

# GREEN'S FUNCTIONS TECHNIQUE FOR STATISTICAL ENSEMBLES

---

LECTURE NOTES

BY

PROF. DR. GERD RÖPKE

&

MATHIAS WINKEL

JUNE 10, 2009



**INSTITUT FÜR PHYSIK**

QUANTUM THEORY & MANY-PARTICLE SYSTEMS  
ROSTOCK UNIVERSITY



# Contents

<b>1</b>	<b>Perturbation theory for statistical ensembles</b>	<b>5</b>
1.1	General relations . . . . .	5
1.2	Calculation of mean values . . . . .	9
1.3	Wick's theorem . . . . .	12
1.4	Example: Hartree-Fock approximation . . . . .	15
<b>2</b>	<b>Thermodynamic Green's functions: Definitions and properties</b>	<b>21</b>
2.1	Definitions . . . . .	21
2.2	Green's function and spectral function . . . . .	27
2.3	Example: Ideal Fermi gas . . . . .	31
<b>3</b>	<b>Perturbation theory for thermodynamic Green's functions</b>	<b>35</b>
3.1	Basic relations . . . . .	35
3.2	Diagrammatic representation of the perturbative series . . . . .	37
3.3	Evaluation of the frequency summation . . . . .	41
3.4	Application: Hartree-Fock approximation . . . . .	44
<b>4</b>	<b>Evaluation of diagrams and partial summation</b>	<b>47</b>
4.1	Mean field and quasi-particle concept . . . . .	47
4.2	Dyson equation and self-energy . . . . .	50
4.3	Screening equation and polarization function . . . . .	53
4.4	Random phase approximation (RPA) . . . . .	59
4.4.1	Static limit $\omega \rightarrow 0$ for a classical plasma: Debye screening . . . . .	61
4.4.2	Long wavelength limit $q \rightarrow 0$ . . . . .	62
4.4.3	Landau damping . . . . .	64
4.5	Vertex equation . . . . .	68
4.6	Single-particle self-energy: consistent approximation . . . . .	70
4.7	Excursus: Dielectric function . . . . .	72
4.8	Bound states . . . . .	75
4.9	Abstract algebraic representation . . . . .	79
4.10	Excursus: Two-particle problem with a separable potential . . . . .	80
<b>5</b>	<b>Diagram technique</b>	<b>87</b>
5.1	Elements of the diagram technique and the chemical picture . . . . .	87
5.2	Cluster expansion for self-energy . . . . .	92
5.3	Cluster-RPA for the polarization function . . . . .	98
5.4	Consistent approximations for the cluster self-energy . . . . .	101
<b>6</b>	<b>Synopsis / Outlook</b>	<b>107</b>
	<b>References</b>	<b>111</b>
	<b>Index</b>	<b>113</b>



# Introduction

During standard lectures on quantum and statistical mechanics, often only ideal systems or systems, that do not show quantum effects, are examined, respectively. However, when treating real many-particle systems, we have to include inter-particle correlations as well as the particles' quantum character.

We will see during this lecture, that such a systematic treatment of many-particle systems is possible in the framework of a perturbation theoretical approach. Alternatively to the perturbation expansions described here, other approaches to calculate correlation functions have been elaborated, such as simulation techniques, in particular path integral approaches, which are not subject of this lecture. They are of advantage if the perturbation is strong, but they do not give analytical expressions, especially in limiting cases.

The rules for a perturbative treatment of quantum many-particle systems are simple but cumbersome. Very efficient new tools have been elaborated: The method of GREEN's functions and diagram techniques. Originally introduced in quantum field theory, these methods have been shown to be very successful in many body theory.

Typical effects besides correlations and screening, that are already present in classical systems, are bound state formation and degeneration in quantum systems. Their treatment via the spectral function, partial summations for quasi-particles, the screened potential and single- and more-particle GREEN's functions will be subject of this lecture.

Due to density effects, not only cluster features but also the single-particle properties are modified. For example, energy levels are broadened, cross-sections are changed or even bound states can be broken up at higher densities (MOTT effect: bound states are dissolved because of screening and/or PAULI blocking). These microscopic phenomena lead to the formation of quasi-particles with shifted energies or effective masses and thus modified spectral functions, to a screened interaction and thus a non-trivial dielectric function, density-density correlation function, and dynamical structure factor, as well as many other exciting effects.

Not only microscopic but also the macroscopic properties are changed by many-particle effects, e.g. the formation of bound states. These strongly modified thermodynamic, kinetic and transport properties can be calculated using GREEN's functions.

In addition, we will introduce a chemical picture, that – as an advancement of the physical one – enables us to treat bound states and free particles on the same footing.

The concepts and methods given here are of significance in different fields of physics such as plasma physics, semiconductor physics, solid state physics, nuclear physics. Special applications such as phase transitions, nonequilibrium processes, or quantum field theory demand a separate special lecture course.

Necessary prerequisites to follow this lecture are standard lectures on quantum and statistical mechanics, in particular:

- knowledge of fundamental concepts of quantum mechanics, including second quantization and
- knowledge of the concepts and methods of statistical mechanics such as thermodynamic relations, equilibrium statistical operator for the grand canonical ensemble, treatment of ideal quantum gases.

These lecture notes have been developed accompanying the winter courses 2007/2008 and 2008/2009 on *Quantum Statistics of Particles and Fields*, that were read at the Institute of Physics of Rostock University by Prof. Dr. Gerd Röpke.

They were based on the scriptum *Greenfunktions-Technik für statistische Gesamtheiten* [SR93], which has been prepared during a WE-HERAEUS summer-school in 1993 by Dr. Holger Stein, and has been in annual use since then.

The material should fill a course of approximately 30 hours of lecture. While section 1 gives an elementary but cumbersome approach to the evaluation of mean values in interacting quantum systems, in sections 2 and 3 the concept of the thermodynamic GREEN's function and its diagrammatic representation is developed. The following section 4 shows the evaluation of the FEYNMAN diagrams and introduces self-energy and polarization function. Finally, sections 5 and 6 present the GREEN's functions calculus' virtue in some higher-level utilization, the chemical picture as a new attainment and an outlook to further applications and enhancements.

Any general theorem or equation of high importance is highlighted by a frame.

Proofs, comments, and additions are written in a smaller font and are marked with a grey line to their side.

We would like to thank Dr. August Wierling for his important contributions to several sections of this work and many valuable discussions as well as Sonja Lorenzen and Dr. Carsten Fortmann for their helpful comments and suggestions.

Rostock,  
May 2009

G. Röpke & M. Winkel

# 1 Perturbation theory for statistical ensembles

## 1.1 General relations

Within the lectures on statistical physics, mostly ideal quantum gases are considered. Their HAMILTONIAN  $H = T+V$  only contains the the single-particle (kinetic) energy

$$T = H^{(1)} = \sum_k E_k c_k^+ c_k \quad \text{with} \quad E_k = \frac{\hbar^2 k^2}{2m} \quad (1.1.1)$$

and does not contain (multi-particle) interaction, i.e.  $V = 0$  holds.

The operators  $c_k$  and  $c_k^+$  are the well-known<sup>1</sup>

fermionic  $a, a^+$

or bosonic  $b, b^+$

annihilation and creation operators with their occupation number  $n_k = c_k^+ c_k$  and their respective commutative relations, such as

$$\begin{aligned} \{a_k, a_{k'}^+\}_+ &= a_k a_{k'}^+ + a_{k'}^+ a_k = \delta_{kk'} \\ [b_k, b_{k'}^+]_- &= b_k b_{k'}^+ - b_{k'}^+ b_k = \delta_{kk'} \text{ , etc.} \end{aligned}$$

Although often the ideal models can be evaluated very comfortably and lead to cohesive results, this picture omits the interaction contribution  $V$ , that is evident in any many-particle system<sup>2</sup>. For example in electrically charged particle systems, we have to consider the COULOMB potential

$$V_{k_1 k_2; k'_1 k'_2} = \frac{e_1 e_2}{\varepsilon_0 \Omega |k_1 - k'_1|^2} \delta_{k_1+k_2, k'_1+k'_2} \delta_{\sigma_1 \sigma'_1} \delta_{\sigma_2 \sigma'_2} \quad (1.1.2)$$

with the normalization volume  $\Omega$ , the respective wave-number vectors  $k_i$  and  $k'_i$  of the incoming and outgoing particles and their spin  $\sigma_i$  and  $\sigma'_i$ . See section 3.2 for a detailed discussion of this FOURIER transformed interaction.

Normally, in theoretical physics we are facing problems that do not lead straightforward to analytically exact solutions, because the interaction of the particles among each other can be arbitrary complex

<sup>1</sup>For a more extensive recapitulation of the calculus of creation and annihilation operators (second quantization), we recommend studying the corresponding chapters in standard textbooks about quantum mechanics. For example, in [Nol03], there is a very detailed derivation of the form (1.1.4) of the standard HAMILTONIAN.

<sup>2</sup>We will later see the reason, why ideal quantum gases are successful in describing interacting systems, such as electrons in metals, after introducing the quasi-particle concept and the chemical picture.

as it is for the considered systems, for example dense plasmas or nuclear matter. In general, we face a HAMILTONIAN of the type

$$H = H^{(1)} + H^{(2)} + \dots \quad (1.1.3)$$

$$= \sum_k E_k c_k^\dagger c_k + \frac{1}{2} \sum_{k_1 k_2, k'_1 k'_2} V_{k_1 k_2, k'_1 k'_2} c_{k_1}^\dagger c_{k_2}^\dagger c_{k'_2} c_{k'_1} + \dots, \quad (1.1.4)$$

consisting of single-, two-, and possibly more-particle contributions. Using the operators of second quantization, any observable can be decomposed in a similar structure.

We regard  $H^{(1)}$  to be diagonal in the single-particle operators. If this is not the case (for example in momentum representation in the case of an external potential) for momentum representation, we have to diagonalize  $H^{(1)}$ , i.e. find a basis, where  $H^{(1)}$  is diagonal by solving the eigenvalue equation.

Averages of operators  $A$  are evaluated with respect to the ensembles characterization by the statistical operator  $\varrho$ :

$$\langle A \rangle = \text{Tr} \{ \varrho A \} . \quad (1.1.5)$$

In the following we will use the grand-canonical ensemble<sup>3</sup>, where the statistical operator is

$$\varrho(T, \Omega, \mu) = e^{-S} \quad (1.1.6)$$

with the entropy operator  $S$ , that satisfies

$$\langle S \rangle = - \langle \ln \varrho \rangle . \quad (1.1.7)$$

A systematic cluster decomposition of the entropy operator with respect to many-particle contributions is considered for the grand statistical operator.

Thus, the entropy is a function of temperature  $T = (k_B \beta)^{-1}$ , volume  $\Omega$  and chemical potential  $\mu$ .

$$S = S^{(0)} + S^{(1)} + S^{(2)} + \dots \quad (1.1.8)$$

$$= \ln Z(T, \Omega, \mu) + \sum_k s_k^{(1)} c_k^\dagger c_k + \sum_{k_1 k_2, k'_1 k'_2} s_{k_1 k_2, k'_1 k'_2}^{(2)} c_{k_1}^\dagger c_{k_2}^\dagger c_{k'_2} c_{k'_1} + \dots . \quad (1.1.9)$$

The summation in  $k$  is running over the usual degrees of freedom, such as momentum  $\hbar \vec{k}$ , spin  $\sigma$ , etc.

Within this cluster decomposition,

$$S^{(0)} = \ln Z(T, \Omega, \mu) \quad \text{with} \quad Z(T, \Omega, \mu) = \text{Tr} \left\{ e^{-(S^{(1)} + S^{(2)})} \right\} \quad (1.1.10)$$

---

<sup>3</sup>Since at least in the thermodynamic limit the different ensembles are equivalent, this choice is arbitrary, but for our calculations the grand-canonical ensemble is more convenient. As soon as phase-transitions appear, the choice of the thermodynamic ensemble would be important. For some more comments on the nonequilibrium case, see section 6.



is a c-number, that guarantees for a correct normalization,

$$S^{(1)} = \sum_k s_k^{(1)} c_k^+ c_k \quad (1.1.11)$$

is the single particle contribution that (in equilibrium) contains the kinetic energy and the chemical potential, and  $S^{(2)}$  a two-particle contribution, which contains two-particle correlations due to the interaction.

In the following, we will exemplarily concentrate on fermionic particles. A generalization to bosonic systems is possible and straightforward.

In the case of an ideal quantum gas, the two- and more-particle correlations in (1.1.9) will vanish and

$$S = S^{(0)} + S^{(1)} = S^{(0)} + \sum_k \beta(E_k - \mu) \quad (1.1.12)$$

is diagonal in momentum representation.

With the statistical operator

$$\varrho = \frac{e^{-\beta(H-\mu N)}}{\text{Tr} \{e^{-\beta(H-\mu N)}\}} \quad (1.1.13)$$

and the evolution operator<sup>4</sup>  $U \propto e^{\frac{i}{\hbar} H \cdot t}$ , the problem of the ideal quantum gas can be seen as solved and all mean values can be evaluated analytically in a closed form.

For example we find

$$N = \sum_k \langle a_k^+ a_k \rangle = \sum_k f_k \quad U = \sum_k E_k \langle a_k^+ a_k \rangle = \sum_k E_k f_k$$

with the FERMI-distribution

$$f_k = \frac{1}{e^{\beta \epsilon_k} + 1} \quad \text{with } \epsilon_k = E_k - \mu$$

in the case of an ideal FERMI gas and the BOSE distribution

$$g_k = \frac{1}{e^{\beta \epsilon_k} - 1}$$

for an ideal BOSE gas.

The wave-number summation can be transformed into an integration via

$$\sum_k \dots \rightarrow (2s+1) \Omega \int \frac{d^3 k}{(2\pi)^3} \dots,$$

where  $\Omega$  is the system volume and  $s$  the particle's spin.

<sup>4</sup>Obviously this time evolution operator is only valid if  $H$  does not explicitly depend on time. In the case of a time-dependent HAMILTONIAN (e.g. in an external potential), a time-ordering procedure has to be included, compare application of the time-ordering operator  $\mathbb{T}[\dots]$  in the following section.

To show the relation to the thermodynamic entropy, we calculate

$$\langle S \rangle \stackrel{(1.1.7)}{=} -\langle \ln \varrho \rangle \stackrel{(1.1.6),(1.1.9)}{=} \left\langle \ln Z(T, \Omega, \mu) + \sum_k \beta(E_k - \mu) \right\rangle \quad (1.1.14)$$

$$= \ln Z(T, \Omega, \mu) + \beta \underbrace{\sum_k \langle E_k \rangle}_{\langle H \rangle = U} - \beta \underbrace{\sum_k \langle \mu \rangle}_{\mu N} \quad (1.1.15)$$

$$= \ln Z(T, \Omega, \mu) + \beta U - \beta \mu N \quad (1.1.16)$$

$$\Rightarrow U - k_B T S - \mu N = -k_B T \ln Z(T, \Omega, \mu) = -p\Omega, \quad (1.1.17)$$

which is the GIBBS-DUHEM-equation.

## 1.2 Perturbation expansion for calculation of mean values

For real quantum gases, two- and possibly more-particle contributions will arise in the exponents of the statistical operator as well as in the time evolution operator<sup>5</sup>.

By expanding the exponential functions into a power series with respect to the interaction  $V$ , the treatment of real quantum gases can be reduced to ideal quantum gases in a perturbation theory.

We use the following relation for operators  $A$  and  $B$ :

$$e^{A+B} = e^A \left( 1 + \int_0^1 d\tau e^{-\tau A} B e^{\tau(A+B)} \right). \quad (1.2.1)$$

Equation (1.2.1) can be proven by introducing two functions

$$F_1(\lambda) = e^{\lambda(A+B)} \quad F_2(\lambda) = e^{\lambda A} \left( 1 + \int_0^\lambda d\tau e^{-\tau A} B e^{\tau(A+B)} \right)$$

and differentiating them with respect to  $\lambda$ :

$$\begin{aligned} \frac{d}{d\lambda} F_1(\lambda) &= (A+B) e^{\lambda(A+B)} \\ &= A F_1(\lambda) + B e^{\lambda(A+B)} \\ \frac{d}{d\lambda} F_2(\lambda) &= A e^{\lambda A} \left( 1 + \int_0^\lambda d\tau e^{-\tau A} B e^{\tau(A+B)} \right) + e^{\lambda A} \left( e^{-\lambda A} B e^{\lambda(A+B)} \right) \\ &= A F_2(\lambda) + B e^{\lambda(A+B)} \end{aligned}$$

Since  $F_1(\lambda)$  and  $F_2(\lambda)$  fulfill the same first-order differential equation and they agree in the special value  $\lambda = 0$ :  $F_1(\lambda = 0) = 1 = F_2(\lambda = 0)$ , they are identical for all values of  $\lambda$ . For  $\lambda = 1$ , equation (1.2.1) follows.

The GIBBS ensemble (and the time evolution operator) contains exponential functions of the form  $e^{A+B}$ . By iterating (1.2.1), a perturbation expansion can be constructed as follows:

$$e^{A+B} = e^A + \int_0^1 d\tau e^{(1-\tau)A} B e^{\tau A} + \int_0^1 d\tau \int_0^\tau d\tau_1 e^{(1-\tau)A} B e^{(\tau-\tau_1)A} B e^{\tau_1 A} + \dots \quad (1.2.2)$$

This is in general the DYSON series that is also known from lectures in quantum physics, especially on time-dependent perturbation theory.

<sup>5</sup>In nonequilibrium, we could define a relevant statistical operator  $\varrho_{\text{rel}}(t)$  with a generalized GIBBS ensemble in an exponential form. See section 6 for further details.

The fact, that the integration over  $\tau_1, \tau_2, \dots$  is running from zero to the predecessor ( $\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \dots$ ) guarantees the correct chronological order, i.e.  $\tau \geq \tau_1 \geq \tau_2 \geq \dots$ . This could also be achieved by introducing a time-ordering operator similar to  $T[\dots]$  in the following chapter.

If  $A$  and  $B$  in (1.2.2) commute, i.e.  $[A, B] = 0$ , the integrals are trivial and the classical case

$$e^{A+B} = e^A \cdot \left( \sum_{m=0}^{\infty} \frac{B^m}{m!} \right) = e^A \cdot e^B$$

holds.

For a further evaluation another important relation can be used: If  $S^{(1)}$  is a single-particle operator of the form

$$S^{(1)} = \sum_k s_k n_k, \quad (1.2.3)$$

with  $n_k = c_k^\dagger c_k$  and the annihilation operator  $c_k$  for fermions ( $a_k$ ) or bosons ( $b_k$ ), the relations

$$e^{S^{(1)}} c_k^\dagger e^{-S^{(1)}} = e^{s_k} c_k^\dagger \quad (1.2.4)$$

and  $e^{S^{(1)}} c_k e^{-S^{(1)}} = e^{-s_k} c_k \quad (1.2.5)$

hold.

The proof can again be performed by introducing a formal parameter  $\lambda$  and differentiating the functions

$$F_1(\lambda) = e^{\lambda S^{(1)}} c_k^\dagger e^{-\lambda S^{(1)}} \quad F_2(\lambda) = e^{\lambda s_k} c_k^\dagger$$

with respect to  $\lambda$ :

$$\begin{aligned} \frac{d}{d\lambda} F_1(\lambda) &= S^{(1)} e^{\lambda S^{(1)}} c_k^\dagger e^{-\lambda S^{(1)}} - e^{\lambda S^{(1)}} c_k^\dagger S^{(1)} e^{-\lambda S^{(1)}} \\ &= e^{\lambda S^{(1)}} [S^{(1)}, c_k^\dagger] e^{-\lambda S^{(1)}} \\ &\stackrel{(1.2.3)}{=} e^{\lambda S^{(1)}} \sum_l [s_l n_l, c_k^\dagger] e^{-\lambda S^{(1)}} \\ &= s_k F_1(\lambda), \end{aligned} \quad (\underline{A})$$

$$\frac{d}{d\lambda} F_2(\lambda) = s_k F_2(\lambda),$$

where in (A) the commutator relation  $[n_l, c_k^\pm]_- = [c_l^\pm c_l, c_k^\pm]_- = \delta_{lk} c_k^\pm$  has been used, that is valid for BOSE as well as for FERMI particles:

$$\begin{aligned} [n_l, c_k^\pm]_- &= c_l^\pm c_l c_k^\pm \pm c_l^\pm c_k^\pm c_l - c_k^\pm c_l^\pm c_l \mp c_l^\pm c_k^\pm c_l \\ &= c_l^\pm \underbrace{[c_l, c_k^\pm]_\pm}_{=\delta_{lk}} - \underbrace{[c_k^\pm, c_l^\pm]_\pm}_{=0} c_l \\ &= \delta_{lk} c_k^\pm \end{aligned}$$

Again  $F_1(\lambda)$  and  $F_2(\lambda)$  fulfill the same first-order differential equation and reach the same value  $F_1(\lambda = 0) = c_k^\pm = F_2(\lambda = 0)$  at  $\lambda = 0$ . Thus they must be identical and (1.2.4) is shown. Proving (1.2.5) works in the same way.

The relations (1.2.4) and (1.2.5) can be utilized for evaluating the time evolution as well as the statistical averaging in (1.2.2), see section 1.4.

For doing so, we would have to expand in terms of multi-particle contributions, which can be expressed by products of creation and annihilation operators. They appear for example in the interaction  $V$ . After inserting a factor of  $1 = e^{-S^{(1)}} e^{S^{(1)}}$  between those operators, the evaluation of such a product can be reduced to applying (1.2.4) and (1.2.5)<sup>6</sup> onto the resulting sandwich structure  $e^{S^{(1)}} A e^{-S^{(1)}}$ . An example of the application of this calculus will be presented in the proof of WICK's theorem in the following section and in the HARTREE-FOCK example in section 1.4.

With the help of the relations (1.2.1), (1.2.4), and (1.2.5) it is possible to simplify the calculation of mean values for a real quantum gas to evaluating correlation functions of an ideal quantum gas. In the framework of our perturbation expansion, correlation functions and averaged operator products of any order can appear.

In the following section we will derive a theorem that can be used for evaluating such high-order correlation functions for ideal quantum systems.

<sup>6</sup>The insertion is valid because  $S^{(1)}$  only contains single-particle contributions that mutually commute.

