

Summary Sec. 2.7: The GW approximation (1)

Remember the important relation between the Inverse of the dielectric function and the ground state energy of a homogeneous gas of interacting electrons:

$$E_0 = 2 \sum_{|\mathbf{k}| \leq k_F} \frac{\hbar^2 k^2}{2m} - \sum_{\mathbf{q}} \int_{\lambda=0}^{e^2} \frac{d\lambda}{\lambda} \left[\frac{2\pi n_0 \lambda}{q^2} + \frac{\hbar}{2\pi} \int_0^\infty d\omega \Im \left(\frac{1}{\kappa_\lambda(\mathbf{q}, \omega)} \right) \right].$$

However, this is only one possibility to calculate E_0 ; another one uses **the one-particle electron Green's function**.

Let's start with the multi-electron Hamiltonian in terms of the second quantization:

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) T(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

with the field operators $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$ and

$$T(\mathbf{r}) = -\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} \quad \text{and} \quad V(\mathbf{r}, \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}.$$

The expectation value of the **kinetic energy operator** with respect to the ground-state wave function $|\Psi_0\rangle$ of the interacting electron gas reads

$$\langle \hat{T} \rangle = \langle \Psi_0 | \hat{T} | \Psi_0 \rangle = \int d^3r \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{r}) T(\mathbf{r}) \hat{\psi}(\mathbf{r}) | \Psi_0 \rangle.$$

Obviously, this expression is similar to the one-particle Green's function for $t' > t$:

$$iG(\mathbf{r}t; \mathbf{r}'t') = - \langle \Psi_0 | \hat{\psi}_H^\dagger(\mathbf{r}'t') \hat{\psi}_H(\mathbf{r}t) | \Psi_0 \rangle.$$

Performing the limits $t' \rightarrow t^+$ and $\mathbf{r}' \rightarrow \mathbf{r}$, one gets

$$\begin{aligned} \lim_{t' \rightarrow t^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} iT(\mathbf{r}) G(\mathbf{r}t; \mathbf{r}'t') &= - \langle \Psi_0 | \hat{\psi}_H^\dagger(\mathbf{r}t^+) T(\mathbf{r}) \hat{\psi}_H(\mathbf{r}t) | \Psi_0 \rangle \\ &= - \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{r}) T(\mathbf{r}) \hat{\psi}(\mathbf{r}) | \Psi_0 \rangle. \end{aligned}$$

By comparing the above equations, one obtains

$$\langle \hat{T} \rangle = -i \int d^3r \lim_{t' \rightarrow t^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} T(\mathbf{r}) G(\mathbf{r}t; \mathbf{r}'t'). \quad (1)$$

- This is by no means a surprise: the expectation value of the **one**-particle operator "kinetic energy" is determined by the **one**-particle electron Green's function.

What's about the expectation value of the operator "potential energy"?

$$\langle \hat{V} \rangle = \frac{1}{2} \int d^3r d^3r' \langle \Psi_0 | \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) | \Psi_0 \rangle .$$

- One might assume that the calculation of the expectation value of such a **two**-particle operator requires a **two**-particle electron-electron Green's function.

In the very important paper V. M. Galitskii and A. B. Migdal, Sov. Phys.-JETP, **7**:96 (1958), these authors showed that this is not the case.

A detailed presentation of Galitskii and Migdal's derivation is given in Sec. 2.7 of my lecture notes. In this summary, I shall give only the result, namely, the important expression

$$\langle \hat{V} \rangle = -\frac{i}{2} \int d^3r \lim_{t' \rightarrow t^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \left(i\hbar \frac{\partial}{\partial t} - T(\mathbf{r}) \right) G(\mathbf{r}t; \mathbf{r}'t'). \quad (2)$$

That means: the potential energy of the interacting electron gas is also fully determined by the one-particle Green's function $G(\mathbf{r}t; \mathbf{r}'t')$.

