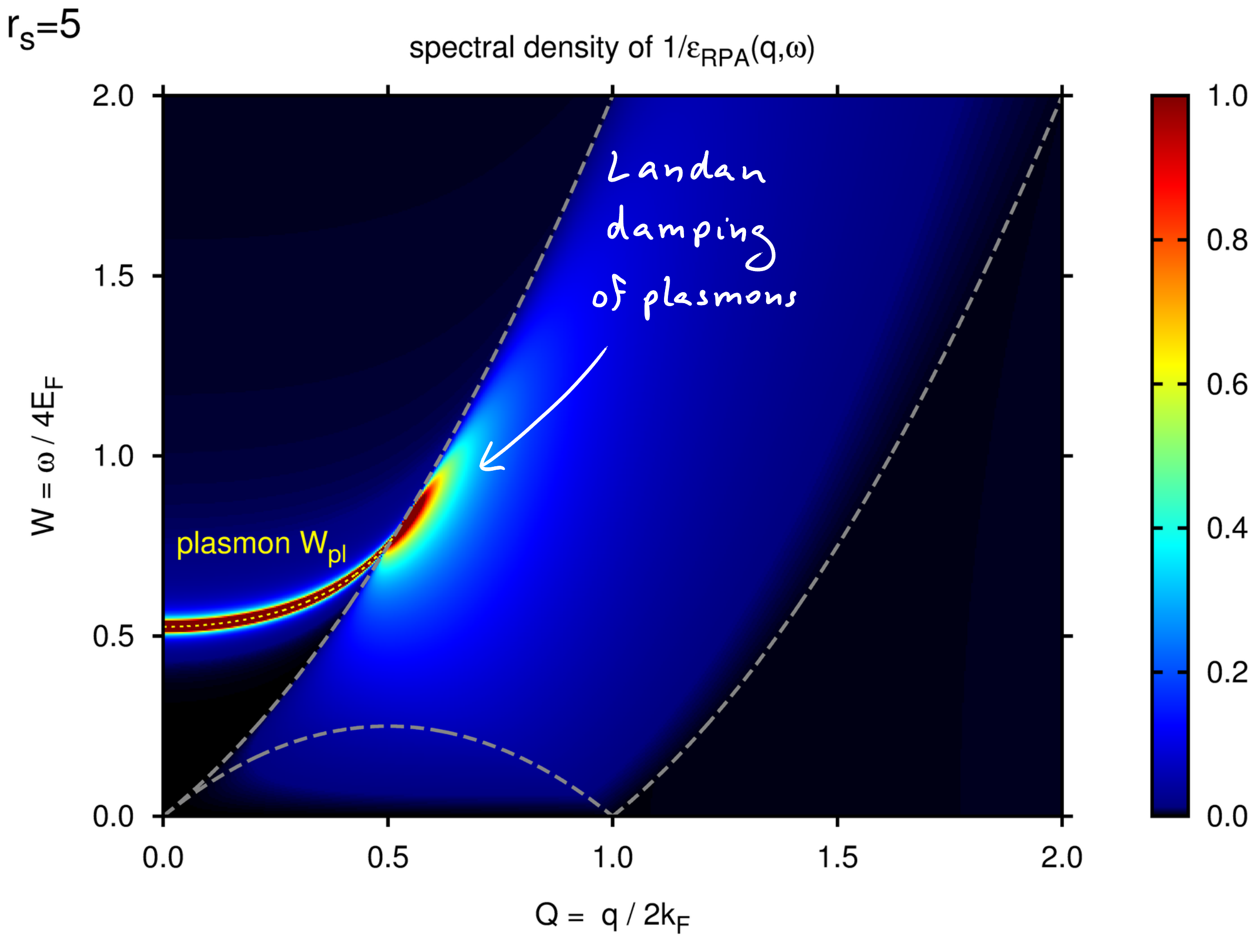
plasmon dispersion obtained by small-q expansion of $\Pi_0(q,\omega)$

$$\tilde{\Pi}_0(q,\omega) = 1 + \frac{1-(Q-\frac{W}{Q})^2}{4Q} \ln\left|\frac{W-Q^2-Q}{W-Q^2+Q}\right| + \frac{1-(Q+\frac{W}{Q})^2}{4Q} \ln\left|\frac{W+Q^2+Q}{W+Q^2-Q}\right| \approx -\frac{2}{3}\left(\frac{Q}{W}\right)^2 - \frac{2}{5}\left(\frac{Q}{W}\right)^4$$

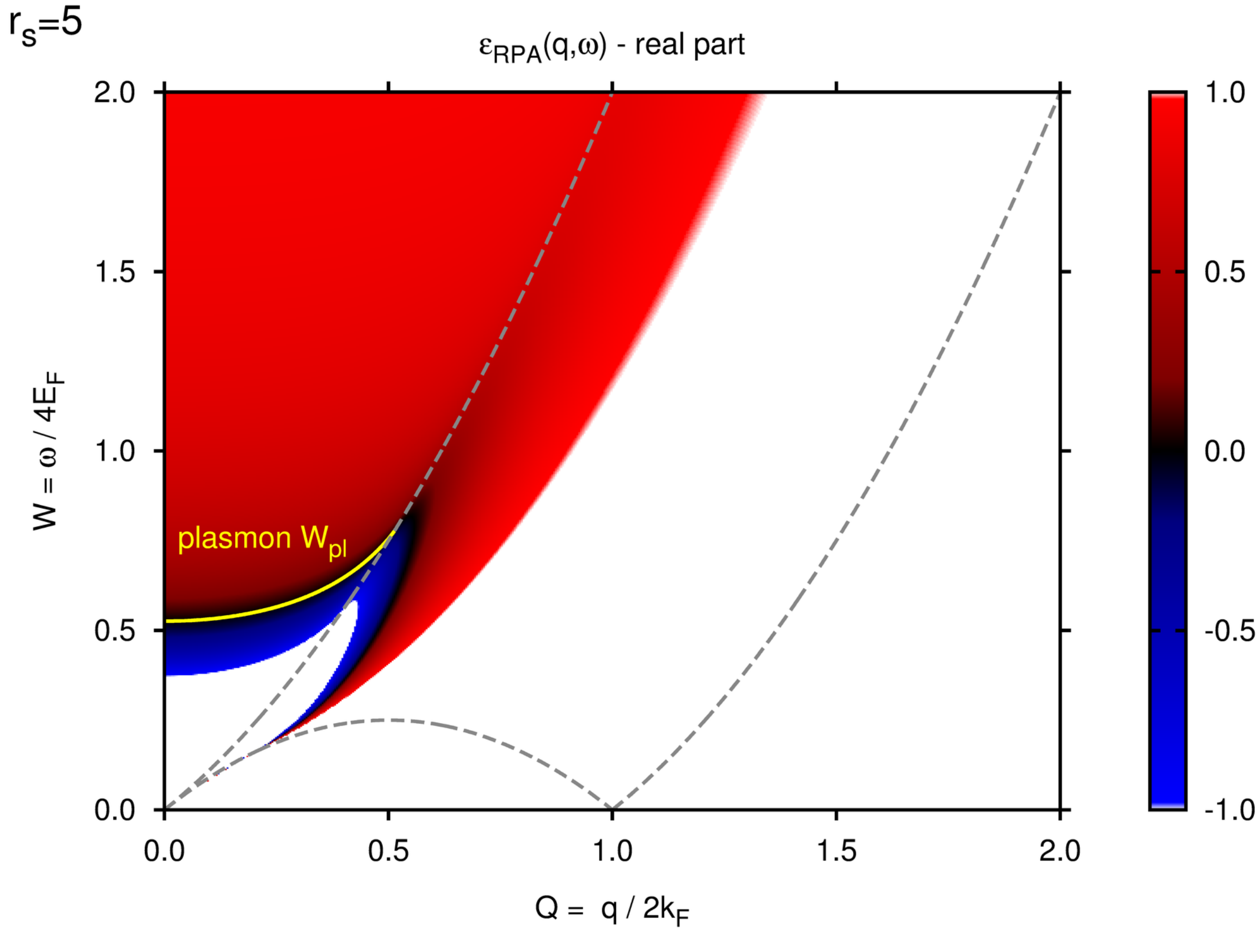
$$\rightarrow \quad \varepsilon_{RPA} \approx 1 - \frac{\omega_{pe}^2(q)}{\omega^2} \quad \text{with} \quad \omega_{pe}(q) = \omega_{pe}(0) + \alpha \frac{\hbar q^2}{2m}$$