### 1.3 Calculation of operator averages for ideal quantum gases and Wick's theorem

While for ideal quantum gases with  $H^{(1)} = \sum_k E_k c_k^\dagger c_k$  – as we have already discussed – the statistical operator is diagonal in the single-particle occupation number and correlation functions can be calculated in a closed form, this is not the case for the general (non-ideal) quantum gas. Here, mean-values of a product of  $s$  operators  $A_i$ , that can be creation or annihilation operators for BOSE ( $b^+, b$ ) or FERMI ( $a^+, a$ ) particles,

$$\text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} \tag{1.3.1}$$

have to be calculated using the free (ideal) statistical operator  $\varrho^0 = e^{-(S^{(0)}+S^{(1)})}$  with  $S^{(1)} = \sum_k s_k^{(1)} c_k^\dagger c_k$  and the partition function of the ideal gas  $Z^0(T, \Omega, \mu) = \text{Tr} \{ e^{-S^{(1)}} \}$  so that  $S^{(0)} = \ln Z^0(T, \Omega, \mu)$ .

The evaluation of (1.3.1) can be performed using WICK's theorem:

$$\text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} = \sum_{\mathfrak{p} = \{\text{all pairings } \{i, j\} \dots \{k, l\}\}} (-1)^{\mathfrak{p}} \prod_{\text{all pairs } \{i, j\} \text{ in } \mathfrak{p}} \langle A_i A_j \rangle, \tag{1.3.2}$$

where  $A_1 \dots A_s$  can be any combination of creation and annihilation operators for BOSE- or FERMI-particles. In the case of fermions, the sign factor  $(-1)^{\mathfrak{p}}$  is positive for an even number of permutations in  $\mathfrak{p}$  and negative for an odd number. For bosons, it is set to one.

With WICK's theorem the evaluation of a high-order correlation functions is reduced to calculating the so-called contractions  $\langle A_i A_j \rangle$ .

In the following, we will concentrate on fermions, however the results can simply be transformed to the bosonic case by exchanging the negative signs and the FERMI functions  $f_i, (1 - f_i)$  with positive signs and BOSE distributions  $g_i, (1 + g_i)$ , respectively.

In (1.3.2), the decomposition of any permutation of the factors in the product  $A_1 A_2 \cdots A_s$  has to be considered as for example in

$$\overbrace{A_1 A_2} \overbrace{A_3 A_4} : \quad (+1) \cdot \langle A_1 A_2 \rangle \cdot \langle A_3 A_4 \rangle \quad [\mathfrak{p} \text{ even}] \tag{1.3.3}$$

$$\overbrace{A_1 A_2 A_3} \overbrace{A_4} : \quad (-1) \cdot \langle A_1 A_3 \rangle \cdot \langle A_2 A_4 \rangle \quad [\mathfrak{p} \text{ odd}] \tag{1.3.4}$$

$$\overbrace{A_1 A_2 A_3} \overbrace{A_4} : \quad (+1) \cdot \langle A_1 A_4 \rangle \cdot \langle A_2 A_3 \rangle \quad [\mathfrak{p} \text{ even}], \tag{1.3.5}$$

where the brackets denote the actual pairings.

Every decomposition into pairs gets a positive sign for an even number of transpositions and a negative one for an odd number of transpositions (character  $\mathfrak{p}$  of the permutation). The sign can simply be deduced by examining the number of crossings of the decomposition-brackets: even  $\rightarrow +1$ , odd  $\rightarrow -1$ .

For bosonic particles, the sign is positive in any case.

The single-particle average  $\langle A_i A_j \rangle$  vanishes if  $A_i$  and  $A_j$  are both annihilation or both creation operators. A non-vanishing result is only obtained in the case of a contraction of an annihilation operator with a creation operator which both affect the same state:

$$\langle a_i^+ a_j \rangle = \delta_{ij} \frac{1}{e^{\beta(E_i - \mu)} + 1} = \delta_{ij} f_i \quad (1.3.6)$$

$$\langle a_i a_j^+ \rangle = \delta_{ij} \frac{1}{e^{-\beta(E_i - \mu)} + 1} = \delta_{ij} (1 - f_i) . \quad (1.3.7)$$

for fermions and

$$\langle b_i^+ b_j \rangle = \delta_{ij} \frac{1}{e^{\beta(E_i - \mu)} - 1} = \delta_{ij} g_i \quad (1.3.8)$$

$$\langle b_i b_j^+ \rangle = \delta_{ij} \frac{1}{e^{-\beta(E_i - \mu)} - 1} = \delta_{ij} (1 + g_i) . \quad (1.3.9)$$

for bosons. Note, that the KRONECKER symbol  $\delta_{ij}$  means coincidence in all single-particle quantum numbers, i.e. besides momentum also spin, species, etc.

Hence, a nonzero result can only be obtained for an even number of operators  $A_i$  comprising the same number of annihilation and creation operators for the appropriate states<sup>7</sup>.

The proof for WICK's theorem is not straightforward but very instructive concerning the construction of (1.3.2).

Examining the fermionic case, at first we calculate

$$\text{Tr} \{ \varrho^0 \{ A_1, A_2 \cdots A_s \}_+ \} = \text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} + \text{Tr} \left\{ \overbrace{\varrho^0 (\varrho^0)^{-1}}^1 A_1 \varrho^0 A_2 \cdots A_s \right\} ,$$

where in the second summand the cyclic invariance of the trace was used and a  $1 = \varrho^0 (\varrho^0)^{-1}$  has been inserted. Considering the underbraced term

$$\begin{aligned} (\varrho^0)^{-1} A_1 \varrho^0 &\stackrel{(1.1.6),(1.1.9)}{=} e^{\sum s_k a_k^+} A_1 e^{-\sum s_k a_k^+} \\ &\stackrel{(1.2.4),(1.2.5)}{=} A_1 e^{\pm s_1} \quad \text{with } s_1 = \beta(E_1 - \mu) , \end{aligned}$$

where the positive sign holds for  $A_1 = a_1^+$  and the negative for  $A_1 = a_1$ , we get

$$\text{Tr} \{ \varrho^0 \{ A_1, A_2 \cdots A_s \}_+ \} = \text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} \cdot [1 + e^{\pm s_1}]$$

or

$$\text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} = \frac{\text{Tr} \{ \varrho^0 \{ A_1, A_2 \cdots A_s \}_+ \}}{1 + e^{\pm s_1}} . \quad (\underline{A})$$

<sup>7</sup>Note that this is not valid for coherent states where the average  $\langle A_i \rangle$  of a single creation operator can be nonzero. However, we will only consider basis states with a defined particle number.

Furthermore, the anticommutator can be evaluated step-by-step:

$$\begin{aligned} \{A_1, A_2 \cdots A_s\}_+ &= \{A_1, A_2\}_+ A_3 \cdots A_s - A_2 \{A_1, A_3\}_+ A_4 \cdots A_s + \dots \\ &\quad \dots + A_2 \cdots A_{s-1} \{A_1, A_s\}_+ . \end{aligned} \quad (\text{B})$$

N.B. the last term is positive in any case, since  $s$  is even.

As an example, we will show (B) for  $s = 4$ :

$$\begin{aligned} \{A_1, A_2 A_3 A_4\}_+ &= A_1 A_2 A_3 A_4 + A_2 A_3 A_4 A_1 \\ &= A_1 A_2 A_3 A_4 + A_2 A_1 A_3 A_4 - A_2 A_1 A_3 A_4 \\ &\quad - A_2 A_3 A_1 A_4 + A_2 A_3 A_1 A_4 + A_2 A_3 A_4 A_1 \\ &= \{A_1, A_2\}_+ A_3 A_4 - A_2 \{A_1, A_3\}_+ A_4 + A_2 A_3 \{A_1, A_4\}_+ . \end{aligned}$$

The expression (B) can be simplified using

$$\{A_i, A_j\}_+ = \delta_{ij} \stackrel{(1.3.6),(1.3.7)}{=} \langle A_i A_j \rangle \cdot (1 + e^{\pm s_i}) :$$

$$\begin{aligned} \{A_1, A_2 \cdots A_s\}_+ &= \langle A_1 A_2 \rangle (1 + e^{\pm s_1}) A_3 \cdots A_s \\ &\quad - \langle A_1 A_3 \rangle (1 + e^{\pm s_1}) A_2 A_4 \cdots A_s + \dots . \end{aligned}$$

As before, the positive sign holds if  $A_i$  is a creation operator and the negative sign if  $A_i$  is an annihilation operator. Hence we get:

$$\begin{aligned} \text{Tr} \{ \varrho^0 \{A_1, A_2 \cdots A_s\}_+ \} &= \langle A_1 A_2 \rangle (1 + e^{\pm s_1}) \text{Tr} \{ \varrho^0 A_3 \cdots A_s \} \\ &\quad - \langle A_1 A_3 \rangle (1 + e^{\pm s_1}) \text{Tr} \{ \varrho^0 A_2 A_4 \cdots A_s \} + \dots . \end{aligned}$$

Now (A) can be further simplified to the recursive expression

$$\text{Tr} \{ \varrho^0 A_1 A_2 \cdots A_s \} = \langle A_1 A_2 \rangle \text{Tr} \{ \varrho^0 A_3 \cdots A_s \} - \langle A_1 A_3 \rangle \text{Tr} \{ \varrho^0 A_2 A_4 \cdots A_s \} + \dots$$

and WICK's theorem (1.3.2) follows iteratively.

WICK's theorem is valid for fermions as well as for bosons and the creation and annihilation operators can be arbitrarily ordered as long as the statistical operator is diagonal (or at least diagonalizable) in the single-particle states.

If the statistical operator contains two- or more-particle-contributions in the exponent, no WICK theorem can be formulated.



## 1.4 Example: Evaluation of equilibrium correlation functions in Hartree-Fock approximation

The determination of equations of state as well as the average population  $\langle n_k \rangle$  for the considered systems is the fundamental problem of many-particle physics. As an example for the application of the calculus shown in this chapter, we will determine an equation of state  $n(\beta, \mu) = \frac{1}{\Omega} \sum_k \langle n_k \rangle$  for a real quantum gas in HARTREE-FOCK-approximation.

Therefore we will use the HAMILTONian<sup>8</sup>

$$H = \sum_{k'} E_{k'} n_{k'} + \frac{1}{2} \sum_{12, 1'2'} V(12, 1'2') a_1^\dagger a_2^\dagger a_{2'} a_{1'} \quad (1.4.1)$$

for computing the expectation value of the population number in the grand-canonical ensemble

$$\langle n_k \rangle = \text{Tr} \{ \varrho n_k \} = \frac{\text{Tr} \{ e^{-\beta(H-\mu N)} n_k \}}{\text{Tr} \{ e^{-\beta(H-\mu N)} \}} \quad \text{with } N = \sum_{k'} n_{k'} , \quad (1.4.2)$$

considering any terms up to first order in the interaction  $V$ .

Using the DYSON series (1.2.2), the exponential function in (1.4.2) can be expanded to

$$\begin{aligned} & e^{-\beta(H-\mu N)} \\ &= e^{-\beta(\sum_{k'} (E_{k'} - \mu) n_{k'} + \frac{1}{2} \sum_{12, 1'2'} V(12, 1'2') a_1^\dagger a_2^\dagger a_{2'} a_{1'})} \quad (\underline{A}) \\ &= e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \\ & \cdot \left( \underbrace{1 + \int_0^1 d\tau e^{\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \left( -\frac{\beta}{2} \sum_{12, 1'2'} V(12, 1'2') a_1^\dagger a_2^\dagger a_{2'} a_{1'} e^{-\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} + \dots \right)}_{\Theta} \right) . \end{aligned}$$

The second summand in brackets can be rewritten to

$$\Theta = -\frac{\beta}{2} \sum_{12, 1'2'} V(12, 1'2') \int_0^1 d\tau e^{\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} a_1^\dagger a_2^\dagger a_{2'} a_{1'} e^{-\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} .$$

We can now insert a  $1 = e^{-\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \cdot e^{\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}}$  between any of the operators  $a_k^{(+)}$  and using (1.2.4), (1.2.5):

$$e^{\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} a_k^{(+)} e^{-\tau \beta \sum_{k'} (E_{k'} - \mu) n_{k'}} = e^{\pm \tau \beta (E_k - \mu)} a_k^{(+)}$$

(with the positive sign for creation and the negative sign for annihilation operators), we find

$$\Theta = -\frac{\beta}{2} \sum_{12, 1'2'} V(12, 1'2') \int_0^1 d\tau e^{\tau \beta (E_1 - \mu)} e^{\tau \beta (E_2 - \mu)} e^{-\tau \beta (E_{2'} - \mu)} e^{-\tau \beta (E_{1'} - \mu)} a_1^\dagger a_2^\dagger a_{2'} a_{1'} .$$

<sup>8</sup>The summation indices  $12, 1'2'$  represent a summation over momentum and spin states as well as any internal quantum number. This notation will often be used within this lecture to simplify notation with more complex expressions containing several different sums over momentum states.

For shorthand notation we write  $\Delta E = E_1 + E_2 - E_{2'} - E_{1'}$ , and after performing the integration, we reach

$$\Theta = \begin{cases} -\frac{\beta}{2} \sum_{12,1'2'} V(12,1'2') a_1^+ a_2^+ a_{2'} a_{1'} \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} & \text{for } \Delta E \neq 0 \\ -\frac{\beta}{2} \sum_{12,1'2'} V(12,1'2') a_1^+ a_2^+ a_{2'} a_{1'} & \text{for } \Delta E = 0. \end{cases} \quad (\text{B})$$

The case  $\Delta E = 0$  had to be considered separately via direct evaluation of the integral. However, it obviously coincides with the limit  $\Delta E \rightarrow 0$  of the case  $\Delta E \neq 0$ . Thus it does not have to be treated separately in the following and (1.4.2) has the form

$$\langle n_k \rangle = \frac{\text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \right\} - \frac{\beta}{2} \sum V \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} a_1^+ a_2^+ a_{2'} a_{1'} n_k \right\}}{\text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \right\} - \frac{\beta}{2} \sum V \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} a_1^+ a_2^+ a_{2'} a_{1'} \right\}},$$

where we dropped the arguments  $12, 1'2'$  in the sums and in the potential.

Identifying  $Z^0 = \text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} \right\}$  as the partition function of the non-interacting system, the expression (for clarity, we will only give the denominator here) becomes

$$\langle n_k \rangle = \frac{\text{numerator}}{Z^0 \left( 1 - \frac{\beta}{2} \sum_{12,1'2'} V(12,1'2') \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \left\{ e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}} a_1^+ a_2^+ a_{2'} a_{1'} \right\} (Z^0)^{-1} \right)}$$

and with the corresponding zeroth-order statistical operator

$$\varrho^0 = \frac{1}{Z^0} e^{-\beta \sum_{k'} (E_{k'} - \mu) n_{k'}}$$

we have

$$\langle n_k \rangle = \frac{\text{Tr} \left\{ \varrho^0 n_k \right\} - \frac{\beta}{2} \sum_{12,1'2'} V(12,1'2') \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \left\{ \varrho^0 a_1^+ a_2^+ a_{2'} a_{1'} n_k \right\}}{1 - \frac{\beta}{2} \sum_{12,1'2'} V(12,1'2') \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \left\{ \varrho^0 a_1^+ a_2^+ a_{2'} a_{1'} \right\}}. \quad (\text{C})$$

For further progress, the traces in numerator and denominator have to be evaluated.

While

$$\text{Tr} \left\{ \varrho^0 n_k \right\} = f_k$$

is trivial, the two other traces will be computed using WICK's theorem (1.3.2) and  $\langle a_i^+ a_j \rangle = \delta_{ij} \cdot f_i$ , compare (1.3.6) and (1.3.7) and remarks there.

- Evaluating  $\text{Tr} \left\{ \varrho^0 a_1^+ a_2^+ a_{2'} a_{1'} \right\}$  in the denominator of (C), we have to consider the following contractions:

$$\begin{aligned} \overbrace{a_1^+ a_2^+ a_{2'} a_{1'}} : & \quad (+1) \cdot \langle a_1^+ a_2^+ \rangle \langle a_{2'} a_{1'} \rangle = 0, \\ \overbrace{a_1^+ a_2^+ a_{2'} a_{1'}} : & \quad (-1) \cdot \langle a_1^+ a_{2'} \rangle \langle a_2^+ a_{1'} \rangle = -\delta_{12'} f_1 \delta_{21'} f_2, \\ \overbrace{a_1^+ a_2^+ a_{2'} a_{1'}} : & \quad (+1) \cdot \langle a_1^+ a_{1'} \rangle \langle a_2^+ a_{2'} \rangle = +\delta_{11'} f_1 \delta_{22'} f_2. \end{aligned}$$

Summing up these contributions, we find

$$\implies \text{Tr} \left\{ \varrho^0 a_1^+ a_2^+ a_{2'} a_{1'} \right\} = (\delta_{11'} \delta_{22'} - \delta_{12'} \delta_{21'}) f_1 f_2.$$

Thus, for the denominator, after performing the sum over  $1'$  and  $2'$  and noting that  $\Delta E = 0$  due to the  $\delta$ -functions and hence  $\frac{e^{\beta\Delta E}-1}{\beta\Delta E} \stackrel{\text{(B)}}{\rightarrow} 1$ , we find

$$\langle n_k \rangle = \frac{\text{numerator}}{1 - \frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2}.$$

The exchange potential  $V(12, 12)_{\text{ex}} = V(12, 12) - V(12, 21)$  denotes the contribution due to a mutual particle exchange. Note, that in the exchange part  $V(12, 21)$ , the spins  $\sigma_1, \sigma_2$  must coincide. Otherwise, the  $\delta$ -functions in the interaction (compare the comments in the interaction on p. 37) give zero.

- For  $\text{Tr} \{ \varrho^0 a_1^+ a_2^+ a_2' a_1' n_k \} = \text{Tr} \{ \varrho^0 a_1^+ a_2^+ a_2' a_1' a_k^+ a_k \}$  in the numerator of (C), the following contractions have to be evaluated:

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (-1) \cdot \delta_{12'} \delta_{21'} \delta_{kk} f_1 f_2 f_k, \quad \text{(D)}$$

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (+1) \cdot \delta_{11'} \delta_{22'} \delta_{kk} f_1 f_2 f_k, \quad \text{(E)}$$

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (+1) \cdot \delta_{1k} \delta_{22'} \delta_{1'k} f_k f_2 (1 - f_k), \quad \text{(F)}$$

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (-1) \cdot \delta_{1k} \delta_{21'} \delta_{2'k} f_k f_2 (1 - f_k), \quad \text{(G)}$$

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (-1) \cdot \delta_{12'} \delta_{2k} \delta_{1'k} f_1 f_k (1 - f_k), \quad \text{(H)}$$

$$a_1^+ a_2^+ a_2' a_1' a_k^+ a_k : \quad (+1) \cdot \delta_{11'} \delta_{2k} \delta_{2'k} f_1 f_k (1 - f_k). \quad \text{(I)}$$

Here, only the non-vanishing contributions, i.e. those, where in any pair an annihilator is connected with a creation operator, are listed. Again, in every case  $\Delta E = 0$  is fulfilled due to the  $\delta$ -functions, so that energy conservation is ensured and  $\frac{e^{\beta\Delta E}-1}{\beta\Delta E} \stackrel{\text{(B)}}{\rightarrow} 1$ .

Now, the fourfold sum in the numerator of (C) can further be simplified to

$$\begin{aligned} & \sum_{12, 1'2'} V(12, 1'2') \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \{ \varrho^0 a_1^+ a_2^+ a_2' a_1' n_k \} \\ &= f_k \sum_{12} \left( \overbrace{-V(12, 21)}^{\text{(D)}} + \overbrace{V(12, 12)}^{\text{(E)}} \right) f_1 f_2 \\ & \quad + f_k (1 - f_k) \sum_2 \left( \overbrace{V(k2, k2)}^{\text{(F)}} - \overbrace{V(k2, 2k)}^{\text{(G)}} \right) f_2 \\ & \quad + f_k (1 - f_k) \sum_1 \left( \overbrace{-V(1k, k1)}^{\text{(H)}} + \overbrace{V(1k, 1k)}^{\text{(I)}} \right) f_1. \end{aligned}$$

Here, we have performed the sums over  $1', 2'$  and 1 or 2, respectively. We can now rename the summation index in the term resulting for (F) and (G) from  $2 \rightarrow 1$ .

Additionally assuming a symmetric interaction  $V(ab, cd) = V(ba, dc)$ , we will exchange the interacting partners in the terms resulting from (H) and (I). Then we get

$$\begin{aligned} & \sum_{12,1'2'} V(12, 1'2') \frac{e^{\beta\Delta E} - 1}{\beta\Delta E} \text{Tr} \{ \rho^0 a_1^+ a_2^+ a_2' a_1' n_k \} \\ &= f_k \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2 + 2 \cdot f_k (1 - f_k) \sum_1 V(k1, k1)_{\text{ex}} f_1. \end{aligned}$$

Bringing everything together, we end up with

$$\langle n_k \rangle = \frac{f_k - \beta f_k (1 - f_k) \sum_1 V(k1, k1)_{\text{ex}} f_1 - \frac{\beta}{2} f_k \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2}{1 - \frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2}. \quad (1.4.3)$$

Since we only want to consider terms of first order in  $V$  we can make use of  $\frac{1}{1+x} = 1 - x + \mathcal{O}(x^2)$ :

$$\begin{aligned} \langle n_k \rangle &= f_k \left( 1 - \beta (1 - f_k) \sum_1 V(k1, k1)_{\text{ex}} f_1 - \frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2 \right) \\ &\quad \times \left( 1 + \frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2 + \mathcal{O}(V^2) \right) \\ &= f_k \left( 1 - \beta (1 - f_k) \sum_1 V(k1, k1)_{\text{ex}} f_1 \right. \\ &\quad \left. - \underbrace{\frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2 + \frac{\beta}{2} \sum_{12} V(12, 12)_{\text{ex}} f_1 f_2}_{=0} + \mathcal{O}(V^2) \right). \end{aligned}$$

The final result is an expression for the single-particle occupation number

$$\langle n_k \rangle = f_k \left( 1 - \beta (1 - f_k) \sum_1 V(k1, k1)_{\text{ex}} f_1 \right), \quad (1.4.4)$$

which can be written in the form

$$\langle n_k \rangle = \frac{1}{e^{\beta(E_k - \mu + \sum_1 V(k1, k1)_{\text{ex}} f_1)} + 1}. \quad (1.4.5)$$

Especially expression (1.4.5) has a very handy structure, that will repeatedly appear in this lecture, for example in section 4.1.

