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.

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

$$\Phi_D[G] = \frac{1}{2} \underbrace{\Sigma_1} \qquad \Sigma_2 \qquad \Sigma_3$$

$$\Sigma_D[G](1,2) = \frac{\delta \Phi_D}{\delta G(2,1)} = \underbrace{\Sigma_1} \qquad + \underbrace{\Sigma_2} \qquad + \underbrace{\Sigma_3} \qquad + \underbrace{\Sigma_3} \qquad + \underbrace{\Sigma_4} \qquad + \underbrace{\Sigma_5} \qquad + \underbrace{$$

n-th order self-energy

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
$$\frac{1}{2\times 3}(\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_2 G + \int \Sigma_3 G) = \frac{1}{2} \ (\int \Sigma_1 G + \int \Sigma_2 G + \int \Sigma_2 G + \int \Sigma_2 G + \int \Sigma_3 G +$$

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

$$\Sigma(1,2) =$$

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

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

Theorem I: The Hxc potential

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

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

Proof:

$$\begin{split} v_{\rm Hxc}[n](1) &= \frac{\delta A_{\rm Hxc}}{\delta n(1)} = -i \int d2d3d4 \frac{\delta \Phi}{\delta G_s(3,2)} \frac{\delta G_s(3,2)}{\delta v_s(4)} \frac{\delta v_s(4)}{\delta n(1)} \\ &= -i \int d2d3d4 \, \Sigma[G_s](2,3) G_s(3,4) G_s(4,2) \chi_s^{-1}(4,1) \end{split} \quad \text{inverse density response function}$$

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

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 $-i\delta\Phi=\int d1\,v_{\mathrm{Hxc}}(1)\delta n(1)$

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

To first order in 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 R(t) this implies

