

# Introduction to Many-body Theory III

## Part III: Linear response and examples

- Conserving approximations and TDDFT
- The 2-particle Green's function and optical spectra
- Linear response
- Examples: Time-dependent screening in an electron gas

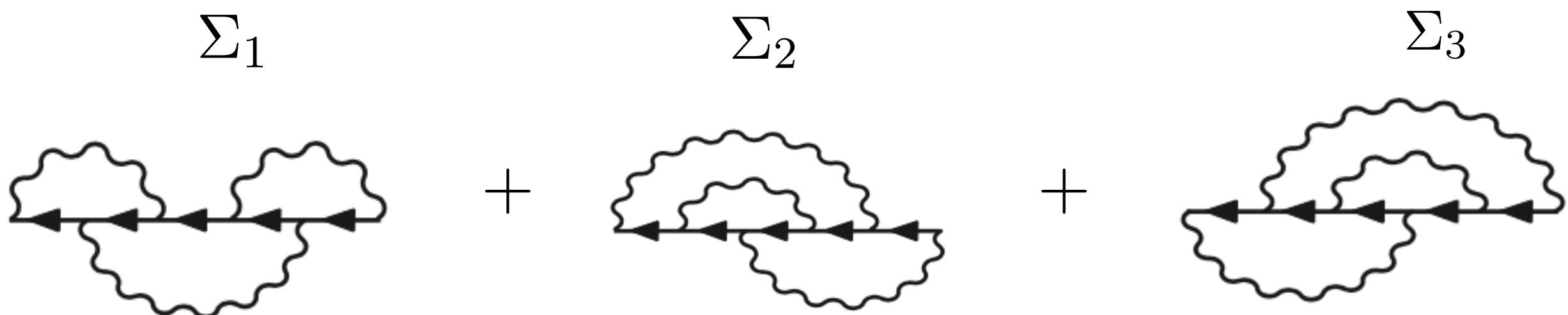
# The Phi-functional

The self-energy can be written as the functional derivative of a so-called Phi-functional.

$$\Sigma(1, 2) = \frac{\delta \Phi}{\delta G(2, 1)}$$


$$\Phi_D[G] = \frac{1}{2} \text{ (diagram: a loop with a wavy line and two straight lines with arrows) }$$

$$\Sigma_D[G](1, 2) = \frac{\delta \Phi_D}{\delta G(2, 1)} = \Sigma_1 + \Sigma_2 + \Sigma_3$$



The Phi-functional can be defined as

$$\Phi[G] = \sum_{n=1}^{\infty} \frac{1}{2n} \int d1 d2 \Sigma^{(n)}[G](1, 2) G(2, 1)$$



Proof:  
Textbook Stefanucci, RvL  
"Nonequilibrium many-body  
theory for quantum systems"

In our example

$$\frac{1}{2 \times 3} \left( \int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G \right) = \frac{1}{2} \text{ (diagram: a loop with a wavy line and two straight lines with arrows) }$$

Approximate self-energies need not be Phi-derivable, for example

$$\Sigma(1, 2) = \text{Diagram}$$

is not a Phi-derivable self-energy

Theorem (Baym): If a self-energy is Phi-derivable and we solve the Dyson equation self-consistently with this self-energy then the conserving laws of energy, momentum and particle number are satisfied

The theorem is a consequence of the invariance of the Phi-functional under space and time translations as well as gauge transformations

It is a many-body version of the Noether theorem

For example: self-consistent GW is a Phi-derivable approximation



# Conserving approximations in TDDFT

Ulf von Barth et al.

“Conserving approximations in TDDFT”, Phys.Rev.B72, 235109 (2005)

We define the Hartree-exchange-correlation action functional by

$$A_{\text{Hxc}}[n] = -i\Phi[G_s[n]]$$

Theorem I: The Hxc potential

$$v_{\text{Hxc}}[n](1) = \frac{\delta A_{\text{Hxc}}}{\delta n(1)}$$

satisfies the linearised Sham-Schlüter equation with a Phi-derivable self-energy

Proof:

$$v_{\text{Hxc}}[n](1) = \frac{\delta A_{\text{Hxc}}}{\delta n(1)} = -i \int d2d3d4 \frac{\delta \Phi}{\delta G_s(3,2)} \frac{\delta G_s(3,2)}{\delta v_s(4)} \frac{\delta v_s(4)}{\delta n(1)}$$



inverse density response function

$$= -i \int d2d3d4 \Sigma[G_s](2,3) G_s(3,4) G_s(4,2) \chi_s^{-1}(4,1)$$

$$\rightarrow \int d1 \chi_s(4,1) v_{\text{Hxc}}(1) = -i \int d2d3d4 G_s(4,2) \Sigma[G_s](2,3) G_s(3,4)$$

which is precisely the LSS equation



Theorem 2: The Hxc potential from the last equation satisfies the zero-force theorem

$$0 = \int d\mathbf{x} n(\mathbf{x}, t) \nabla v_{\text{Hxc}}(\mathbf{x}, t)$$

Proof:

We use the relation  $-i\delta\Phi = \int d1 v_{\text{Hxc}}(1) \delta n(1)$

and use that the Phi-functional is invariant under the coordinate change  $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}(t)$

To first order in  $\mathbf{R}(t)$  we have  $\delta n(\mathbf{r}, t) = n(\mathbf{r} + \mathbf{R}(t), t) - n(\mathbf{r}, t) = \mathbf{R}(t) \cdot \nabla n(\mathbf{r}, t)$

and therefore

$$0 = -i\delta\Phi = \int d1 v_{\text{Hxc}}(1) \delta n(1) = \int dt_1 d\mathbf{r}_1 v_{\text{Hxc}}(\mathbf{r}_1, t_1) \mathbf{R}(t_1) \cdot \nabla n(\mathbf{r}_1, t_1)$$

but since this is valid for arbitrary  $\mathbf{R}(t)$  this implies

$$0 = \int d\mathbf{r} v_{\text{xc}}(\mathbf{r}, t) \nabla n(\mathbf{r}, t) \quad \longrightarrow \quad 0 = \int d\mathbf{x} n(\mathbf{x}, t) \nabla v_{\text{Hxc}}(\mathbf{x}, t)$$

# The 2-particle Green's function

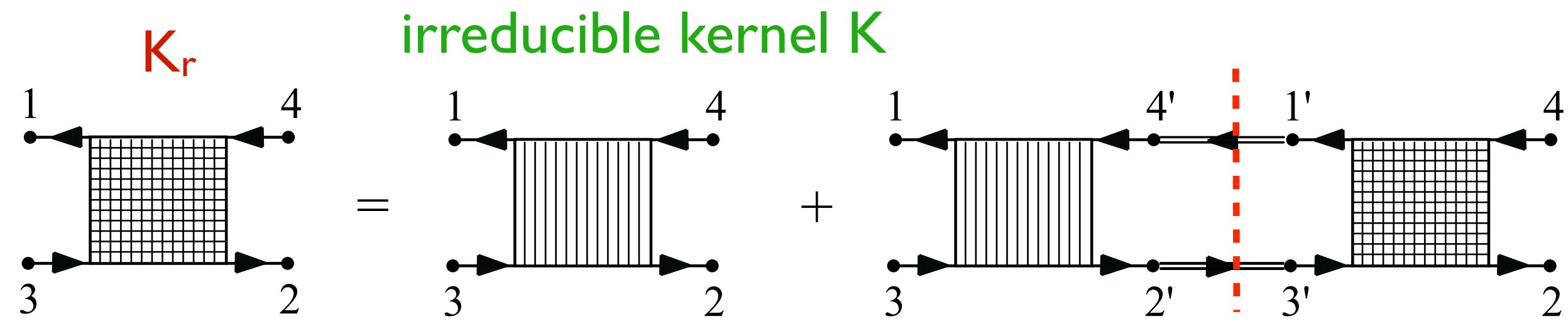
We can expand the two-particle Green's function using Wick's theorem

$$G_2(a, b; c, d)$$

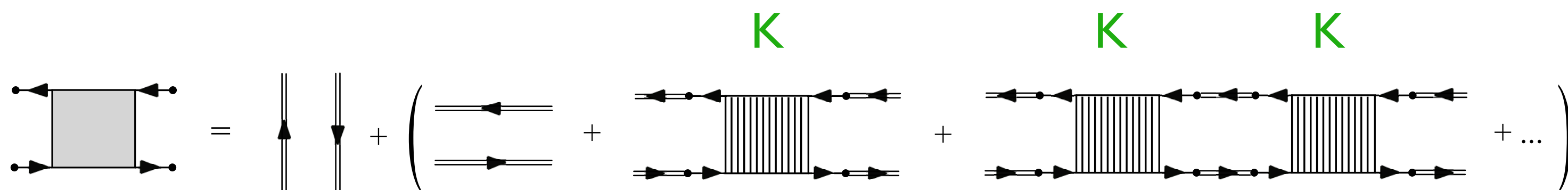
$$= \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int v(1; 1') \dots v(k; k') \begin{vmatrix} G_0(a; c) & G_0(a; d) & \dots & G_0(a; k'^+) \\ G_0(b; c) & G_0(b; d) & \dots & G_0(b; k'^+) \\ \vdots & \vdots & \ddots & \vdots \\ G_0(k'; c) & G_0(k'; d) & \dots & G_0(k'; k'^+) \end{vmatrix}_{\pm}}{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int v(1; 1') \dots v(k; k') \begin{vmatrix} G_0(1; 1^+) & G_0(1; 1'^+) & \dots & G_0(1; k'^+) \\ G_0(1'; 1^+) & G_0(1'; 1'^+) & \dots & G_0(1'; k'^+) \\ \vdots & \vdots & \ddots & \vdots \\ G_0(k'; 1^+) & G_0(k'; 1'^+) & \dots & G_0(k'; k'^+) \end{vmatrix}_{\pm}}$$

Again only connected diagrams contribute. In the same way as before non-connected diagrams cancel and we can expand in G-skeletons by removing self-energy insertions