Equation (1.4.5) can be expanded in terms of  $V$  with the shorthand notation  $\Delta E^{\text{HF}} = \sum_1 V(k1, k1)_{\text{ex}} f_1$ :

$$\begin{aligned} \frac{1}{e^{\beta(E_k - \mu + \Delta E^{\text{HF}})} + 1} &= \frac{1}{e^{\beta(E_k - \mu)} e^{\beta \Delta E^{\text{HF}}} + 1} \\ &= \frac{1}{e^{\beta(E_k - \mu)} (1 + \beta \Delta E^{\text{HF}} + \mathcal{O}(\Delta E^{\text{HF}})^2) + 1} \\ &= \frac{1}{(e^{\beta(E_k - \mu)} + 1) \left( 1 + \underbrace{\frac{e^{\beta(E_k - \mu)}}{e^{\beta(E_k - \mu)} + 1}}_{1 - f_k} \beta \Delta E^{\text{HF}} + \mathcal{O}(\Delta E^{\text{HF}})^2 \right)}. \end{aligned}$$

Using  $\frac{1}{1+x} = 1 - x + \mathcal{O}(x^2)$  we get

$$= f_k \left( 1 - \beta \Delta E^{\text{HF}} (1 - f_k) + \mathcal{O}(\Delta E^{\text{HF}})^2 \right),$$

which is the same expression as (1.4.4).

Thus, we have finally found, that in HARTREE-FOCK approximation, the ideal expression  $\langle n_k \rangle^{\text{id}} = f_k$  is extended by a term  $\propto V$ :  $\langle n_k \rangle^{\text{HF}} = f_k (1 - \beta (1 - f_k) \Delta E^{\text{HF}})$  with  $\Delta E^{\text{HF}} = \sum_1 V(k1, k1)_{\text{ex}} f_1$ .

This correction can be interpreted as an energy shift like in (1.4.5), where we could introduce a quasi-particle energy  $E_k^{\text{HF}} = E_k + \Delta E^{\text{HF}}$ :

$$\langle n_k \rangle^{\text{HF}} = \frac{1}{e^{\beta(E_k^{\text{HF}} - \mu)} + 1}. \quad (1.4.6)$$

Corresponding terms will appear in the equation of state  $n^{\text{HF}}(\beta, \mu) = \frac{1}{\Omega} \sum_k \langle n_k \rangle^{\text{HF}}$ , which can also be interpreted as the effect of a mean field and an exchange term.

Because we only have considered terms up to first order in  $V$ , the equation of state in this approximation requires the interaction to be weak. However, as shown below, it is applicable in several cases, for example the electron gas in metals, for solids and semiconductors, or simple models of nuclear matter where the interaction is strong<sup>9</sup>. The advantage of this picture is the possibility, to include the strong correlations into mean-field by partial summation of an infinite number of contributions, see chapter 4.

In the case of a stronger interaction, the HARTREE-FOCK approximation is not sufficient and higher order terms have to be included. Often the summation of an infinite number of contributions is necessary, which leads to a very confusing perturbation calculus and makes a more effective representation necessary. Such an efficient approach will be shown in the following two chapters, which introduces the technique of GREEN's functions and their diagrammatic representation as a new concept.

<sup>9</sup>Since for inhomogeneous system the momentum states cannot be used as eigenstates, the single-particle states have to be determined in a HARTREE-FOCK potential in a self consistent way.



## 2 Thermodynamic Green's functions: Definitions and properties

### 2.1 Definitions

As already introduced in classical statistics, the reduced distribution functions (density matrices) of many-body systems contain any information about the systems' properties and evolution. In the one- and two-particle case, these density matrices are the two-point correlation function (one particle density matrix) with an additional dependence on the parameter  $\tau$ :

$$\langle a_1^+(\tau_1) a_{1'}(\tau_{1'}) \rangle = \text{Tr} \{ \rho a_1^+(\tau_1) a_{1'}(\tau_{1'}) \} \quad (2.1.1)$$

and the four-point correlation function (two-particle density matrix)

$$\langle a_1^+(\tau_1) a_2^+(\tau_2) a_{2'}(\tau_{2'}) a_{1'}(\tau_{1'}) \rangle = \text{Tr} \{ \rho a_1^+(\tau_1) a_2^+(\tau_2) a_{2'}(\tau_{2'}) a_{1'}(\tau_{1'}) \} \quad (2.1.2)$$

with the statistical operator  $\rho$  and the entropy operator  $S$ :

$$\rho = \frac{e^{-\beta(H-\mu N)}}{\text{Tr} \{ e^{-\beta(H-\mu N)} \}} = e^{-S}. \quad (2.1.3)$$

The dependence on  $\tau$  is given by the modified HEISENBERG picture:

$$A(\tau) = e^{\tau(H-\mu N)} A e^{-\tau(H-\mu N)}. \quad (2.1.4)$$

These matrices are special cases of more general averages of time-ordered field operators, which are referred to as GREEN's functions.<sup>1</sup>

In general,

$$G_1(1\tau_1, 1'\tau_{1'}) = -\text{Tr} \{ \rho T [a_1(\tau_1) a_{1'}^+(\tau_{1'})] \} \quad (2.1.5)$$

is the single-particle (two-point) GREEN's function,

$$G_2(1\tau_1, 2\tau_2, 1'\tau_{1'}, 2'\tau_{2'}) = -\text{Tr} \{ \rho T [a_1(\tau_1) a_2(\tau_2) a_{2'}^+(\tau_{2'}) a_{1'}^+(\tau_{1'})] \} \quad (2.1.6)$$

the two-particle GREEN's function, etc.

<sup>1</sup>The formalism can also be applied to a general GIBBS-ensemble (relevant statistical operator in nonequilibrium), using the GREEN's functions technique, that will be presented in the following sections. For some further details and keywords, see section 6.

The parameters  $\tau_i, \tau_{i'}$  traverse  $0 \leq \tau_i, \tau_{i'} \leq \beta$ .

The  $\mathbb{T}[\dots]$ -product denotes an ordering of the factors according to the value of the parameter  $\tau$ , so that the creation operator with smallest value of  $\tau$  will appear right and growing parameter values of  $\tau$  are arranged left. Furthermore, for fermions  $\mathbb{T}[\dots]$  contains a sign factor of  $(-1)^{\mathfrak{p}}$ , where  $\mathfrak{p}$  represents the number of transpositions needed for restoring the operators' original order.

For fermions  $\mathbb{T}[\dots]$  holds

$$\mathbb{T} [a_1(\tau_1)a_{1'}^+(\tau_{1'})] = \begin{cases} a_1(\tau_1)a_{1'}^+(\tau_{1'}) & \text{for } \tau_{1'} < \tau_1 \\ -a_{1'}^+(\tau_{1'})a_1(\tau_1) & \text{for } \tau_1 < \tau_{1'} \end{cases} ,$$

and thus

$$G_1(1\tau_1, 1'\tau_{1'}) = \begin{cases} -\text{Tr} \{ \varrho a_1(\tau_1)a_{1'}^+(\tau_{1'}) \} & \text{for } \tau_{1'} < \tau_1 \\ \text{Tr} \{ \varrho a_{1'}^+(\tau_{1'})a_1(\tau_1) \} & \text{for } \tau_1 < \tau_{1'} \end{cases} .$$

For bosons, the sign is positive in both cases.

Sometimes<sup>2</sup>, the thermodynamic GREEN's function is introduced with imaginary times in the HEISENBERG picture, using the HAMILTONIAN instead of the entropy operator:

$$A(t) = e^{\frac{i}{\hbar}tH} A e^{-\frac{i}{\hbar}tH}$$

with  $0 \geq \text{Im} \{t\} > -i\hbar\beta$ .

Expressions resulting from this notation differ by a factor of  $(-i\hbar)$  and the chemical potential  $\mu$  is missing in the exponent compared with the grand canonical statistical operator. This results in modified MATSUBARA frequencies  $z_\nu^{\text{KB}} = \frac{\pi\nu}{-i\hbar} + \frac{\mu}{\hbar}$ , which also depend on the chemical potential. Compare (2.1.21) for our definition of the MATSUBARA frequencies.

According to

$$G_1(1\tau_1, 1'\tau_{1'}) = \Theta(\tau_1 - \tau_{1'}) G_1^>(1\tau_1, 1'\tau_{1'}) + \Theta(\tau_{1'} - \tau_1) G_1^<(1\tau_1, 1'\tau_{1'}) , \quad (2.1.7)$$

where  $\Theta(\tau)$  is the HEAVISIDE step-function

$$\Theta(\tau) = \begin{cases} 0 & \text{for } \tau \leq 0 \\ 1 & \text{for } \tau > 0 \end{cases} , \quad (2.1.8)$$

the GREEN's function can be related to the two-point correlation functions of the form

$$G_1^>(1\tau_1, 1'\tau_{1'}) = -\text{Tr} \{ \varrho a_1(\tau_1)a_{1'}^+(\tau_{1'}) \} \quad (2.1.9)$$

$$G_1^<(1\tau_1, 1'\tau_{1'}) = \text{Tr} \{ \varrho a_{1'}^+(\tau_{1'})a_1(\tau_1) \} . \quad (2.1.10)$$

---

<sup>2</sup>For example in [KB62] and [Ric81]



Thus, there is a close connection between  $G_1^{\lessgtr}$  and the density matrices  $\langle a_{1'}^+(\tau_{1'})a_1(\tau_1) \rangle$ .

Since we are investigating thermodynamic systems in equilibrium state, the absolute 'time' does not play a role. While at the moment,  $\tau$  looks like a time parameter, it can also be related to temperature or entropy respectively. The respective properties for  $t$  are also valid for  $\tau$ . In thermodynamic equilibrium, the GREEN's and correlation functions only depend on  $\tau_1$  and  $\tau_{1'}$  in the form  $\tau_1 - \tau_{1'}$ :

$$G_1(1\tau_1, 1'\tau_{1'}) \equiv G_1(11', \tau) = \begin{cases} G_1^>(11', \tau) & \text{for } \tau > 0 \\ G_1^<(11', \tau) & \text{for } \tau < 0 \end{cases} \quad (2.1.11)$$

$$= G_1(1\tau_1 - \tau_{1'}, 1'0) = G_1(1\tau, 1'0) = G_1(10, 1' - \tau) \quad (2.1.12)$$

with the new parameter  $\tau = \tau_1 - \tau_{1'}$  running through  $-\beta \leq \tau \leq \beta$ .

Equation (2.1.11) can be proven by using the invariance of  $\text{Tr}\{\}$  under cyclic permutation of its arguments.

Because the statistical operator  $\varrho$  of the grand canonical ensemble commutes with  $e^{-\beta(H-\mu N)}$ , we make use of the invariance of  $\text{Tr}\{\dots\}$  under cyclic permutations of its operands to write

$$\begin{aligned} G_1^>(1\tau_1, 1'\tau_{1'}) &\stackrel{(2.1.9),(2.1.4)}{=} -\text{Tr} \left\{ \varrho e^{\tau_1(H-\mu N)} a_1 e^{-\tau_1(H-\mu N)} e^{\tau_{1'}(H-\mu N)} a_{1'}^+ e^{-\tau_{1'}(H-\mu N)} \right\} \\ &= -\text{Tr} \left\{ \varrho e^{(\tau_1-\tau_{1'})(H-\mu N)} a_1 e^{-(\tau_1-\tau_{1'})(H-\mu N)} a_{1'}^+ \right\} \\ &\equiv G_1^>(1\tau_1 - \tau_{1'}, 1'0) \quad \text{with } \tau_1 - \tau_{1'} > 0 \end{aligned}$$

and in the same way

$$\begin{aligned} G_1^<(1\tau_1, 1'\tau_{1'}) &\stackrel{(2.1.10),(2.1.4)}{=} \text{Tr} \left\{ \varrho a_{1'}^+ e^{(\tau_1-\tau_{1'})(H-\mu N)} a_1 e^{-(\tau_1-\tau_{1'})(H-\mu N)} \right\} \\ &\equiv G_1^<(1\tau_1 - \tau_{1'}, 1'0) \quad \text{with } \tau_1 - \tau_{1'} < 0. \end{aligned}$$

With (2.1.11), we already introduced the new notation

$$G_1(1\tau, 1'0) = G_1(11', \tau) . \quad (2.1.13)$$

Now we can write

$$G_1^>(11', \tau) = -\text{Tr} \left\{ \varrho e^{\tau(H-\mu N)} a_1 e^{-\tau(H-\mu N)} a_{1'}^+ \right\} = -\langle a_1(\tau) a_{1'}^+ \rangle \quad (2.1.14)$$

$$= -\text{Tr} \left\{ \varrho a_1 e^{-\tau(H-\mu N)} a_{1'}^+ e^{\tau(H-\mu N)} \right\} = -\langle a_1 a_{1'}^+(-\tau) \rangle \quad (2.1.15)$$

$$G_1^<(11', \tau) = \text{Tr} \left\{ \varrho e^{-\tau(H-\mu N)} a_{1'}^+ e^{\tau(H-\mu N)} a_1 \right\} = \langle a_{1'}^+(-\tau) a_1 \rangle \quad (2.1.16)$$

$$= \text{Tr} \left\{ \varrho a_{1'}^+ e^{\tau(H-\mu N)} a_1 e^{-\tau(H-\mu N)} \right\} = \langle a_{1'}^+ a_1(\tau) \rangle . \quad (2.1.17)$$

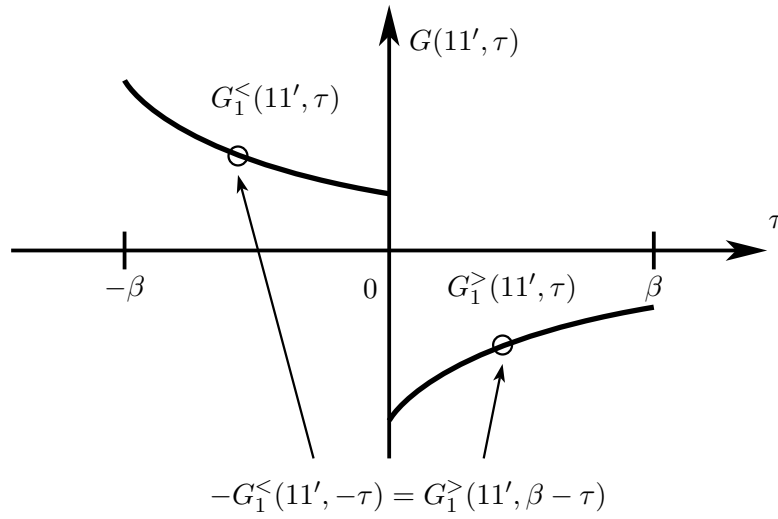
The KUBO-MARTIN-SCHWINGER (KMS-)condition is an important property of the thermodynamical GREEN's function. It connects  $G_1(11', -\tau)$  with  $G_1(11', \beta - \tau)$  for  $0 \leq \tau \leq \beta$  to a quasi-periodicity relation:

$$G_1(11', \beta - \tau) = -G_1(11', -\tau) \quad (2.1.18)$$

or

$$G_1^>(11', \beta - \tau) = -G_1^<(11', -\tau). \quad (2.1.19)$$

Thus, the thermodynamic GREEN's function  $G_1(11', \tau)$  is determined by only knowing  $G_1^>(11', \tau)$ , i.e. its behavior in the interval  $0 \leq \tau \leq \beta$  or  $G_1^<(11', \tau)$  for  $-\beta \leq \tau \leq 0$ , respectively.



Schematic plot of the thermodynamic GREEN's function, eq. (2.1.7), for an ideal FERMION gas. For detailed calculations, see section 2.3.

The KMS-condition can again simply be proven by utilizing the invariance of  $\text{Tr}\{\dots\}$  under cyclic permutations. Knowing that for  $\tau \geq 0$

$$G(11', \tau) \stackrel{(2.1.7), (2.1.10)}{=} -\text{Tr} \left\{ \varrho e^{\tau(H-\mu N)} a_1 e^{-\tau(H-\mu N)} a_{1'}^+ \right\}$$

with  $\varrho = \frac{1}{Z} e^{-\beta(H-\mu N)}$  and  $\beta - \tau \geq 0$ , we get

$$\begin{aligned} G(11', \beta - \tau) &= -\text{Tr} \left\{ \frac{1}{Z} e^{-\beta(H-\mu N)} e^{(\beta-\tau)(H-\mu N)} a_1 e^{-(\beta-\tau)(H-\mu N)} a_{1'}^+ \right\} \\ &= -\frac{1}{Z} \text{Tr} \left\{ e^{-\tau(H-\mu N)} a_1 e^{-(\beta-\tau)(H-\mu N)} a_{1'}^+ \right\} \\ &= -\text{Tr} \left\{ \frac{1}{Z} e^{-(\beta-\tau)(H-\mu N)} a_{1'}^+ e^{-\tau(H-\mu N)} a_1 \right\} \\ &= -\text{Tr} \left\{ \varrho e^{\tau(H-\mu N)} a_{1'}^+ e^{-\tau(H-\mu N)} a_1 \right\} \\ &= -\text{Tr} \left\{ \varrho a_{1'}^+ a_1(-\tau) \right\} \stackrel{(2.1.17), (2.1.7)}{=} -G_1(11', -\tau) . \end{aligned}$$

Due to the KMS-condition, that implies quasi-periodicity, it is possible to decompose  $G_1$  in terms of a FOURIER expansion of the form

$$G_1(11', \tau) = \frac{1}{\beta} \sum_{\nu} G_1(11', iz_{\nu}) e^{-iz_{\nu}\tau} \quad (2.1.20)$$

with the MATSUBARA frequencies  $z_{\nu}$  which are defined by (2.1.18):

$$z_{\nu} = \frac{\pi\nu}{\beta}, \quad \nu = \pm 1, \pm 3, \dots \text{ for fermions.} \quad (2.1.21)$$

For bosons there is a similar periodicity condition as (2.1.18) but without alternating sign. That is why the MATSUBARA frequencies in the bosonic case are given with even  $\nu = 0, \pm 2, \dots$ . Although within this lecture we will primarily deal with fermions, we will also make use of even MATSUBARA frequencies in some special cases.

We can directly show that (2.1.20) agrees with the KMS-condition (2.1.18) by putting in (2.1.21):

$$\begin{aligned} G_1(11', \beta - \tau) &\stackrel{(2.1.20)}{=} \frac{1}{\beta} \sum_{\nu} G_1(11', iz_{\nu}) \underbrace{e^{-i\pi\nu}}_{=-1 \text{ } (\nu \text{ odd})} e^{i\frac{\pi\nu}{\beta}\tau} \\ &= -\frac{1}{\beta} \sum_{\nu} G_1(11', iz_{\nu}) e^{i\frac{\pi\nu}{\beta}\tau} \\ &\stackrel{(2.1.20)}{=} -G_1(11', -\tau) . \end{aligned}$$

The inverse transformation is given by

$$G_1(11', iz_{\nu}) = \int_0^{\beta} d\tau G_1(11', \tau) e^{iz_{\nu}\tau} . \quad (2.1.22)$$

Equation (2.1.22) can be shown by some simple calculation:

$$\begin{aligned} \int_0^\beta d\tau G_1(11', \tau) e^{iz_\nu \tau} &\stackrel{(2.1.20)}{=} \int_0^\beta d\tau e^{iz_\nu \tau} \frac{1}{\beta} \sum_{\nu'} G_1(11', iz_{\nu'}) e^{-iz_{\nu'} \tau} \\ &= \frac{1}{\beta} \sum_{\nu'} G_1(11', iz_{\nu'}) \int_0^\beta d\tau e^{-i(z_{\nu'} - z_\nu) \tau}. \end{aligned}$$

While for  $z_{\nu'} \neq z_\nu$  we can make use of  $e^{-i(z_{\nu'} - z_\nu)\beta} = 1$ , because  $(z_{\nu'} - z_\nu)\beta$  is an even multiple of  $\pi$ :

$$\int_0^\beta d\tau e^{-i(z_{\nu'} - z_\nu) \tau} = \frac{\overbrace{e^{-i(z_{\nu'} - z_\nu)\beta} - 1}^{(2.1.21)_1}}{-i(z_{\nu'} - z_\nu)} = 0,$$

in the case of  $z_{\nu'} = z_\nu$ , the denominator is zero and the expression is indefinite. In that case the integral is

$$\int_0^\beta d\tau e^{-i(z_{\nu'} - z_\nu) \tau} = \int_0^\beta d\tau 1 = \beta.$$

Thus we can write

$$\int_0^\beta d\tau e^{-i(z_{\nu'} - z_\nu) \tau} = \beta \cdot \delta_{z_\nu, z_{\nu'}}$$

and finally have

$$\int_0^\beta d\tau G_1(11', \tau) e^{iz_\nu \tau} = \frac{1}{\beta} \sum_{\nu'} G_1(11', iz_{\nu'}) \beta \cdot \delta_{z_\nu, z_{\nu'}} = G_1(11', iz_\nu),$$

so that (2.1.22) is proven.

While we introduced the thermodynamic GREEN's function as some kind of useful definition, we recommend considering additional literature, where a straightforward construction and extended discussion of these definitions is performed. Two feasible examples are [Mah90] and [FW71].

## 2.2 Green's function and spectral function

The frequency dependent GREEN's function is closely connected to another important function which is called the spectral function. It can be obtained by analytic continuation of the thermodynamic GREEN's function into the complex plane.