classical result $\sqrt{\frac{n_0 e^2}{m \varepsilon_0}}$

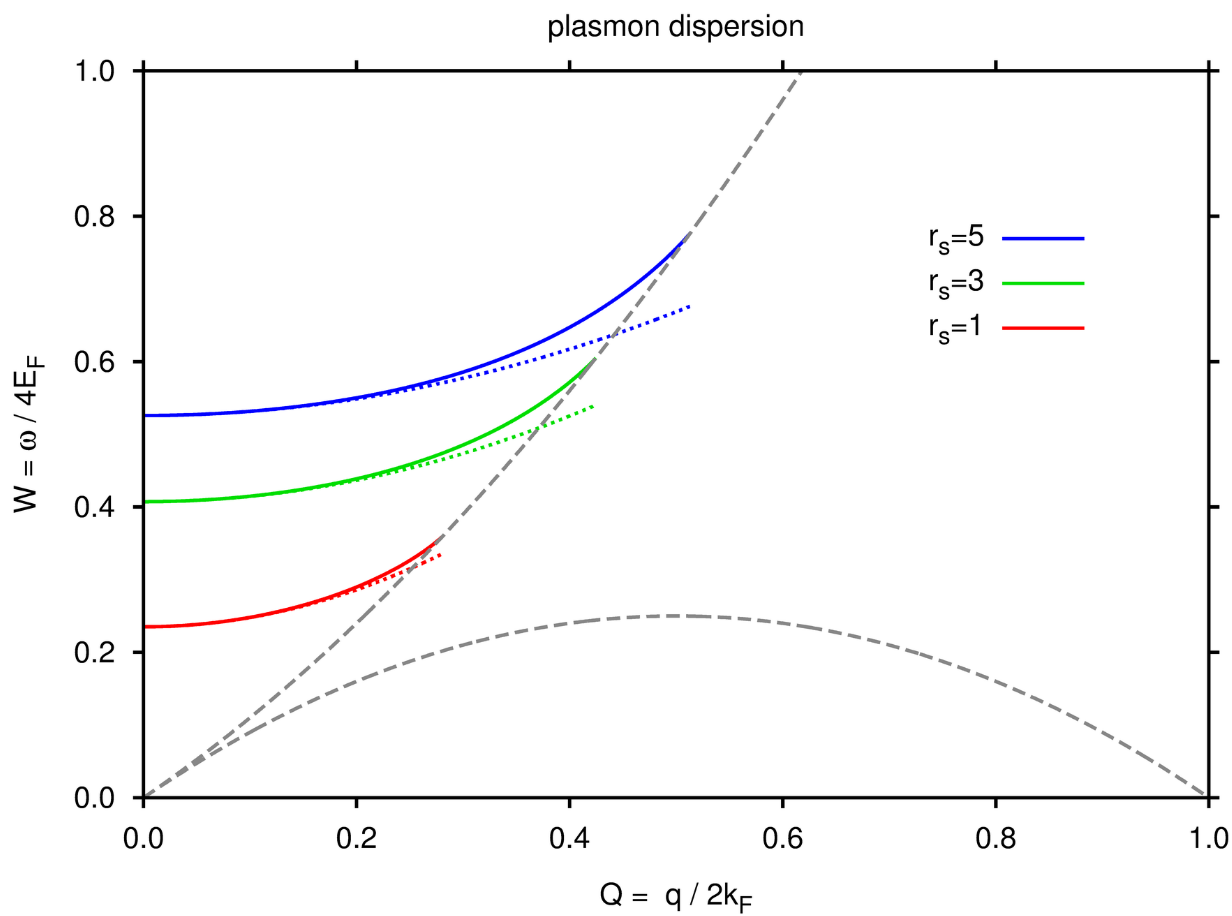
$\alpha_{FE} = \frac{3}{10} \frac{E_F}{\hbar \omega_{pe}}$ (free electrons)



r_s=5
spectral density of $1/\varepsilon_{RPA}(q,\omega)$
Landau damping of plasmons
plasmon W_{pl}
$W = \omega / 4E_F$
$Q = q / 2k_F$
0.0
0.5
1.0
1.5
2.0
0.2
0.4
0.6
0.8



r_s=5
$\varepsilon_{RPA}(q,\omega)$ - real part
plasmon W_{pl}
$W = \omega / 4E_F$
$Q = q / 2k_F$
2.0
1.5
1.0
0.5
0.0
0.0
0.5
1.0
1.5
2.0
1.0
0.5
0.0
-0.5
-1.0


plasmon dispersion
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
W = ω / 4E_F
Q = q / 2k_F
r_s=5
r_s=3
r_s=1

- Comparison to classical hydrodynamics of the charged electron fluid

1) Euler equation $\frac{d\rho\bar{v}}{dt} = \frac{\partial\rho\bar{v}}{\partial t} + (\bar{v}\cdot\nabla)\rho\bar{v} = \bar{F}$ force density $(-\nabla p + \text{others})$

linearized eq. for electrons in electric field $m\frac{\partial n\bar{v}}{\partial t} = -\nabla p - en\bar{E}$

electron density

2) continuity equation $\frac{\partial n}{\partial t} + \nabla\cdot(n\bar{v}) = 0$

3) electric field due to deviations $\delta n = n - n_0$ from homog. density : $\nabla\cdot\bar{E} = -\frac{e(n-n_0)}{\varepsilon_0}$

assuming small $\delta n, \bar{E}$, and $\bar{v}$: $mn_0\frac{\partial\bar{v}}{\partial t} = -\frac{\partial p}{\partial n}\nabla n - en_0\bar{E}$ $\qquad \frac{\partial\delta n}{\partial t} + n_0\nabla\cdot\bar{v} = 0$

divergence + cont. eq.