Consequently, using Eqs. (1) and (2), one gets the result

$$E_0 = \langle \hat{T} \rangle + \langle \hat{V} \rangle = -\frac{i}{2} \int d^3r \lim_{t' \rightarrow t^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \left(i\hbar \frac{\partial}{\partial t} + T(\mathbf{r}) \right) G(\mathbf{r}t; \mathbf{r}'t'). \quad (3)$$

The results given in the Eqs. (1)-(3) are valid both for spatially inhomogeneous and homogeneous electron gases. However, in the homogeneous case (jellium), Eq. (3) can be considerably simplified by using the FT

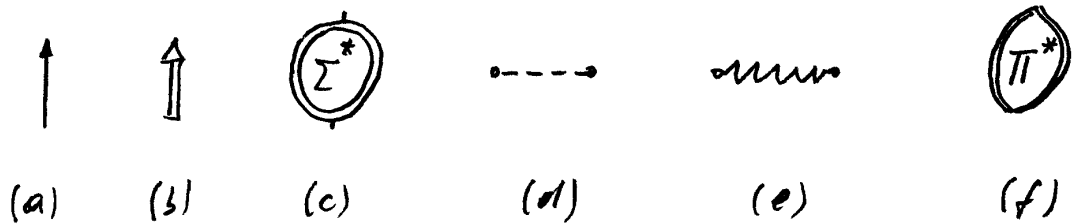
$$G(\mathbf{r}t; \mathbf{r}'t') = \frac{1}{2\pi\Omega} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} d\omega e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} e^{-i\omega(t-t')} G(\mathbf{k}, \omega).$$

After a short calculation, one obtains the result for *jellium*

$$E_0 = -\frac{i}{2} \lim_{\eta \rightarrow 0^+} \frac{1}{2\pi} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} d\omega e^{i\omega\eta} \left(\frac{\hbar^2 k^2}{2m} + \hbar\omega \right) G(\mathbf{k}, \omega). \quad (4)$$

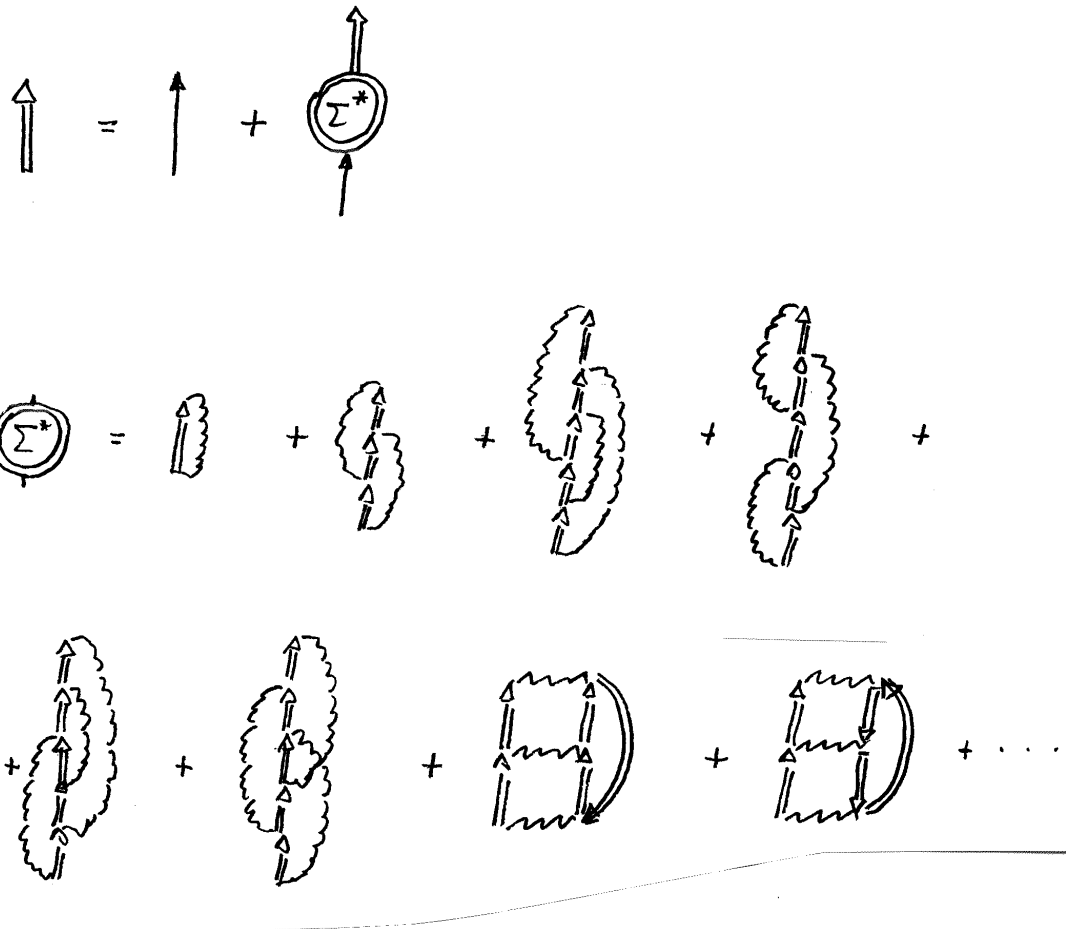
A milestone: **L. Hedin, Phys. Rev. 139, A796 (1965)**