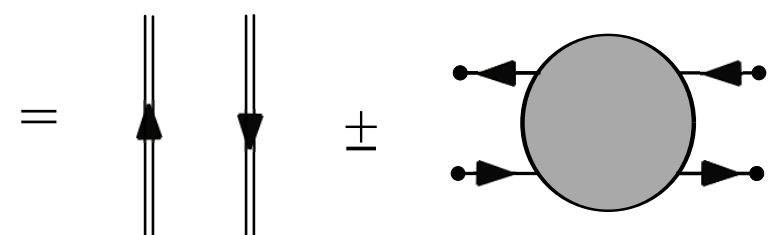


$$K_r(1, 2; 3, 4) = K(1, 2; 3, 4) \pm \int K(1, 2'; 3, 4') G(4'; 1') G(3'; 2') K_r(1', 2; 3', 4)$$

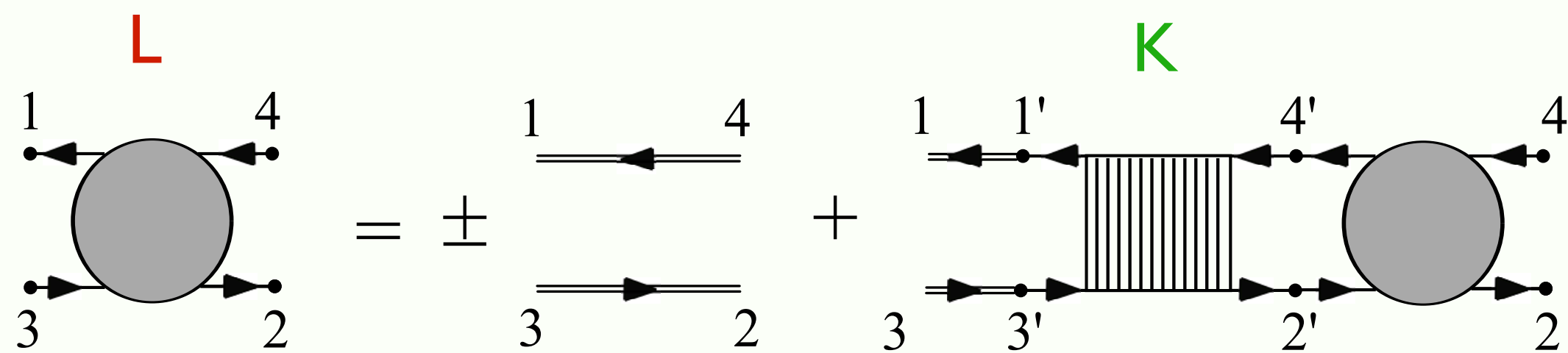


$G_2$

$L$



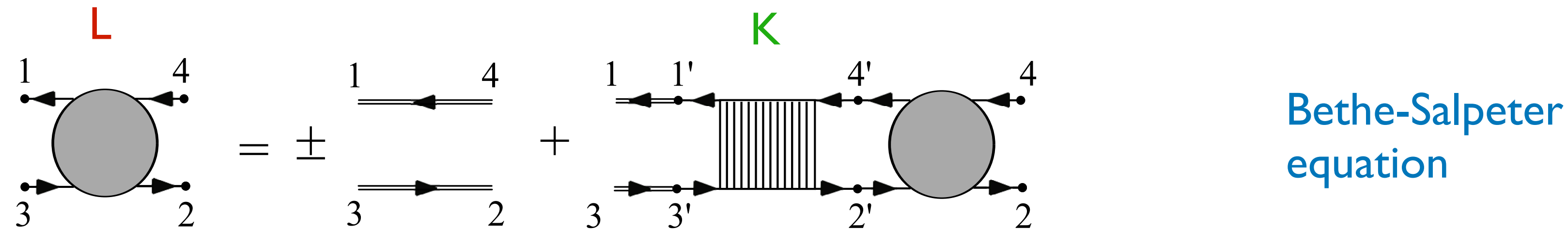
$$L(1, 2; 3, 4) \equiv \pm [G_2(1, 2; 3, 4) - G(1; 3)G(2; 4)]$$



Bethe-Salpeter equation

$$L(1, 2; 3, 4) = G(1; 4)G(2; 3) \pm \int G(1; 1')G(3'; 3)K(1', 2'; 3', 4')L(4', 2; 2', 4)$$

To find the 2-particle Green's function we have to solve the Bethe-Salpeter equation



$$L(1, 2; 3, 4) = G(1; 4)G(2; 3) \pm \int G(1; 1')G(3'; 3)K(1', 2'; 3', 4')L(4', 2; 2', 4)$$

If we expand the self-energy in G-skeletonic diagrams then the following important relation is valid

$$K(1, 2; 3, 4) = \pm \frac{\delta \Sigma(1; 3)}{\delta G(4; 2)}$$

One can prove this diagrammatically

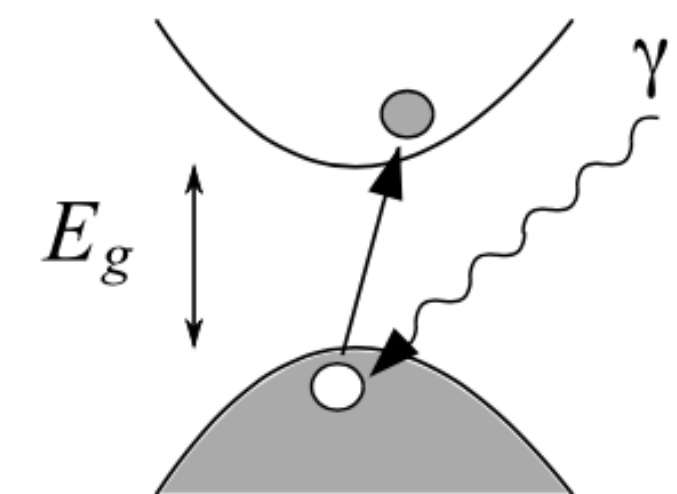
Let us give an example

$$\Sigma_{\text{HF}}(1; 3) = \text{[Diagram 1]} + \text{[Diagram 2]} \xrightarrow{\text{K}} \pm \frac{\delta \Sigma_{\text{HF}}(1; 3)}{\delta G(4; 2)} = \text{[Diagram 3]} + \text{[Diagram 4]}$$

K

The Bethe-Salpeter equation is then given by

This equation is relevant for describing excitons in semiconductors



# Linear response functions

$$\langle \hat{n}(\mathbf{x}, t) \rangle = \frac{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \hat{n}(\mathbf{x}, t) \right\}}{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \right\}}$$

If we make the variation  $\hat{H}(z) \rightarrow \hat{H}(z) + \delta\hat{V}(z)$  then  $\delta\hat{V}(z) = \int d\mathbf{x} \hat{n}(\mathbf{x}) \delta v(\mathbf{x}z)$

$$\delta \langle \hat{n}(\mathbf{x}, t) \rangle = -i \int_{\gamma} dz_1 \frac{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \hat{n}(\mathbf{x}, t) \delta\hat{V}(z_1) \right\}}{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \right\}} + i \langle \hat{n}(\mathbf{x}, t) \rangle \int_{\gamma} dz_1 \frac{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \delta\hat{V}(z_1) \right\}}{\text{Tr } \mathcal{T} \left\{ e^{-i \int_{\gamma} d\bar{z} \hat{H}(\bar{z})} \right\}}$$

which can be rewritten as

$$\delta n(1) = \int d2 \chi(1, 2) \delta v(2)$$

$$\chi(1, 2) = -i [ \langle \mathcal{T} \{ \hat{n}_H(1) \hat{n}_H(2) \} \rangle - n(1)n(2) ]$$



There is a close relation between the density response function and the Bethe-Salpeter equation. We have

$$\begin{aligned} L(1, 2; 1', 2') &= - [G_2(1, 2; 1', 2') - G(1, 1')G(2, 2')] \\ &= \langle \mathcal{T} \{ \hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}_H^\dagger(2')\hat{\psi}_H^\dagger(1') \} \rangle - \langle \mathcal{T} \{ \hat{\psi}_H(1)\hat{\psi}_H^\dagger(1') \} \rangle \langle \mathcal{T} \{ \hat{\psi}_H(2)\hat{\psi}_H^\dagger(2') \} \rangle \end{aligned}$$

and therefore

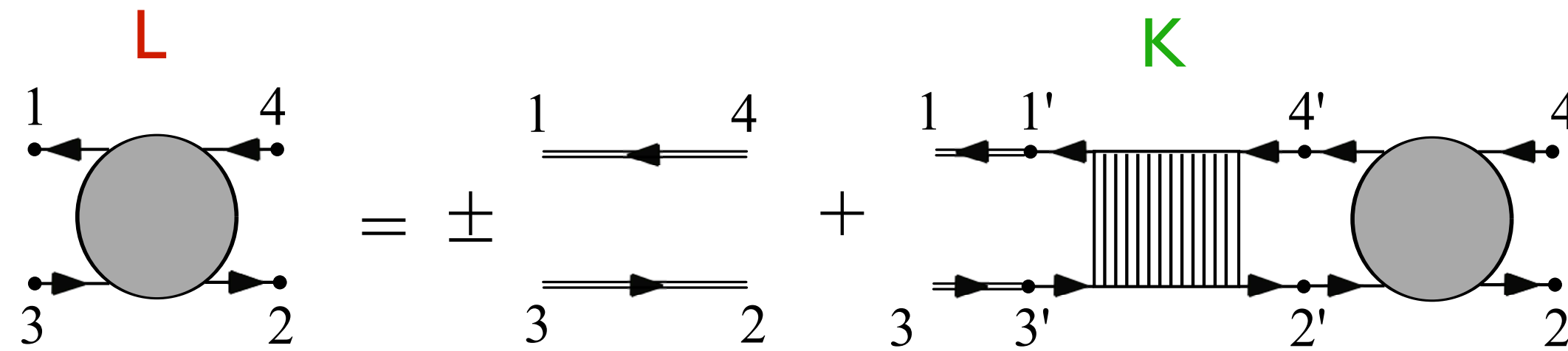
$$\chi(1, 2) = -i [ \langle \mathcal{T} \{ \hat{n}_H(1)\hat{n}_H(2) \} \rangle - n(1)n(2) ] = -i L(1, 2; 1^+, 2^+)$$