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

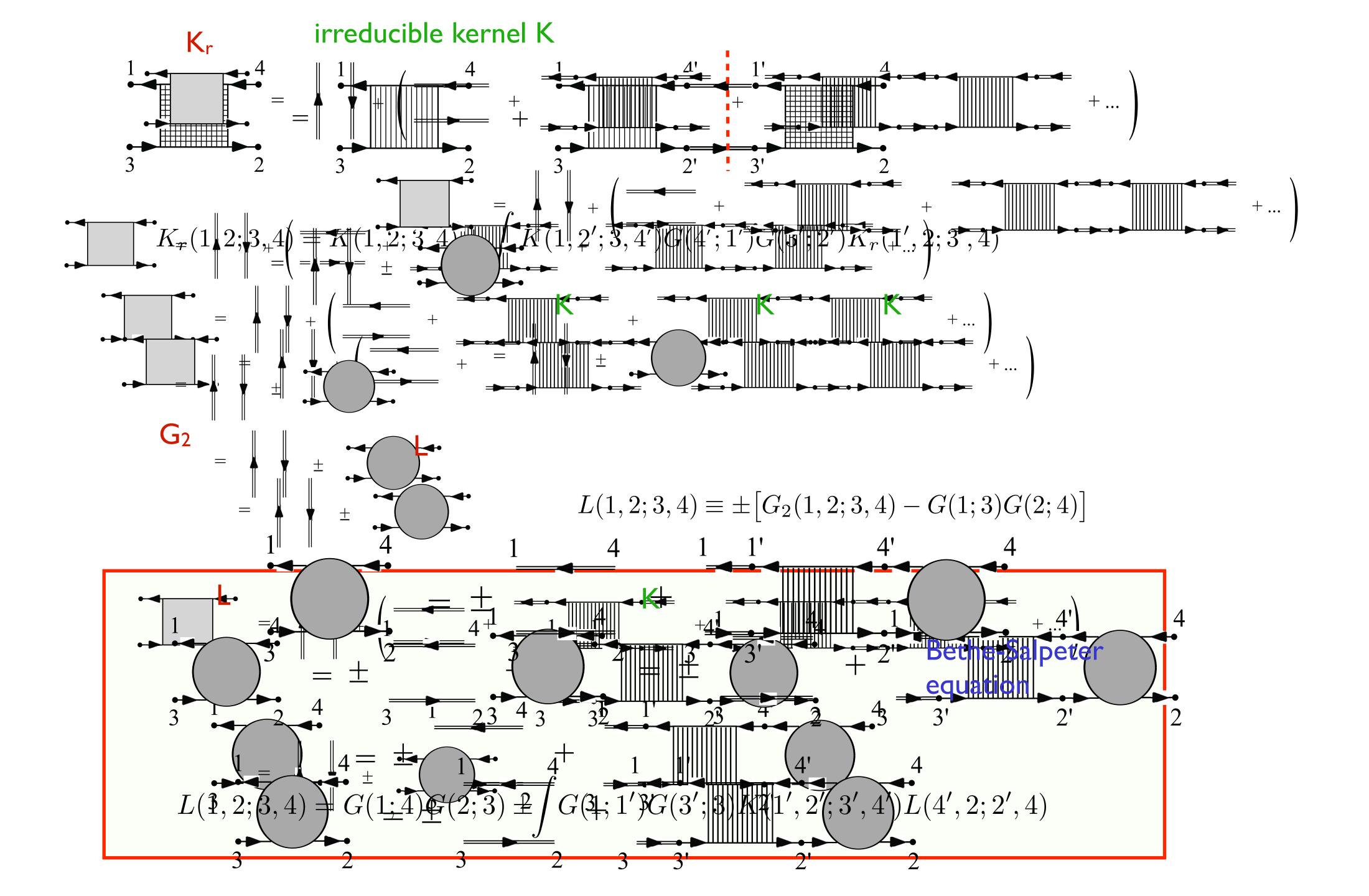
The 2-particle Green's function

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

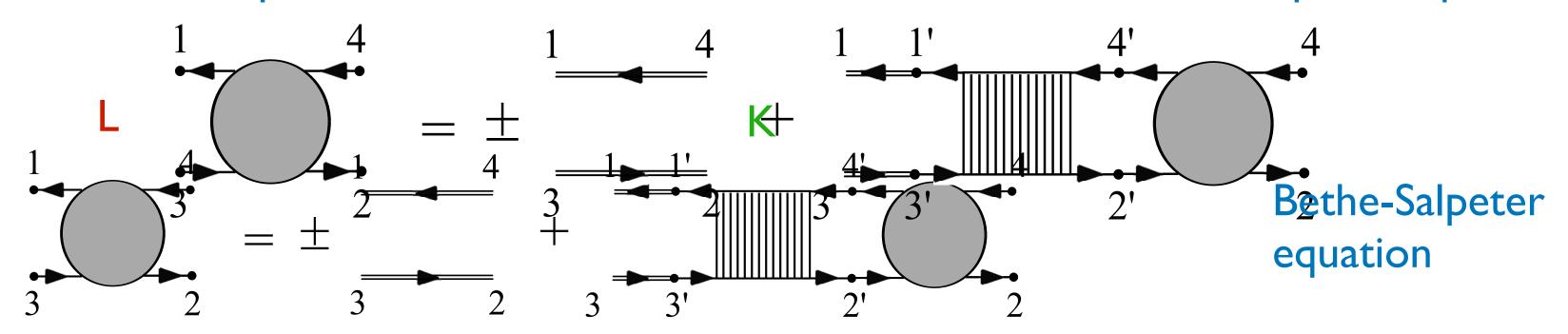
$$G_{2}(a,b;c,d) = \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^{k} \int v(1;1') \dots v(k;k') \begin{vmatrix} G_{0}(a;c) & G_{0}(a;d) & \dots & G_{0}(a;k'^{+}) \\ G_{0}(b;c) & G_{0}(b;d) & \dots & G_{0}(b;k'^{+}) \\ \vdots & \vdots & \ddots & \vdots \\ G_{0}(k';c) & G_{0}(k';d) &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

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

$$G_2(1,2;3,4) = G(1;3)G(2;4) \pm G(1;4)G(2;3)$$
 noninteracting form
$$+ \int G(1;1')G(3';3)K_r(1',2';3',4')G(4';4)G(2;2')$$



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

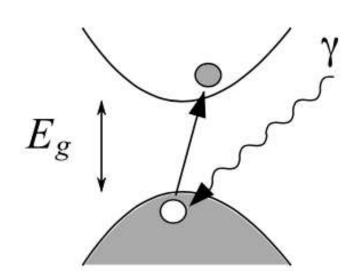
$$1 \overline{3}$$
 $1 \overline{3}$

Let us give an example

The Bethe-Salpeter equation is then given by

$$\frac{1}{3} + \frac{4}{3} = -\frac{1}{3} + \frac{4}{3} + \frac{1}{2!} + \frac{4}{3!} + \frac{1}{2!} + \frac{4}{3!} + \frac{1}{3!} + \frac{2!}{2!} + \frac{4}{3!} + \frac{1}{3!} + \frac{2!}{3!} + \frac{2!}{3!$$

This equation is relevant for describing excitons in semiconductors



Linear response functions

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

If we make the variation then

$$\hat{H}(z) \to \hat{H}(z) + \delta \hat{V}(z)$$

$$\hat{H}(z) \rightarrow \hat{H}(z) + \delta \hat{V}(z)$$
 $\delta \hat{V}(z) = \int d\mathbf{x} \, \hat{n}(\mathbf{x}) \, \delta v(\mathbf{x}z)$

$$\delta\langle \hat{n}(\mathbf{x},t)\rangle = -i\int_{\gamma} dz_{1} \frac{\operatorname{Tr} \mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\,\hat{H}(\bar{z})}\hat{n}(\mathbf{x},t)\delta\hat{V}(z_{1})\right\}}{\operatorname{Tr} \mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\,\hat{H}(\bar{z})}\right\}} + i\langle \hat{n}(\mathbf{x},t)\rangle\int_{\gamma} dz_{1} \frac{\operatorname{Tr} \mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\,\hat{H}(\bar{z})}\delta\hat{V}(z_{1})\right\}}{\operatorname{Tr} \mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\,\hat{H}(\bar{z})}\right\}}$$

which can be rewritten as

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

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

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

$$L(1,2;1',2') = -\left[G_2(1,2;1',2') - G(1,1')G(2,2')\right]$$

$$= \langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}_H^{\dagger}(2')\hat{\psi}_H^{\dagger}(1')\right\}\rangle - \langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^{\dagger}(1')\right\}\rangle\langle \mathcal{T}\left\{\hat{\psi}_H(2)\hat{\psi}_H^{\dagger}(2')\right\}\rangle$$

and therefore

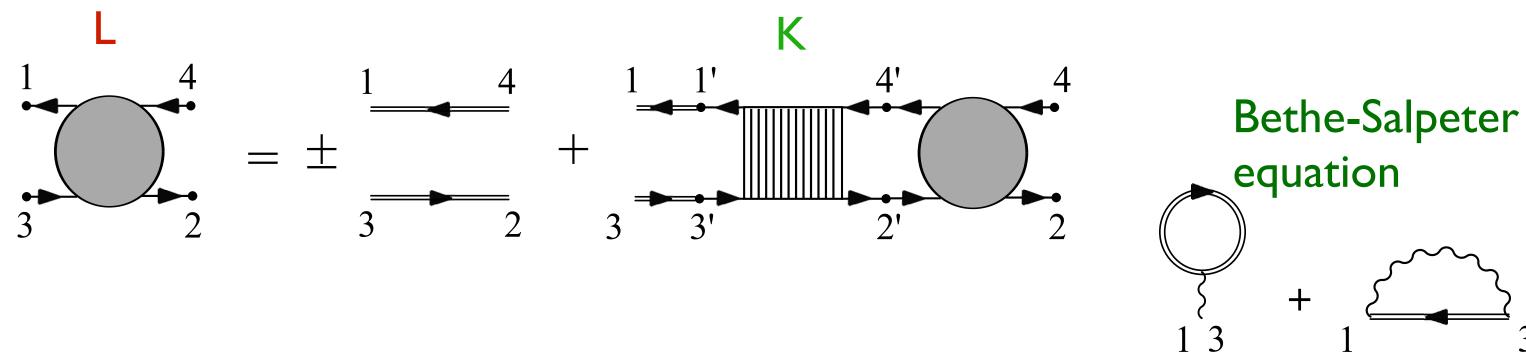
$$\chi(1,2) = -i \left[\langle \mathcal{T} \{ \hat{n}_H(1) \hat{n}_H(2) \} \rangle - n(1)n(2) \right] = -i L(1,2;1^+,2^+)$$