- L. Hedin's famous paper **New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem** offers the theoretical basis for many actual investigations concerning electrons in solid-state media.
- In this paper, the exact calculation of the one-particle Green's function of electrons is based on the self-consistent solution of a system of four equations.
- In the following, these equations are presented in form of Feynman diagrams where the elements of this graphical representation are well-known:



- (a) non-interacting Green's function
- (b) interacting Green's function
- (c) (proper) selfenergy insertion,
based on interacting Green's functions
- (d) (bare) Coulomb potential
- (e) effective (dynamic) interaction potential
- (f) (proper) polarization insertion,
based on interacting Green's functions

- The first two of Hedin's equations are the **Dyson equation** of an interacting electron, where the interaction is defined by a **proper selfenergy insertion**:



- **Note:** the selfenergy insertion is **completely interacting**, i.e., it contains exclusively **interacting** Green's functions and **effective** interaction lines.
- These interaction lines are defined by Hedin's equations three and four, i.e., in the well-known form



- where the **proper polarization insertion** looks like

- **Note:** the polarization insertion is also completely interacting, i.e., it contains exclusively interacting Green's functions and effective interaction lines.

Historically, about twenty years passed by from the "invention" of Hedin's formulas until their first applications in solid state physics (≈ 1985). The reason for that is simple: the numerical evaluation of these equations is rather complicated and requires a lot of computer power.

Approximations to Hedin's concept:

- One great problem concerning the evaluation of Hedin's formulas is the **complicated structure** of the proper selfenergy $\Sigma^{pr}(\mathbf{q}, \omega)$ and the proper polarization function $\Pi^{pr}(\mathbf{q}, \omega)$.
- **Therefore, a significant simplification is to be expected if these functions are approximated by their first terms.**
- For the polarization function, this means



This approximation can be denoted an **extended RPA**: "extended" means that the electron-hole bubble consists of two **interacting** Green's functions.

- The corresponding simplification of the proper selfenergy, namely

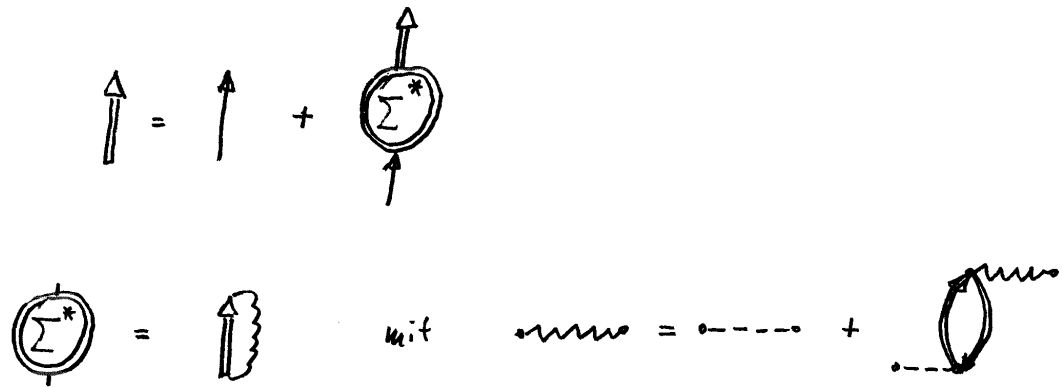


has already be proposed by Hedin himself. This approximation means a "product" of a full-interacting Green's function (G) and of an effective interaction potential (W) and is therefore called a

GW Approximation (GWA)

- Since about 1990, the GWA has been used for numerous applications concerning both homogeneous and inhomogeneous electron gases in solid-state media. It can really be denoted **the state-of-the-art method of modern solid-state physics.**