In combination with the Bethe-Salpeter equation we can then further derive that

$$\chi(1, 2) = P(1, 2) + \int d3d4 P(1, 3) w(3, 4) \chi(4, 2)$$

A diagrammatic expansion of the polarisability therefore directly gives an approximation for the density response function

# Random Phase Approximation and plasmons

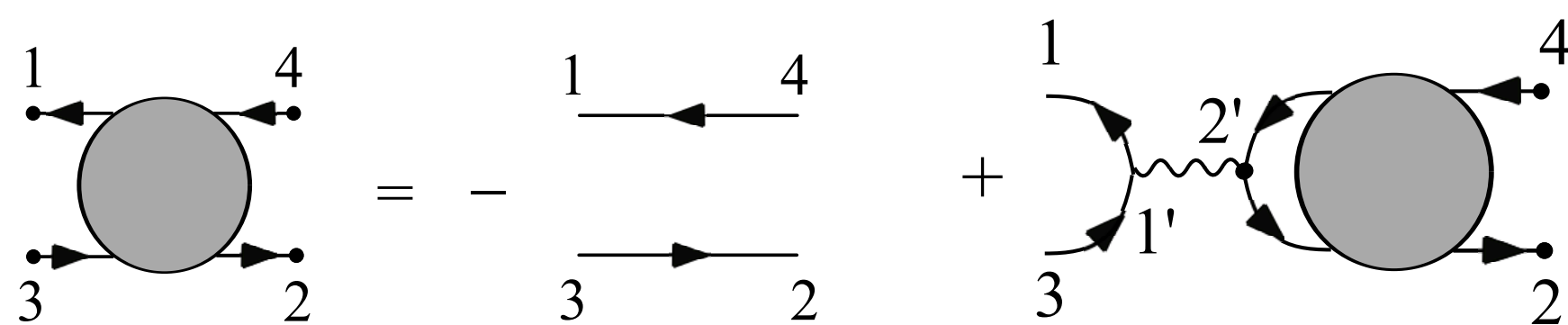


Bethe-Salpeter equation

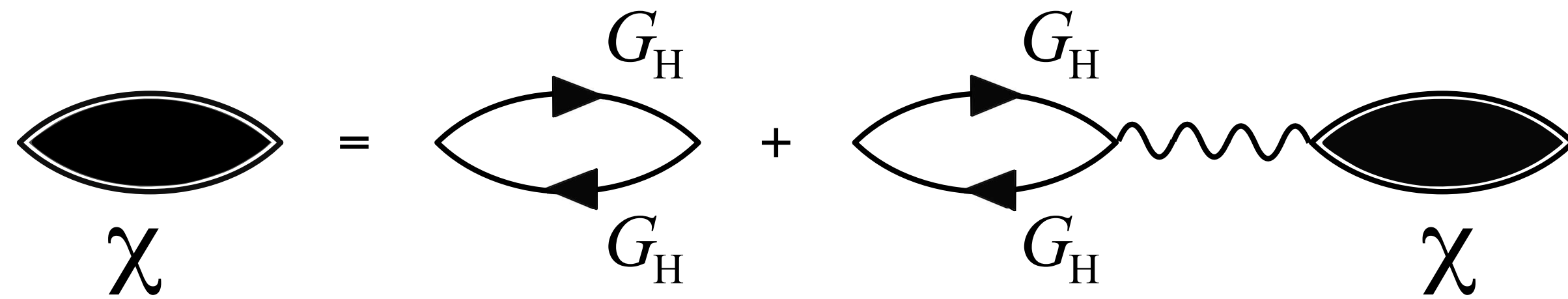
If we calculate the Bethe-Salpeter from the Hartree self-energy

$$\Sigma_H = \text{[Hartree self-energy diagram]} \longrightarrow K_H(1, 2; 3, 4) = -\frac{\delta \Sigma_H(1, 3)}{\delta G(4, 2)} = \text{[Hatched box diagram]}$$

then the Bethe-Salpeter equation becomes



From  $\chi(1, 2) = -i L(1, 2; 1^+, 2^+)$  it then follows



if we take the retarded component of this expression and Fourier transform then we find

$$\chi^R(\mathbf{x}_1, \mathbf{x}_2; \omega) = \chi_0^R(\mathbf{x}_1, \mathbf{x}_2; \omega) + \int d\mathbf{x}_3 d\mathbf{x}_4 \chi_0^R(\mathbf{x}_1, \mathbf{x}_3; \omega) v(\mathbf{x}_3, \mathbf{x}_4) \chi^R(\mathbf{x}_4, \mathbf{x}_2; \omega)$$

This approximation for the density response function is also known as the **Random Phase Approximation (RPA)**.

A better name is the **Time-Dependent Hartree Approximation** (it amounts to TDDFT with zero xc-kernel)

Let us now take the case of the homogeneous electron gas. Since the system is translational invariant we can write

$$\sum_{\sigma\sigma'} \chi^{\text{R}}(\mathbf{x}, \mathbf{x}'; \omega) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \chi^{\text{R}}(\mathbf{p}, \omega)$$

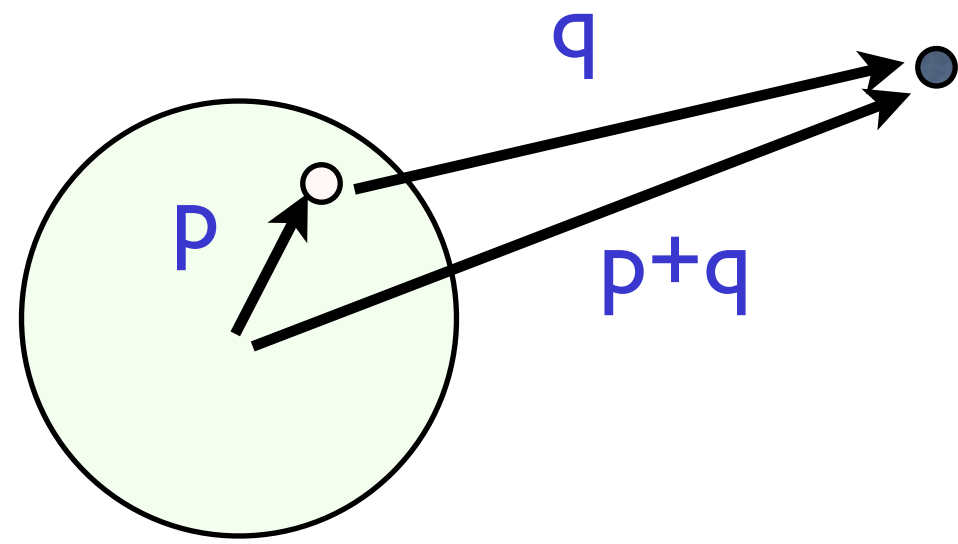
$$\chi^{\text{R}}(\mathbf{q}, \omega) = \frac{\chi_0^{\text{R}}(\mathbf{q}, \omega)}{1 - \tilde{v}_{\mathbf{q}} \chi_0^{\text{R}}(\mathbf{q}, \omega)}, \quad \tilde{v}_{\mathbf{q}} = \frac{4\pi}{q^2} \quad \leftarrow \begin{array}{l} \text{Fourier transform} \\ \text{Coulomb potential} \end{array}$$



The RPA response function has poles at the poles of  $\chi_0(\mathbf{q}, \omega)$  and when

$$1 - \tilde{v}_{\mathbf{q}} \chi_0(\mathbf{q}, \omega) = 0$$

The extra pole corresponding to this condition is known as the plasmon and corresponds to a collective mode of the electron gas

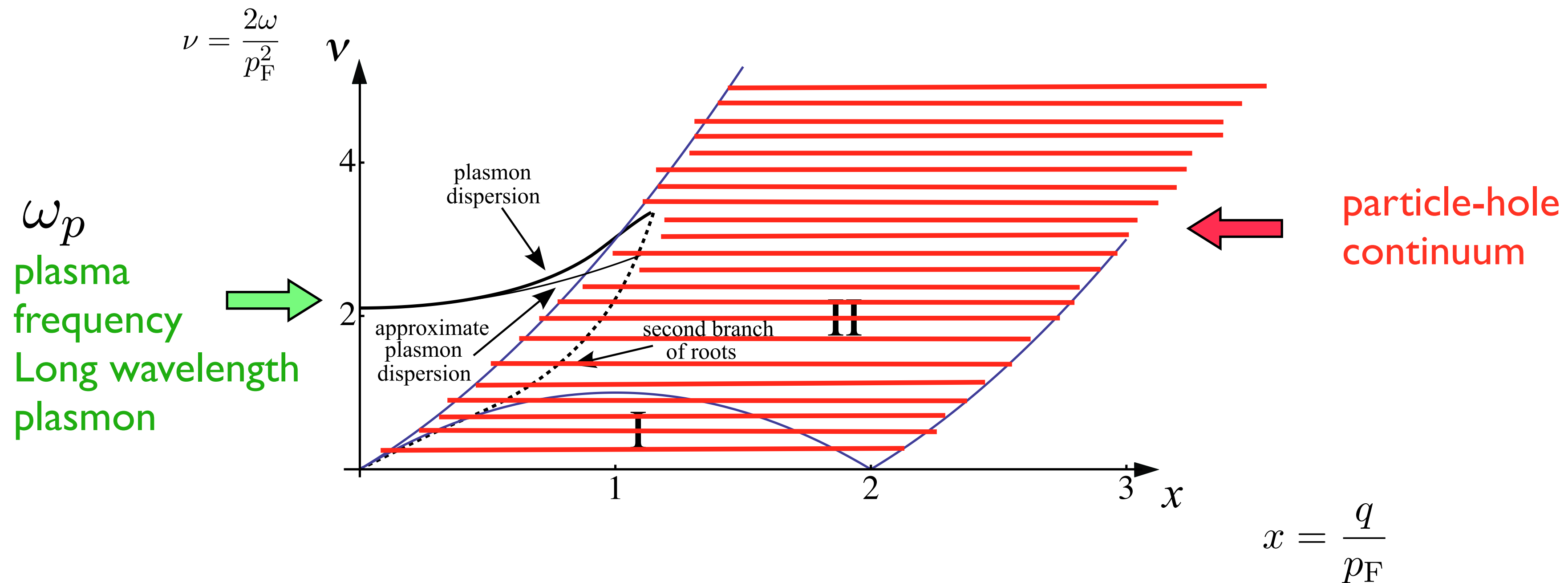


Fermi sphere  
with radius  $p_F$

$$\epsilon = \frac{(\mathbf{p} + \mathbf{q})^2}{2} - \frac{\mathbf{p}^2}{2} = \frac{\mathbf{q}^2}{2} + |\mathbf{p}||\mathbf{q}| \cos \theta$$

$$\frac{q^2}{2} - q p_F \leq \epsilon \leq \frac{q^2}{2} + q p_F \quad q = |\mathbf{q}|$$