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



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

$$\Sigma_{H} = \begin{cases} K_{H}(1,2;3,4) = -\frac{\delta\Sigma_{H}(1,3)}{\delta G(4,2)} = \begin{cases} 1 & 4 \\ 3 & 2 \end{cases} \end{cases}$$

then the Bethe-Salpeter equation becomes

$$\frac{1}{3} = -\frac{1}{3} + \frac{4}{3}$$

$$\frac{1}{2} = -\frac{4}{3}$$

$$\frac{1}{2} = -\frac{4}{3}$$

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

$$\chi^{\mathrm{R}}(\mathbf{x}_{1}, \mathbf{x}_{2}; \omega) = \chi^{\mathrm{R}}_{0}(\mathbf{x}_{1}, \mathbf{x}_{2}; \omega) + \int d\mathbf{x}_{3} d\mathbf{x}_{4} \, \chi^{\mathrm{R}}_{0}(\mathbf{x}_{1}, \mathbf{x}_{3}; \omega) v(\mathbf{x}_{3}, \mathbf{x}_{4}) \chi^{\mathrm{R}}(\mathbf{x}_{4}, \mathbf{x}_{2}; \omega)$$

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

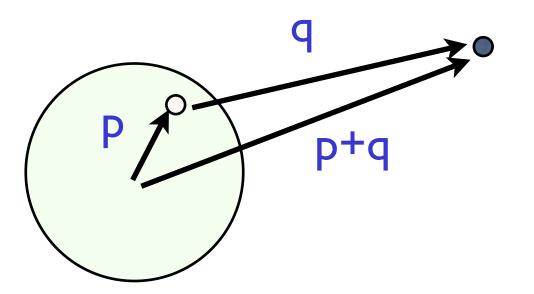
$$\sum_{\mathbf{q},\mathbf{q}'} \chi^{\mathrm{R}}(\mathbf{x},\mathbf{x}';\omega) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \chi^{\mathrm{R}}(\mathbf{p},\omega)$$

$$\chi^{\mathrm{R}}(\mathbf{q},\omega) = \frac{\chi^{\mathrm{R}}_{0}(\mathbf{q},\omega)}{1-\tilde{v}_{\mathbf{q}}\chi^{\mathrm{R}}_{0}(\mathbf{q},\omega)}, \qquad \tilde{v}_{\mathbf{q}} = \frac{4\pi}{q^{2}} \qquad \qquad \text{Fourier transform Coulomb potential}$$

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

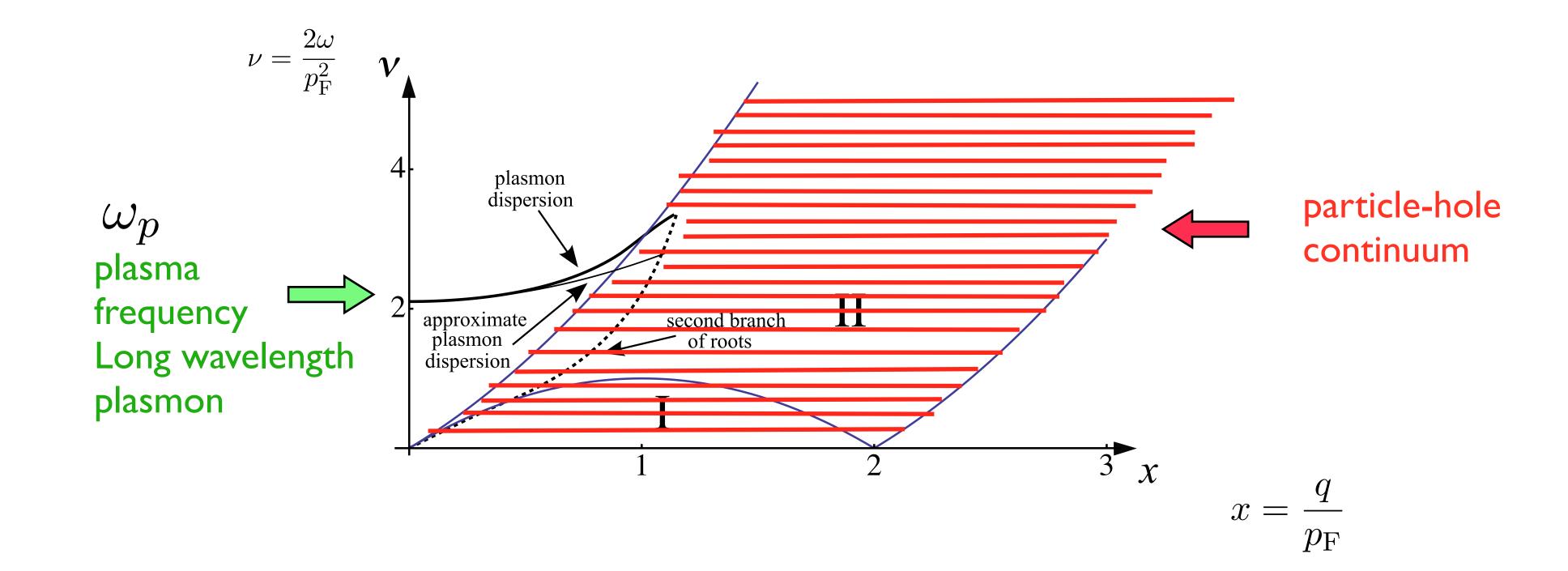


Fermi sphere with radius pf

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

$$\frac{q^2}{2} - q p_{\mathrm{F}} \le \epsilon \le \frac{q^2}{2} + q p_{\mathrm{F}} \qquad q = |\mathbf{q}|$$

The particle-hole excitations lie between two parabolas in the q- ω plane



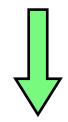
Sudden creation of a positive charge (such as in the creation of a core-hole)