With the eigenstates  $|n\rangle$  for the grand canonical operator

$$(H - \mu N) |n\rangle = \epsilon_n |n\rangle , \quad (2.2.1)$$

the single-particle spectral density is defined as

$$I_1(11', \omega) = 2\pi \frac{1}{Z} \sum_{m,n} \delta(\epsilon_n - \epsilon_m - \omega) e^{-\beta\epsilon_n} \langle n | a_{1'}^+ | m \rangle \langle m | a_1 | n \rangle . \quad (2.2.2)$$

It is the FOURIER transform of  $G_1^<$ :

$$\langle a_{1'}^+ a_1(\tau) \rangle = G_1^<(11', \tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} I_1(11', \omega') e^{-\omega'\tau} , \quad (2.2.3)$$

while it also satisfies

$$\langle a_1(\tau) a_{1'}^+ \rangle = -G_1^>(11', \tau) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{\beta\omega'} I_1(11', \omega') e^{-\omega'\tau} . \quad (2.2.4)$$

Equation (2.2.3) can be shown by utilizing (2.2.1) and using that  $e^{(H-\mu N)} |n\rangle = e^{\epsilon_n} |n\rangle$ , which follows directly from the eigenvalue equation by performing a TAYLOR expansion:

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} I_1(11', \omega') e^{-\omega'\tau} \\ \stackrel{(2.2.2)}{=} & \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \cdot \frac{1}{Z} \sum_{m,n} e^{-\beta\epsilon_n} \langle n | a_{1'}^+ | m \rangle \langle m | a_1 | n \rangle 2\pi \delta(\epsilon_n - \epsilon_m - \omega') e^{-\omega'\tau} \\ = & \sum_{m,n} \frac{e^{-\beta\epsilon_n}}{Z} \langle n | a_{1'}^+ | m \rangle \langle m | a_1 | n \rangle \cdot \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-\omega'\tau} 2\pi \delta(\epsilon_n - \epsilon_m - \omega') \\ = & \sum_{m,n} \frac{e^{-\beta\epsilon_n}}{Z} \langle n | a_{1'}^+ | m \rangle \langle m | a_1 | n \rangle e^{\tau(\epsilon_m - \epsilon_n)} \\ = & \sum_{m,n} \frac{e^{-\beta\epsilon_n}}{Z} \langle n | a_{1'}^+ | m \rangle \overbrace{\langle m | e^{\tau\epsilon_m} \rangle}^{\langle m | e^{\tau(H-\mu N)} \rangle} a_1 \overbrace{e^{-\tau\epsilon_n} | n \rangle}^{e^{-\tau(H-\mu N)} | n \rangle} \\ = & \sum_n \frac{e^{-\beta\epsilon_n}}{Z} \langle n | a_{1'}^+ e^{\tau(H-\mu N)} a_1 e^{-\tau(H-\mu N)} | n \rangle \\ \stackrel{(2.1.17)}{=} & \langle a_{1'}^+ a_1(\tau) \rangle = G_1^<(11', \tau) . \end{aligned}$$

The proof for (2.2.4) works in the same way but with exchanged  $m$  and  $n$ :

$$\begin{aligned}
 & \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{\beta\omega'} I_1(11', \omega') e^{-\omega'\tau} \\
 \stackrel{(2.2.2)}{=} & \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{\beta\omega'} \cdot \frac{1}{Z} \sum_{m,n} e^{-\beta\epsilon_n} \langle n | a_{1'}^+ | m \rangle \langle m | a_1 | n \rangle 2\pi\delta(\epsilon_n - \epsilon_m - \omega') e^{-\omega'\tau} \\
 = & \frac{1}{Z} \sum_{m,n} \overbrace{e^{\beta\omega'} \cdot e^{-\beta\epsilon_n}}^{e^{-\beta\epsilon_m}} \overbrace{\langle m | e^{\tau\epsilon_m}}^{\langle m | e^{\tau(H-\mu N)} a_1} \overbrace{e^{-\tau\epsilon_n} | n \rangle}^{e^{-\tau(H-\mu N)} | n \rangle} \langle n | a_{1'}^+ | m \rangle \\
 \stackrel{(2.1.15)}{=} & \langle a_1(\tau) a_{1'}^+ \rangle = -G_1^>(11', \tau) .
 \end{aligned}$$

For the MATSUBARA GREEN's function (2.1.20), the following important connection arises:

$$G_1(11', iz_\nu) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} (1 + e^{\beta\omega'}) \frac{I_1(11', \omega')}{iz_\nu - \omega'} . \quad (2.2.5)$$

Starting from (2.1.22) and using (2.1.7), we can write

$$\begin{aligned}
 G_1(11', iz_\nu) & \stackrel{(2.1.22), (2.1.7)}{=} \int_0^\beta d\tau \left( \Theta(\tau) G_1^>(11', \tau) + \underbrace{\Theta(-\tau) G_1^<(11', \tau)}_{=0, \text{ because } \tau > 0} \right) e^{iz_\nu\tau} \\
 & \stackrel{(2.2.4)}{=} - \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \underbrace{\int_0^\beta d\tau e^{\tau(iz_\nu - \omega')}}_{-\frac{e^{-\beta\omega'} + 1}{iz_\nu - \omega'}} I_1(11', \omega') e^{\beta\omega'} \quad (\underline{A}) \\
 & = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} (e^{\beta\omega'} + 1) \frac{I_1(11', \omega')}{iz_\nu - \omega'}
 \end{aligned}$$

In  $(\underline{A})$  we made use of  $\frac{z_\nu\beta}{\pi}$  being odd and thus  $e^{iz_\nu\beta} = -1$ .

Since we know the value of  $G_1(11', iz_\nu)$  in an infinite number of distinct points on the complex plane, we can analytically continue (2.2.5) into the whole complex  $z$ -plane<sup>3</sup>:

$$G_1(11', z) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A_1(11', \omega')}{z - \omega'} \quad (2.2.6)$$

with the spectral function

$$A_1(11', \omega) = (1 + e^{\beta\omega}) I_1(11', \omega). \quad (2.2.7)$$

Again, we emphasize that this is the expression for the fermionic case. For bosonic particles, the sign in (2.2.7) has to be swapped.

The integral is of CAUCHY type. It defines an analytic function in the upper half-plane  $\text{Im}\{z\} > 0$  and the lower half-plane  $\text{Im}\{z\} < 0$ . On the real axis  $\text{Im}\{z\} = 0$ , there is a branch cut with singularities at  $z = \omega$ .

$G_1$  can be computed with the DIRAC identity

$$\frac{1}{\omega \pm i\varepsilon} = \mp i\pi\delta(\omega) + \frac{\mathcal{P}}{\omega} \quad (2.2.8)$$

with the principal value  $\mathcal{P}$ . With the replacement  $z \rightarrow \omega \pm i\varepsilon$  and the implicit convention  $\varepsilon \searrow 0$ , the following important equation shows

$$G_1(11', \omega - i\varepsilon) - G_1(11', \omega + i\varepsilon) = 2i\text{Im}\{G_1(11', \omega - i\varepsilon)\} \quad (2.2.9)$$

$$= iA_1(11', \omega) \quad (2.2.10)$$

It can be proven with a straightforward calculation, using (2.2.8) in (2.2.6):

$$\begin{aligned} G_1(11', \omega \pm i\varepsilon) &\stackrel{(2.2.6)}{=} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A_1(11', \omega')}{\omega \pm i\varepsilon - \omega'} \\ &\stackrel{(2.2.8)}{=} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left[ \frac{\mathcal{P} A_1(11', \omega')}{\omega - \omega'} \mp i\pi\delta(\omega - \omega') A_1(11', \omega') \right] \\ &= \underbrace{\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left[ \frac{\mathcal{P} A_1(11', \omega')}{\omega - \omega'} \right]}_{\text{Re}\{G_1(11', \omega \pm i\varepsilon)\}} \mp \underbrace{\frac{1}{2} A_1(11', \omega)}_{\text{Im}\{G_1(11', \omega \pm i\varepsilon)\}} \cdot i. \end{aligned}$$

<sup>3</sup>Strictly spoken, the analytic continuation is well-defined only if the infinite number of points has a finite accumulation point.

Hence we can see, that the discontinuity of the imaginary part of the GREEN's function at the real axis is given by the spectral function or, the other way around, we can determine  $A_1(11', \omega)$  by examining  $\text{Im}\{G(11', z)\}$  at the real axis.

The commutator relation leads to

$$G_1^>(11', \tau = 0) - G_1^<(11', \tau = 0) = -\delta_{11'} \quad (2.2.11)$$

as well as the normalization constraint for the spectral function (sum rule)

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Im}\{G_1(11', \omega' - i\varepsilon)\} d\omega' = 1. \quad (2.2.12)$$

Proving (2.2.11) is a straightforward utilization of the equations (2.1.15) to (2.1.17) and the (anti-) commutator relation for fermions:

$$\begin{aligned} G_1^>(11', \tau = 0) - G_1^<(11', \tau = 0) &= -\langle a_1 a_{1'}^+ \rangle - \langle a_{1'}^+ a_1 \rangle \\ &= -\{a_1, a_{1'}^+\}_+ \\ &= -\delta_{11'} . \end{aligned}$$

With all the knowledge from this section – especially (2.2.10), (2.2.6) and (2.2.3), we can use the method of thermodynamic GREEN's functions to calculate physical properties of interacting quantum systems according to the following scheme:

1. We calculate  $G_1(11', iz_\nu)$ . An appropriate perturbation theory for doing so will be given later.
2.  $G_1(11', z)$  is the analytic continuation of the MATSUBARA GREEN's function into the complex  $z$ -plane.
3. We compute the spectral function  $A_1(11', \omega)$  via

$$A_1(11', \omega) = 2\text{Im}\{G_1(11', \omega - i\varepsilon)\} . \quad (2.2.13)$$

4. From the spectral function we calculate the spectral density  $I_1(11', \omega)$ :

$$I_1(11', \omega) = \frac{A_1(11', \omega)}{1 + e^{\beta\omega}} . \quad (2.2.14)$$

5. The correlation functions are obtained by integration, for example through (2.2.3):

$$\langle a_{1'}^+ a_1(\tau) \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} I_1(11', \omega) e^{-\omega\tau} . \quad (2.2.15)$$

6. Equations of state ( $f(\omega) = \frac{1}{e^{\beta\omega} + 1}$ ):

$$\text{e.g. } n(\beta, \mu) = \frac{1}{\Omega} \sum_1 \langle a_1^+ a_1 \rangle = \int \frac{d\omega}{2\pi} f(\omega) A_1(11, \omega) . \quad (2.2.16)$$

7. Thermodynamic potential (contains all equilibrium properties):

$$\text{e.g. } J(T, \Omega, \mu) = -p(T, \mu) \Omega = - \int_{-\infty}^{\mu} d\mu' n(\mu', T) \Omega . \quad (2.2.17)$$



## 2.3 Example: Thermodynamic Green's function for the ideal Fermi gas

In this section, we will discuss the example of an ideal FERMION gas. While the case of a HAMILTONIAN without any interaction contribution has already been addressed in earlier lectures on statistical physics, this example is very instructive for getting used to the GREEN's functions formalism.

With the HAMILTONIAN

$$H - \mu N = \sum_1 \epsilon_1 a_1^\dagger a_1 \quad \epsilon_1 = E_1 - \mu = \frac{\hbar^2 k_1^2}{2m} - \mu, \quad (2.3.1)$$

we have the statistical operator of the ideal FERMION gas

$$\varrho^0 = \frac{e^{-\beta(H-\mu N)}}{\text{Tr} \{e^{-\beta(H-\mu N)}\}} = \frac{e^{-\beta \sum_1 \epsilon_1 a_1^\dagger a_1}}{\text{Tr} \{e^{-\beta \sum_1 \epsilon_1 a_1^\dagger a_1}\}}. \quad (2.3.2)$$

Although some steps are obvious in this simple example, we will strictly follow the steps from the previous section to explicitly show their application.

Step 1:

Since we did not introduce a perturbation theory for the thermodynamic GREEN's function up to now, we have to derive  $G_1^0(11', iz_\nu)$  from fundamental principles.

From an earlier section of this lecture, we know that the  $\tau$ -dependence of  $a^{(+)}$  for an ideal gas is given by

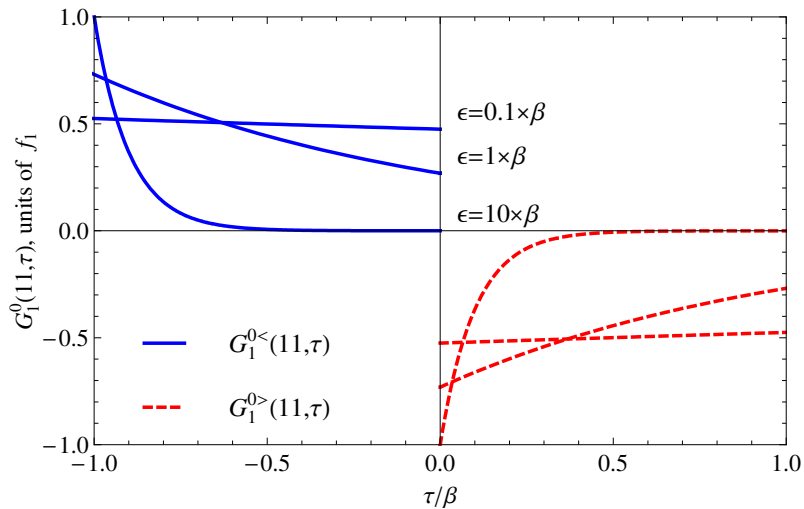
$$a_1(\tau) \stackrel{(1.2.5)}{=} a_1 e^{-\epsilon_1 \tau} \quad a_1^\dagger(\tau) \stackrel{(1.2.4)}{=} a_1^\dagger e^{\epsilon_1 \tau}. \quad (\text{A})$$

Thus all correlation functions can be given:

$$G_1^{0<}(11', \tau) \stackrel{(2.1.17)}{=} \langle a_1^\dagger(-\tau) a_1 \rangle \stackrel{(\text{A})}{=} e^{-\epsilon_1 \tau} f_1 \delta_{11'}$$

$$G_1^{0>}(11', \tau) \stackrel{(2.1.15)}{=} -\langle a_1(\tau) a_1^\dagger \rangle \stackrel{(\text{A})}{=} -e^{-\epsilon_1 \tau} (1 - f_1) \delta_{11'}$$

$$G_1^0(11', \tau) \stackrel{(2.1.7), (2.1.11)}{=} [\Theta(-\tau) f_1 - \Theta(\tau) (1 - f_1)] e^{-\epsilon_1 \tau} \delta_{11'}. \quad (\text{B})$$



GREEN's function  $G_1^0(11, \tau)$  of the ideal FERMION gas according to (B) for single-particle energies  $\epsilon_1 = 0.1\beta, \beta, 10\beta$  and  $-\beta \leq \tau \leq \beta$ .

The FOURIER-transform of the GREEN's-function (B) can be obtained via (2.1.22):

$$\begin{aligned}
 G_1^0(11', iz_\nu) &\stackrel{(2.1.22)}{=} \int_0^\beta d\tau G_1(11', \tau) e^{iz_\nu \tau} \\
 &\stackrel{(B)}{=} \int_0^\beta d\tau \left( \underbrace{\Theta(-\tau) f_1}_{\text{vanishes due to } \tau > 0} - \Theta(\tau) (1 - f_1) \right) e^{-\epsilon_1 \tau} \delta_{11'} e^{iz_\nu \tau} \\
 &= -\frac{\delta_{11'}}{iz_\nu - \epsilon_1} \left( e^{(iz_\nu - \epsilon_1)\beta} - 1 \right) \cdot (1 - f_1) = \frac{\delta_{11'}}{iz_\nu - \epsilon_1}, \quad (C)
 \end{aligned}$$

where we made use of  $\frac{z_\nu \beta}{\pi}$  being odd and thus  $e^{iz_\nu \beta} = -1$ .

Step 2:

The analytic continuation of the single-particle free propagator (C) is

$$G_1^0(11', z) = \frac{\delta_{11'}}{z - \epsilon_1}. \quad (D)$$

Step 3:

Thus, the imaginary part of  $G_1^0$  results to

$$\begin{aligned}
 \text{Im} \{G_1^0(11', \omega - i\varepsilon)\} &\stackrel{(D)}{=} \text{Im} \left\{ \frac{\delta_{11'}}{(\omega - \epsilon_1) - i\varepsilon} \right\} \\
 &\stackrel{(2.2.8)}{=} \text{Im} \left\{ +i\pi\delta(\omega - \epsilon_1) + \frac{\mathcal{P}}{\omega - \epsilon_1} \right\} \delta_{11'} = \pi\delta(\omega - \epsilon_1) \delta_{11'}, \quad (E)
 \end{aligned}$$

where the principal value of the integral has been omitted since it only contributes to the real part.

With (E), we find for the spectral function

$$A_1(11', \omega) \stackrel{(2.2.13)}{=} 2\pi\delta(\omega - \epsilon_1) \delta_{11'}. \quad (F)$$

Step 4:

The spectral density is

$$I_1(11', \omega) \stackrel{(2.2.14), (F)}{=} \frac{2\pi\delta(\omega - \epsilon_1) \delta_{11'}}{1 + e^{\beta\omega}}. \quad (G)$$

Step 5:

As an example for a correlation function we evaluate the single-particle occupation number

$$\langle a_1^+ a_1 \rangle \stackrel{(2.2.15), (G)}{=} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{2\pi\delta(\omega - \epsilon_1) \delta_{11'}}{e^{\beta\omega} + 1} = \delta_{11'} f_1 \quad (H)$$

Step 6:

With the correlation function (H) we have an equation of state via:

$$n(\beta, \mu) \stackrel{(H)}{=} \frac{1}{\Omega} \sum_1 \langle a_1^+ a_1 \rangle = \frac{1}{\Omega} \sum_1 f_1. \quad (I)$$

The equation of state

$$n(\beta, \mu) \stackrel{\text{(I)}}{=} \frac{1}{\Omega} \sum_1 f_1 = (2s+1) \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\epsilon_k} + 1}, \quad (2.3.3)$$

that we have found with our calculus is the well-known result from statistical mechanics for the ideal FERMI gas.

As an important result from this example we have found an expression for the single-particle free propagator:

$$G_1^0(11', iz_\nu) \stackrel{\text{(C)}}{=} \frac{\delta_{11'}}{iz_\nu - \epsilon_1}. \quad (2.3.4)$$

Further, the spectral function

$$A_1(11', \omega) \stackrel{\text{(F)}}{=} 2\pi\delta(\omega - \epsilon_1)\delta_{11'} \quad (2.3.5)$$

has a  $\delta$ -like singularity at  $\omega = \epsilon_1$ .



# 3 Perturbation theory for thermodynamic Green's functions

## 3.1 Basic relations

Since we are examining many-particle systems with interaction, we need to construct a perturbation theory for the GREEN's function. Within this and the following sections we will concentrate on fermions. The appropriate expressions for bosonic particles will only be given in some special cases. However, the generalization of the calculus to arbitrary spin is straightforward.

With a decomposition of the entropy operator  $S$  of the form

$$S = S^{(0)} + S^{(1)} + S^{(2)} , \quad (3.1.1)$$

$$S^{(1)} = \beta \sum_1 (E_1 - \mu) a_1^\dagger a_1 , \quad (3.1.2)$$

$$S^{(2)} = \beta \frac{1}{2} \sum_{12,1'2'} V(12,1'2') a_1^\dagger a_2^\dagger a_{2'} a_{1'} , \quad (3.1.3)$$

that we already introduced with (1.1.9), we can perform an expansion with respect to the two-particle contributions in the statistical operator

$$\varrho = e^{-S} = e^{-(S^{(0)}+S^{(1)}+S^{(2)})} . \quad (3.1.4)$$

While in the previous chapters, the parameter  $\tau$  was of the dimension of the inverse energy and  $0 \leq \tau \leq \beta$ , we will now consider the more general case of a dimensionless parameter with  $0 \leq \tau \leq 1$ .

We have to consider the complete evolution as it was given with equation (2.1.4):

$$A(\tau) = e^{S\tau} A(0) e^{-S\tau} . \quad (3.1.5)$$

For constructing a perturbation theory for the GREEN's function, we treat  $S^{(2)}$  as the perturbation and introduce an interaction picture by means of

$$A(\tau) = U_I(0, \tau) A_I(\tau) U_I(\tau, 0) , \quad (3.1.6)$$

$$\text{where } A_I(\tau) = e^{(S^{(0)}+S^{(1)})\tau} A(0) e^{-(S^{(0)}+S^{(1)})\tau} = e^{S^{(1)}\tau} A(0) e^{-S^{(1)}\tau} \quad (3.1.7)$$

is the 'evolution' of the unperturbed system. Using (1.2.4) and (1.2.5),  $A_I(\tau)$  can further be simplified, since it only contains creation and annihilation operators. The 'evolution' operator in interaction representation has the form

$$U(\tau, \tau') = e^{S^{(1)}\tau} e^{S(\tau-\tau')} e^{-S^{(1)}\tau'} \quad (3.1.8)$$

and can be decomposed with respect to  $S^{(2)}$ , compare eq. (1.2.2):

$$U(\tau, \tau') = \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \cdots \int_{\tau'}^{\tau} d\tau_n \mathbb{T} [S^{(2)}(\tau_1) \dots S^{(2)}(\tau_n)] \quad (3.1.9)$$

as  $\tau$ -ordered product in terms of a DYSON series<sup>1</sup>.

In full analogy with (1.1.6) and (1.1.9),  $S^{(0)} = \ln Z(T, \Omega, \mu)$  cares for an appropriate normalization of the statistical operator  $\varrho$ .

Now, a perturbation theory for thermodynamic GREEN's function can be constructed by expanding any exponential function in

$$G_1(1\tau, 1'\tau') = -\text{Tr} \left\{ \varrho \mathbb{T} [a_1(\tau) a_1^\dagger(\tau')] \right\} \quad \text{with} \quad \varrho = \frac{e^{-(S^{(1)}+S^{(2)})}}{\text{Tr} \left\{ e^{-(S^{(1)}+S^{(2)})} \right\}} \quad (3.1.12)$$

in numerator and denominator with respect to  $S^{(2)}$ , that is contained in the statistical operator  $\varrho$  as well as in every 'evolution' operator via (3.1.6). A division by the denominator results in a power series in  $S^{(2)}$  with elements of a certain structure. Any of these elements can be illustrated by a diagram, whereas the FOURIER-representation is especially advantageous, since due to homogeneity in space and 'time', energy and momentum are conserved (as long as there is no external potential).