The GWA: Feynman and mathematical representation:



$$G(\mathbf{k}, \omega) = G^0(\mathbf{k}, \omega) + G(\mathbf{k}, \omega) \Sigma^{pr}(\mathbf{k}, \omega) G^0(\mathbf{k}, \omega)$$

$$\Sigma^{pr}(\mathbf{k}, \omega) \approx \frac{i}{\hbar(2\pi)^4} \int d^3q d\sigma G(\mathbf{k} - \mathbf{q}, \omega - \sigma) W(\mathbf{q}, \sigma) \quad (5)$$

$$W(\mathbf{q}, \omega) = V(\mathbf{q}) + W(\mathbf{q}, \omega) \Pi^{pr}(\mathbf{q}, \omega) V(\mathbf{q})$$

$$\Pi^{pr}(\mathbf{q}, \omega) \approx -\frac{2i}{\hbar(2\pi)^4} \int d^3q_1 d\sigma G(\mathbf{q}_1, \sigma) G(\mathbf{q}_1 - \mathbf{q}, \sigma - \omega)$$

- In the literature, the neglected terms of the selfenergy function and the polarization function are used to be called **vertex corrections**.

These corrections will - at least in principle - be discussed in some further sections of this lecture.

- Despite the strong simplifications of Hedin's formulas due to neglecting the vertex corrections, the numerical treatment of Eqs. (5) is still a rather complicated job. Therefore, in the literature, further simplifications are discussed, especially under the names **GW₀** and **G₀W₀**.
- The meaning of these abbreviations can be easily understood by comparing the diagrams above and the Eqs. (5) with the following:

$G W_0$:

$$G(\mathbf{k}, \omega) = G^0(\mathbf{k}, \omega) + G(\mathbf{k}, \omega) \Sigma^{pr}(\mathbf{k}, \omega) G^0(\mathbf{k}, \omega)$$

$$\Sigma^{pr}(\mathbf{k}, \omega) \approx \frac{i}{\hbar(2\pi)^4} \int d^3q d\sigma G(\mathbf{k} - \mathbf{q}, \omega - \sigma) W(\mathbf{q}, \sigma) \quad (6)$$

$$W(\mathbf{q}, \omega) = V(\mathbf{q}) + W(\mathbf{q}, \omega) \Pi_0^{pr}(\mathbf{q}, \omega) V(\mathbf{q})$$

$$\Pi_0^{pr}(\mathbf{q}, \omega) \approx -\frac{2i}{\hbar(2\pi)^4} \int d^3q_1 d\sigma G^0(\mathbf{q}_1, \sigma) G^0(\mathbf{q}_1 - \mathbf{q}, \sigma - \omega)$$

$G_0 W_0$:

$$G(\mathbf{k}, \omega) = G^0(\mathbf{k}, \omega) + G(\mathbf{k}, \omega) \Sigma^{pr}(\mathbf{k}, \omega) G^0(\mathbf{k}, \omega)$$

$$\Sigma^{pr}(\mathbf{k}, \omega) \approx \frac{i}{\hbar(2\pi)^4} \int d^3q d\sigma G^0(\mathbf{k} - \mathbf{q}, \omega - \sigma) W(\mathbf{q}, \sigma) \quad (7)$$

$$W(\mathbf{q}, \omega) = V(\mathbf{q}) + W(\mathbf{q}, \omega) \Pi_0^{pr}(\mathbf{q}, \omega) V(\mathbf{q})$$

$$\Pi_0^{pr}(\mathbf{q}, \omega) \approx -\frac{2i}{\hbar(2\pi)^4} \int d^3q_1 d\sigma G^0(\mathbf{q}_1, \sigma) G^0(\mathbf{q}_1 - \mathbf{q}, \sigma - \omega)$$

GW studies on jellium:

- [1] U. von Barth and B. Holm, *Self-consistent GW_0 results for the electron gas: Fixed screened potential W_0 within the random-phase approximation*, Phys. Rev. **54**, 8411 (1996).
- [2] B. Holm and U. von Barth, *Fully self-consistent GW self-energy of the electron gas*, Phys. Rev. **57**, 2108 (1998).
- [3] B. Holm, *Total energies from GW calculations*, Phys. Rev. Lett. **83**, 788 (1999)
- [4] P. Garcia-Gonzalez and R. W. Godby, *Self-consistent calculation of total energies of the electron gas using many-body perturbation theory*, Phys. Rev. B **63**, 075112 (2001).

We shall now discuss some important applications of G_0W_0 , GW_0 , and GW on the homogeneous electron gas. The calculated Green's functions are inserted into Eq. (4), and the corresponding correlation energies (= ground state energies minus Hartree-Fock contributions) are compared with other theoretical results.