The particle-hole excitations lie between  
two parabolas in the  $q$ - $\omega$  plane



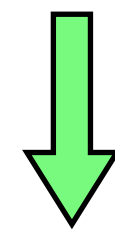
Sudden creation of a positive charge (such as in the creation of a core-hole)

$$\delta V(\mathbf{x}, t) = \theta(t) \frac{Q}{r} = \int \frac{d\mathbf{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i\mathbf{q}\cdot\mathbf{r} - i\omega t} \delta V(\mathbf{q}, \omega)$$

$$\delta V(\mathbf{q}, \omega) = \frac{4\pi Q}{q^2} \frac{i}{\omega + i\eta} = \tilde{v}_{\mathbf{q}} Q \frac{i}{\omega + i\eta}.$$

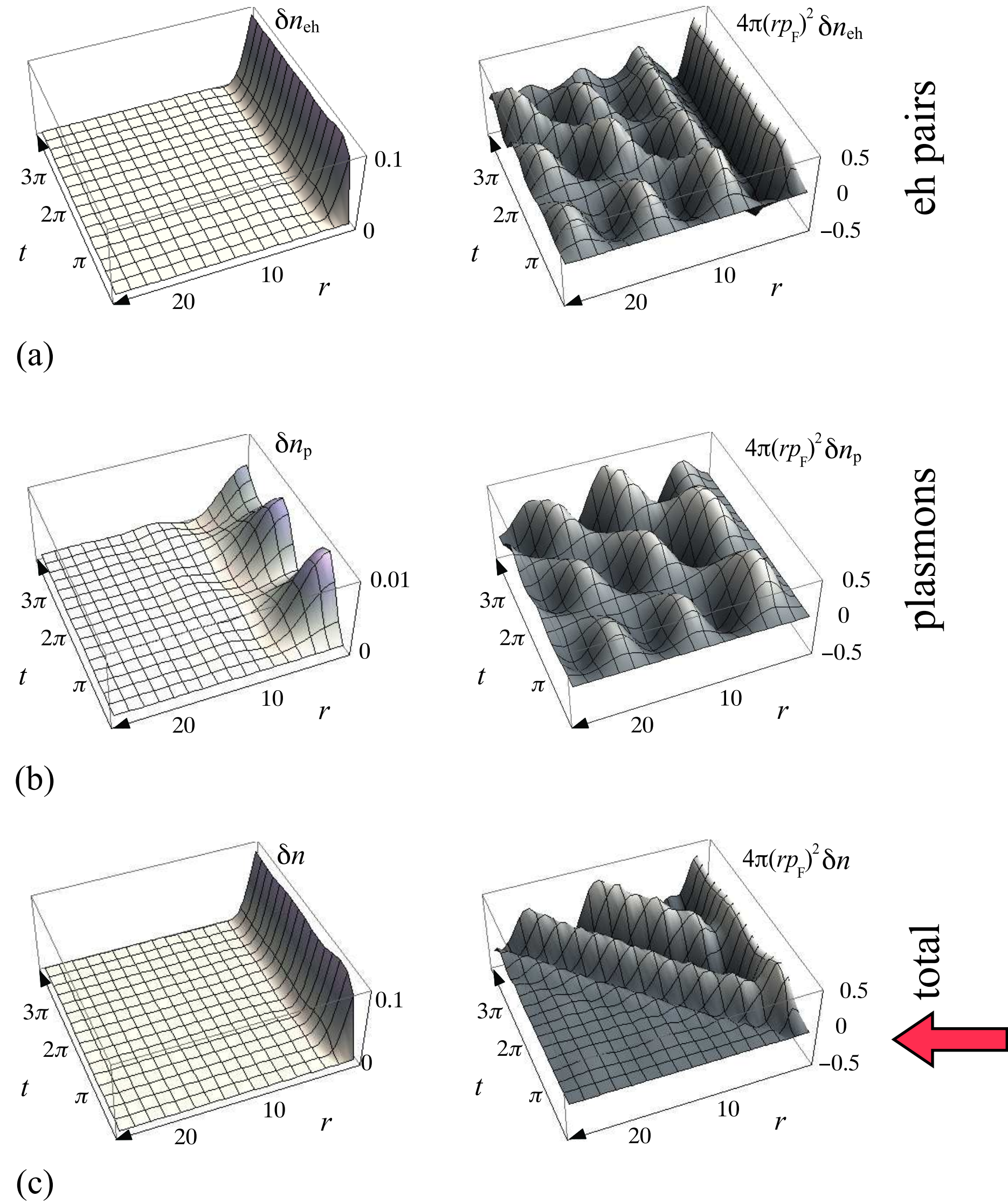
We can calculate the induced density change from the RPA response function. A few manipulations lead to

$$\delta n(\mathbf{r}, t) = -\frac{16\pi Q}{(2\pi)^4} \frac{1}{r} \int_0^\infty dq q \sin qr \int_0^\infty d\omega \operatorname{Im} \chi^{\text{RPA}}(q, \omega) \tilde{v}_{\mathbf{q}} \frac{1 - \cos \omega t}{\omega}$$



The integral can be split into a contribution from particle-hole excitations and a contribution from the plasmon





The positive charge is screened at a time-scale of the inverse plasmon frequency

Figure 15.7: This figure shows the 3D plot of the transient density in an electron gas with  $r_s = 3$  induced by the sudden creation of a point-like positive charge  $Q = 1$  in the origin at  $t = 0$ . The contribution due to the excitation of electron-hole pairs (a) and plasmons (b) is, for clarity, multiplied by  $4\pi(rp_F)^2$  in the plots to the right. Panel (c) is simply the sum of the two contributions. Units:  $r$  is in units of  $1/p_F$ ,  $t$  is in units of  $1/\omega_p$  and all densities are in units of  $p_F^3$ .



In the long time limit we have

$$\delta n_s(\mathbf{r}) \equiv \lim_{t \rightarrow \infty} \delta n(\mathbf{r}, t) = -\frac{Q}{2\pi^2} \frac{1}{r} \int_0^\infty dq q \sin(qr) \tilde{v}_{\mathbf{q}} \chi^R(\mathbf{q}, 0)$$

has spatial oscillations  
known as Friedel oscillations

Suppose now that  $Q = q = -1$  is the same as the electron charge. The total density change due to this test charge is

$$q \delta n_{\text{tot}}(\mathbf{r}) = q[\delta(\mathbf{r}) + \delta n_s(\mathbf{r})]$$

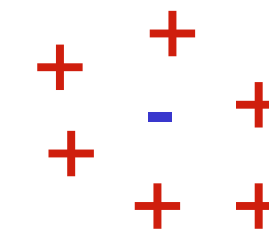
The interaction energy between this charge and a generic electron is

$$e_{\text{int}}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \delta n_{\text{tot}}(\mathbf{r}')$$

$$e_{\text{int}}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \left[ \delta(\mathbf{r}) + \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}'} \tilde{v}_{\mathbf{q}} \chi^R(\mathbf{q}, 0) \right]$$

$$= \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} [\tilde{v}_{\mathbf{q}} + \tilde{v}_{\mathbf{q}}^2 \chi^R(\mathbf{q}, 0)]$$

$$= \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} W^R(\mathbf{q}, 0) \xrightarrow{r \rightarrow \infty} \frac{e^{-r/\lambda_{\text{TF}}}}{r}$$



In the static limit  $W$  describes the interaction between a test charge and an electron

## Linear response: Take home message

- We can derive a diagrammatic expansion for the linear response function from the diagrammatic rules for the 2-particle Green's function
- The linear response function gives direct information on neutral excitation spectra such as measured in optical absorption experiments
- The random phase approximation to the linear response function describes the phenomena of plasmon excitation in metallic systems
- The screening of a an added charge in the electron gas happens at a time-scale of the inverse plasmon frequency

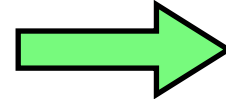
## Spectral properties of an electron gas : GW

We have seen that the spectral function describes the energy distribution of excitations upon addition or removal of an electron. We therefore expect to see both plasmon and particle-hole excitations when we do a photo-emission experiment on an electron gas ( or electron gas like metals such a sodium )

### Dyson equation

$$G^R(\mathbf{q}, \omega) = g^R(\mathbf{q}, \omega) + g^R(\mathbf{q}, \omega)\Sigma^R(\mathbf{q}, \omega)G^R(\mathbf{q}, \omega)$$

$$g^R(\mathbf{q}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{q}} + i\eta} \quad \epsilon_{\mathbf{q}} = \frac{|\mathbf{q}|^2}{2}$$

  $G^R(\mathbf{q}, \omega) = \frac{g^R(\mathbf{q}, \omega)}{1 - g^R(\mathbf{q}, \omega)\Sigma^R(\mathbf{q}, \omega)} = \frac{1}{\omega - \epsilon_{\mathbf{q}} - \Sigma^R(\mathbf{q}, \omega)}$