The expansion is very similar to time dependent perturbation theory from earlier lectures in quantum mechanics<sup>2</sup>, where for example transition rates between two states  $m$  and  $n$  in first and second order resulted to

$$w_{mn}^{(1)} = \frac{1}{\hbar^2} \left| \int_{t_0}^t dt' \underbrace{\langle \Psi_m | H' | \Psi_n \rangle}_{\cong V_{mn}} \underbrace{e^{\frac{i}{\hbar}(E_n - E_m)(t' - t_0)}}_{\cong G_1^0(mn)} \right|^2$$

$$w_{mn}^{(2)} = \frac{1}{\hbar^4} \left| \sum_k \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' e^{-i\omega_{nk}t'} V_{nk}(t') e^{-i\omega_{km}t''} V_{km}(t) \right|^2$$

When moving from coordinate space to momentum space via FOURIER transformation, the convolution integrals become simple products:

$$w_{mn}^{(1)} \propto \frac{1}{\hbar^2} |V_{mn} G_1^0(mn)|^2$$

$$w_{mn}^{(2)} \propto \frac{1}{\hbar^4} \left| \sum_k V_{mk} V_{kn} G_1^0(mk) G_1^0(kn) \right|^2$$

$$\vdots$$

These products can be effectively evaluated using FEYNMAN graphs.

<sup>1</sup> Instead of the nested integral

$$\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3 \dots \int_0^{\tau_{n-1}} d\tau_n A(\tau_1) B(\tau_2) C(\tau_3) \dots N(\tau_n), \quad (3.1.10)$$

we consider the full integral

$$\frac{1}{n!} \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 \int_0^\tau d\tau_3 \dots \int_0^\tau d\tau_n \mathbb{T} [A(\tau_1) B(\tau_2) C(\tau_3) \dots N(\tau_n)]. \quad (3.1.11)$$

The  $n!$  arrangements of the arguments  $\tau_1 \dots \tau_n$  can be brought to the original order  $\tau_1 \geq \tau_2 \geq \dots \geq \tau_n$  by renaming the integration variables while the time-ordering operator  $\mathbb{T}[\dots]$  guarantees the correct order of the operator product.

<sup>2</sup>For further details in time-dependent perturbation theory, consider any standard textbook on Quantum Mechanics.

## 3.2 Diagrammatic representation of the perturbative series

The perturbative expressions for the GREEN's functions will become unhandy when considering higher orders in the potential. That is why an effective and clear diagrammatic representation has been developed. Using the fact that the convolution integrals in coordinate space become simple products in FOURIER space, we can represent the perturbation theory up to arbitrary orders by constructing appropriate FEYNMAN diagrams.

The

- free single-particle GREEN's function

$$\underbrace{G_1^0(11', iz_\nu)}_{\text{Diagram}} \quad G_1^0(11', iz_\nu) \stackrel{(2.3.4)}{=} \frac{\delta_{11'}}{iz_\nu - \epsilon_1} \quad (3.2.1)$$

For homogeneous systems,  $G_1^0(11', iz_\nu)$  is diagonal in the single particle quantum numbers 11':  $G_1^0(11', iz_\nu) \propto \delta_{11'}$ . Thus, in the following we will often omit the second argument for convenience and just write  $G_1^0(1, iz_\nu)$ .

- and the interaction

$$\underbrace{V(\vec{q}, i\omega_\lambda)}_{\text{Diagram}} \quad V(\vec{q}) = \frac{1}{\Omega} \int d^3r e^{i\vec{q}\vec{r}} V(\vec{r}) \quad (3.2.2)$$

are parts of this diagram technique.

The representation for the interaction  $V$ , we give here, is just a shorthand notation. In the very general case we have to use  $V(12, 1'2')$ .

However, if there is no explicit dependence of the interaction on time (homogeneity in time), energy conservation holds and the interaction takes the form  $V(12, 1'2') \delta_{z_{\nu_1} + z_{\nu_2}, z_{\nu_1'} + z_{\nu_2'}}$ , i.e. it solely depends on  $\omega_\lambda = z_{\nu_1} - z_{\nu_1'}$ . If it is also local in time (instantaneous), the dependence on  $\omega_\lambda$  is also removed and the interaction is non-dispersive.

It is important to mention, that  $\omega_\lambda$  – as the difference of two odd MATSUBARA frequencies in the fermionic and two even frequencies in the bosonic case – corresponds to an even frequency. Thus, the interaction has bosonic character. For spin conserving interaction – as we only consider here – the expression reduces to

$$V(12, 1'2') = V(\vec{k}_1\vec{k}_2, \vec{k}_1'\vec{k}_2') \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} .$$

The ( $k$ -dependent) interaction in FOURIER space depends on the interaction in coordinate space via

$$\begin{aligned} V(\vec{k}_1\vec{k}_2, \vec{k}_1'\vec{k}_2') &= \langle k_1'k_2' | V | k_1k_2 \rangle \\ &= \int d^3\vec{r}_1 \int d^3\vec{r}_2 \int d^3\vec{r}_1' \int d^3\vec{r}_2' \langle k_1' | r_1' \rangle \langle k_2' | r_2' \rangle \langle r_1'r_2' | V | r_1r_2 \rangle \langle k_2 | r_2 \rangle \langle k_1 | r_1 \rangle \end{aligned}$$

with  $\langle r|k\rangle = \Omega^{-1/2} e^{i\vec{k}\vec{r}}$ :

$$\begin{aligned} &= \frac{1}{\Omega^2} \int d^3\vec{r}_1 \int d^3\vec{r}_2 \int d^3\vec{r}_{1'} \int d^3\vec{r}_{2'} e^{-i\vec{k}_{1'}\vec{r}_{1'}} e^{-i\vec{k}_{2'}\vec{r}_{2'}} V(\vec{r}_1\vec{r}_2, \vec{r}_{1'}\vec{r}_{2'}) e^{i\vec{k}_2\vec{r}_2} e^{i\vec{k}_1\vec{r}_1} \\ &= \frac{1}{\Omega^2} \int d^3\vec{r}_1 \int d^3\vec{r}_2 \int d^3\vec{r}_{1'} \int d^3\vec{r}_{2'} e^{i(\vec{k}_1\vec{r}_1 + \vec{k}_2\vec{r}_2 - \vec{k}_{1'}\vec{r}_{1'} - \vec{k}_{2'}\vec{r}_{2'})} V(\vec{r}_1\vec{r}_2, \vec{r}_{1'}\vec{r}_{2'}) , \end{aligned}$$

where  $k$  represents a wave-number and  $\Omega$  the normalization volume. For local interactions,  $V(\vec{r}_1\vec{r}_2, \vec{r}_{1'}\vec{r}_{2'}) = V(\vec{r}_1\vec{r}_2) \delta(\vec{r}_1 - \vec{r}_{1'}) \delta(\vec{r}_2 - \vec{r}_{2'})$  holds:

$$V(\vec{k}_1\vec{k}_2, \vec{k}_{1'}\vec{k}_{2'}) = \frac{1}{\Omega^2} \int d^3\vec{r}_1 \int d^3\vec{r}_2 e^{i([\vec{k}_1 - \vec{k}_{1'}]\vec{r}_1 + [\vec{k}_2 - \vec{k}_{2'}]\vec{r}_2)} V(\vec{r}_1\vec{r}_2) .$$

If the potential only depends on the relative vector between the interacting particles (homogeneity in space):  $V(\vec{r}_1\vec{r}_2) = V(\vec{r}_1 - \vec{r}_2)$ , we can transform one integration to relative coordinates and evaluate the other one:

$$\begin{aligned} &V(\vec{k}_1\vec{k}_2, \vec{k}_{1'}\vec{k}_{2'}) \\ &= \frac{1}{\Omega^2} \int d^3(\vec{r}_1 - \vec{r}_2) e^{i[\vec{k}_1 - \vec{k}_{1'}](\vec{r}_1 - \vec{r}_2)} V(\vec{r}_1 - \vec{r}_2) \underbrace{\int d^3\vec{r}_2 e^{i[\vec{k}_1 - \vec{k}_{1'} + \vec{k}_2 - \vec{k}_{2'}]\vec{r}_2}}_{\Omega \cdot \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_{1'} + \vec{k}_{2'}}} \\ &= \frac{1}{\Omega} \int d^3(\vec{r}_1 - \vec{r}_2) e^{i[\vec{k}_1 - \vec{k}_{1'}](\vec{r}_1 - \vec{r}_2)} V(\vec{r}_1 - \vec{r}_2) \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_{1'} + \vec{k}_{2'}} . \end{aligned}$$

Thus, we see, that due to the locality and homogeneity in space, momentum conservation is ensured.

For the COULOMB potential, we find

$$\begin{aligned} V(\vec{r}_1\vec{r}_2, \vec{r}_{1'}\vec{r}_{2'}) &= \frac{e_1 e_2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} \delta(\vec{r}_1 - \vec{r}_{1'}) \delta(\vec{r}_2 - \vec{r}_{2'}) \quad \text{and} \\ V(\vec{k}_1\vec{k}_2, \vec{k}_{1'}\vec{k}_{2'}) &= \frac{e_1 e_2}{\Omega\epsilon_0 |\vec{k}_1 - \vec{k}_{1'}|^2} \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_{1'} + \vec{k}_{2'}} \end{aligned}$$

As a shorthand notation we will often use  $q = |\vec{k}_1 - \vec{k}_{1'}|$  and

$$V_{12}(q) = \frac{e_1 e_2}{\Omega\epsilon_0 q^2} .$$

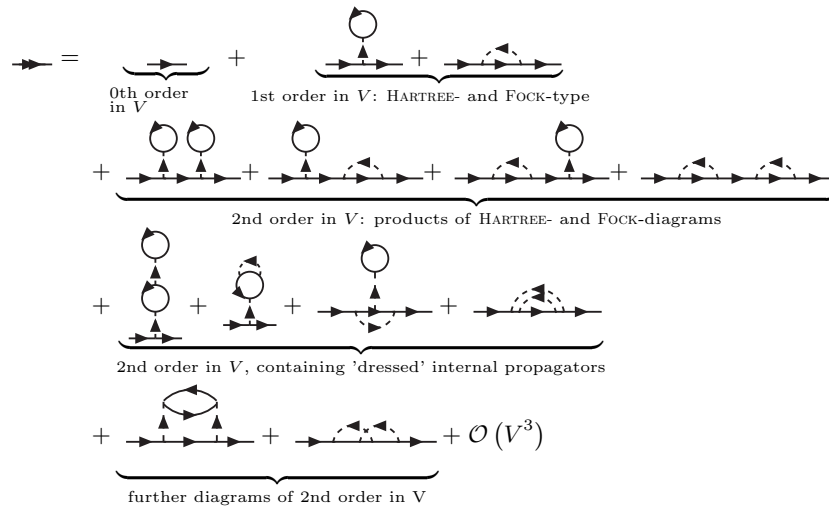
Note, that when introducing a vertex function (see section 4.3), the particle's charges as well as the KRONECKER symbols that ensure spin, momentum, and species conservation can also be defined to be part of the vertex, see equation (4.3.3). Then, the interaction  $V(q) = \frac{1}{\Omega\epsilon_0 q^2}$  indeed looks like a particle (photon) propagator, compare (3.2.1).



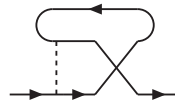
For developing correct and useful diagrams, several rules<sup>3</sup> have to be applied. These cannot be derived directly but checked on lowest orders.

1. Draw any connected diagrams which are not topologically equivalent. Otherwise equivalent diagrams would erroneously be counted multiple times. In particular for  $G_1$  in  $n$ -th order in  $V$ :
  - $n$  interaction lines
  - $(2n + 1)$  free-particle lines (otherwise we would not have a closed and connected diagram)

For getting an overview of the contributions of the three lowest orders to  $G_1$  we show the first constituents of the decomposition of the so-called 'full propagator'  $\rightarrow$ , that represents  $G_1$ :




A diagram like



does for example not appear, since it is topologically equivalent to the FOCK diagram



Also diagrams of the form  are not allowed because they are disconnected.

Furthermore the formalism can also be adapted to two- and more-particle GREEN's functions. In the two-particle case this would look like

$$\overline{G_2^{\text{1add}}} = \overline{\text{---}} + \overline{\text{---}} + \overline{\text{---}} + \overline{\text{---}} + \overline{\text{---}} + \overline{\text{---}} + \mathcal{O}(V^3) .$$

The two-particle GREEN's function will be addressed in section 4.8, where bound states are discussed.

<sup>3</sup>These rules are taken from [FW71]. For further details, we recommend consulting this monograph. A strict derivation would need topological arguments which are usually not available.

2. Every line is assigned a direction and a MATSUBARA frequency as well as a wave number vector. For any vertex (point where lines touch) conservation of energy (frequency) and momentum (wave number vector) apply.
3. Every interaction line is given a factor of  $V(q, i\omega_\lambda)$ , see equation (3.2.2) and any free-particle line is assigned a factor  $G_1^0(11', iz_\nu)$ , see equation (3.2.1)
4. A summation/integration over all  $n$  independent internal frequencies and wave number vectors has to be performed.
5. For every frequency summation and wave number integration, we have to multiply with  $-\frac{\Omega}{\beta} \left(\frac{1}{2\pi}\right)^3$ . The volume part of this factor is already known from the transition from discrete momentum summation to integration in quantum mechanics ( $\sum_k \dots \rightarrow \Omega \int \frac{d^3k}{(2\pi)^3} \dots$ ). It compensates the volume  $\Omega$  in the interaction. The energy part preserves the dimension of  $\frac{1}{\text{energy}}$  for the diagram, since any propagator itself contributes the same unit.  
 Additionally, for ensuring the correct spin summation, we have to multiply with  $(2s + 1)$  for every degree of freedom in a spin coordinate  $s$ . For any closed fermion line a multiplication with  $(-1)$  has to be introduced.
6. If a fermion propagator begins and ends at the same interaction line (as it is the case in the HARTREE and FOCK diagrams above), a convergence factor of  $e^{iz_\nu\eta}$  with the implicit convention  $\eta \searrow 0$  is introduced. As usual, the limit  $\eta \searrow 0$  has to be performed after any other limit has been computed.

### 3.3 Evaluation of the frequency summation

The direct summation over the MATSUBARA frequencies is only possible at high temperatures where only few summands contribute. However, the sum can be transformed into an integration using the FERMI function  $f(z) = \frac{1}{e^{\beta z} + 1}$  for fermionic particles and the BOSE function  $g(z) = \frac{1}{e^{\beta z} - 1}$  in the bosonic case, respectively.

We consider an arbitrary function  $h(z)$  which is analytic in the complex  $z$ -plane with exception of a set of distinct poles  $\{z_h\}$ . Especially at the MATSUBARA frequencies  $iz_\mu$  and in their environment, analyticity has to be ensured.

Then, the summation over the MATSUBARA frequencies can be simplified with

$$\sum_{z_\mu} h(iz_\mu) = -\frac{\beta}{2\pi i} \int_{\mathcal{C}_1} dz f(z) h(z) \quad (3.3.1)$$

with the integration contour  $\mathcal{C}_1$  enclosing the MATSUBARA frequencies. The function  $f(z)$  is analytic in the whole  $z$ -plane with the exception of singularities at the MATSUBARA frequencies  $iz_\mu$ . For odd frequencies (fermionic case), the FERMI function is an appropriate choice, while for even frequencies (bosonic case), the BOSE function is applicable.

For example for the single particle GREEN's function  $h(z) = G_1^0(\vec{k}, z) \stackrel{(3.2.1)}{=} \frac{1}{z - \epsilon_k}$ , equation (3.3.1) can be used to evaluate the frequency sum

$$\lim_{\eta \searrow 0} \sum_{z_\mu} G_1^0(\vec{k}, iz_\mu) \cdot e^{iz_\mu \eta} = \lim_{\eta \searrow 0} \sum_{z_\mu} \frac{e^{iz_\mu \eta}}{iz_\mu - \epsilon_k} = \begin{cases} \beta f(\epsilon_k) & \text{for fermions} \\ -\beta g(\epsilon_k) & \text{for bosons.} \end{cases} \quad (3.3.2)$$

Note, that the series expansion of the FERMI and BOSE distribution is given in [Mah90], section 3.1 *Green's Functions at Finite Temperatures - Introduction* as

$$f(\epsilon_k) = \frac{1}{e^{\beta \epsilon_k} + 1} = \frac{1}{2} + \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1) \frac{i\pi}{\beta} - \epsilon_k}$$

$$g(\epsilon_k) = \frac{1}{e^{\beta \epsilon_k} - 1} = -\frac{1}{2} + \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{2n \frac{i\pi}{\beta} - \epsilon_k}.$$

The additional summand  $\pm 1/2$  becomes relevant in numerical evaluation of the MATSUBARA sum and high-temperature expansions.

We will prove (3.3.1) in general and directly show (3.3.2) in the fermionic case. The algorithm for doing so is a straightforward application of the residue theorem, that is well-known from complex analysis:

$$\frac{1}{2\pi i} \int_{\mathcal{C}} F(z) dz = \sum_a \text{Res}_a F(z) \tag{A}$$

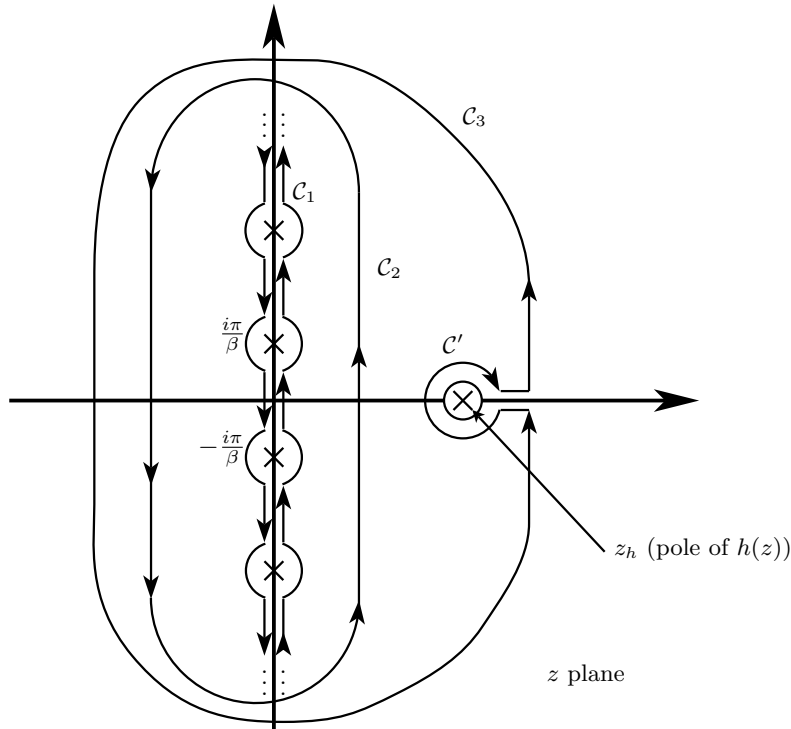
for closed curves  $\mathcal{C}$  with the residues at any pole  $a$  of  $F(z)$  within  $\mathcal{C}$ . Using  $h(z) = \frac{e^{z\eta}}{z-x}$  and  $f(z) = \frac{1}{e^{\beta z} + 1}$  with  $x \in \mathbb{R}$ , it is obvious that  $F(z) := h(z) \cdot f(z)$  has singularities at  $z = iz_\nu = i\frac{\pi\nu}{\beta}$  with  $\nu = \pm 1, \pm 3, \dots$ :

$$f(iz_\nu) = \frac{1}{\underbrace{e^{i\pi\nu}}_{-1} + 1} = \infty$$

with the residues  $-\frac{1}{\beta} \cdot h(iz_\nu)$  and a simple pole at  $z = x$ , where  $h(z = x) = \infty$ . with the residue  $f(x) \cdot e^{x\eta}$ .

Thus, taking a look at the picture, equation (A) can be utilized as following:

$$\sum_{z_\mu} h(iz_\mu) = -\frac{\beta}{2\pi i} \int_{\mathcal{C}_1} dz f(z)h(z)$$



The contour  $\mathcal{C}_1$  can be expanded via  $\mathcal{C}_2$  to  $\mathcal{C}_3$  as long as  $h(z)$  remains analytic. Note, that the antiparallel paths cancel each other. Since – according to JORDAN's lemma – contributions of large arcs vanish, we are left with the integration along  $\mathcal{C}'$ , that encloses the simple pole of  $h(z)$  at  $z = x$ . The application of JORDAN's lemma is restricted to functions that vanish fast enough with  $|z| \rightarrow \infty$ .

In our example this is guaranteed by the convergence factor, that thus plays an essential role. If we have to sum over a product of two or more propagators, the function  $h(z)$  vanishes faster than  $\propto 1/z$  for  $|z| \rightarrow \infty$  and the convergence factor is not necessary.

$$\sum_{z_\mu} h(iz_\mu) = -\frac{\beta}{2\pi i} \int_{\mathcal{C}'} dz F(z)$$

The residue of  $g(z)$  at  $z = x$  is  $f(x) \cdot e^{x\eta}$ , so that

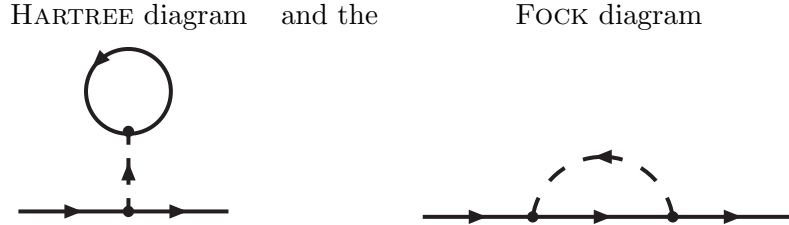
$$-\frac{1}{2\pi i} \int_{\mathcal{C}'} dz F(z) \stackrel{(\Delta)}{=} f(x) \cdot e^{x\eta}$$

(N.B. the direction of  $\mathcal{C}'$  is mathematically negative) and thus

$$\sum_{z_\mu} h(iz_\mu) = \beta f(x) \cdot e^{x\eta} \stackrel{\eta \geq 0}{=} \beta f(x) .$$

### 3.4 Application of the diagram rules: Hartree-Fock approximation

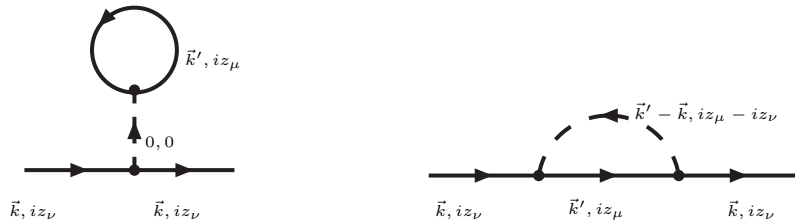
We will now apply the diagram rules to the two diagrams that are of lowest (first) order in  $V$ , the so-called



Both diagrams consist of  $n = 1$  interaction lines and contain  $2n + 1 = 3$  free-particle lines. They are connected and not topologically equivalent (i.e. cannot be transformed into each other without changing internal connections). Thus, these two diagrams fulfill the first rule from the previous section.