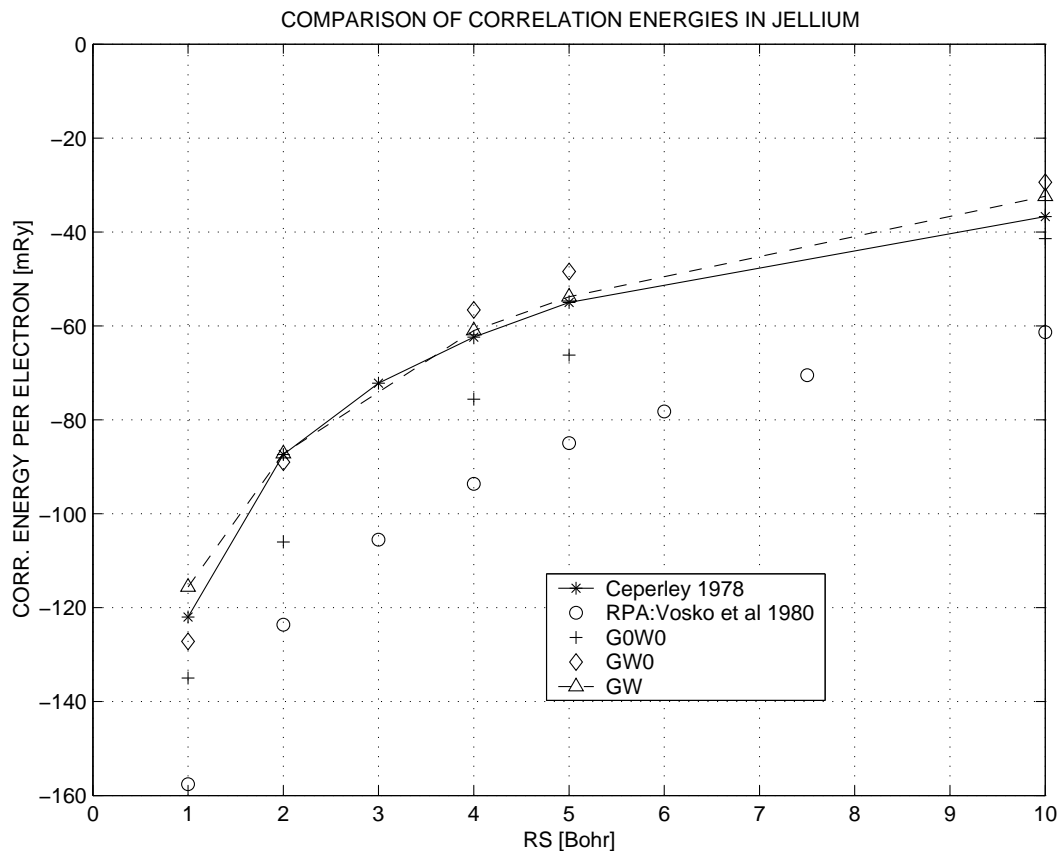
In the following table, we show a comparison between QMC data (Ceperley and Alder 1980) and GW results from Ref. [3]:

TABLE: The correlation energy per electron for different GW schemes, compared to Quantum Monte Carlo data.

r_s	GOWO	GW0	GW	QMC
2.0	-0.101	-0.0825	-0.0901	-0.0897
4.0	-0.0718	-0.0578	-0.0640	-0.0638
	(13 %	9 %	0.3 %)	

- For both values of r_s , the differences of the GW results to QMC significantly decrease for $G_0W_0 \rightarrow GW_0 \rightarrow GW$.
- The agreement between GW and QMC is almost perfect.

This conclusion is also supported by further GW results:



Theoretically obtained correlation energies in *jellium*.

The figure contains QMC results by Ceperley (1978), RPA results by Vosko et al (1980), and self-consistent G_0W_0 , GW_0 and GW data by Garcia-Gonzalez and Godby (2001), Ref. [4].