We calculate the self-energy in the GW approximation using noninteracting Green's function we find

$$\Sigma^{\lessgtr}(p, \omega) = \frac{i}{(2\pi)^3 p} \int d\omega' \int_0^\infty dk k G^{\lessgtr}(k, \omega') \int_{|k-p|}^{k+p} dq q W^{\gtrless}(q, \omega' - \omega)$$

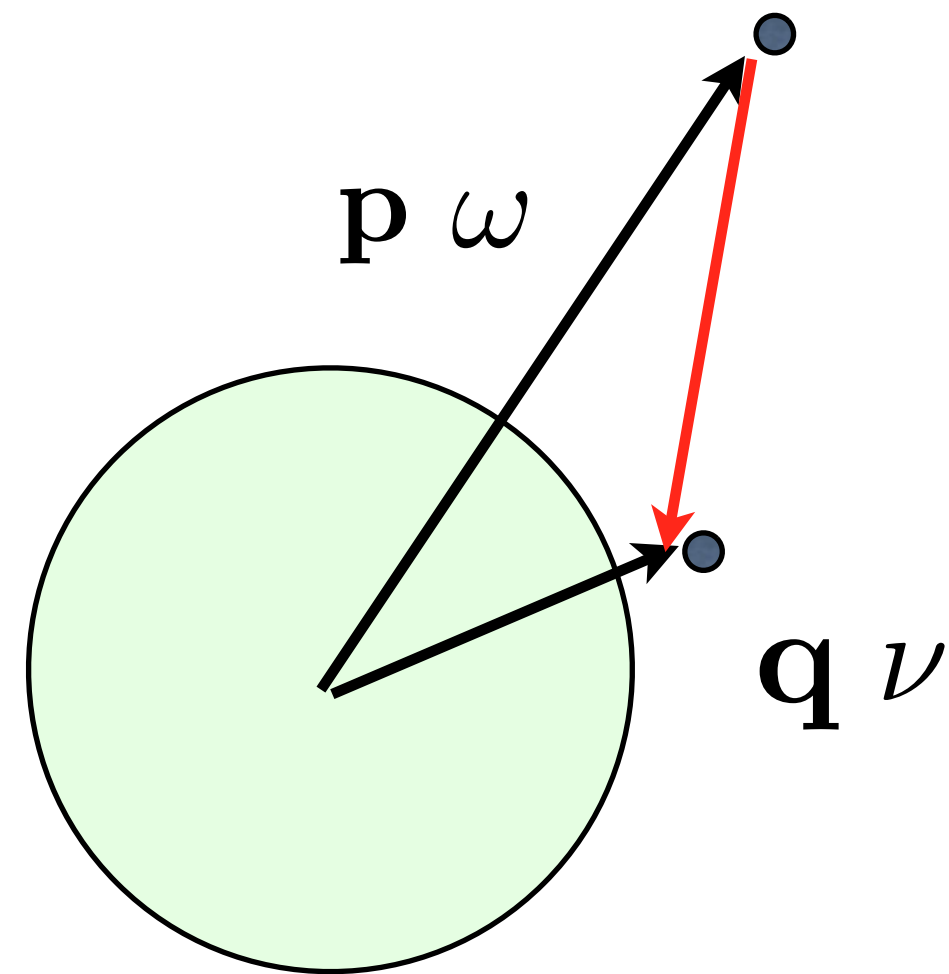
The greater and lesser self-energies describe scattering rates for added or removed particles with energy  $\omega$  and momentum  $p$

The self-energy vanishes when  $\omega \rightarrow \mu$  due to the fact an added particle can maximally lose energy  $\omega - \mu$  as states below the Fermi energy are occupied

$$i(\Sigma^>(\mathbf{q}, \omega) - \Sigma^<(\mathbf{q}, \omega)) = -2 \text{Im} \Sigma^R(\mathbf{q}, \omega) = \Gamma(\mathbf{q}, \omega)$$

$$\lim_{\omega \rightarrow \mu} \text{Im} \Sigma^R(\mathbf{q}, \omega) = 0 \quad \Sigma^R(\mathbf{q}, \omega) = \Lambda(\mathbf{q}, \omega) - \frac{i}{2} \Gamma(\mathbf{q}, \omega)$$

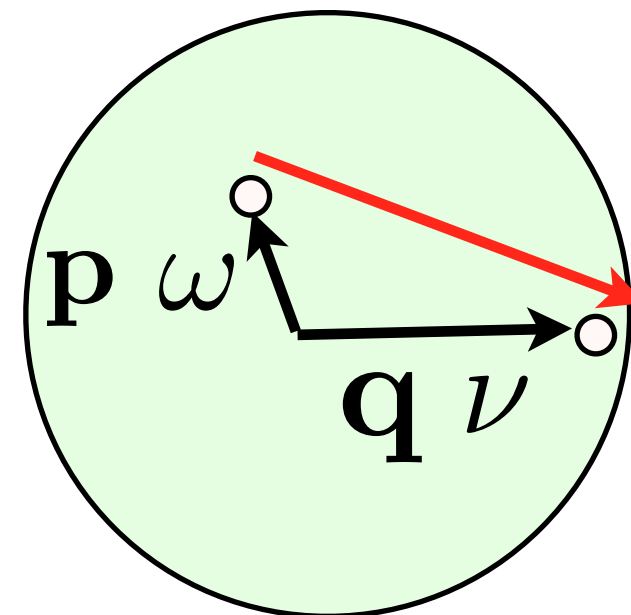
## Scattering processes



Loss of energy by a particle.  
Scattering rate given by  $i\Sigma^>(\mathbf{p}, \omega)$

Only relevant when  $p \geq p_F$

A plasmon can be excited  
only when  $\omega \geq \mu + \omega_p$



Absorption of energy by a hole.  
Scattering rate given by  $-i\Sigma^<(\mathbf{p}, \omega)$

Only relevant when  $p \leq p_F$

A plasmon can be absorbed  
only when  $\omega \leq \mu - \omega_p$

Absorption of plasmons  
by hole states

Energy loss to plasmons  
by particle states

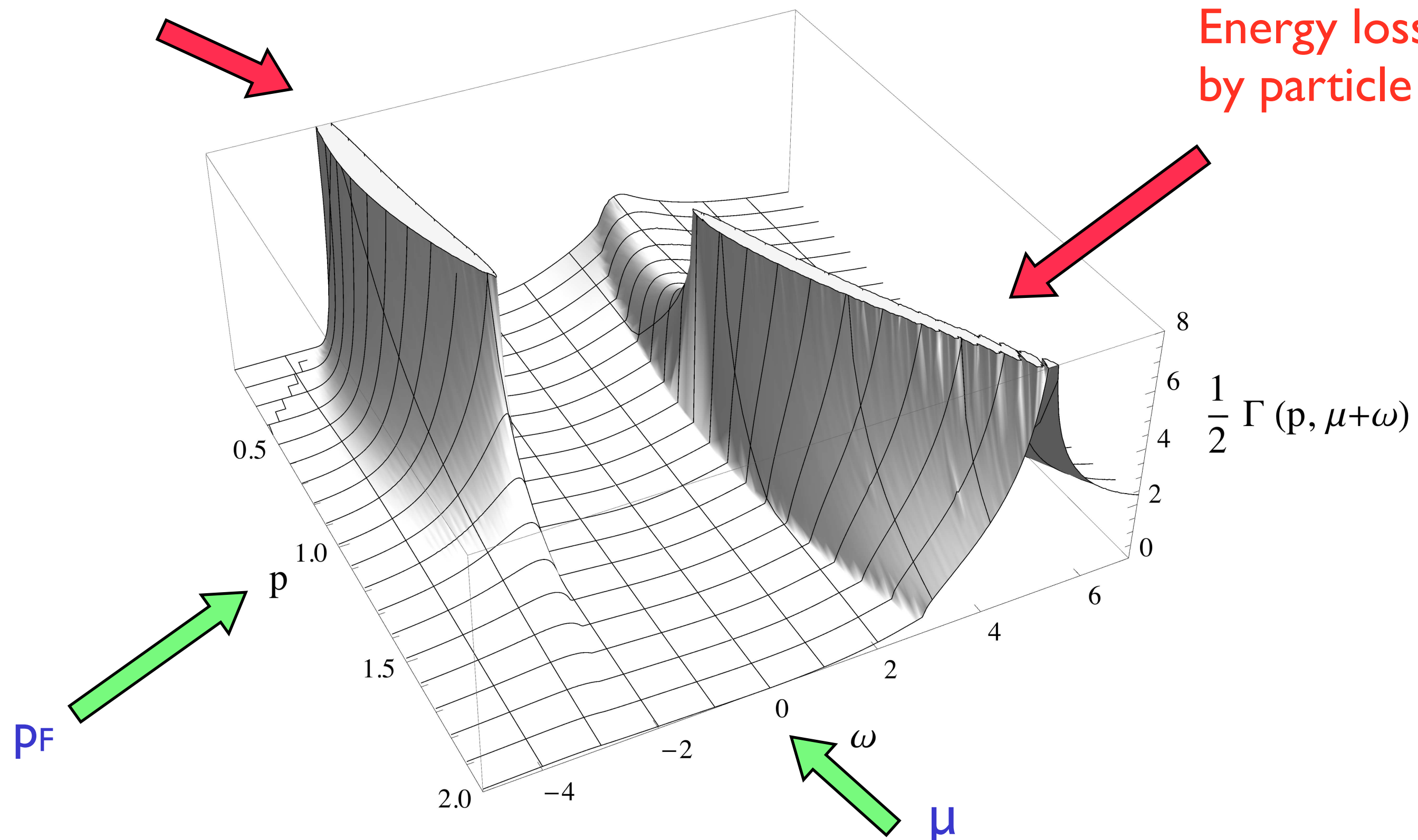


Figure 15.9: The imaginary part of the retarded self-energy  $-\text{Im}[\Sigma^R(p, \omega + \mu)] = \Gamma(p, \omega + \mu)/2$  for an electron gas at  $r_s = 4$  within the  $G_0W_0$  approximation as a function of the momentum and energy. The momentum  $p$  is measured in units of  $p_F$  and the energy  $\omega$  and the self-energy in units of  $\epsilon_{p_F} = p_F^2/2$ .