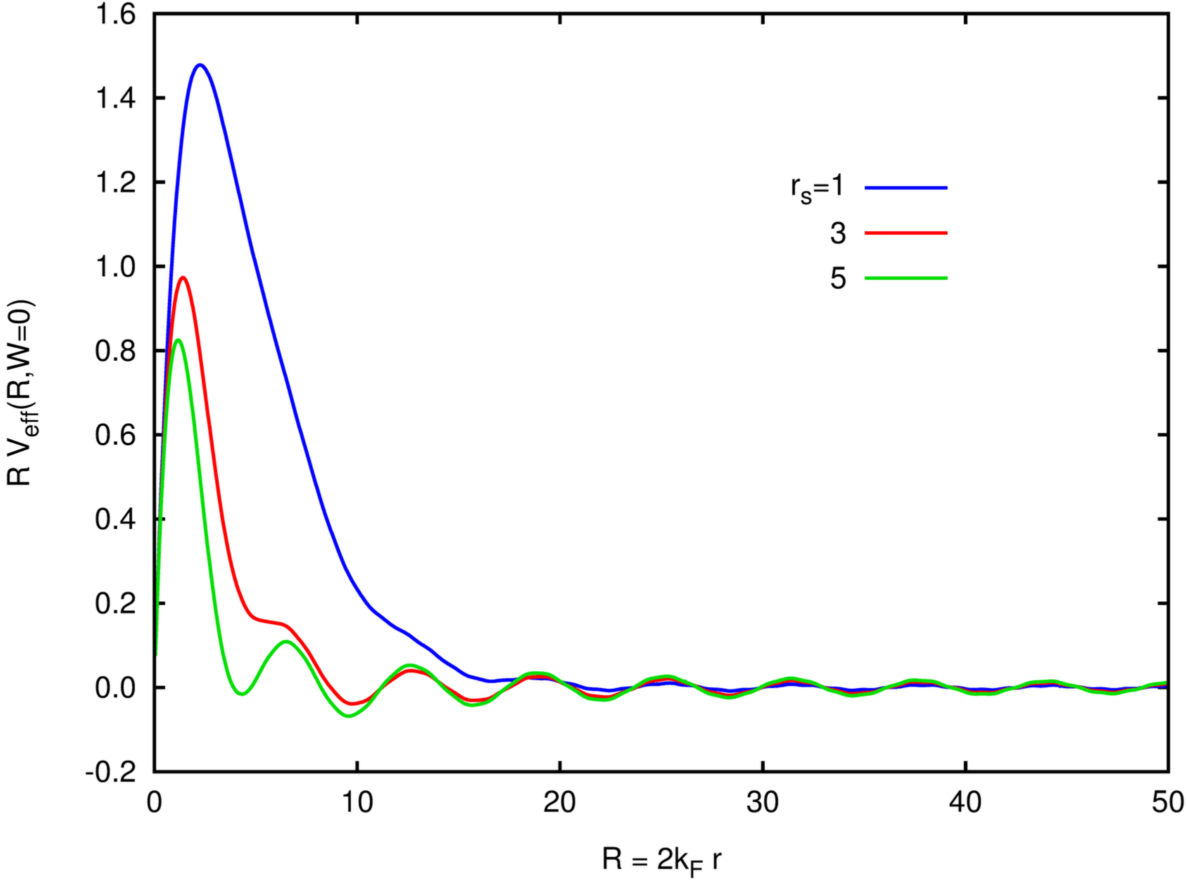
$$m\frac{\partial^2\delta n}{\partial t^2} - \frac{\partial p}{\partial n}\nabla^2\delta n - en_0\nabla\cdot\bar{E} = 0$$

last term $+\frac{e^2 n_0}{\varepsilon_0}\delta n$

wave-like solution

$$\delta n \sim e^{i(\bar{q}\cdot\bar{r} - \omega t)} \rightarrow \omega^2(q) = \frac{n_0 e^2}{m\varepsilon_0} + \frac{1}{m}\frac{\partial p}{\partial n}q^2$$

(quadratic dispersion of electron plasma waves)


1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
0
10
20
30
40
50
$R\ V_{eff}(R,W=0)$
$R = 2k_F\ r$
$r_s=1$
3
5

c) Quasiparticle renormalization

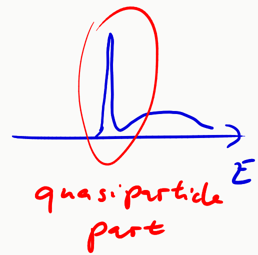
- Dyson's equation for GF continued to the real axis

$$G_{ret}(k,E) = \frac{1}{E-(\varepsilon_k-\mu)-\Sigma_{ret}(k,E)} \qquad \text{bare GF: } \frac{1}{E-(\varepsilon_k-\mu)+i0^+}$$

! E measured from the chemical potential μ (to be determined selfconsistently)

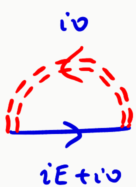
- spectral function

$$A(k,E) = -\frac{1}{\pi}\,\mathrm{Im}\,G_{ret}(k,E) = \frac{1}{\pi}\,\frac{-\mathrm{Im}\,\Sigma}{(E-\varepsilon_k+\mu-\mathrm{Re}\,\Sigma)^2+(\mathrm{Im}\,\Sigma)^2}$$