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

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

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

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



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

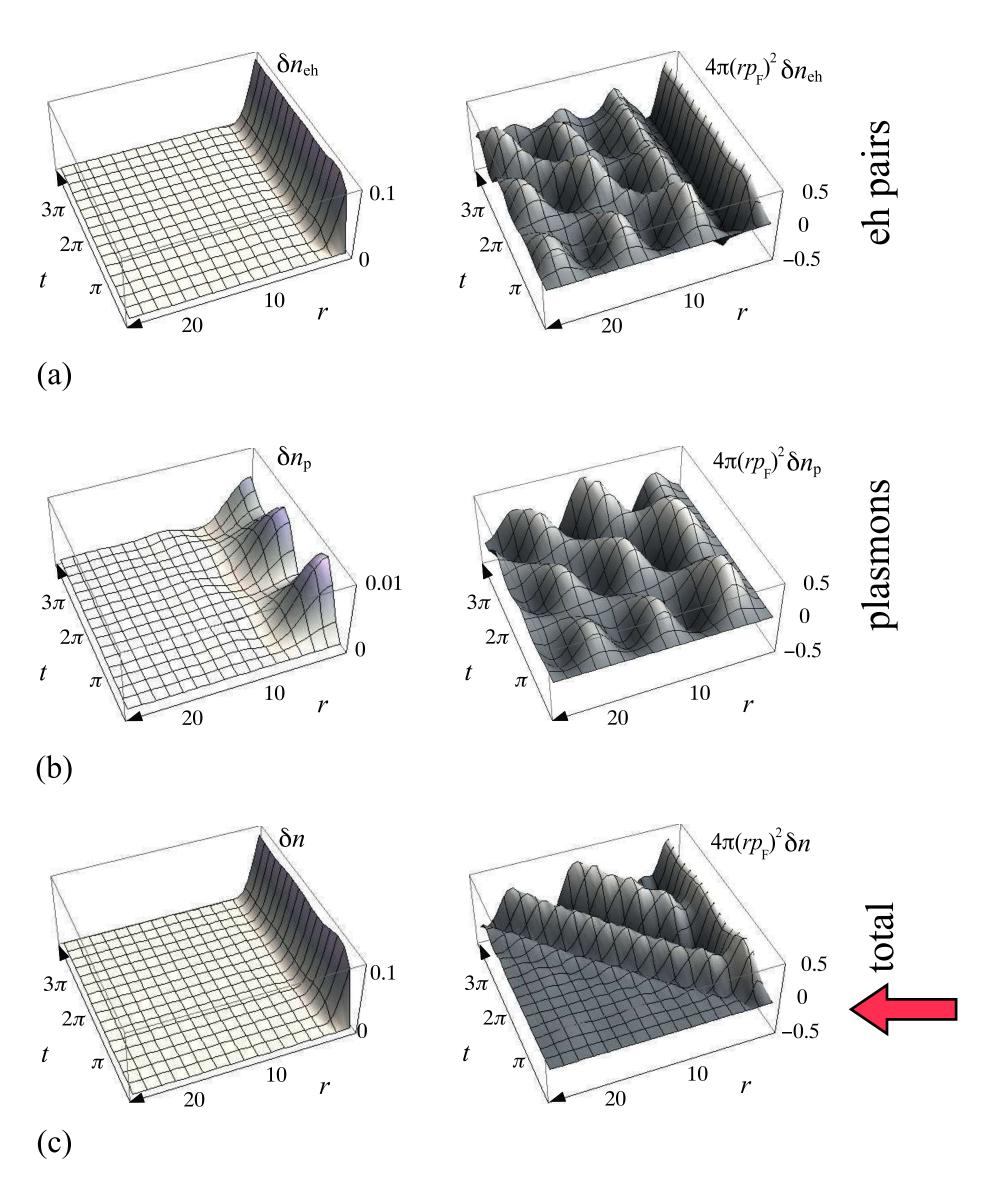


Figure 15.7: This figure shows the 3D plot of the transient density in an electron gas with $r_s=3$ induced by the sudden creation of a point-like positive charge Q=1 in the origin at t=0. The contribution due to the excitation of electron-hole pairs (a) and plasmons (b) is, for clarity, multiplied by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

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

In the long time limit we have

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

has spatial oscillations known as Friedel oscillations

Suppose now that Q=q=-1 is the same a 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

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

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

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

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

In the static limit W describes the interaction between a test charge an 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 photoemission experiment on an electron gas (or electron gas like metals such a sodium)

Dyson equation

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

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

$$\epsilon_{\mathbf{q}} = \frac{|\mathbf{q}|^{2}}{2}$$

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

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

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

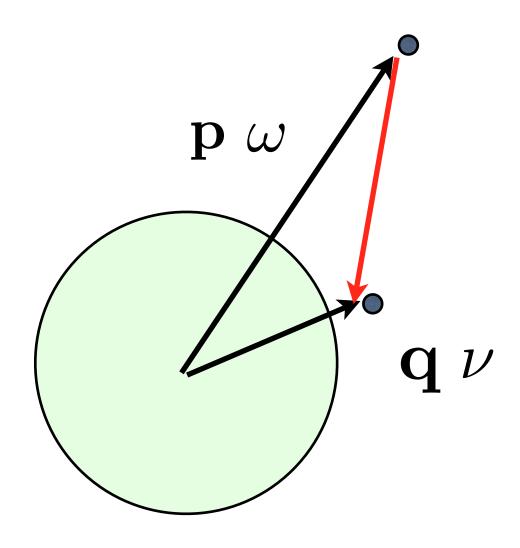
The greater and lesser self-energies describe scattering rates for added or removed particles with energy ω and momentum p

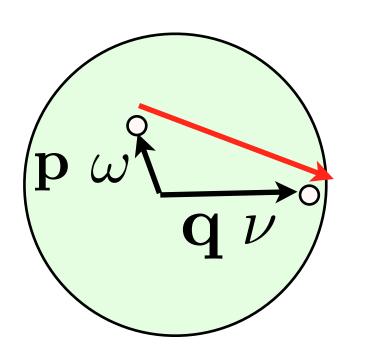
The self-energy vanishes when $\omega \to \mu$ due to the fact an added particle can maximally lose energy $\omega - \mu$ as states below the Fermi energy are occupied