Additionally, there is no third first-order diagram in  $V$ .

Applying the second rule is straightforward: Caring for conservation of energy and wave-number at any vertex, we just add arbitrary MATSUBARA frequencies and wave number vectors (N.B. the interaction has bosonic character, since it carries even frequencies in both cases):



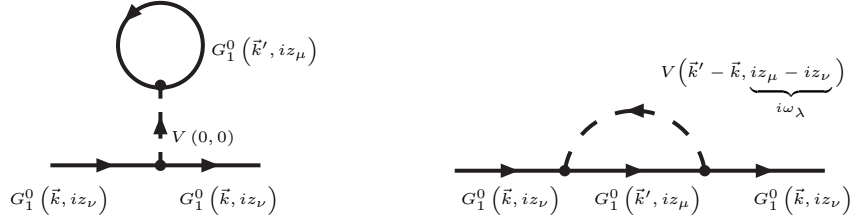
The diagram lines are now replaced with the interaction potential

$$V(\vec{q}, i\omega_\lambda) = \frac{1}{\Omega} \int d^3\vec{r} e^{i\vec{q}\vec{r}} V(\vec{r}) \overset{\text{COULOMB interaction, compare section 3.2}}{=} \frac{e_1 e_2}{\Omega \epsilon_0 q^2} \quad (3.4.1)$$

and the free-particle propagator

$$G_1^0(\vec{k}, iz_\nu) = \frac{1}{iz_\nu - \epsilon_{\vec{k}}} \quad \epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \mu \quad (3.4.2)$$

with the appropriate coefficients (rule 3):



After combining the summations and integrations from rule 4 and the prefactors of rule 5, we get

$$\begin{aligned}
 \text{Diagram 1} &= -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 (-2s+1)^1 \sum_{z_\mu} \int d^3 \vec{k}' G_1^0(\vec{k}, iz_\nu) \cdot G_1^0(\vec{k}', iz_\mu) \\
 &\quad \cdot G_1^0(\vec{k}, iz_\nu) \cdot V(0,0)
 \end{aligned} \tag{3.4.3}$$

$$\begin{aligned}
 \text{Diagram 2} &= -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 (-2s+1)^0 \sum_{z_\mu} \int d^3 \vec{k}' G_1^0(\vec{k}, iz_\nu) \cdot G_1^0(\vec{k}', iz_\mu) \\
 &\quad \cdot G_1^0(\vec{k}, iz_\nu) \cdot V(\vec{k}' - \vec{k}, i\omega_\lambda)
 \end{aligned} \tag{3.4.4}$$

Since the MATSUBARA frequency summations would not converge, according to rule 6, we have to introduce a convergence factor of  $e^{iz_\nu \eta}$  in both cases:

$$\begin{aligned}
 \text{Diagram 1} &= \lim_{\eta \searrow 0} -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 (-2s+1)^1 \sum_{z_\mu} \int d^3 \vec{k}' G_1^0(\vec{k}, iz_\nu) \cdot G_1^0(\vec{k}', iz_\mu) \\
 &\quad \cdot e^{iz_\mu \eta} \cdot G_1^0(\vec{k}, iz_\nu) \cdot V(0,0)
 \end{aligned} \tag{3.4.5}$$

$$\begin{aligned}
 &= \lim_{\eta \searrow 0} -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 (-2s+1)^1 \sum_{z_\mu} \int d^3 \vec{k}' \frac{1}{iz_\nu - \epsilon_k} \cdot \frac{1}{iz_\mu - \epsilon_{k'}} \\
 &\quad \cdot e^{iz_\mu \eta} \cdot \frac{1}{iz_\nu - \epsilon_k} \cdot V(0,0)
 \end{aligned} \tag{3.4.6}$$

and

$$\begin{aligned}
 \text{Diagram 2} &= \lim_{\eta \searrow 0} -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 \sum_{z_\mu} \int d^3 \vec{k}' G_1^0(\vec{k}, iz_\nu) \cdot G_1^0(\vec{k}', iz_\mu) \\
 &\quad \cdot e^{iz_\mu \eta} \cdot G_1^0(\vec{k}, iz_\nu) \cdot V(\vec{k}' - \vec{k}, i\omega_\lambda)
 \end{aligned} \tag{3.4.7}$$

$$\begin{aligned}
 &= \lim_{\eta \searrow 0} -\frac{1}{\beta} \left( \frac{1}{2\pi} \right)^3 \sum_{z_\mu} \int d^3 \vec{k}' \frac{1}{iz_\nu - \epsilon_k} \cdot \frac{1}{iz_\mu - \epsilon_{k'}} \\
 &\quad \cdot e^{iz_\mu \eta} \cdot \frac{1}{iz_\nu - \epsilon_k} \cdot V(\vec{k}' - \vec{k}, i\omega_\lambda)
 \end{aligned} \tag{3.4.8}$$

These expressions can further be simplified using (3.3.2), i.e.  $\lim_{\eta \searrow 0} \sum_{z_\mu} \frac{e^{iz_\mu \eta}}{iz_\mu - \epsilon_k} = \beta f(\epsilon_k)$ . Additionally, we can omit the frequency coefficient in the interaction, since the instantaneous COULOMB potential only depends on the momentum, compare (3.2.2) and comments there.

Finally, we find the contributions of the

HARTREE diagram

$$\begin{aligned} & \text{Diagram: } \begin{array}{c} \text{Circular loop } G_1^0(\vec{k}', iz_\mu) \\ \uparrow V(0,0) \\ \text{Horizontal line } G_1^0(\vec{k}, iz_\nu) \end{array} \\ & \text{Equation: } \begin{array}{c} \text{Diagram} = \frac{1}{iz_\nu - \epsilon_k} \cdot \underbrace{(2s+1)}_n \int \frac{d^3 \vec{k}'}{(2\pi)^3} f(\epsilon_{k'}) \cdot V(0) \cdot \frac{1}{iz_\nu - \epsilon_k} \end{array} \end{aligned} \quad (3.4.9)$$

and the

FOCK diagram

$$\begin{aligned} & \text{Diagram: } \begin{array}{c} \text{Dashed line } V(\vec{k}' - \vec{k}, iz_\mu - iz_\nu) \\ \text{Horizontal line } G_1^0(\vec{k}, iz_\nu) \quad G_1^0(\vec{k}', iz_\mu) \quad G_1^0(\vec{k}, iz_\nu) \end{array} \\ & \text{Equation: } \begin{array}{c} \text{Diagram} = -\frac{1}{iz_\nu - \epsilon_k} \cdot \int \frac{d^3 \vec{k}'}{(2\pi)^3} f(\epsilon_{k'}) \cdot V(\vec{k}' - \vec{k}) \cdot \frac{1}{iz_\nu - \epsilon_k} \end{array} \end{aligned} \quad (3.4.10)$$

Obviously, the HARTREE diagram has an additional degree of freedom due to its closed particle loop. It is removed by spin summation, that leads to the prefactor  $(2s+1)$ . In the FOCK diagram the particle's spin is fixed by the  $\delta$  functions in the potential ( $\delta_{\sigma_1 \sigma_{1'}} \rightarrow \delta_{\sigma_1 \sigma_2}$  after particle exchange) and  $\delta_{\sigma_2 \sigma_{2'}}$  in the GREEN's function. Thus, the factor  $(2s+1)$  is missing there and the negative sign is preserved. For the COULOMB potential  $V(q) \propto 1/q^2$ , the term  $V(0)$  in the HARTREE expression is divergent. However, in real systems (that are electrically neutral), we have to consider a mixture of different species  $c$  in addition to the spin variable  $\sigma$ . The summation over positive and negatively charged species leads to a mutual compensation and the HARTREE diagram does not give any contribution. For a screened interaction (see section 4.3),  $V^s(0,0)$  is not singular any longer.



# 4 Evaluation of diagrams and partial summation

## 4.1 Mean field and quasi-particle concept

Due to their similar structure, the HARTREE and FOCK contributions can be combined in one diagram class:

$$\begin{aligned}
 & \text{Diagram 1} + \text{Diagram 2} \\
 &= \frac{1}{iz_\nu - \epsilon_k} \cdot \underbrace{\left[ \int \frac{d^3 k'}{(2\pi)^3} \left( (2s+1)V(0) - V(\vec{k}' - \vec{k}) \right) f(\epsilon_{k'}) \right]}_{\equiv \Sigma_1^{\text{HF}}(\vec{k})} \cdot \frac{1}{iz_\nu - \epsilon_k} \quad (4.1.1)
 \end{aligned}$$

$$= G_1^0(\vec{k}, iz_\nu) \cdot \Sigma_1^{\text{HF}}(\vec{k}) \cdot G_1^0(\vec{k}, iz_\nu) \quad (4.1.2)$$

$$= \text{Diagram 1} \cdot \left( \text{Diagram 1} + \text{Diagram 2} \right) \cdot \text{Diagram 1} \quad (4.1.3)$$

In fact, the second diagram can be interpreted as an exchange contribution to the first one. Their contribution leads to an energy shift, that can be seen as being caused by mutual particle exchange.

In the following, we will especially concentrate in the COULOMB interaction. Note, that we have omitted the species summation. Considering the full expression including the species, the propagator terms would carry a species conserving factor  $\delta_{cd}$  and we would have to sum over all species:  $\sum_{cd}$ . As already mentioned, for charge-neutral systems, with this summation, the HARTREE-diagram vanishes, since positive and negative charges compensate for each other.

Even for small  $\Sigma_1^{\text{HF}}$ , the perturbation expansion does not converge near the poles  $\omega = \epsilon_k$  of the free propagator  $G_1^0$ . This behavior is due to the insufficiency of the mathematical methods that were applied until now. The real physical behavior does not show a discontinuity. Thus, higher orders of diagrams have to be taken into account in a so-called 'partial summation'. That is, only diagrams of a certain structure but up to arbitrary orders, are included. To exemplify this, we will calculate the self-energy in HARTREE-FOCK-approximation, i.e. we will perform a partial summation of self-energy contributions considering only diagrams of HARTREE- and FOCK-type up to arbitrary orders.

This leads to the single-particle GREEN's function in HARTREE-FOCK approximation. Collecting all orders of HARTREE and FOCK diagrams together, we can formally write

$$G_1^{\text{HF}}(\vec{k}, iz_\nu) = \frac{1}{iz_\nu - \epsilon_{\vec{k}} - \Sigma_1^{\text{HF}}(\vec{k})} \quad (4.1.4)$$

$$\text{with } \Sigma_1^{\text{HF}}(\vec{k}) = \text{[diagram: a circle with an arrow pointing up] + \text{[diagram: a triangle with an arrow pointing up]} , \quad (4.1.5)$$

which results from a straightforward application of the geometric series.

The proof for (4.1.4) is straightforward:

$$\begin{aligned} G_1^{\text{HF}} &= \text{[diagram: a horizontal line with an arrow pointing right]} + \left( \text{[diagram: a horizontal line with an arrow pointing right and a circle with an arrow pointing up above it]} + \text{[diagram: a horizontal line with an arrow pointing right and a triangle with an arrow pointing up above it]} \right) + \left( \text{[diagram: a horizontal line with an arrow pointing right and two circles with arrows pointing up above it]} + \text{[diagram: a horizontal line with an arrow pointing right and two triangles with arrows pointing up above it]} + \text{[diagram: a horizontal line with an arrow pointing right and one circle with an arrow pointing up above it and one triangle with an arrow pointing up above it]} \right) + \dots \\ &= \text{[diagram: a horizontal line with an arrow pointing right]} \cdot \left[ 1 + \left( \text{[diagram: a circle with an arrow pointing up]} + \text{[diagram: a triangle with an arrow pointing up]} \right) + \left( \text{[diagram: two circles with arrows pointing up]} + \text{[diagram: two triangles with arrows pointing up]} + \text{[diagram: one circle with an arrow pointing up and one triangle with an arrow pointing up]} \right) + \dots \right] \\ &= \text{[diagram: a horizontal line with an arrow pointing right]} \cdot \left[ 1 + \underbrace{\left( \text{[diagram: a circle with an arrow pointing up]} + \text{[diagram: a triangle with an arrow pointing up]} \right)}_{(\Sigma_1^{\text{HF}} \cdot G_1^0)} + \underbrace{\left( \text{[diagram: two circles with arrows pointing up]} + \text{[diagram: two triangles with arrows pointing up]} + \text{[diagram: one circle with an arrow pointing up and one triangle with an arrow pointing up]} \right)^2}_{(\Sigma_1^{\text{HF}} \cdot G_1^0)^2} + \dots \right] \\ &= \text{[diagram: a horizontal line with an arrow pointing right]} \cdot \left[ 1 + (\Sigma_1^{\text{HF}} \cdot G_1^0) + (\Sigma_1^{\text{HF}} \cdot G_1^0)^2 + \dots \right] . \end{aligned}$$

Making use of the geometric series  $\frac{1}{1-x} \approx 1 + x + x^2 + \dots$ , we get

$$\begin{aligned} &= \text{[diagram: a horizontal line with an arrow pointing right]} \cdot \frac{1}{1 - \Sigma_1^{\text{HF}} \cdot G_1^0} = G_1^0 \cdot \frac{1}{1 - \Sigma_1^{\text{HF}} \cdot G_1^0} \\ &= \frac{1}{(G_1^0)^{-1} - \Sigma_1^{\text{HF}}} = \frac{1}{iz_\nu - \epsilon_1 - \Sigma_1^{\text{HF}}} . \end{aligned}$$

From (4.1.1) it is obvious, that  $\Sigma_1^{\text{HF}}(\vec{k})$  is a real quantity, i.e.  $\text{Im} \left\{ \Sigma_1^{\text{HF}}(\vec{k}) \right\} = 0$ . Equation (4.1.4) shows that if all orders of HARTREE and FOCK diagrams are taken into account,  $\Sigma_1^{\text{HF}}$  is an energy shift in  $\epsilon_1$ , that moves the pole of  $G_1^0 \rightarrow G_1^{\text{HF}}$ . Although in general,  $\Sigma$  will have complex values, in the case of the HARTREE-FOCK approximation,  $\Sigma_1^{\text{HF}}$  is real and just shifts the pole along the real axis. Thus, the same terms as for ideal quantum gases arise. Simply the free-particle's energy  $\epsilon_1$  is replaced by the HARTREE-FOCK energy  $\epsilon_1 + \Sigma_1^{\text{HF}}$ .

Knowing  $G_1^{\text{HF}}$ , we can now perform the full thermodynamic program from section 2.2. Since

$$G_1^{\text{HF}}(11', iz_\nu) = \frac{\delta_{11'}}{iz_\nu - (\epsilon_1 + \Sigma_1^{\text{HF}})}$$

only has a pole of the order 1, the analytic continuation is as simple as

$$G_1^{\text{HF}}(11', z) = \frac{\delta_{11'}}{z - (\epsilon_1 + \Sigma_1^{\text{HF}})}.$$

The corresponding spectral function is

$$\begin{aligned} A^{\text{HF}}(1, \omega) &= \lim_{\eta \searrow 0} i \left( G_1^{\text{HF}}(11', \omega + i\eta) - G_1^{\text{HF}}(11', \omega - i\eta) \right) \\ &= \lim_{\eta \searrow 0} i \left( \frac{1}{\omega + i\eta - (\epsilon_1 + \Sigma_1^{\text{HF}})} - \frac{1}{\omega - i\eta - (\epsilon_1 + \Sigma_1^{\text{HF}})} \right) \\ &\stackrel{(2.2.8)}{=} i \left( \mathcal{P} \frac{1}{\omega - (\epsilon_1 + \Sigma_1^{\text{HF}})} - i\pi\delta(\omega - (\epsilon_1 + \Sigma_1^{\text{HF}})) \right) \\ &\quad - \mathcal{P} \frac{1}{\omega - (\epsilon_1 + \Sigma_1^{\text{HF}})} - i\pi\delta(\omega - (\epsilon_1 + \Sigma_1^{\text{HF}})) \\ &= 2\pi\delta(\omega - (\epsilon_1 + \Sigma_1^{\text{HF}})). \end{aligned}$$

Thus, in comparison with the non-interacting spectral function  $A(1, \omega) = 2\pi\delta(\omega - \epsilon_1)$ , the HARTREE-FOCK spectral function  $A^{\text{HF}}$  is shifted by  $\Sigma_1^{\text{HF}}$  but keeps its  $\delta$ -character. In the special case of  $\Sigma_1^{\text{HF}} = 0$ , the well-known result of a free particle holds.

With the spectral function we can now compute the occupation number

$$\begin{aligned} \langle a_1^\dagger a_1 \rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A^{\text{HF}}(1, \omega) f(\omega) \\ &= f(\epsilon_1 + \Sigma_1^{\text{HF}}) \end{aligned}$$

and the density

$$\begin{aligned} n(\beta, \mu) &= \frac{1}{\Omega} \sum_1 \langle a_1^\dagger a_1 \rangle \\ &= \frac{1}{\Omega} \sum_1 f(\epsilon_1 + \Sigma_1^{\text{HF}}) \end{aligned}$$

as an example for any other thermodynamic variable. This result is consistent with a result we would get when performing elementary perturbation theory in HARTREE-FOCK approximation, see section 1.4.

We see, that the divergences when expanding  $G_1$  near the pole, are cured. The solution is a simple shift of the pole, which cannot be obtained by expansion at the unperturbed pole.

## 4.2 Dyson equation and self-energy

The method of partial summation of special diagram classes can be generalized. When considering the sum of all irreducible diagrams with one incoming and one outgoing vertex that don't disintegrate if one propagator of a free fermion is cut, we are facing a new diagram element:

$$\begin{aligned}
 \Sigma_1(1, iz_\nu) = & \\
 \underbrace{\text{---}\Sigma\text{---}} = & \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} \\
 & + \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} + \mathcal{O}(V^3), \quad (4.2.1)
 \end{aligned}$$

which is called 'single-particle self-energy'.

The first two terms describe the HARTREE-FOCK contribution

$$\Sigma_1^{\text{HF}}(1, iz_\nu) = \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---} \quad (4.2.2)$$

With the self-energy, we can define a 'full propagator'  $\text{---}\text{---}\text{---}$ , that iteratively includes contributions of the self-energy  $\underbrace{\text{---}\Sigma\text{---}}$ :

$$\begin{aligned}
 \text{---}\text{---}\text{---} &= \text{---}\text{---}\text{---} + \text{---}\text{---}\text{---}\text{---}\text{---}\text{---} + \text{---}\text{---}\text{---}\text{---}\text{---}\text{---}\text{---}\text{---} + \dots \quad (4.2.3) \\
 &= \text{---}\text{---}\text{---} \left( 1 + \text{---}\text{---}\text{---}\text{---}\text{---}\text{---} + \text{---}\text{---}\text{---}\text{---}\text{---}\text{---}\text{---}\text{---} + \dots \right) \\
 &= \text{---}\text{---}\text{---} \cdot \frac{1}{1 - \text{---}\text{---}\text{---}\text{---}\text{---}\text{---}} \\
 &= G_1^0(1, iz_\nu) \frac{1}{1 - \Sigma_1(1, iz_\nu) G_1^0(1, iz_\nu)} \\
 &= \frac{1}{G_1^0(1, iz_\nu)^{-1} - \Sigma_1(1, iz_\nu)}
 \end{aligned}$$

$$\Rightarrow G_1(1, iz_\nu) = \frac{1}{iz_\nu - \epsilon_1 - \Sigma_1(1, iz_\nu)}. \quad (4.2.4)$$

Relation (4.2.3) is the DYSON equation, we already introduced earlier, compare (1.2.2). It can also be used to define the single-particle self-energy and calculate the single-particle full propagator in a self consistent way:

$$\begin{array}{c} \longrightarrow \\ \longleftarrow \end{array} = \begin{array}{c} \longrightarrow \\ \longleftarrow \end{array} + \begin{array}{c} \longrightarrow \\ \longleftarrow \end{array} \begin{array}{c} \curvearrowright \\ \Sigma \\ \curvearrowleft \end{array} \begin{array}{c} \longrightarrow \\ \longleftarrow \end{array} \quad (4.2.5)$$

The self-energy just appears like an energy shift in the free particle propagator. In the previous section we already saw, that when considering only diagrams of the HARTREE and FOCK type, the spectral function is  $\delta$ -shaped, but shifted along the frequency axis (compare figure 1). However, since  $\Sigma_1(1, iz_\nu)$  is in general a dynamic (frequency-dependent) and complex variable, the  $\delta$ -like spectral function of the free-particle is becoming more complicated (figures 1 and 2):

$$\begin{aligned} G_1(1, iz_\nu) &= \frac{1}{iz_\nu - \epsilon_1 - \text{Re}\{\Sigma_1(1, iz_\nu)\} - i\text{Im}\{\Sigma_1(1, iz_\nu)\}}, & (4.2.6) \\ A_1(1, \omega) &\stackrel{(2.2.10)}{=} \lim_{\epsilon \searrow 0} 2\text{Im}\{G_1(1, \omega - i\epsilon)\} \\ &= \lim_{\epsilon \searrow 0} 2\text{Im}\left\{\frac{1}{\omega - \epsilon_1 - \text{Re}\{\Sigma_1(1, \omega - i\epsilon)\} - i(\text{Im}\{\Sigma_1(1, \omega - i\epsilon)\} - \epsilon)}\right\} \\ &= \lim_{\epsilon \searrow 0} 2\frac{\text{Im}\{\Sigma_1(1, \omega - i\epsilon)\}}{[\omega - \epsilon_1 - \text{Re}\{\Sigma_1(1, \omega - i\epsilon)\}]^2 + [\text{Im}\{\Sigma_1(1, \omega - i\epsilon)\} - \epsilon]^2} & (4.2.7) \end{aligned}$$

In general, the spectral function can be arbitrary complex. In the case of  $\text{Im}\{\Sigma_1(1, \omega)\}$  being independent of the frequency  $\omega$ , this is a LORENTZian profile with the width  $2\text{Im}\{\Sigma_1(1, \omega)\}$ .

