Introduction to Many-body Theory III

Part III: Linear response and examples

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

The 2-particle Green's function

We can further 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 + $\int G(1;1')G(3';3)K_{r}(1',2';3',4')G(4';4)G(2;2')$





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







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



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



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

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

It is not hard to prove this diagrammatically

Let us give some examples



Κ



What about the W-skeletons? Remember that $= \cdots + \cdots \xrightarrow{P}$ Let us look at the reducible kernel again interaction line reducible $= \frac{1}{3} \frac{4}{2} + \frac{1}{3}$ Kr $+ \frac{1}{3} + \frac{4}{2} + \frac{1}{2} + \frac{1}{3} + \frac{$ $+ \underbrace{\underbrace{5}}_{2} \underbrace{4}_{2} \underbrace{4}_{2} \underbrace{1}_{2} \underbrace{4}_{2} \underbrace{4}_{2} \underbrace{1}_{2} \underbrace{4}_{2} \underbrace{4}_{2} \underbrace{4}_{2} \underbrace{1}_{2} \underbrace{1}_{2} \underbrace{4}_{2} \underbrace{4}_{2} \underbrace{1}_{2} \underbrace{1}_$

If we remove from K_r all interaction line reducible we obtain a new kernel \tilde{K}_r



The reducible kernel can again be expanded in a G-line irreducible one



 $\tilde{K}(1,2;3,4) = K(1,2;3,4) - i\delta(1;3)\delta(2;4)v(1;2)$

The polarizability can then be expressed as

$$= i \qquad P(1,2) = -i \int d4 G(1,3) G(4,1) \Gamma(3,4;2)$$

where we defined the vertex function as



 $\Gamma(1,2;3) = \delta(1,2^+)\delta(3,2) - \int d(4567)\,\tilde{K}(1,5;2,4)\,G(4,6)\,G(7,5)\,\Gamma(6,7;3)$

For the kernel $\, \tilde{K} \,$ the following relation is valid

$$\tilde{K}(1,2;3,4) = -\frac{\delta \Sigma_{\rm xc}(1,3)}{\delta G(4,2)}$$

as follows from a diagrammatic proof

The equation for the vertex therefore becomes

$$\Gamma(1,2;3) = \delta(1;2^+)\delta(3;2) + \int d4d5d6d7 \,\frac{\delta\Sigma_{\rm xc}(1;2)}{\delta G(4;5)} \,G(4;6)G(7;5)\Gamma(6,7;3)$$

If we can further express the vertex in terms of the vertex we have a closed set of functional differential equations

By a diagrammatic derivation we can also show that the self-energy can be expressed in terms of the vertex

$$\Sigma(1;2) = \frac{3}{1 \ 2} + i \qquad \frac{3}{1 \ 4} 2$$

$$\Sigma(1;2) = \pm i \,\delta(1;2) \int d3 \,v(1;3) G(3;3^+) + i \int d3d4 \,W(1;3) G(1;4) \Gamma(4,2;3)$$

Let us collect all the equations that we derived

Hedin's equations



2-particle Green's function and Hedin's equations: Take home message

- For the 2-particle Green's function we can derive an equation with a reducible kernel, known as the Bethe-Salpeter equation.
- The reducible kernel is the functional derivative of the self-energy with respect to the Green's function.
- From the diagrammatic rules we can derive a set of functional differential equations relating the vertex, the Dyson and the Bethe-Salpeter equation. These equations are known as the Hedin equations.
- The Hedin equations can be iterated in various ways to generate different perturbation series.
 It is not known whether all skeleton diagrams are generated once by such a procedure.

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

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

which can be rewritten as

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

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

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

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

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



Bethe-Salpeter equation

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

then the Bethe-Salpeter equation becomes



From $\chi(1,2) = -iL(1,2;1^+,2^+)$ 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

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

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

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

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

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

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

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

The interaction energy between this charge and a generic electron is

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

$$\begin{aligned} e_{\text{int}}(\mathbf{r}) &= \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \left[\delta(\mathbf{r}) + \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}'} \,\tilde{v}_{\mathbf{q}} \,\chi^{\text{R}}(\mathbf{q}, 0) \right] \\ &= \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \left[\tilde{v}_{\mathbf{q}} + \tilde{v}_{\mathbf{q}}^2 \chi^{\text{R}}(\mathbf{q}, 0) \right] \\ &= \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} W^{\text{R}}(\mathbf{q}, 0) \xrightarrow[r \to \infty]{} \frac{e^{-r/\lambda_{\text{TF}}}}{r} \end{aligned}$$

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

- 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 so 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

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

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

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

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

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

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 $p \ge p_{\rm F}$

 $\begin{array}{lll} \mbox{A plasmon can be excited} \\ \mbox{only when} & \omega \geq \mu + \omega_p \end{array}$

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

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 $-\text{Im}[\Sigma^{\text{R}}(p,\omega+\mu)] = \Gamma(p,\omega+\mu)/2$ 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 $\epsilon_{p_{\text{F}}} = p_{\text{F}}^2/2$.

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 $q = p_{\rm F}$, $\omega = \mu$

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

(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 $G_0 W_0$ 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.

Some recent results beyond GW

Y.Pavlyukh, A.-M. Uimonen, G.Stefanucci, RvL, arXiv. 1607.04309

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.

Things we did not talk about

- Feynman diagrams for the grand canonical potential and the action. Luttinger-Ward functionals, variational principles
- Connections to TDDFT and TD current DFT :
 - Diagrammatic expansion of xc-kernel
 - Sham-Schlüter equation and TDOEP
- General initial states
- Bethe-Salpeter and excitons, Lehmann representation
- Non-equilibrium phenomena and the Kadanoff-Baym equations (quantum transport)
- Conserving approximations and Ward identities
- Open quantum systems, T-matrix, superconductivity, phonons, Bose condensates,.....etc.