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

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

Scattering processes





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

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

Only relevant when $p \ge p_{\mathrm{F}}$

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

Only relevant when $p \le p_{\rm F}$

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

Absorption of plasmons by hole states

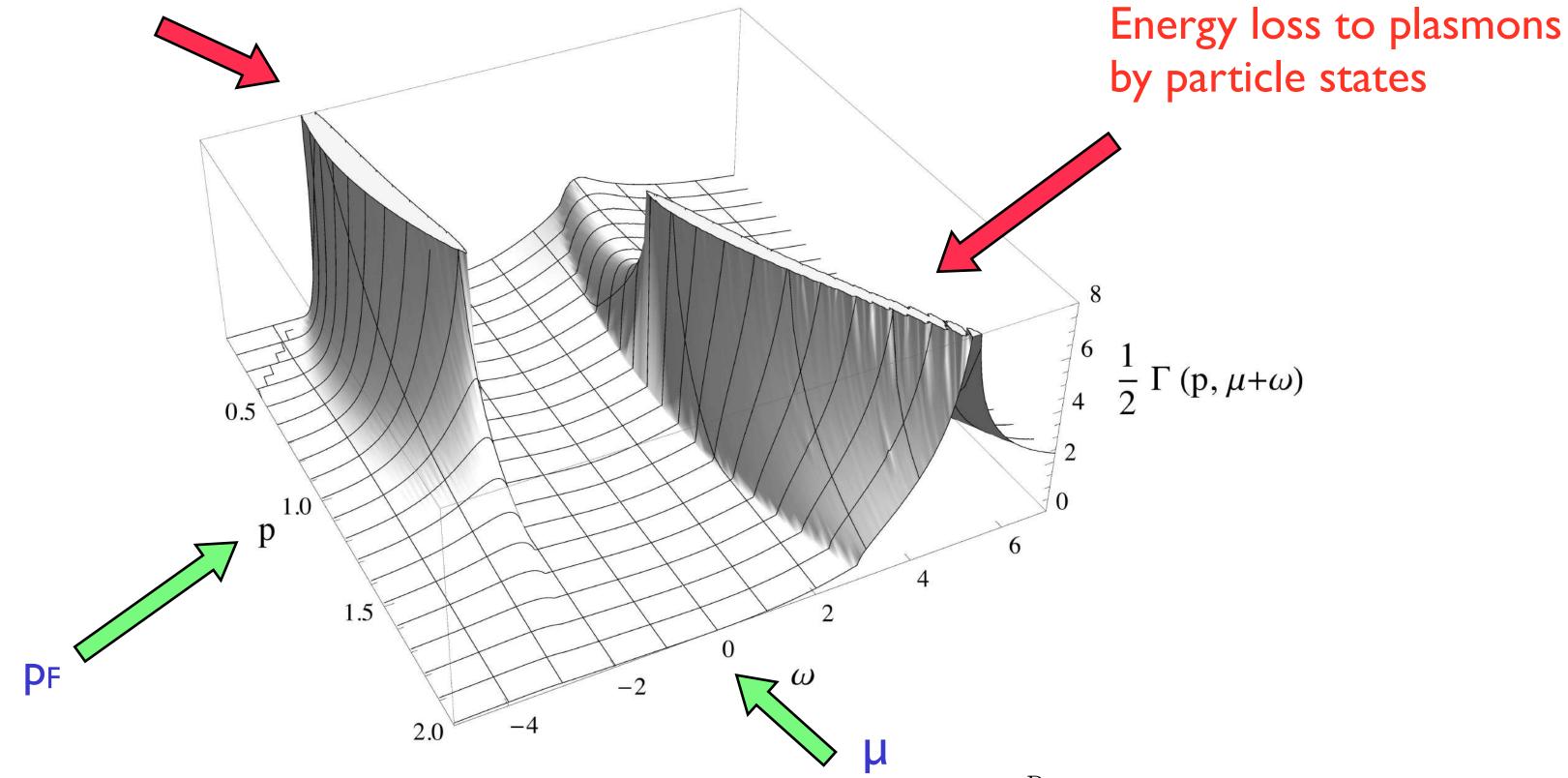


Figure 15.9: The imaginary part of the retarded self-energy $-\mathrm{Im}[\Sigma^{\mathrm{R}}(p,\omega+\mu)]=\Gamma(p,\omega+\mu)/2$ for an electron gas at $r_s=4$ within the G_0W_0 approximation as a function of the momentum and energy. The momentum p is measured in units of p_{F} and the energy ω and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