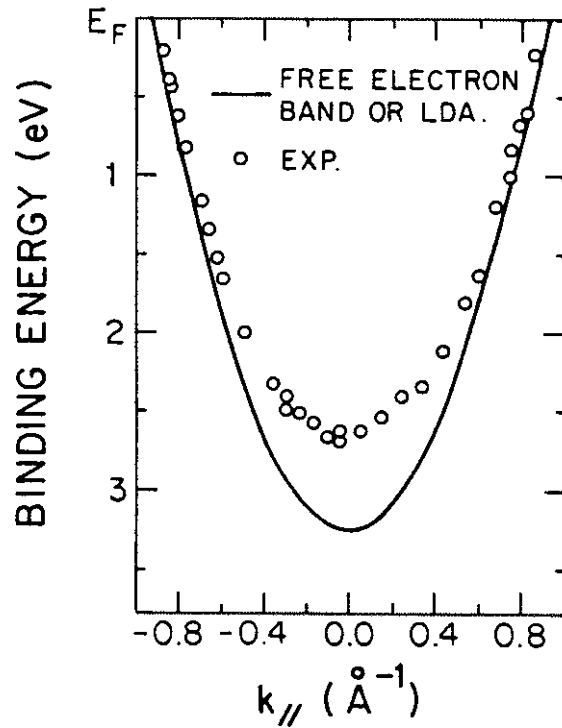
- **No surprise: the theoretical results are the better the less approximations are included into the GW process.**

BUT

- **The following discussion about the quasiparticle dispersion of the sodium 3s valence band shows that one has to be very careful with such general statements.**

The experimental situation,

based on ARPES measurements by Lyo and Plummer, Phys. Rev. Lett. **60**, 1558 (1988):



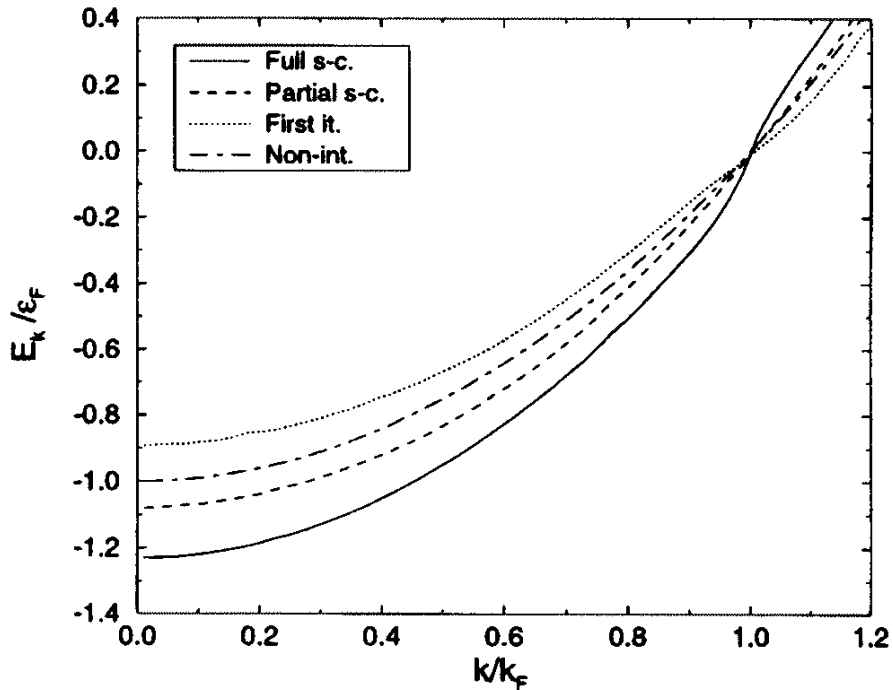
ARPES-measured quasiparticle dispersion of the sodium 3s valence band, compared to a free-electron or LDA band.

- The "free electron" or "LDA" bandwidth of the *occupied* 3s states is 3.23 eV.
- The corresponding, ARPES-measured "quasiparticle" bandwidth is 2.68 eV.
- That means a - surprisingly large - **band narrowing of $\approx 17\%$** .

If one accepts the hypothesis that this band narrowing is caused by multi-particle correlations, one should expect that "better and better" theoretical descriptions of such correlations (e.g., $G_0W_0 \rightarrow GW_0 \rightarrow GW$) will show a "more and more" significant reduction of the Na 3s bandwidth.

The theoretical situation,

based on G_0W_0 , GW_0 , and GW calculations by Holm and von Barth, Ref. [2]:



The dispersion E_k of the 3s valence band of sodium. In this figure, the following notations are used: *Non-int.* = free electron, *First it.* = G_0W_0 , *Partial s-c.* = GW_0 , *Full s-c.* = GW .