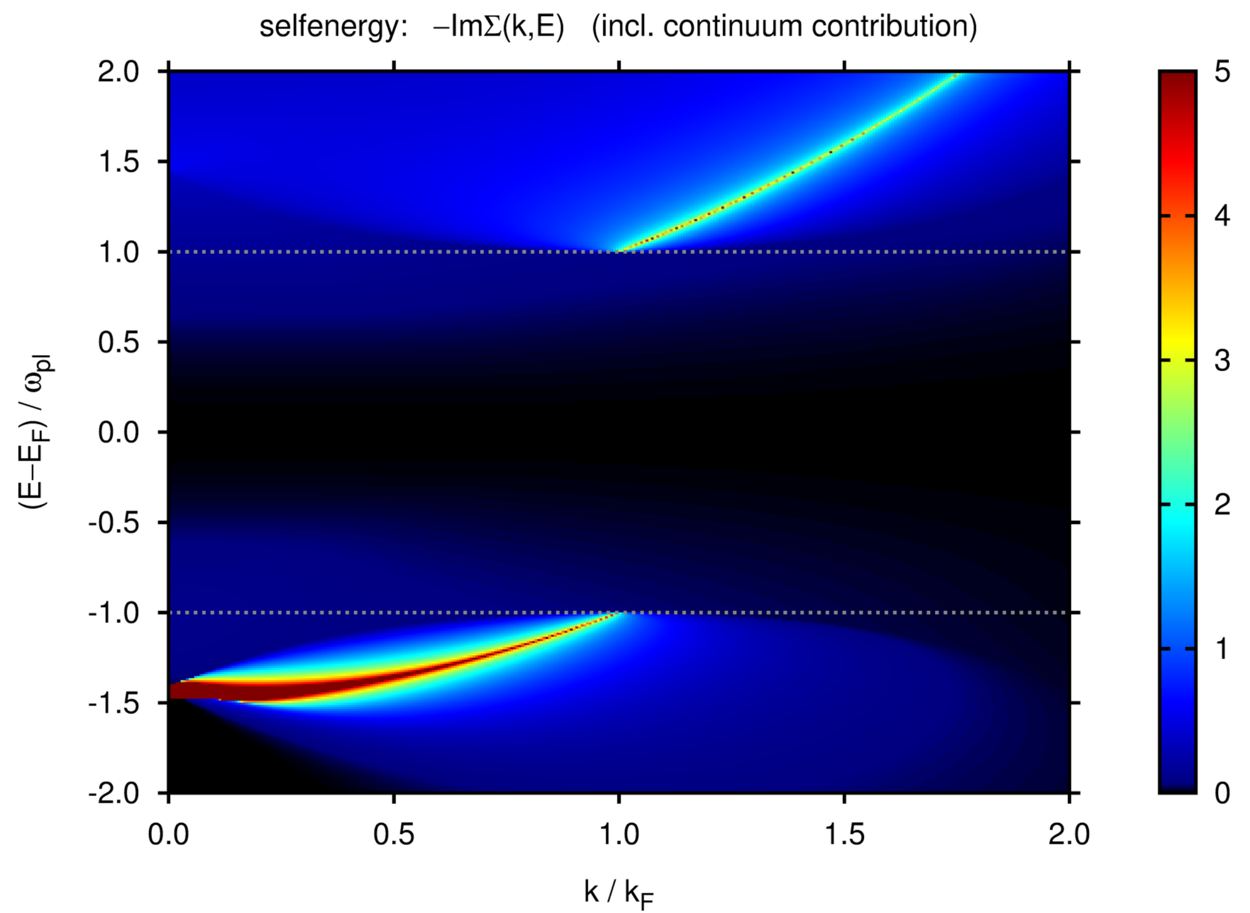


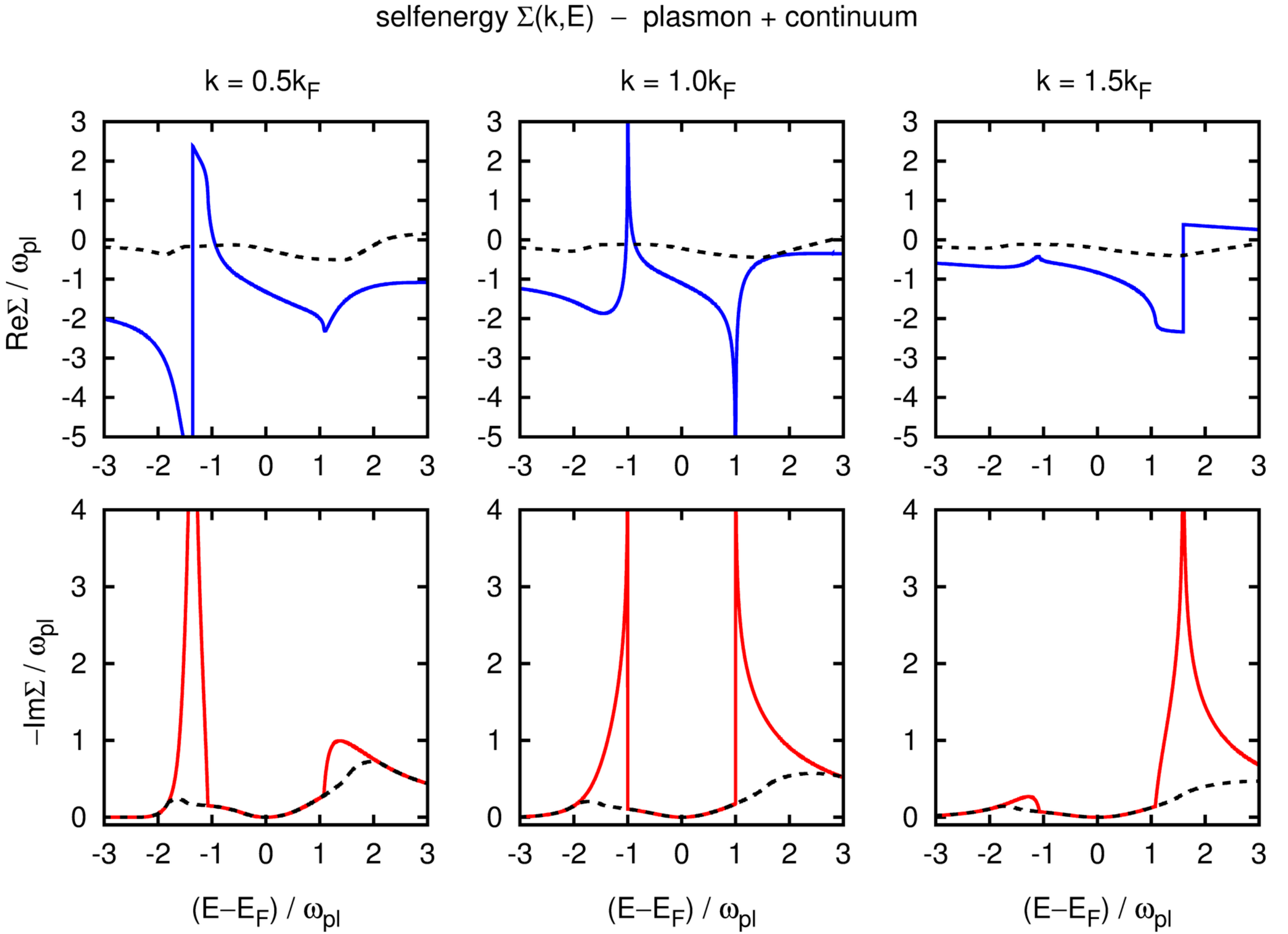
- RPA selfenergy

Σ =



contains plasmon contribution and a continuum one
- dominant
- characteristic energy shift $\hbar\omega_p$