If the width of the spectral profile and thus  $\text{Im}\{\Sigma_1(1, \omega)\}$  is negligibly small, the propagator (4.2.4) takes the form

$$G_1(1, \omega) = \frac{1}{\omega - \epsilon_1 - \text{Re}\{\Sigma_1(1, \omega)\}}. \quad (4.2.8)$$

Thus, we have an energy shift to a new quasi particle energy

$$E_1^{\text{qu.}} = \epsilon_1 + \text{Re}\{\Sigma_1(1, \omega)\}|_{\omega=E_1^{\text{qu.}}}. \quad (4.2.9)$$

This quasi-particle energy justifies the introduction of a quasi-particle concept, where we renormalize the particle mass to restore the original free particle's propagator structure<sup>1</sup>:

$$G_1(1, \omega) = \frac{1}{\omega - \frac{\hbar^2 p^2}{2m^*}} \quad \text{with} \quad \frac{1}{m^*} = \frac{\partial^2}{\partial(\hbar p)^2} E_1^{\text{qu.}}. \quad (4.2.10)$$

<sup>1</sup>See [KKER86], section 4.3.2. *Self-Energy in  $V^s$ -Approximation*, for explicit results for the effective mass.

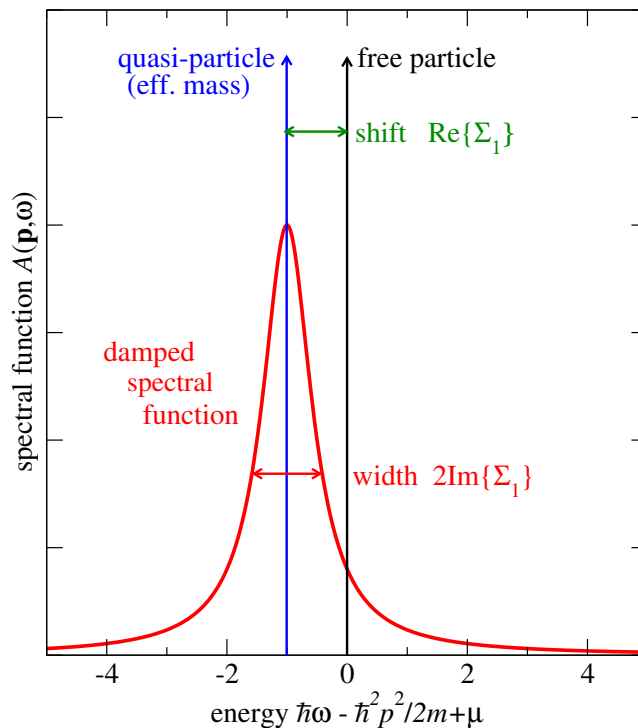


FIGURE 1: Spectral function at fixed momentum  $p$  in different approximations of the self-energy. While the spectral function of a free particle and a particle with inclusion of the HARTREE-FOCK self-energy is  $\delta$ -shaped, the spectral function for complex (but  $\omega$ -independent) self-energy has a LORENTZIAN profile<sup>2</sup>.

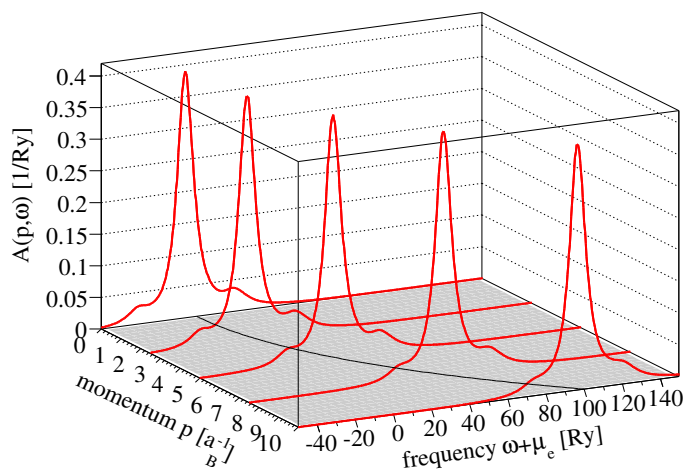


FIGURE 2: Spectral function for a plasma under solar core conditions (density  $n = 7 \times 10^{25} \text{ cm}^{-3}$  and temperature  $k_B T = 1000 \text{ eV}$ ) as a function of momentum and energy. The black line on the bottom plane represents the free dispersion relation  $\hbar\omega = \epsilon_p = \frac{\hbar^2 p^2}{2m} - \mu$ .<sup>3</sup>

<sup>2</sup>Figure with kind permission by C. FORTMANN.

<sup>3</sup>For further details, see [For08], which is a very recent and very detailed work on the spectral function of Coulomb systems. Additionally, we recommend [For09] for further studies.

### 4.3 Screening equation and polarization function

Until now, we have only considered self-energy corrections of the single-particle propagator  $G_1$ . The reason, why  $G_1$  factorizes and can be treated by a geometrical series, is the conservation of momentum. In general, e.g. in an external potential, a matrix equation or integral equation has to be solved.

We will now examine, whether the approach of introducing a self-energy  $\Sigma_1(1, z)$  can also be generalized to the interaction

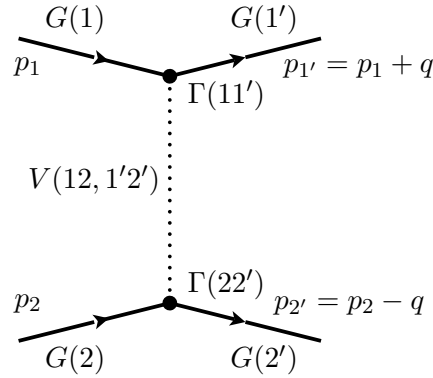
$$V(1, 2; 1', 2') = V(p_1 \sigma_1 c_1 i z_{\mu_1}, p_2 \sigma_2 c_2 i z_{\mu_2}; p_{1'} \sigma_{1'} c_{1'} i z_{\mu_{1'}}, p_{2'} \sigma_{2'} c_{2'} i z_{\mu_{2'}}), \quad (4.3.1)$$

where  $p_i$  are the momenta of the incoming,  $p_{i'}$  those of the outgoing particles and  $\sigma_i$  and  $c_i$  their respective spin and species.

A diagram fragment containing interaction has a structure, which consists of three general elements:

- the particle propagators  $G_1(1, i z_\nu)$  and  $G_1(2, i z_\nu)$  with species  $c_1$  and  $c_2$ , where  $G(1, z) = \frac{1}{z - \epsilon_1}$  respectively,
- the vertices  $\Gamma(11') \propto e_1$  and  $\Gamma(22') \propto e_2$  and
- the 'interaction propagator'  $V(1, 2; 1', 2')$ , that will be generalized to the photon as an interaction particle in quantum electrodynamics, where it is a general 4-point and -frequency function. Note, that the numbers  $1, 2, 1', 2'$  include all single-particle properties (momentum, spin, species, energy/MATSUBARA frequency). However, as we already discussed in section 3.2, in our applications the dependence on frequency vanishes (non-dispersive interaction).

An instantaneous interaction does not depend on  $\omega_\lambda$  and thus is non-dispersive.



We consider a spin- and species-conserving interaction, that is local ( $r_1 = r_{1'}, r_2 = r_{2'}$ ) and thus solely depends on the relative distance  $|\vec{r}_2 - \vec{r}_1|$  so that momentum is conserved. After FOURIER transform, with  $q = p_1 - p_{1'}$ , we have

$$V(12, 1'2') = \sum_q \underbrace{e_1 \delta_{\sigma_1 \sigma_{1'}} \delta_{c_1 c_{1'}} \delta_{p_1 + q, p_{1'}}}_{\Gamma(11')} V(q) \underbrace{e_2 \delta_{\sigma_2 \sigma_{2'}} \delta_{c_2 c_{2'}} \delta_{p_2 - q, p_{2'}}}_{\Gamma(22')}, \quad (4.3.2)$$

see also the comments on the interaction in section 3.2. When omitting the spin-, species-, and momentum-conserving  $\delta$  functions, the COULOMB interaction in FOURIER space has a very simple structure:

$$V_{ab}(q) = \Gamma_a V(q) \Gamma_b = e_a \frac{1}{\Omega \varepsilon_0 q^2} e_b. \quad (4.3.3)$$

Equation (4.3.3) is the FOURIER transform of the COULOMB potential in coordinate space:

$$V_{ab}(r) = \frac{e_a e_b}{4\pi \varepsilon_0} \cdot \frac{1}{r}$$

$$V_{ab}(q) = \lim_{\eta \searrow 0} \frac{1}{\Omega} \int d^3 \vec{r} V_{ab}(r) e^{-\eta r} e^{-i\vec{q}\vec{r}} = \lim_{\eta \searrow 0} \frac{e_a e_b}{\Omega \varepsilon_0 (\eta^2 + q^2)} = \frac{e_a e_b}{\Omega \varepsilon_0 q^2}$$

The factor  $e^{-\eta r}$  had to be introduced to guarantee convergence of the integral.

Although for now, we treat the photon propagator and the vertices as a monolithic interaction  $V_{ab}(q)$ , it is important to keep in mind that in general, the photon propagator is charge-neutral and the vertices can be separated from the interaction.

Due to homogeneity of space, momentum is conserved along any propagator. This holds for the classical particle propagators with momentum  $p$  as well as for the photon propagators, that carry the transfer momentum  $q$ .

In full analogy with the DYSON equation, that relates the single-particle propagator to the self-energy, we can construct the so-called screening equation, that defines an interaction-self-energy (effective mass operator), which is called the polarization function  $\Pi(\vec{q}, iz_\mu)$ :

$$V_{ab}^s(q, iz_\mu) = V_{ab}(q) + \sum_{cd} V_{ac}(q) \Pi_{cd}(q, iz_\mu) V_{db}^s(q, iz_\mu) \quad (4.3.4)$$

$$\text{wavy} = \text{---} + \text{---} \circlearrowleft \text{---} + \text{---} \circlearrowright \text{---} + \text{---} \circlearrowleft \text{---} \circlearrowright \text{---} + \dots = \text{---} \circlearrowleft \text{---} \text{wavy} \quad (4.3.5)$$

The polarization function  $\Pi(\vec{q}, iz_\mu)$  is the sum of all irreducible diagrams:

$$\text{---} \circlearrowleft \text{---} = \text{---} \circlearrowright \text{---} + \text{---} \text{---} + \text{---} \text{---} + \text{---} \text{---} + \text{---} \text{---} + \text{---} \text{---} + \dots \quad (4.3.6)$$



N.B. the polarization function does not include diagrams, that would disintegrate if an interaction line, that connects incoming and outgoing particles channels, is cut through. These diagrams, for example


(4.3.7)

are already considered in (4.3.5) with (4.3.6) and would be double-counted otherwise.

Since the frequency of the polarization function is either the difference of two even or two odd MATSUBARA frequencies, it corresponds to even MATSUBARA frequencies. Thus, it has bosonic character.

While in coordinate space the screening equation would be a rather complicated matrix-integral equation, in momentum space it reduces to an algebraic matrix equation because the transferred momentum  $q$  is conserved along an interaction path from incoming to outgoing particle channels and the respective integrals collapse.

The matrix character of (4.3.4) results from the fact that interaction contributions with any particle species that fulfill the appropriate conservation laws are allowed, i.e. the polarization function represents any of these species.

If the polarization function is diagonal in the particle species<sup>4</sup>,

$$\Pi_{cd}(q, iz_\mu) = \Pi_{cc}(q, iz_\mu) \delta_{cd}, \quad (4.3.8)$$

the screened interaction can be simplified to

$$V_{ab}^s(q, iz_\mu) = \frac{V_{ab}(q)}{1 - \sum_c V_{cc}(q) \Pi_{cc}(q, iz_\mu)} \equiv \frac{V_{ab}(q)}{\varepsilon(q, iz_\mu)} \quad (4.3.9)$$

with the newly defined (longitudinal) dielectric function

$$\varepsilon(q, iz_\mu) = 1 - \sum_c V_{cc}(q) \Pi_{cc}(q, iz_\mu). \quad (4.3.10)$$

<sup>4</sup>If this is not the case, i.e.  $\Pi_{cd}$  contains off-diagonal elements, (4.3.4) has to be solved as a matrix equation.

Showing equation (4.3.9) is straightforward:

$$\begin{aligned} V_{ab}^s(q, iz_\mu) &= V_{ab}(q) + \sum_{cd} V_{ac}(q) \Pi_{cd}(q, iz_\mu) \delta_{cd} V_{db}^s(q, iz_\mu) \\ &= V_{ab}(q) + \sum_c e_a V(q) e_c \Pi_{cc}(q, iz_\mu) e_c V^s(q, iz_\mu) e_b, \end{aligned}$$

where we separated the vertices from the interaction. We can now reorder the factors and rejoin them to

$$\begin{aligned} &= V_{ab}(q) + \sum_c V_{cc}(q) \Pi_{cc}(q, iz_\mu) V_{ab}^s(q, iz_\mu), \\ V_{ab}^s(q, iz_\mu) \left[ 1 - \sum_c V_{cc}(q) \Pi_{cc}(q, iz_\mu) \right] &= V_{ab}(q) \\ V_{ab}^s(q, iz_\mu) &= \frac{V_{ab}(q)}{1 - \sum_c V_{cc}(q) \Pi_{cc}(q, iz_\mu)}. \end{aligned}$$

We should keep in mind, that the interaction between two charges occurs via the scalar and vector potential as well. The division of the interaction into a scalar and a vectorial part is, however, arbitrary and depending on the chosen gauge condition. Considering the vectorial part of the interaction, we do not face scalar quantities any longer. Instead,  $V$  is a vector and the polarization function  $\Pi$  a  $3 \times 3$  matrix. However, if space is homogeneous, we can assume the interaction to have a transversal component and the polarization function can be split up into a transversal part  $\Pi_t$  and a longitudinal part  $\Pi_l$ . Then, for the transversal part, we find an analogous relation to (4.3.9):

$$V_t^s(q, iz_\mu) = \frac{V_t}{1 - V_t \Pi_t}. \quad (4.3.11)$$

This equation explicitly demonstrates, that only the transversal part of the polarization function contributes to the (transversal) photon propagator very similar to the self-energy.<sup>5</sup> However, when considering the propagation of light through a solid, the assumption of a homogeneous space does not hold. Instead, it is periodic and the matrix form of the polarization function  $\Pi$  may be more complicated. Then, such a closed algebraic solution will in general not be possible. Instead, (4.3.4) has to be interpreted as a matrix equation for the respective spatial components of the polarization function and the interaction.<sup>6</sup>

<sup>5</sup>An even more general discussion of the screening equation can for example be found in [Mah90], section 2.10.: *Photon Green's Functions*.

<sup>6</sup>For further details, see [Mah90], section 2.10.: *Photon Green's Functions*, especially the comments on equations (2.10.10) and following.

For showing (4.3.11), we separate the dependence on the direction of  $\vec{q}$  in the polarization function and in the interaction to decompose them into transversal and longitudinal part:

$$\Pi_{cd} = \left( \delta_{cd} - \frac{q_c q_d}{q^2} \right) \Pi_t + \frac{q_c q_d}{q^2} \Pi_l \quad V_{ac}^s = \left( \delta_{ac} - \frac{q_a q_c}{q^2} \right) V_t^s$$

Note, that the indices do not represent particle species here, but are space indices, e.g.  $q_c$  is a component of the vector  $\vec{q}$ , etc.

The explicit dependence on  $|\vec{q}|$  has been omitted for convenience and as already stated,  $V_l$  vanishes because the photons are transversal.

These expressions are inserted into (4.3.4), so that the sum is

$$\sum_{cd} \left[ \left( \delta_{ac} \delta_{cd} - \delta_{ac} \frac{q_c q_d}{q^2} - \delta_{cd} \frac{q_a q_c}{q^2} + \frac{q_a q_c q_c q_d}{q^4} \right) V_t \Pi_t \right. \\ \left. + \left( \delta_{ac} \frac{q_c q_d}{q^2} - \frac{q_a q_c q_c q_d}{q^4} \right) V_l \Pi_l \right] \left( \delta_{db} - \frac{q_d q_b}{q^2} \right) V_t^s$$

and after performing the sum over  $c$  and  $d$ , we find

$$= \sum_d \left( \delta_{ad} - \frac{q_a q_d}{q^2} \right) V_t \Pi_t \left( \delta_{db} - \frac{q_d q_b}{q^2} \right) V_t^s = \left( \delta_{ab} - \frac{q_a q_b}{q^2} \right) V_t \Pi_t V_t^s,$$

so that for the full expression (4.3.4), we have

$$\left( \delta_{ab} - \frac{q_a q_b}{q^2} \right) V_t^s = \left( \delta_{ab} - \frac{q_a q_b}{q^2} \right) V_t + \left( \delta_{ab} - \frac{q_a q_b}{q^2} \right) V_t \Pi_t V_t^s.$$

This equation is only generally true if it holds for the scalar coefficients:

$$V_t^s = V_t + V_t \Pi_t V_t^s.$$

This is (4.3.11).

The spectral representation of the screened interaction is

$$V_{ab}^s(q, z) = V_{ab}(q) \left[ 1 + \int \frac{d\omega}{\pi} \text{Im} \{ \varepsilon^{-1}(q, \omega - i\eta) \} \cdot \frac{1}{z - \omega} \right]. \quad (4.3.12)$$

The proof for (4.3.12) can be performed using DIRAC's identity (2.2.8) for the imaginary and real part separately. For doing so, we analytically continue  $V_{ab}^s(q, z)$  with  $z \rightarrow \Omega - i\varepsilon$  in (4.3.12):

$$V_{ab}^s(q, \Omega - i\varepsilon) = V_{ab}(q) \left[ 1 + \int \frac{d\omega}{\pi} \text{Im} \{ \varepsilon^{-1}(q, \omega - i\eta) \} \cdot \frac{1}{\Omega - i\varepsilon - \omega} \right]$$

and apply (2.2.8), keeping in mind, that  $V_{ab}(q)$  is real-valued:

$$\begin{aligned} \text{Im} \{ V_{ab}^s(q, \Omega - i\varepsilon) \} &= V_{ab}(q) \int \frac{d\omega}{\pi} \text{Im} \{ \varepsilon^{-1}(q, \omega - i\eta) \} \cdot (+\pi \delta(\Omega - \omega)) \\ &= V_{ab}(q) \text{Im} \{ \varepsilon^{-1}(q, \Omega - i\eta) \} \\ \text{Re} \{ V_{ab}^s(q, \Omega - i\varepsilon) \} &= V_{ab}(q) \underbrace{\left[ 1 + \mathcal{P} \int \frac{d\omega}{\pi} \text{Im} \{ \varepsilon^{-1}(q, \omega - i\eta) \} \cdot \frac{1}{\Omega - \omega} \right]}_{\text{Re} \{ \varepsilon^{-1}(q, \Omega) \}}, \end{aligned} \quad (\underline{A})$$

where in  $(\underline{A})$  the well-known KRAMERS-KRONIG relation<sup>7</sup>, for the dielectric function has been used.

Bringing real and imaginary part together, we have

$$V_{ab}^s(q, \Omega - i\varepsilon) = V_{ab}(q) \cdot \varepsilon^{-1}(q, \Omega - i\varepsilon),$$

which is (4.3.9).

The screened interaction is especially important for systems with charged particles. Since the COULOMB interaction  $V(q) \sim 1/q^2$  is long-ranged, the perturbation series can diverge. This is avoided by the screening effect, performing partial summations of the respective contributions.

---

<sup>7</sup>See for example [LPL84], § 82 *The analytic properties of the function  $\varepsilon(\omega)$* .

## 4.4 Lowest order approximation for the polarization function: RPA

We will now examine the lowest order summand of the polarization function  $\Pi(\vec{q}, iz_\mu)$  in  $V$  for a single-species system, e.g. electrons in a positive background. It leads to the free-particle approximation that is called 'random phase approximation' (RPA):

$$\Pi^{\text{RPA}}(\vec{q}, iz_\mu) = \vec{q}, iz_\mu \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \vec{q}, iz_\mu = (2s+1)\Omega \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{p-q}) - f(\epsilon_p)}{iz_\mu + \epsilon_{p-q} - \epsilon_p} \quad (4.4.1)$$

For proving (4.4.1), we will examine the following constellation:

$$\Pi^{\text{RPA}}(\vec{q}, iz_\mu) = \begin{array}{c} \vec{p}-\vec{q}, iz_\lambda - iz_\mu = iz_{\lambda'} \\ \vec{q}, iz_\mu \\ \vec{p}, iz_\lambda \end{array}$$

It is interesting to mention that, since  $iz_\lambda$  and  $iz_{\lambda'}$  carry fermionic character (odd MATSUBARA frequencies),  $iz_\mu = iz_\lambda - iz_{\lambda'}$  must be an even frequency and thus must have bosonic character. Consequently, the possible quasi-particle that will be related to this 'bubble' must be a boson. According to the diagram rules from section 3.2 we get

$$\Pi^{\text{RPA}}(\vec{q}, iz_\mu) = -\frac{\Omega}{\beta}(2s+1)(-1) \int \frac{d^3p}{(2\pi)^3} \sum_{z_\lambda} \frac{1}{iz_\lambda - \epsilon_p} \cdot \frac{1}{iz_\lambda - iz_\mu - \epsilon_{p-q}}.$$

After performing the partial fraction decomposition

$$\begin{aligned} \frac{1}{iz_\lambda - \epsilon_p} \cdot \frac{1}{iz_\lambda - iz_\mu - \epsilon_{p-q}} &= \frac{1}{-iz_\mu - \epsilon_{p-q} + \epsilon_p} \left( \frac{1}{iz_\lambda - \epsilon_p} - \frac{1}{iz_\lambda - iz_\mu - \epsilon_{p-q}} \right) \\ \rightarrow \sum_{z_\lambda} \frac{1}{iz_\lambda - \epsilon_p} \cdot \frac{1}{iz_\lambda - iz_\mu - \epsilon_{p-q}} &= \frac{1}{\dots} \left( \underbrace{\sum_{z_\lambda} \frac{1}{iz_\lambda - \epsilon_p}}_{\beta f(\epsilon_p)} - \underbrace{\sum_{z_\lambda} \frac{1}{iz_\lambda - iz_\mu - \epsilon_{p-q}}}_{\beta f(iz_\mu + \epsilon_{p-q})} \right), \end{aligned}$$

the second summand can be simplified using  $z_\mu = \pm \frac{\pi\mu}{\beta}$  with even  $\mu$

$$f(iz_\mu + \epsilon_{p-q}) = \frac{1}{e^{\beta(iz_\mu + \epsilon_{p-q})} + 1} = \frac{1}{\underbrace{e^{\pm i\pi\mu}}_{=1} e^{\beta(\epsilon_{p-q})} + 1} = f(\epsilon_{p-q})$$

and thus, equation (4.4.1) can be shown by just inserting into  $\Pi^{\text{RPA}}(\vec{q}, iz_\mu)$ :

$$\Pi^{\text{RPA}}(\vec{q}, iz_\mu) = (2s+1)\Omega \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{p-q}) - f(\epsilon_p)}{iz_\mu + \epsilon_{p-q} - \epsilon_p}$$

Now, with the analytic continuation  $iz_\mu \rightarrow z = \hbar(\omega + i\eta)$ ,  $\eta \rightarrow 0$ , the dielectric function (compare equation (4.3.9)) with the particle species index  $c$  in random phase approximation evaluates to

$$\varepsilon^{\text{RPA}}(q, \hbar\omega) = 1 - \sum_c V_{cc}(q) \Pi_{cc}^{\text{RPA}}(q, \hbar(\omega + i0)) \quad (4.4.2)$$

$$= 1 - \sum_c V_{cc}(q) (2s_c + 1) \Omega \int \frac{d^3p}{(2\pi)^3} \frac{f(\epsilon_{c,p-q}) - f(\epsilon_{c,p})}{\hbar(\omega + i0) + \epsilon_{c,p-q} - \epsilon_{c,p}}. \quad (4.4.3)$$

The small perturbation  $+i0$  has to be introduced to avoid the pole at  $\hbar\omega = \epsilon_{c,p} - \epsilon_{c,p-q}$ . We will later see that it leads to the LANDAU damping which results from the particles interacting with the plasma waves. Of course, the selection of the 'retarded' solution needs some further discussion, that is not given here.