For the spectral function this implies the following

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

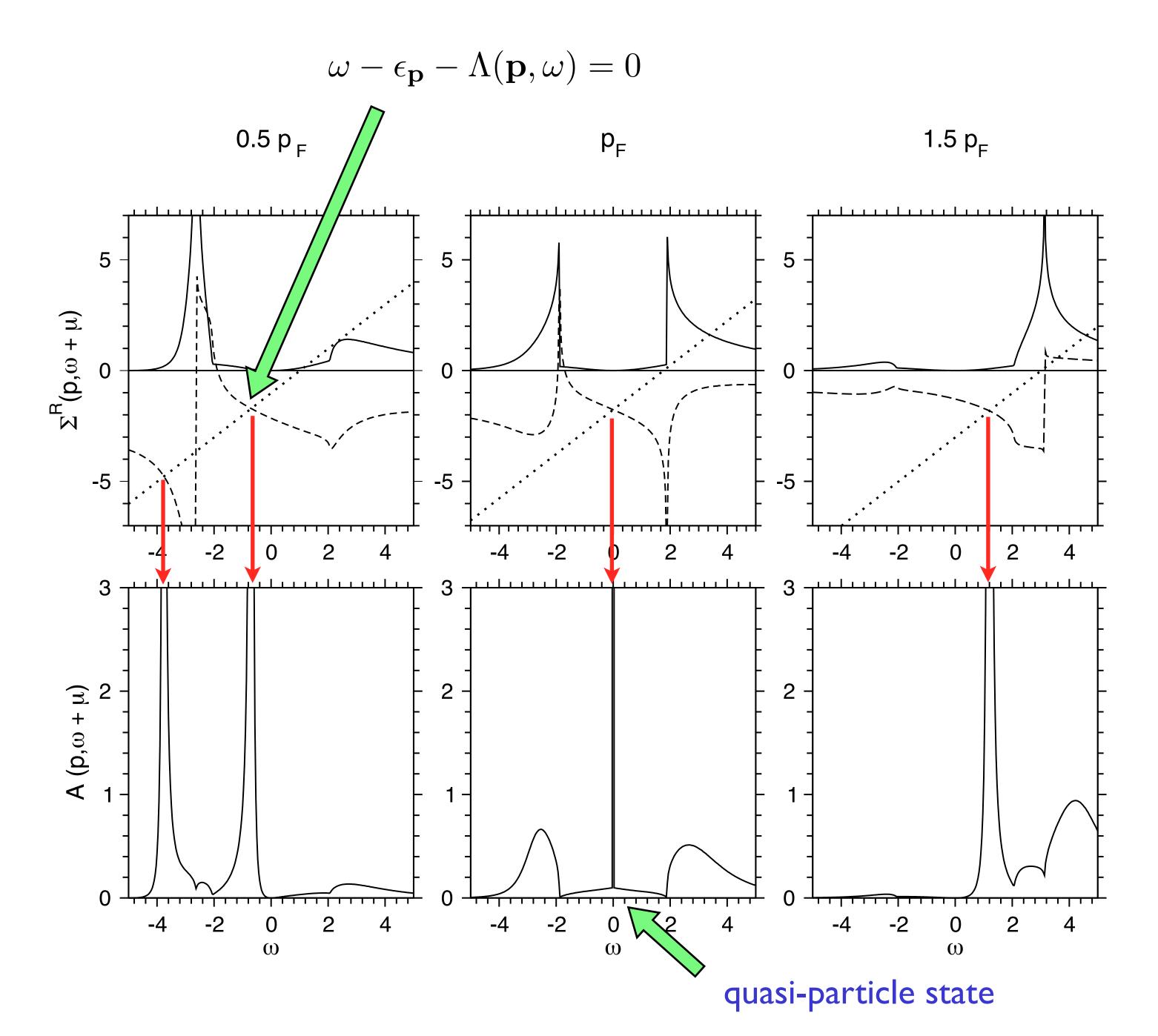
If $\Gamma({\bf q},\omega)$ is small then the spectral function can only become large ($\sim 1/\Gamma$) when

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

The Luttinger-Ward theorem tells that this happens when $q=p_{
m F}\;,\;\omega=\mu$

$$\mu - \epsilon_{p_{\rm F}} - \Lambda(p_{\rm F}, \mu) = 0$$

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



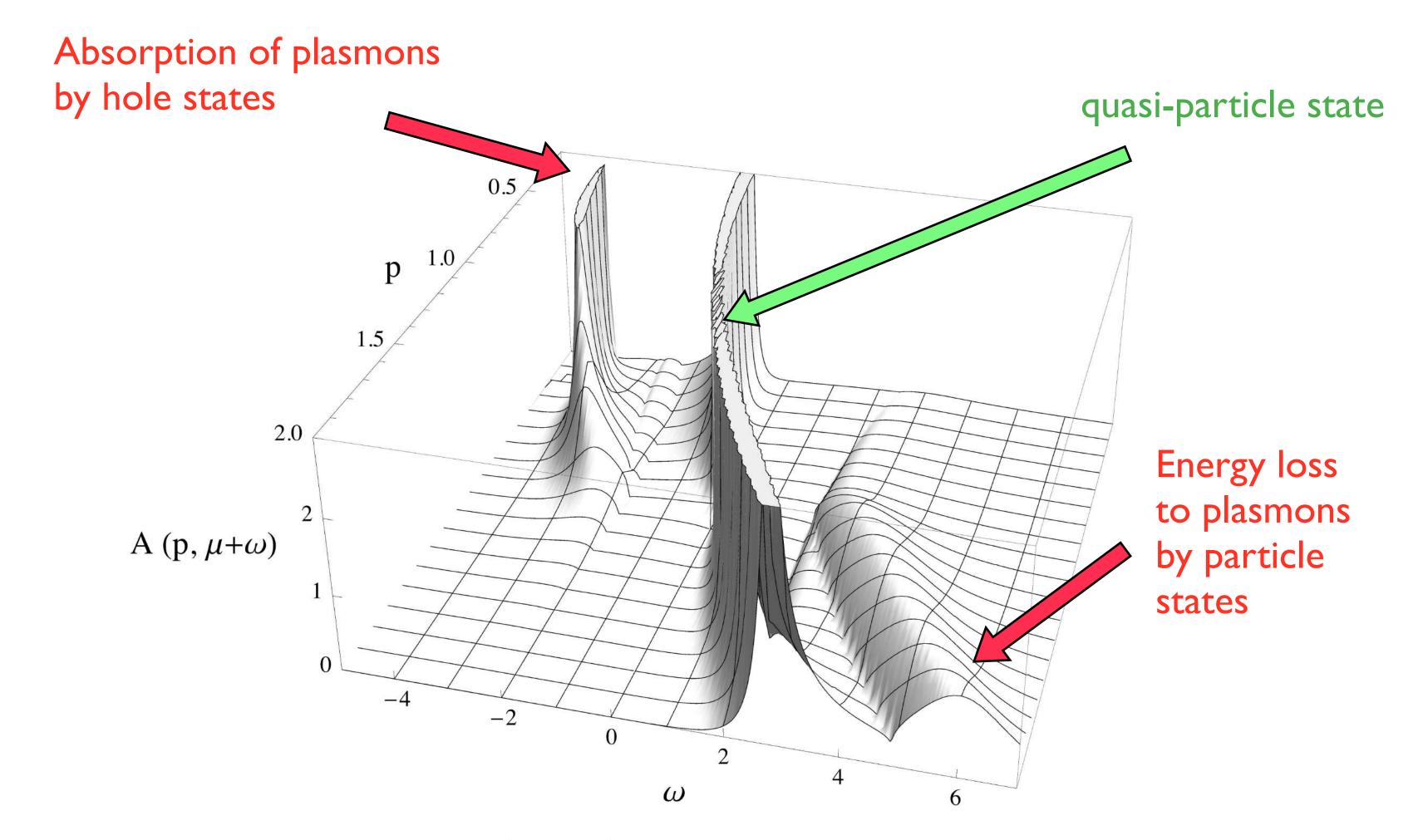
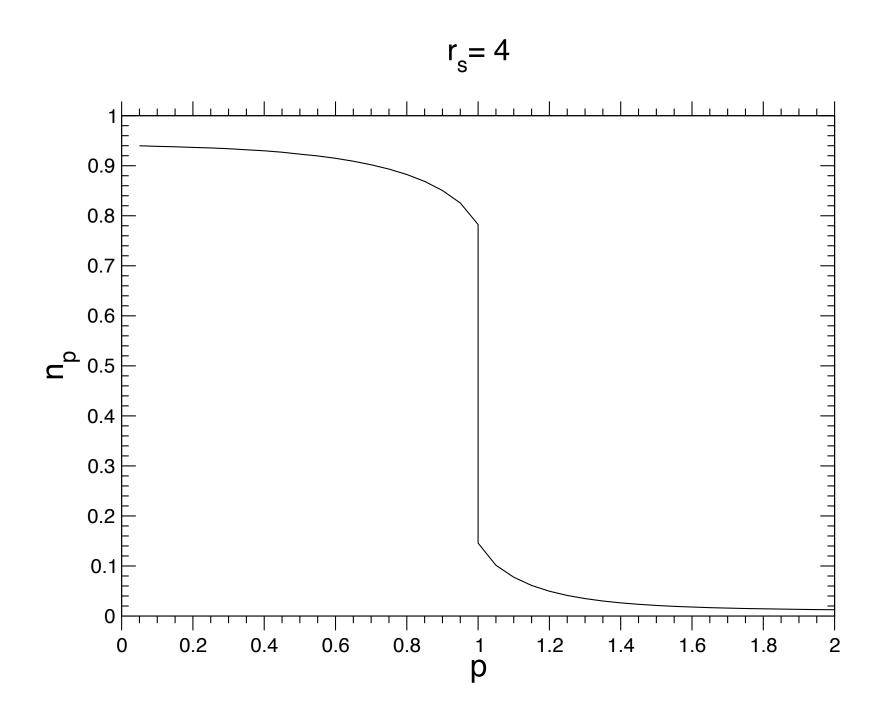