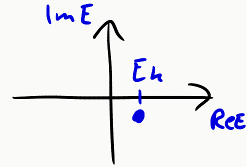

selfenergy: −ImΣ(k,E) (incl. continuum contribution)
(E−E_F) / ω_pl
k / k_F
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4
5



selfenergy Σ(k,E) – plasmon + continuum
k = 0.5k_F
k = 1.0k_F
k = 1.5k_F
ReΣ / ω_pl
−ImΣ / ω_pl
(E−E_F) / ω_pl

- pole of the GF determines the quasiparticle energy and lifetime

$$E_k - (\varepsilon_k - \mu) - \mathrm{Re}\,\Sigma(k, E_k) = 0 \qquad \text{(pole equation)}$$



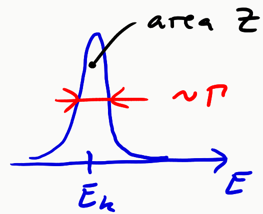
expansion around pole

$$A(k,E) \approx \frac{1}{\pi} \frac{-(\mathrm{Im}\,\Sigma)_{E_k}}{\left[\left(1 - \frac{\partial \mathrm{Re}\,\Sigma}{\partial E}\right)_{E_k} (E - E_k)\right]^2 + (\mathrm{Im}\,\Sigma)^2_{E_k}}$$

to be compared to

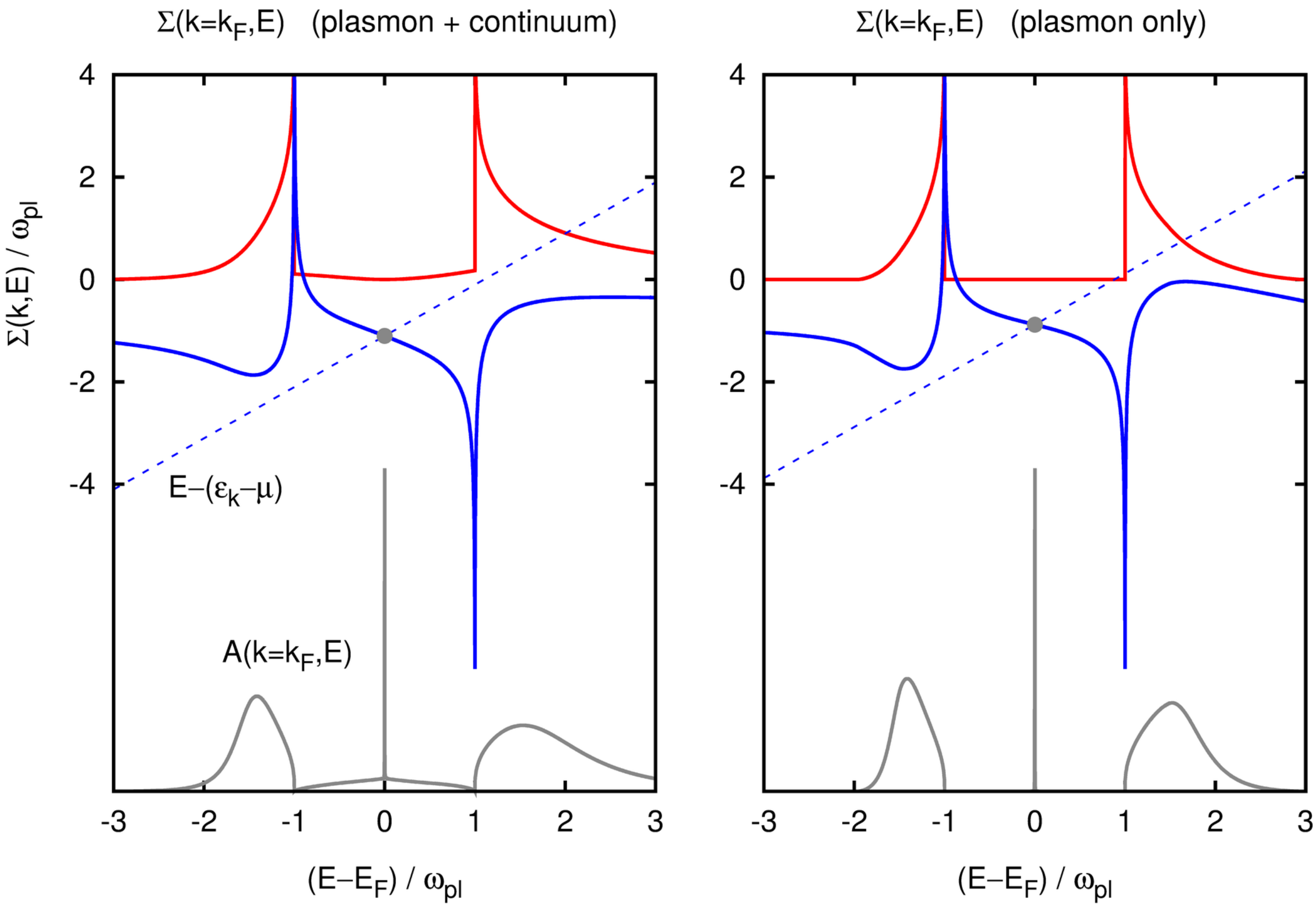
$$A(k,E) \approx Z \, \frac{1}{\pi} \frac{\Gamma}{(E - E_k)^2 + \Gamma^2} \qquad \text{goes to } Z\,\delta(E - E_k) \text{ for } \Gamma \to 0$$

$$Z = \left(1 - \frac{\partial \mathrm{Re}\,\Sigma}{\partial E}\bigg|_{E_k}\right)^{-1} \qquad \text{... quasiparticle weight}$$