For the spectral function this implies the following

$$A(\mathbf{q}, \omega) = -2 \operatorname{Im} G^R(\mathbf{q}, \omega) = \frac{\Gamma(\mathbf{q}, \omega)}{(\omega - \epsilon_{\mathbf{q}} - \Lambda(\mathbf{q}, \omega))^2 + \left(\frac{\Gamma(\mathbf{q}, \omega)}{2}\right)^2}$$

If  $\Gamma(\mathbf{q}, \omega)$  is small then the spectral function can only become large ( $\sim 1/\Gamma$ ) when

$$\omega - \epsilon_{\mathbf{q}} - \Lambda(\mathbf{q}, \omega) = 0$$

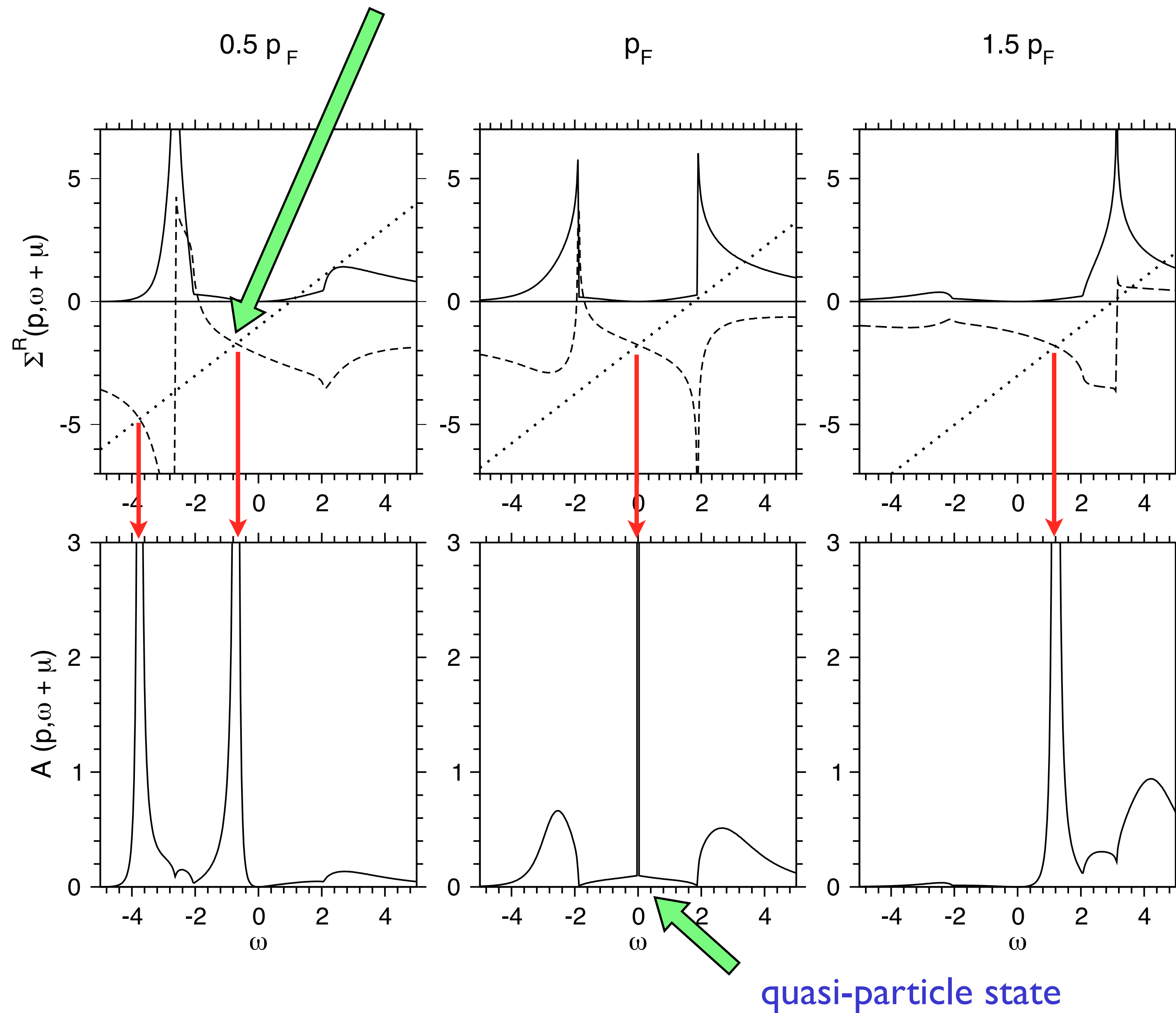
The **Luttinger-Ward theorem** tells that this happens when  $q = p_F$ ,  $\omega = \mu$

$$\mu - \epsilon_{p_F} - \Lambda(p_F, \mu) = 0$$

(not explained in these lectures, requires a derivation of the Luttinger-Ward functional, see G.Stefanucci, RvL, Nonequilibrium Many-Body Theory of Quantum Systems)



$$\omega - \epsilon_{\mathbf{p}} - \Lambda(\mathbf{p}, \omega) = 0$$



Absorption of plasmons  
by hole states

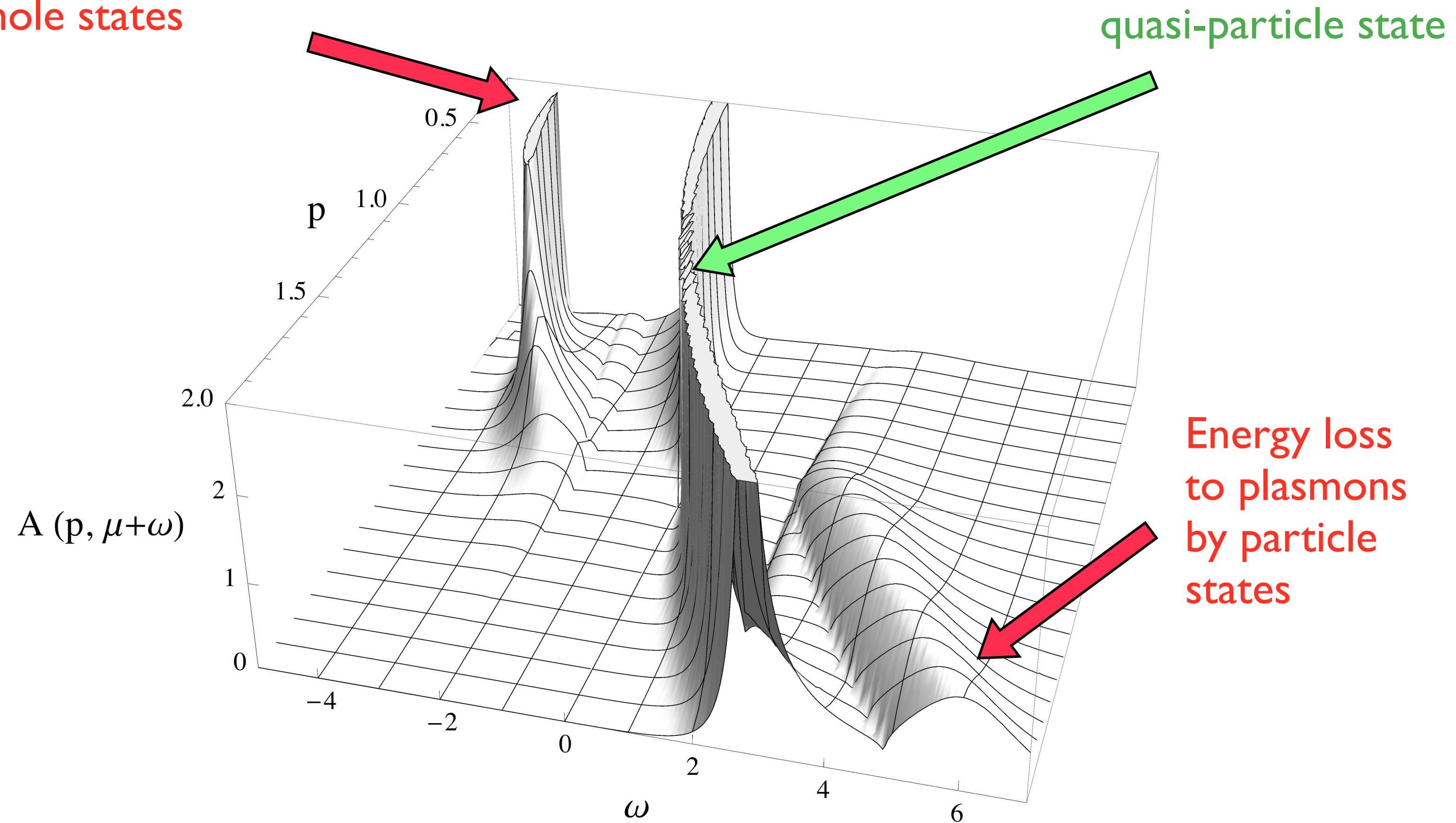
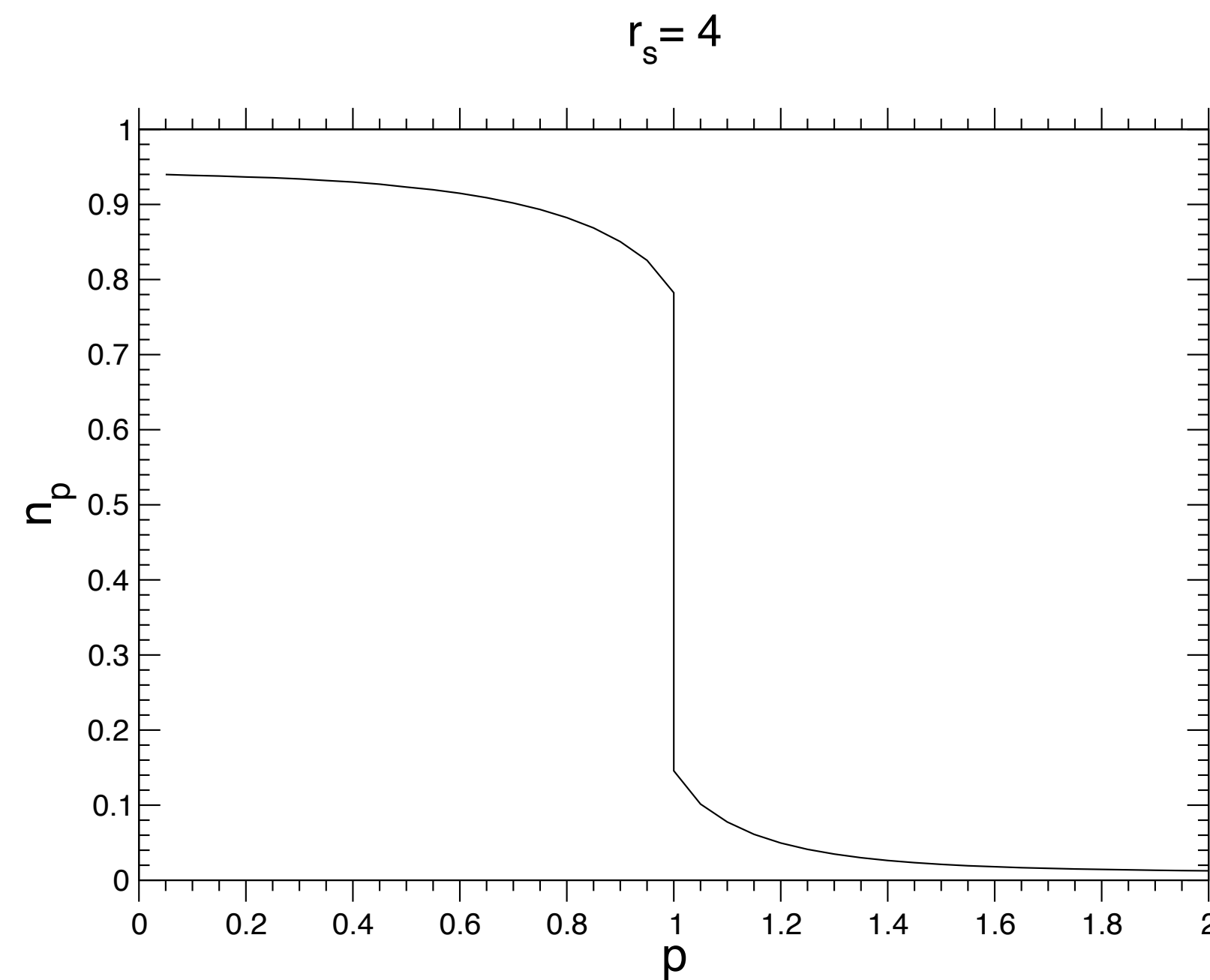