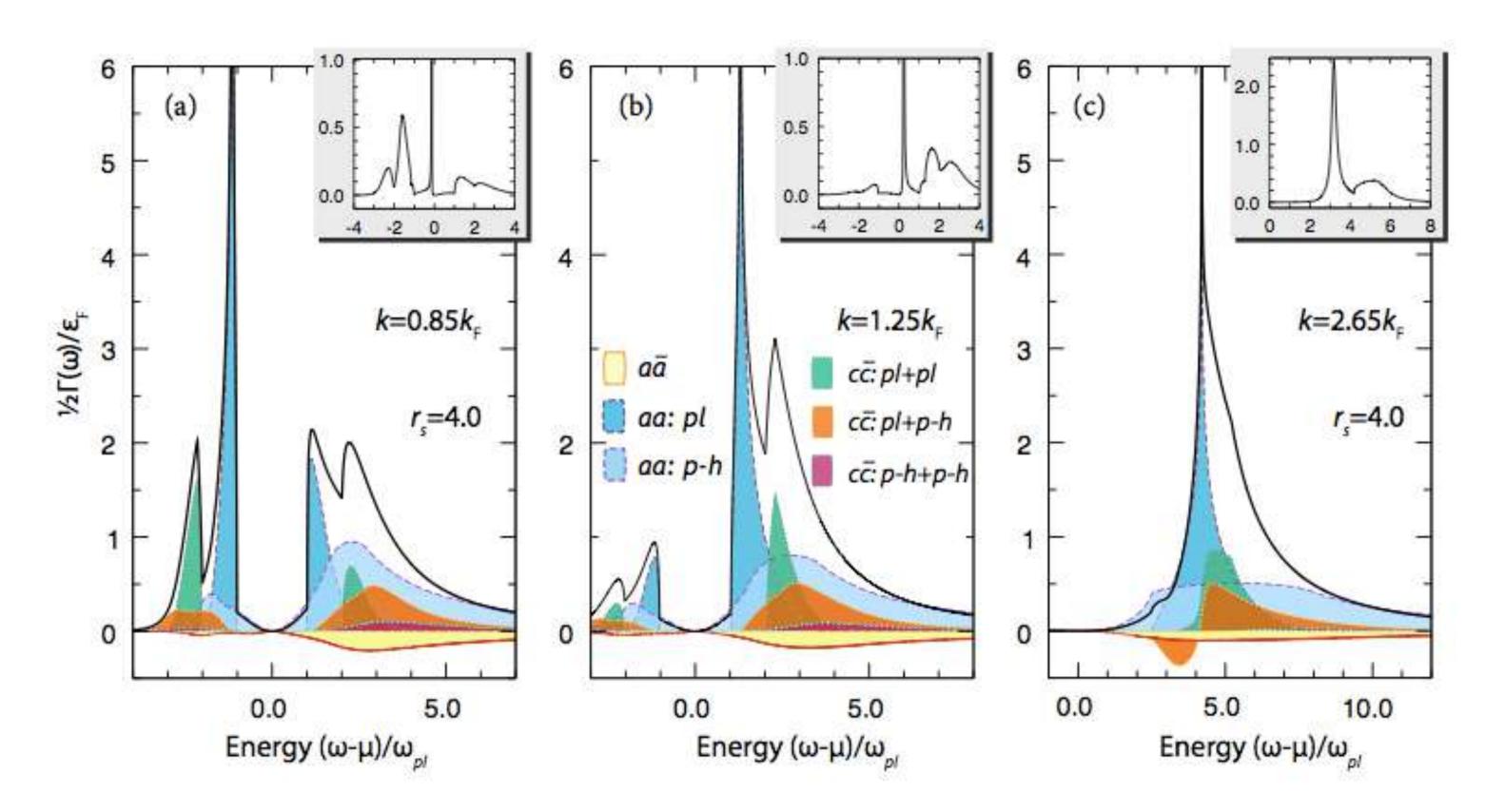
Figure 15.12: The spectral function $A(p,\mu+\omega)$ as a function of the momentum and energy for an electron gas at $r_s=4$ within the G_0W_0 approximation. The momentum p is measured in units of $p_{\rm F}$ and the energy ω and the spectral function in units of $\epsilon_{p_{\rm F}}=p_{\rm F}^2/2$.