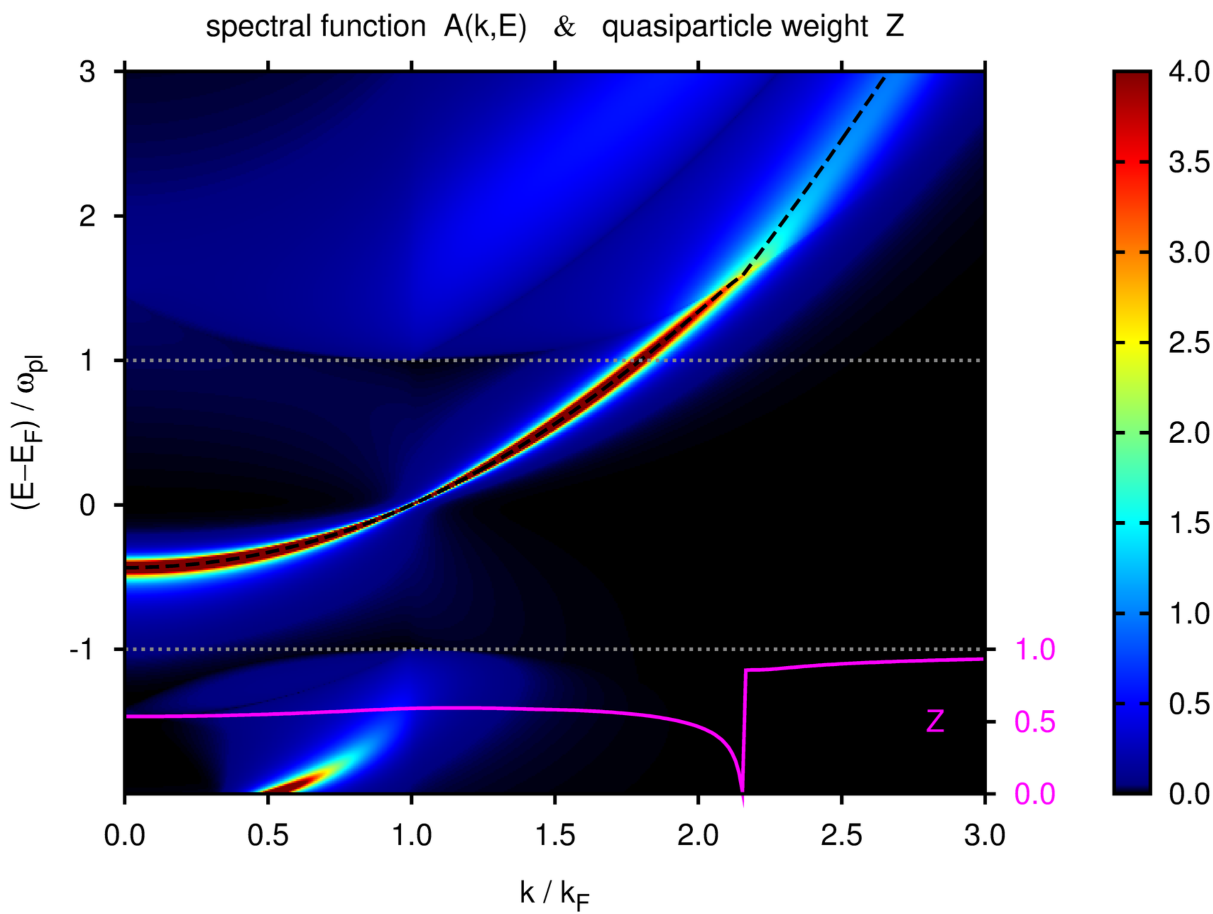


$$\Gamma = \tau^{-1} = \frac{1}{\hbar} Z \, |\mathrm{Im}\,\Sigma|_{E_k} \qquad \text{... quasiparticle decay rate (inverse lifetime)}$$

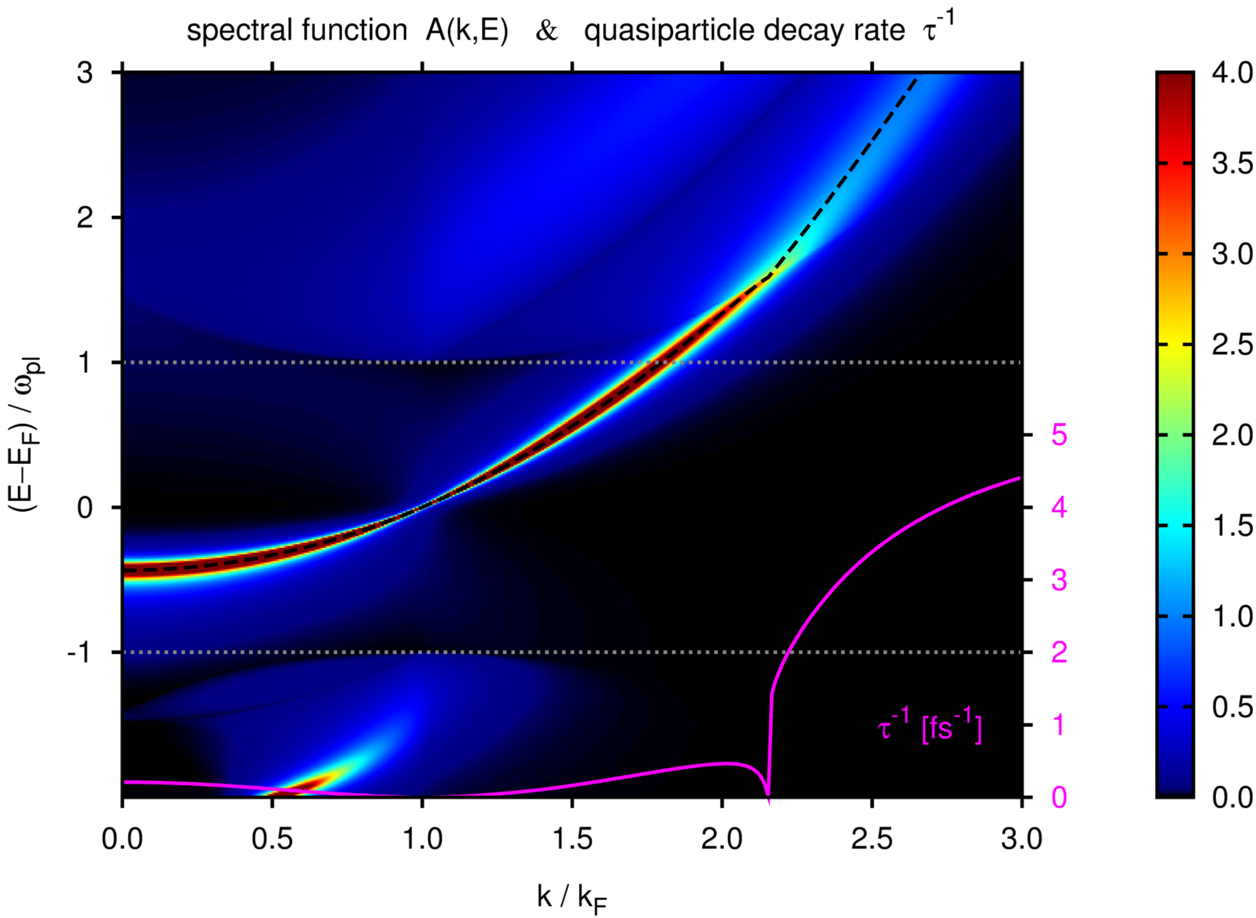
(& effective mass from $E_k \approx \frac{k_F}{m^*}(k - k_F)$)