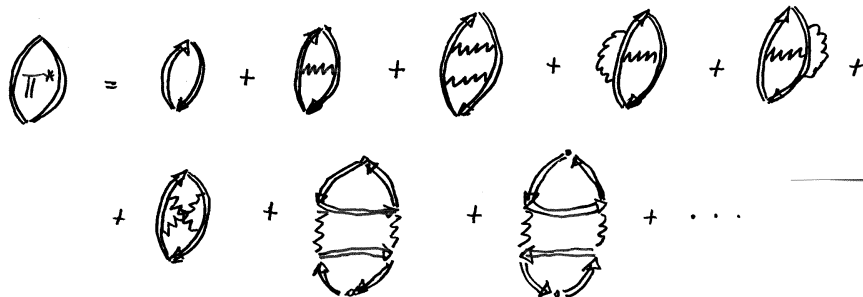
We give now some original quotations out of Ref. [2]:

- *Experiments show that the bandwidths of simple metals are of the order of 10% more narrow as compared to the results of band-structure calculations employing a local and energy-independent potential, i.e., like that of the LDA.*
- *Thus, there was originally some hope that a GW calculation would cure this problem – and a non-self-consistent G_0W_0 calculation for the electron gas does indeed produce a more narrow bandwidth although not narrow enough....*
- *Therefore, it was disappointing to find that a partially self-consistent GW_0 calculation gives a bandwidth larger than of noninteracting electrons.*
- *... even more disappointing to see that the fully self-consistent procedure actually makes the problem even worse.*

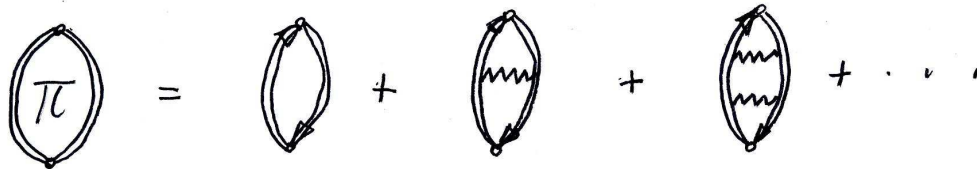
Summary Sec. 2.7.1: Vertex corrections and local-field factors

The main topic of this section is to discuss connections between two very important quantities of theoretical electron theory, namely, the **local-field factor** F - introduced in Sec. 2.6 - and the **vertex corrections** which appear in Hedin's system of equations.

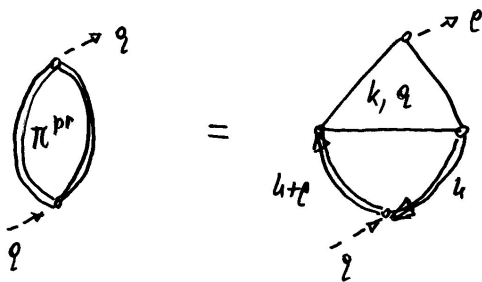
Remember the Feynman expansion of the polarisation:



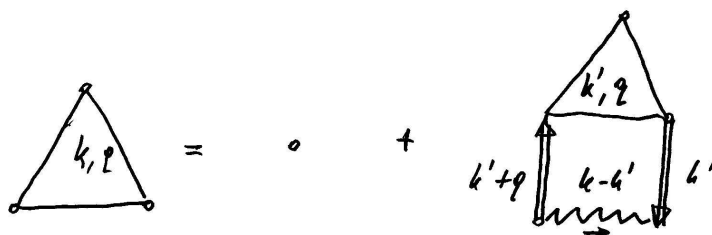
One immediately observes that this sum of diagrams includes **the Hubbard expansion**



which can more conveniently be written in the form



with



The last figure defines **Hubbard's vertex correction** which is - for graphical reasons - often called the **ladder summation vertex**. The first term of this recurrence relation means that the "vertex triangle" degenerates to a "vertex point".

Mathematically, the last two figures correspond to

$$\Pi^H(q) = -\frac{2i}{(2\pi)^4\hbar} \int d^4k G(k) G(k+q) \Gamma^H(k, q) \quad (8)$$

and

$$\Gamma^H(k, q) = 1 + \frac{i}{(2\pi)^4\hbar} \int d^4k' \Gamma^H(k', q) G(k') G(k'+q) W(k-k'),$$

where the quantities k, q etc. mean the four-component vectors $k \equiv \mathbf{k}; \omega, q \equiv \mathbf{q}; \omega'$ etc.