The momentum distribution in the electron gas is given by

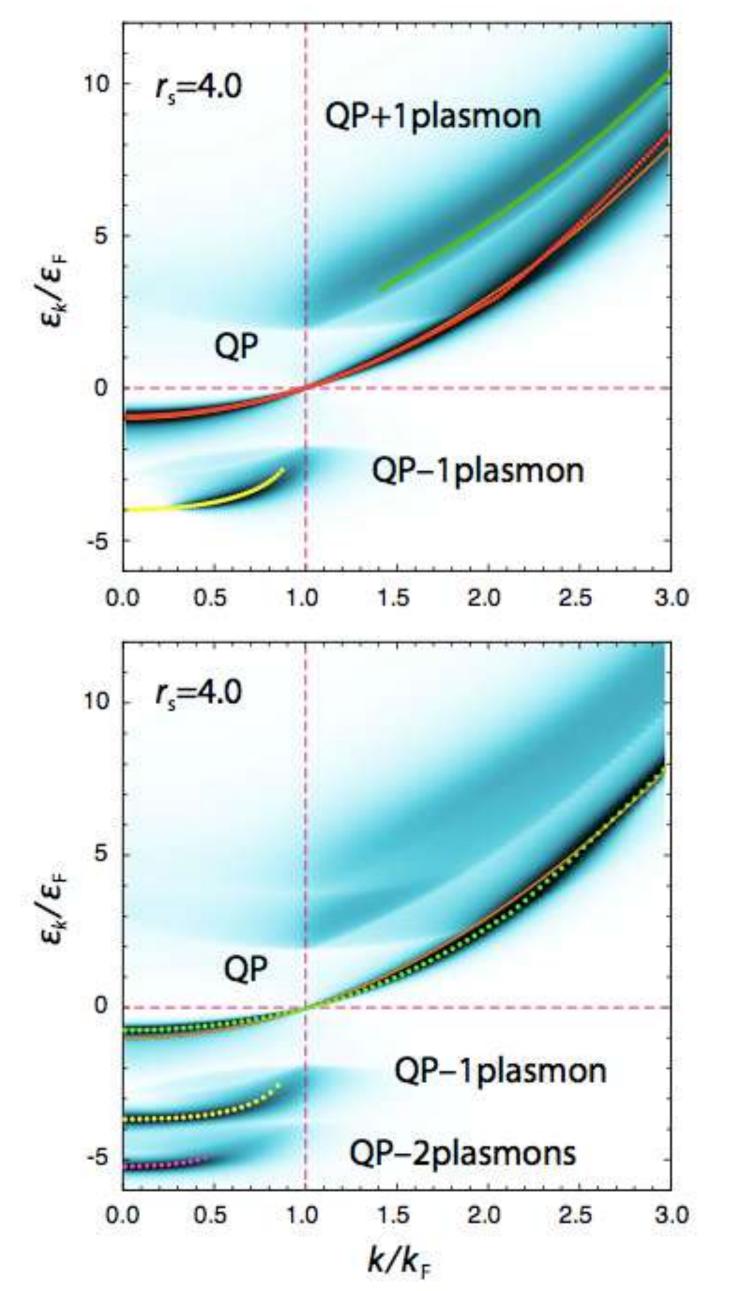
$$n_p = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(p, \omega)$$

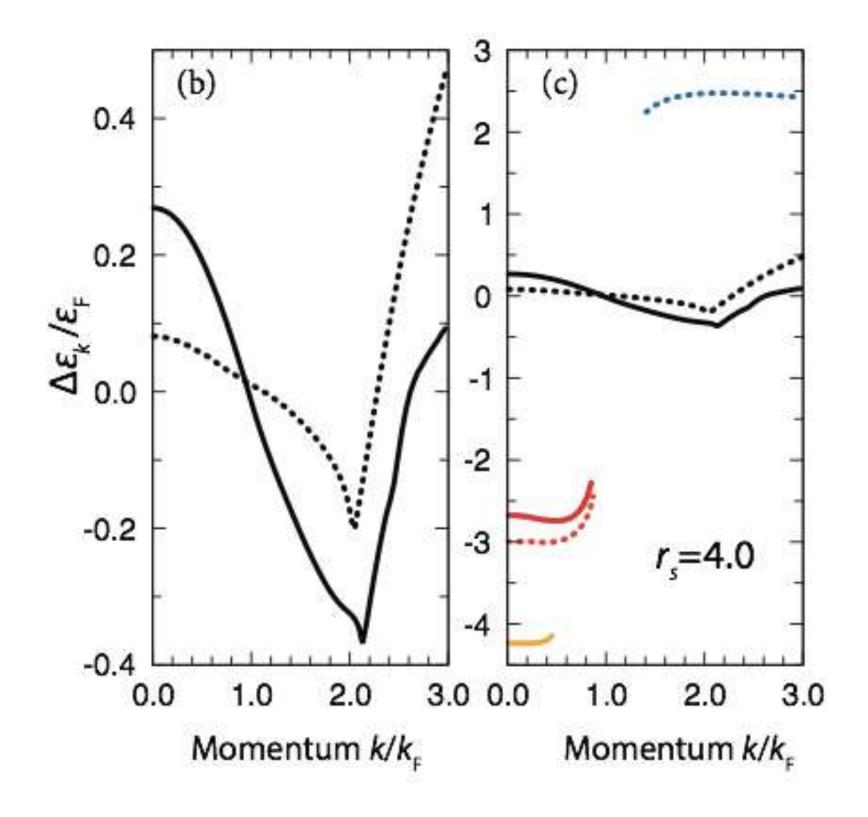
Due to the appearance of a delta peak in the spectral function at the Fermi momentum p_F the momentum distribution jumps discontinuously at the Fermi momentum. The jump is the strength of the quasi-particle peak.





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:
 - I) 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.