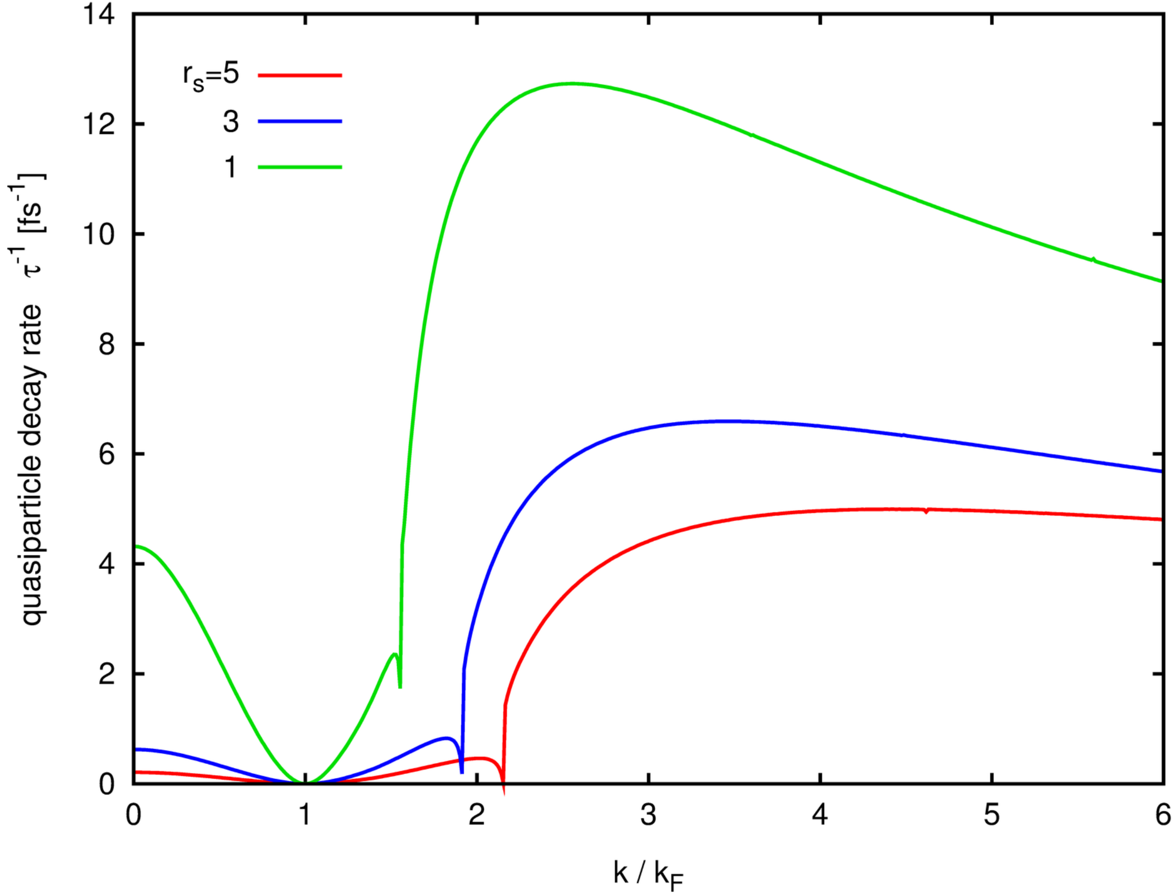


Σ(k=k_F,E) (plasmon + continuum)
Σ(k=k_F,E) (plasmon only)
Σ(k,E) / ω_pl
E−(ε_k−μ)
A(k=k_F,E)
(E−E_F) / ω_pl
(E−E_F) / ω_pl



spectral function A(k,E) & quasiparticle weight Z
(E−E_F) / ω_pl
k / k_F
Z
3
2
1
0
-1
0.0
0.5
1.0
1.5
2.0
2.5
3.0
1.0
0.5
0.0
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

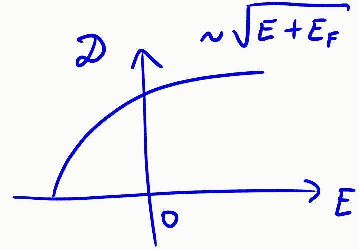

spectral function A(k,E) & quasiparticle decay rate τ^-1
(E–E_F) / ω_pl
k / k_F
τ^-1 [fs^-1]
3
2
1
0
-1
0.0
0.5
1.0
1.5
2.0
2.5
3.0
5
4
3
2
1
0
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0



quasiparticle decay rate τ^-1 [fs^-1]
k / k_F
r_s=5
3
1
0
2
4
6
8
10
12
14
0
1
2
3
4
5
6

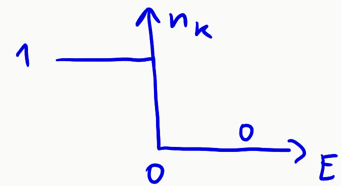
- density of states

$$\mathcal{D}(E) = \frac{1}{\Omega}\sum_{k\sigma} A(k,E) \qquad \text{bare} \quad \sum_{k\sigma}\delta[E-(\varepsilon_k-\mu)]$$



- occupation

$$n_{k\sigma} = \int_{-\infty}^{\infty} A(k,E)\, n_F(E)\, dE \overset{T=0}{\approx} \int_{-\infty}^{0} A(k,E)\, dE$$