Obviously, the simplest approximation to Γ^H means a neglect of vertex corrections, and the corresponding polarization insertion reduces to the RPA.

For the rather simplified form of Hubbard's vertex correction, namely for $G \rightarrow G_0$ and $W(\mathbf{k}, \omega) \rightarrow V(\mathbf{q})$, one gets

$$\Gamma_0^H(k, q) = 1 + \frac{i}{(2\pi)^4\hbar} \int d^4k' \Gamma_0^H(k', q) G_0(k') G_0(k'+q) V(\mathbf{k}-\mathbf{k}').$$

Insertion into Eq. (8) obtains

$$\Pi_0^H(q) = -\frac{2i}{(2\pi)^4\hbar} \int d^4k G_0(k) G_0(k+q) \Gamma_0^H(k, q). \quad (9)$$

Remember the corresponding formula earlier discussed in this lecture:

$$\Pi_0^H(q) = \frac{\Pi_0^{RPA}(q)}{1 + V(\mathbf{q}) F_H(\mathbf{q}) \Pi_0^{RPA}(q)} \quad (10)$$

where $F_H(\mathbf{q})$ means **Hubbard's (static) local-field factor**.

With some mathematical effort [see e.g. Singwi et al., Phys. Rev. 176, 589 (1968)] one can prove that the equations (9) and (10) are equivalent for

$$\begin{aligned}
F_H(\mathbf{q}) = & \frac{9}{32} \left(\frac{q}{k_F} \right)^2 \left\{ \frac{2}{105} \left[24 \left(\frac{k_F}{q} \right)^2 + 44 + \left(\frac{q}{k_F} \right)^2 \right] \right. \\
& - 2 \frac{k_F}{q} \left[\frac{8}{35} \left(\frac{k_F}{q} \right)^2 - \frac{4}{15} + \frac{1}{6} \left(\frac{q}{k_F} \right)^2 \right] \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \\
& \left. + \left(\frac{q}{k_F} \right)^2 \left[\frac{1}{210} \left(\frac{q}{k_F} \right)^2 - \frac{2}{15} \right] \ln \left| \frac{q^2 - 4k_F^2}{q^2} \right| \right\} \\
& \approx \frac{q^2}{2(q^2 + k_F^2)}.
\end{aligned}$$

In a similar way, vertex corrections can also be included into the selfenergy function Σ .

How do vertex corrections influence the GW results?

The following data are taken from a paper of E.L. Shirley [*Self-consistent GW and higher-order calculations of electron states in metals*, Phys. Rev. B **54**, 7758 (1996)].

Here we find *ab initio* calculations of the occupied bandwidth of various homogeneous electron gases ($r_S = 2-5$ Bohr units), obtained by GW calculations of different level (G_0W_0 and GW) and also by taking account to **vertex corrections to the selfenergy function**:

Remember: Photoemission experiments of Lyo and Plummer (1988) yielded for sodium ($r_s = 3.96$ Bohr units) a band narrowing of 17 %:

(for $r_s=4$ Bohr)	Holm-Barth 1998	Shirley 1996
non-interacting electrons	1.00	1.00
GWO	0.90	0.81
GW	1.08	1.02
GW + vertex corr		0.82

Some quotations from Shirley's paper:

- *One can speculate that simultaneous neglect of renormalization (= self-consistency (HS)) and vertex corrections produces two, largely canceling errors in the behavior of the selfenergy.*
- *While a non-selfconsistent, low-order GW treatment reduces occupied bandwidths by 10-30 % (compared to independent-electron theory), self-consistency leads to overall increased bandwidths.*
- *Subsequent inclusion of the next-order term (=vertex term (HS)) in Sigma restores reduced bandwidths which agree well with experiment.*

BUT:

During the last years, several papers were published where the band narrowing **is in principle disbelieved**. The argumentation is that this effect appears due to **an erraneous evaluation of the photoemission data**:

H. Yasuhara, S. Yoshinaga, and M. Higuchi, *Why is the Bandwidth of Sodium Observed to be Narrower in Photoemission Experiments?*,

Phys. Rev. Lett. **83**, 3250 (1999).

W. Ku, A.G. Eguiluz, and E.W. Plummer, *Comment on Yasuhara's paper*,

Phys. Rev. Lett. **85**, 2410 (2000).