Figure 15.12: The spectral function  $A(p, \mu + \omega)$  as a function of the momentum and energy for an electron gas at  $r_s = 4$  within the  $G_0W_0$  approximation. The momentum  $p$  is measured in units of  $p_F$  and the energy  $\omega$  and the spectral function in units of  $\epsilon_{p_F} = p_F^2/2$ .

The momentum distribution in the electron gas is given by

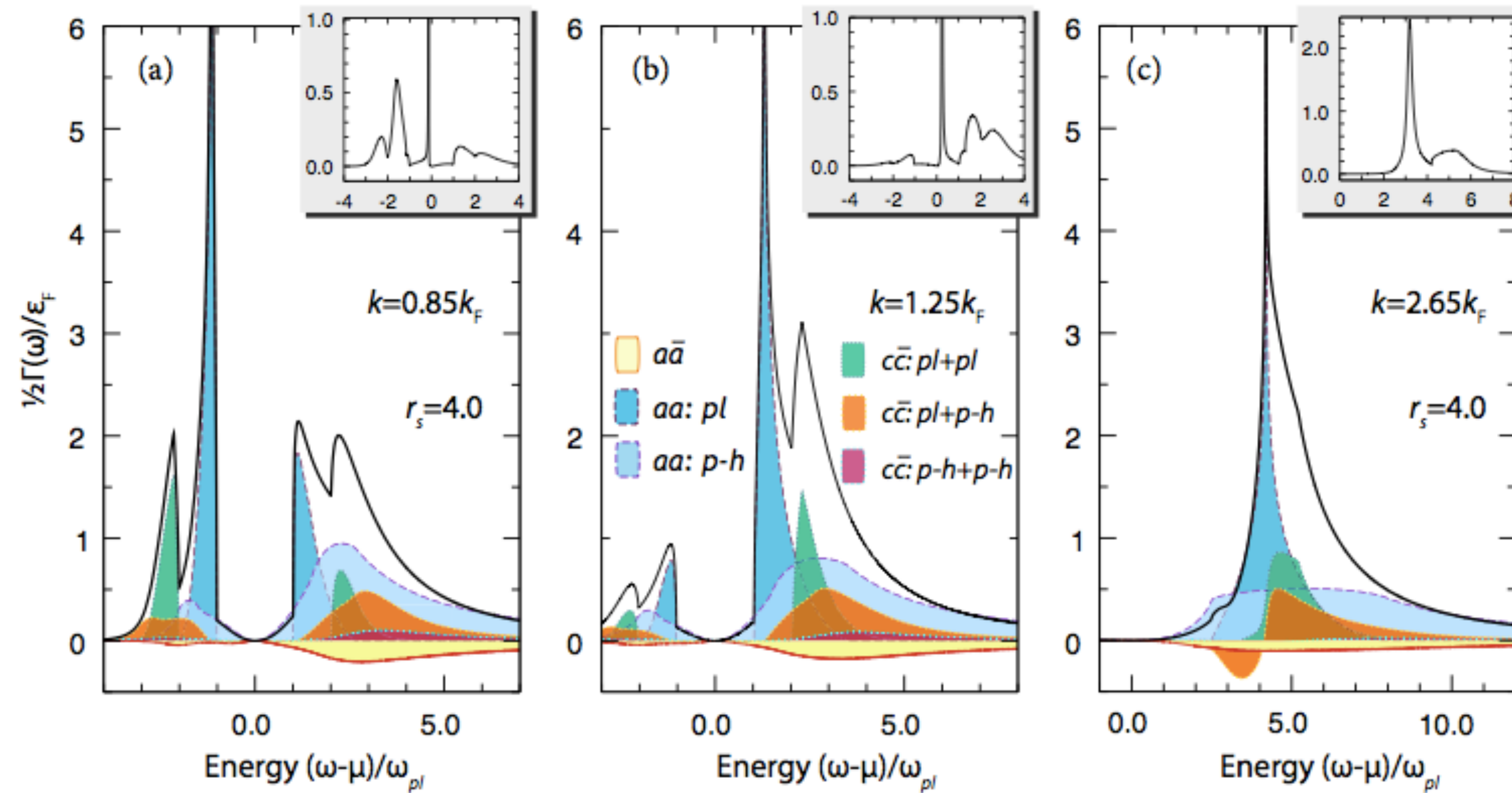
$$n_p = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(p, \omega)$$

Due to the appearance of a delta peak in the spectral function at the Fermi momentum  $p_F$  the momentum distribution jumps discontinuously at the Fermi momentum. The jump is the strength of the quasi-particle peak.