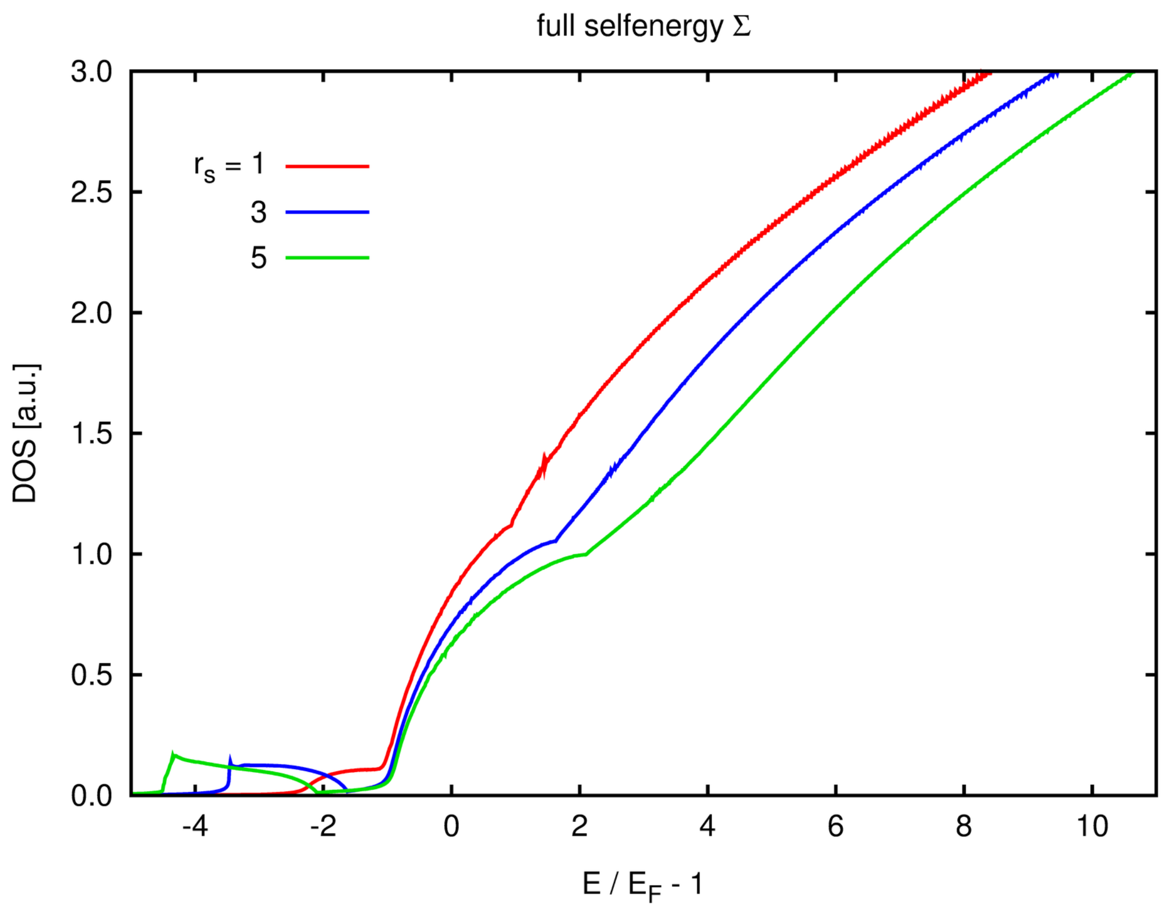


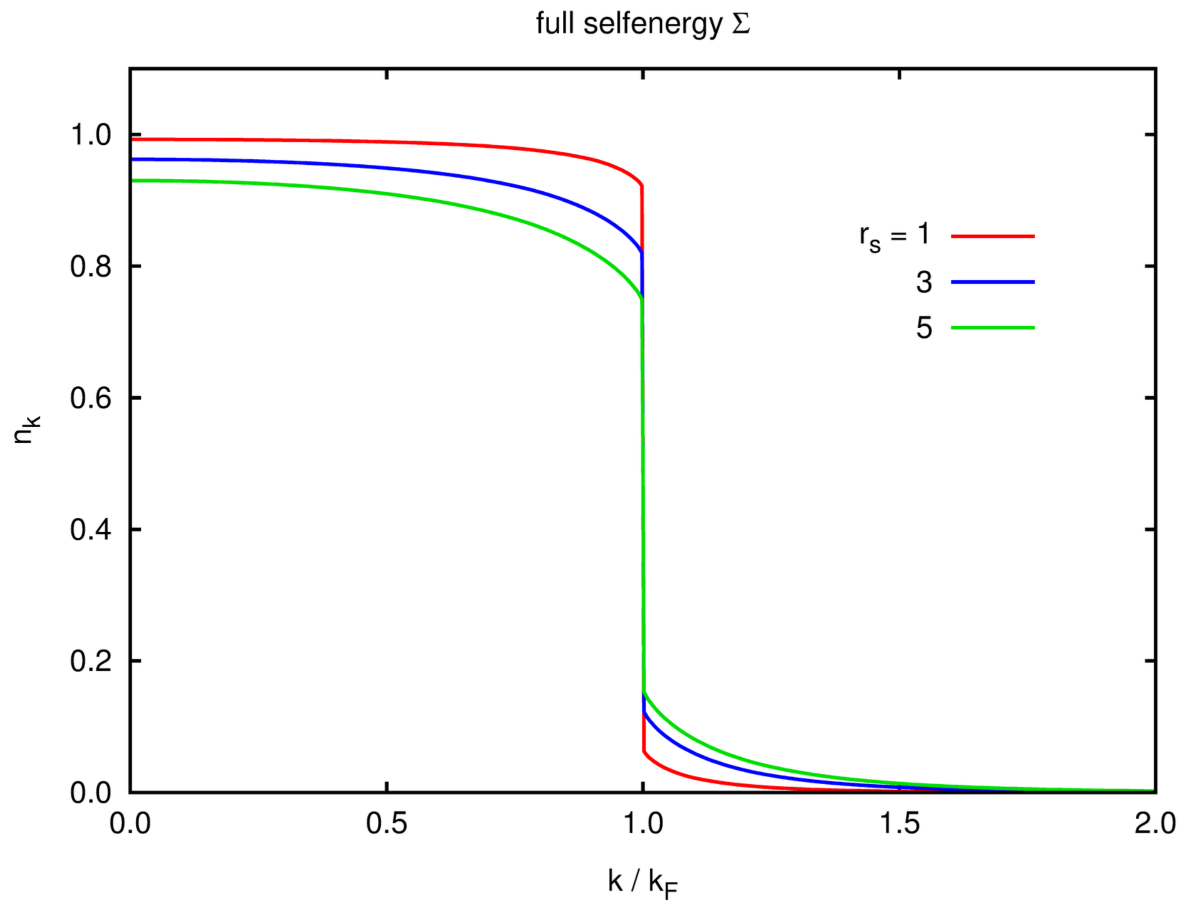
- chemical potential needs to be selfconsistently adjusted to have $n_0 = \frac{1}{\Omega}\sum_{k\sigma} n_{k\sigma}$

- occupation n_k shows a step at k_F indicating the Fermi surface

Luttinger theorem: volume enclosed by the Fermi surface remains constant

$\rightarrow$ in our spherically symmetric case, k_F is preserved


full selfenergy Σ
DOS [a.u.]
E / E_F - 1
r_s = 1
3
5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-4
-2
0
2
4
6
8
10


full selfenergy Σ
1.0
0.8
0.6
0.4
0.2
0.0
n_k
0.0
0.5
1.0
1.5
2.0
k / k_F
r_s = 1
3
5