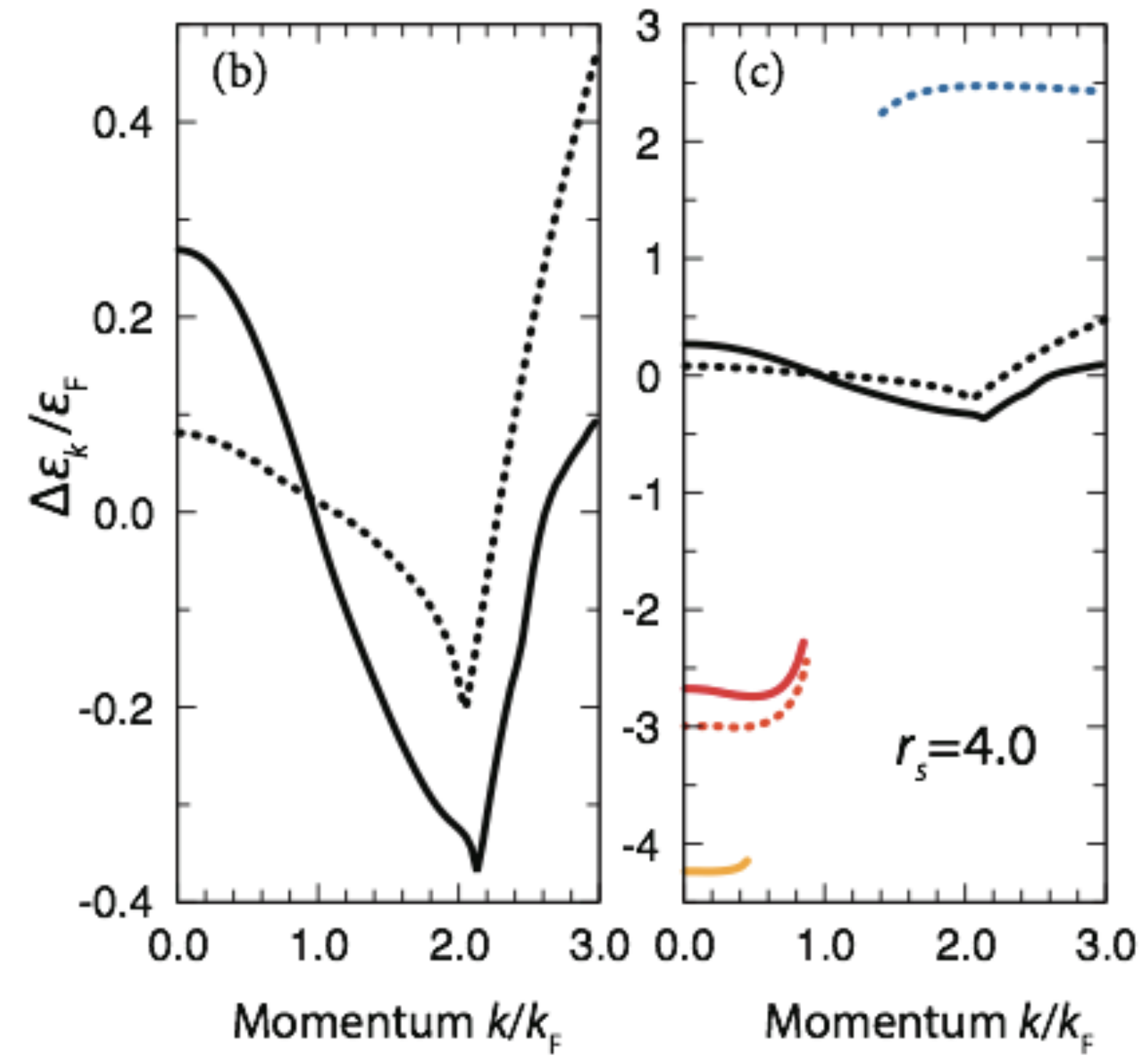
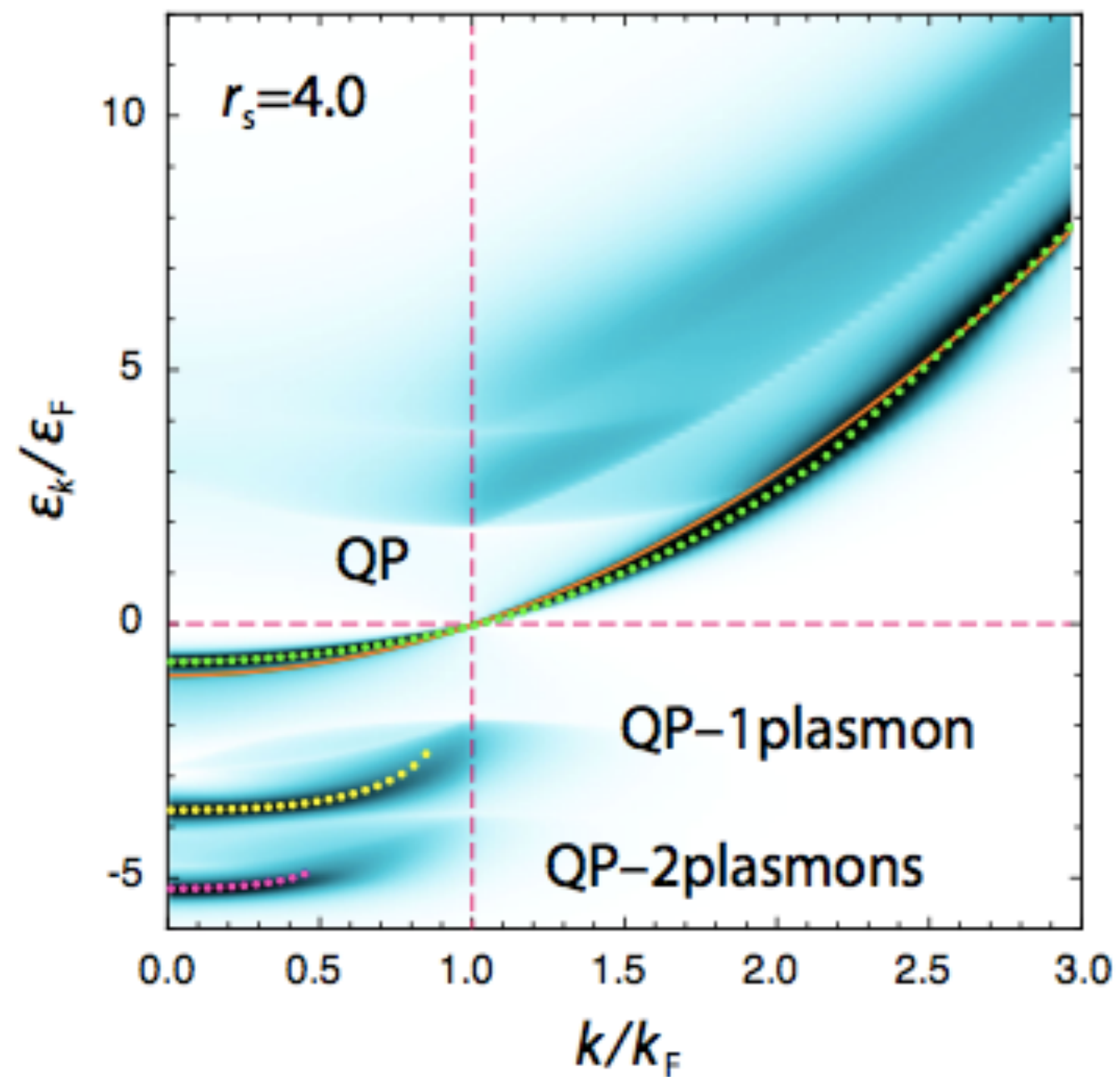
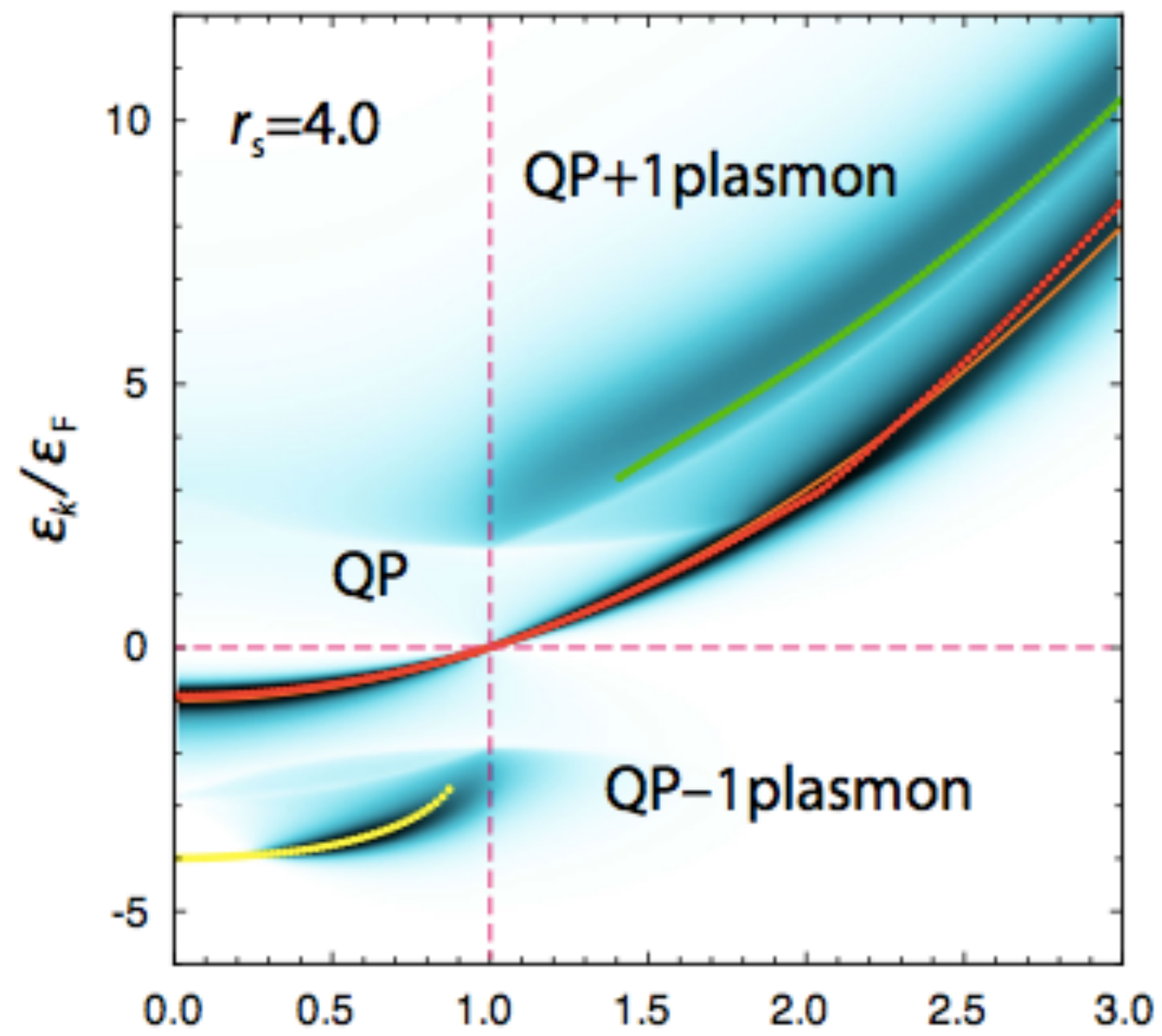
# Beyond GW

Y.Pavlyukh, A.-M. Uimonen,  
G.Stefanucci, RvL, PRL 2016



Due to negative corrections around the chemical potential in the rate function, vertex corrections sharpen the quasi-particle peak as compared to  $G_0W_0$





Vertex corrections:

- Reduce the band width by 27 percent (sc GW increases by 20 percent)
- Wash out the plasmon above the chemical potential
- Reduce the first plasmon energy

## Spectral properties of the electron gas: Take home message

- By addition or removal of an electron we create particle-hole and plasmon excitations
- The self-energy at the Fermi-surface vanishes due to phase-space restrictions. This has various consequences:
  - 1) The momentum distribution of the electron gas jumps discontinuously at the Fermi momentum
  - 2) Quasi-particles at the Fermi surface have an infinite life-time.
- The GW approximation gives extra plasmon structure in the spectral function due to plasmons
- Multiple-plasmons excitations (satellites) are beyond GW and require vertex corrections.

**That's all folks!**