Since (4.4.3) is an important approximate result for the dielectric function  $\varepsilon(q, \hbar\omega)$ , its limits have been intensively investigated and will be examined in the following three sections<sup>8</sup>.

The dielectric function in RPA-approximation includes the interaction in lowest order and is valid for arbitrary degeneracy. For classical plasmas and low frequencies, it leads to DEBYE-screening, while for strongly degenerate plasmas ( $T \rightarrow 0$ ), the static limit is called THOMAS-FERMI-approximation.

In the long-wavelength limit ( $q \rightarrow 0$ ), the so-called plasmon-resonance appears, that results from the collective excitation of the electrons in matter.

From the imaginary part of the dielectric function, we can derive the LANDAU damping.

---

<sup>8</sup>A more detailed discussion of the dielectric function in RPA approximation can be found in [AB84]. Additionally, we recommend consulting the books [KKER86] and [Mah90] for further studies.

#### 4.4.1 Static limit $\omega \rightarrow 0$ for a classical plasma: Debye screening

In the static case  $\omega \rightarrow 0$ , the DEBYE screening can be derived in the classical limit:

$$\lim_{\omega \rightarrow 0} \varepsilon^{\text{RPA}}(q, \hbar\omega) = 1 + \frac{\kappa^2}{q^2} \quad \text{with} \quad \kappa^2 = \sum_c \frac{e_c^2 n_c}{\varepsilon_0 k_B T} \quad (4.4.4)$$

Note, that  $\kappa = 1/r_D$  is the inverse DEBYE screening length. The corresponding screened potential is

$$\lim_{\omega \rightarrow 0} V^s(q, \omega) = \frac{V(q)}{1 + \frac{\kappa^2}{q^2}}. \quad (4.4.5)$$

The correspondence of (4.4.5) with the DEBYE potential  $V^D(r)$  in coordinate space can be shown via FOURIER transformation:

$$\begin{aligned} V^D(r) &= \frac{e_1 e_2}{4\pi\varepsilon_0} \cdot \frac{e^{-\kappa r}}{r} \\ V^D(q) &= \frac{1}{\Omega} \int d^3\vec{r} V^D(r) e^{-i\vec{q}\vec{r}} = \frac{e_1 e_2}{\Omega\varepsilon_0 (\kappa^2 + q^2)} = \frac{e_1 e_2}{\Omega\varepsilon_0 q^2} \cdot \frac{1}{1 + \frac{\kappa^2}{q^2}} \end{aligned}$$

The screening parameter  $\kappa$  (inverse screening length) leads to a faster vanishing potential for  $r \rightarrow \infty$  than the bare COULOMB potential. The screening effect in a plasma results from the electron cloud, surrounding the ions and partially compensating for the effect of their charge on remote charged particles.

We will show (4.4.4) in the classical approximation  $f(\epsilon_{c,p}) = e^{-\beta(E_{c,p} - \mu_c)}$  that is only valid for non-degeneracy and according low density, i.e.  $\frac{n_c \Lambda_c^3}{2s_c + 1} = e^{\beta\mu_c} \ll 1$ . The thermal wavelength of the particle species  $c$  is  $\Lambda_c = \sqrt{\frac{2\pi\hbar^2}{m_c k_B T}}$ .

$$\begin{aligned} f(\epsilon_{c,p-q}) - f(\epsilon_{c,p}) &= e^{-\beta(E_{c,p-q} - \mu_c)} - e^{-\beta(E_{c,p} - \mu_c)} \\ &= e^{-\beta(E_{c,p} - \mu_c)} \left( \underbrace{e^{-\beta(E_{c,p-q} - E_{c,p})}}_{\approx 1 - \beta\Delta + \mathcal{O}(\Delta^2)} - 1 \right) \\ &\approx -f(\epsilon_{c,p}) \beta\Delta. \end{aligned}$$

Here we have implicitly presumed  $\hbar \rightarrow 0$  (classical limit), hence  $\hbar q \rightarrow 0$  and thus  $\Delta \rightarrow 0$ .

Using this result and the COULOMB potential  $V(q) = \frac{e_c^2}{\Omega \epsilon_0 q^2}$ , we can write

$$\begin{aligned}
 & \lim_{\omega \rightarrow 0} \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \\
 (4.4.3) \quad & \stackrel{=}{=} \lim_{\omega \rightarrow 0} \left[ 1 - \sum_c \frac{e_c^2}{\Omega \epsilon_0 q^2} (2s_c + 1) \int \frac{\Omega}{(2\pi)^3} d^3p f(\epsilon_{c,p}) \underbrace{\frac{-\beta \Delta}{\hbar(\omega + i0) + \Delta}}_{\rightarrow -\beta} \right] \\
 & = 1 + \frac{1}{q^2} \underbrace{\sum_c \frac{e_c^2 \beta}{\epsilon_0} (2s_c + 1) \int \frac{d^3p}{(2\pi)^3} f(\epsilon_{c,p})}_{n_c} .
 \end{aligned}$$

Equation (4.4.5) is just (4.3.9) with the dielectric function  $\varepsilon$  from (4.4.4).

#### 4.4.2 Long wavelength limit $q \rightarrow 0$

In the long wavelength limit  $q \rightarrow 0$ , a modification of the  $\omega$  dependence results. The effective photon mass parameter is the plasma frequency  $\omega_{\text{pl}}$ . This is the frequency of collective oscillations of the free electron density. The excitation quanta of these oscillations are called plasmons:

$$\lim_{q \rightarrow 0} \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) = 1 - \frac{\omega_{\text{pl}}^2}{\omega^2} \quad \text{with} \quad \omega_{\text{pl}}^2 = \sum_c \frac{e_c^2 n_c}{\epsilon_0 m_c} \quad (4.4.6)$$

so that the screened potential reads

$$\lim_{q \rightarrow 0} V^s(q, \omega) = \frac{V(q)}{1 - \frac{\omega_{\text{pl}}^2}{\omega^2}} . \quad (4.4.7)$$

For  $\omega \approx \omega_{\text{pl}}$ , the real part of the dielectric function vanishes and the screened potential grows without bounds. This is the plasmon resonance, where the free electrons of the matter are resonantly driven to collective oscillations.



Since here we are only interested in the real part of the dielectric function, we can use the DIRAC identity (2.2.8) for simplifying (4.4.3) and then neglect the imaginary term:

$$\begin{aligned}
 & \lim_{q \rightarrow 0} \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \\
 &= 1 - \lim_{q \rightarrow 0} \sum_c \frac{e_c^2}{\varepsilon_0 q^2} (2s_c + 1) \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} \frac{f(\epsilon_{c,p-q}) - f(\epsilon_{c,p})}{\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}} - \cancel{i\pi\delta(\dots)} \dots \\
 &= 1 + \lim_{q \rightarrow 0} \sum_c \frac{e_c^2 (2s_c + 1)}{\varepsilon_0 q^2} \left( \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} \frac{f(\epsilon_{c,p})}{\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}} \right. \\
 & \quad \left. - \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} \frac{f(\epsilon_{c,p-q})}{\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}} \right)
 \end{aligned}$$

In the second integral we can substitute  $p' := p - q$ , rename  $p := p'$  and rejoin the two integrals:

$$= 1 + \lim_{q \rightarrow 0} \sum_c \frac{e_c^2 (2s_c + 1)}{\varepsilon_0 q^2} \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} \left( \frac{f(\epsilon_{c,p})}{\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}} - \frac{f(\epsilon_{c,p})}{\hbar\omega + \epsilon_{c,p} - \epsilon_{c,p+q}} \right).$$

The term in brackets can be simplified as follows:

$$\begin{aligned}
 & \frac{1}{\hbar\omega} \left[ \frac{1}{1 + \frac{1}{\hbar\omega} (\epsilon_{c,p-q} - \epsilon_{c,p})} - \frac{1}{1 + \frac{1}{\hbar\omega} (\epsilon_{c,p} - \epsilon_{c,p+q})} \right] \\
 &= \frac{1}{\hbar\omega} \left[ \frac{1}{1 + \frac{\hbar}{\omega} \left( \frac{(\vec{p}-\vec{q})^2}{2m_c} - \frac{\vec{p}^2}{2m_c} \right)} - \frac{1}{1 + \frac{\hbar}{\omega} \left( \frac{\vec{p}^2}{2m_c} - \frac{(\vec{p}+\vec{q})^2}{2m_c} \right)} \right] \\
 &= \frac{1}{\hbar\omega} \left[ \frac{1}{1 + \frac{\hbar}{\omega m_c} \left( -\vec{p}\vec{q} + \frac{\vec{q}^2}{2} \right)} - \frac{1}{1 + \frac{\hbar}{\omega m_c} \left( -\frac{\vec{q}^2}{2} - \vec{p}\vec{q} \right)} \right].
 \end{aligned}$$

Since we are examining the limit  $q \rightarrow 0$ , we can use  $\frac{1}{1-x} = 1 + x + x^2 + \mathcal{O}(x^3)$

$$\begin{aligned}
 & \approx \frac{1}{\hbar\omega} \left[ 1 - \frac{\hbar}{\omega m_c} \left( -\vec{p}\vec{q} + \frac{\vec{q}^2}{2} \right) + \frac{\hbar^2}{(\omega m_c)^2} \left( -\vec{p}\vec{q} + \frac{\vec{q}^2}{2} \right)^2 \right. \\
 & \quad \left. - 1 + \frac{\hbar}{\omega m_c} \left( -\frac{\vec{q}^2}{2} - \vec{p}\vec{q} \right) - \frac{\hbar^2}{(\omega m_c)^2} \left( -\frac{\vec{q}^2}{2} - \vec{p}\vec{q} \right)^2 + \dots \right] \\
 &= -\frac{1}{\hbar\omega} \left[ \frac{\hbar q^2}{\omega m_c} + \mathcal{O}(q^3) \right].
 \end{aligned}$$

Now we can resume our computation with

$$\begin{aligned}
 \lim_{q \rightarrow 0} \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) &= 1 - \lim_{q \rightarrow 0} \sum_c \frac{e_c^2}{\varepsilon_0 q^2} \frac{1}{\hbar\omega} \frac{\hbar q^2}{\omega m_c} \underbrace{(2s_c + 1) \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} f(\epsilon_{c,p})}_{n_c} \\
 &= 1 - \frac{1}{\omega^2} \underbrace{\sum_c \frac{e_c^2 n_c}{\varepsilon_0 m_c}}_{\omega_{\text{pl}}^2}
 \end{aligned}$$

### 4.4.3 Effect of the infinitesimal imaginary part: Landau damping

In (4.4.3) an infinitely small imaginary part had to be introduced for handling the discontinuity due to a pole at  $\hbar\omega = \epsilon_{c,p} - \epsilon_{c,p-q}$ . An analysis of its impact leads to a damping of the form

$$\text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} = \sum_c \frac{e_c^2 m_c^2 (2s_c + 1)}{4\pi \varepsilon_0 \beta \hbar^4 q^3} \ln \left| \frac{1 + e^{-\beta \left( \frac{\hbar^2}{2m_c} \left( \frac{m_c \omega}{\hbar q} - \frac{q}{2} \right)^2 - \mu_c \right)}}{1 + e^{-\beta \left( \frac{\hbar^2}{2m_c} \left( \frac{m_c \omega}{\hbar q} + \frac{q}{2} \right)^2 - \mu_c \right)}} \right|. \quad (4.4.8)$$

Again we start our examination with the dielectric function  $\varepsilon^{\text{RPA}}(q, \hbar(\omega + i0))$  from (4.4.3) and the COULOMB potential  $V(q) = \frac{e_c^2}{\varepsilon_0 q^2}$ , but now we are interested in the imaginary part and thus take the second summand from the DIRAC identity (2.2.8):

$$\begin{aligned} & \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} \\ &= - \sum_c (-\pi) \frac{e_c^2}{\varepsilon_0 q^2} (2s_c + 1) \int \frac{d^3 p}{(2\pi)^3} [f(\epsilon_{c,p-q}) - f(\epsilon_{c,p})] \delta(\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}) \\ &= - \sum_c (-\pi) \frac{e_c^2}{\varepsilon_0 q^2} (2s_c + 1) \left[ \int \frac{d^3 p}{(2\pi)^3} f(\epsilon_{c,p-q}) \delta(\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}) \right. \\ & \quad \left. - \int \frac{d^3 p}{(2\pi)^3} f(\epsilon_{c,p}) \delta(\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}) \right]. \end{aligned}$$

In the first integral we can substitute  $p' := p - q$  and rename  $p := p'$ :

$$\begin{aligned} &= - \sum_c (-\pi) \frac{e_c^2}{\varepsilon_0 q^2} (2s_c + 1) \int \frac{d^3 p}{(2\pi)^3} f(\epsilon_{c,p}) [\delta(\hbar\omega + \epsilon_{c,p} - \epsilon_{c,p+q}) \\ & \quad - \delta(\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p})]. \end{aligned}$$

Using  $\delta(\alpha x) = \frac{1}{|\alpha|} \delta(x)$ ,  $\epsilon_{c,p} = \frac{\hbar^2 p^2}{2m_c}$  and  $\epsilon_{c,p \pm q} = \frac{\hbar^2 (\vec{p} \pm \vec{q})^2}{2m_c} = \frac{\hbar^2 (\vec{p}^2 \pm 2pq \cos \theta + \vec{q}^2)}{2m_c}$ , we can restructure the arguments of the  $\delta$  functions

$$\delta(\hbar\omega + \epsilon_{c,p-q} - \epsilon_{c,p}) = \frac{m_c}{\hbar^2 pq} \delta \left( \cos \theta - \frac{m_c \omega}{\hbar pq} - \frac{q}{2p} \right) \equiv \frac{m_c}{\hbar^2 pq} \delta_1,$$

as well as

$$\delta(\hbar\omega + \epsilon_{c,p} - \epsilon_{c,p+q}) = \frac{m_c}{\hbar^2 pq} \delta \left( \cos \theta - \frac{m_c \omega}{\hbar pq} + \frac{q}{2p} \right) \equiv \frac{m_c}{\hbar^2 pq} \delta_2.$$

After transforming to spherical coordinates, we get

$$\begin{aligned} & \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} \\ &= - \sum_c (-\pi) \frac{e_c^2}{\varepsilon_0 q^2} 2\pi \frac{(2s_c + 1)}{(2\pi)^3} \int_0^\infty dp \int_{-1}^1 d \cos \theta p^2 f(\epsilon_{c,p}) \frac{m_c}{\hbar^2 p q} [\delta_2 - \delta_1]. \end{aligned}$$

Since  $\cos \theta \in [-1; 1]$ , the two  $\delta$  functions only contribute if

$$\left| \frac{m_c \omega}{\hbar p q} \pm \frac{q}{2p} \right| \leq 1 \quad \Leftrightarrow \quad \left| \frac{m_c \omega}{\hbar q} \pm \frac{q}{2} \right| \leq p$$

holds, respectively. This just changes the limits in the two  $p$ -integrations:

$$\begin{aligned} & \text{Im} \{ \varepsilon(q, \hbar(\omega + i0)) \} \\ &= - \sum_c (-2\pi^2) \frac{e_c^2 m_c}{\varepsilon_0 \hbar^2 q^3} \frac{(2s_c + 1)}{(2\pi)^3} \left[ \int_{\left| \frac{m_c \omega}{\hbar q} - \frac{q}{2} \right|}^\infty dp p f(\epsilon_{c,p}) - \int_{\left| \frac{m_c \omega}{\hbar q} + \frac{q}{2} \right|}^\infty dp p f(\epsilon_{c,p}) \right]. \end{aligned}$$

We can now collect the integrals, insert the FERMI distribution and perform the integration:

$$\begin{aligned} &= - \sum_c (-2\pi^2) \frac{e_c^2 m_c}{\varepsilon_0 \hbar^2 q^3} \frac{(2s_c + 1)}{(2\pi)^3} \int_{\left| \frac{m_c \omega}{\hbar q} - \frac{q}{2} \right|}^{\left| \frac{m_c \omega}{\hbar q} + \frac{q}{2} \right|} dp \frac{p}{1 + e^{\beta \left( \frac{\hbar^2 p^2}{2m_c} - \mu_c \right)}} \\ &= - \sum_c (-2\pi^2) \frac{e_c^2 m_c}{\varepsilon_0 \hbar^2 q^3} \frac{(2s_c + 1)}{(2\pi)^3} \left( -\frac{m_c}{\hbar^2 \beta} \right) \left[ \ln \left| 1 + e^{-\beta \left( \frac{\hbar^2 p^2}{2m_c} - \mu_c \right)} \right| \right]_{\left| \frac{m_c \omega}{\hbar q} - \frac{q}{2} \right|}^{\left| \frac{m_c \omega}{\hbar q} + \frac{q}{2} \right|} \\ &= - \sum_c \frac{e_c^2 m_c^2}{4\pi \varepsilon_0 \beta \hbar^4 q^3} (2s_c + 1) (-1) \ln \left| \frac{1 + e^{-\beta \left( \frac{\hbar^2}{2m_c} \left( \frac{m_c \omega}{\hbar q} - \frac{q}{2} \right)^2 - \mu_c \right)}}{1 + e^{-\beta \left( \frac{\hbar^2}{2m_c} \left( \frac{m_c \omega}{\hbar q} + \frac{q}{2} \right)^2 - \mu_c \right)}} \right|. \end{aligned}$$

This is (4.4.8).

In the limit of vanishing degeneracy and with only one particle species, eq. (4.4.8) leads to the classical LANDAU damping that results from the energy-transfer from the longitudinal plasma-mode to the electrons. In contrast to many other coupled-oscillator problems, this coupling is phase-matching, i.e. there is no phase-shift between the plasma mode and the electronic movement.

$$\text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} \Big|_{e^{\beta\mu} \ll 1} = \frac{m \omega_{\text{pl}}^2}{\hbar q^3} \sqrt{\frac{2\pi m}{k_B T}} \cdot e^{-\frac{\beta}{2} \left( \frac{m\omega^2}{q^2} - \frac{\hbar^2 q^2}{4m} \right)} \sinh \left( \frac{\beta \hbar \omega}{2} \right). \quad (4.4.9)$$

Vanishing degeneracy means low densities and thus  $1 \gg e^{\beta\mu_c} = \frac{n_c \Lambda_c^3}{2s_c + 1}$ . In this case, after converting the  $\ln(\dots)$  of a quotient into a difference of logarithms, we can expand the  $\ln(\dots)$  functions in (4.4.8) using  $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots = x + \mathcal{O}(x^2)$  for  $x \ll 1$

$$\begin{aligned} & \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} \Big|_{e^{\beta\mu_c} \ll 1} \\ &= \sum_c \frac{e_c^2 m_c^2 (2s_c + 1)}{4\pi \varepsilon_0 \beta \hbar^4 q^3} \underbrace{e^{\beta\mu_c}}_{\frac{n_c \Lambda_c^3}{2s_c + 1}} \cdot e^{-\frac{\beta}{2} \left( \frac{m_c \omega^2}{q^2} - \frac{\hbar^2 q^2}{4m_c} \right)} \underbrace{\left[ e^{\frac{\beta \hbar \omega}{2}} - e^{-\frac{\beta \hbar \omega}{2}} \right]}_{2 \cdot \sinh \left( \frac{\beta \hbar \omega}{2} \right)} \\ &= \sum_c \frac{e_c^2 m_c^2 n_c \Lambda_c^3}{2\pi \varepsilon_0 \beta \hbar^4 q^3} \cdot e^{-\frac{\beta}{2} \left( \frac{m_c \omega^2}{q^2} - \frac{\hbar^2 q^2}{4m_c} \right)} \sinh \left( \frac{\beta \hbar \omega}{2} \right) \end{aligned}$$

Now we can insert the thermal wavelength  $\Lambda_c = \sqrt{\frac{2\pi \hbar^2}{m_c k_B T}}$  and  $\beta = \frac{1}{k_B T}$

$$= \sum_c \frac{e_c^2 m_c n_c}{\varepsilon_0 \hbar q^3} \sqrt{\frac{2\pi}{m_c k_B T}} \cdot e^{-\frac{\beta}{2} \left( \frac{m_c \omega^2}{q^2} - \frac{\hbar^2 q^2}{4m_c} \right)} \sinh \left( \frac{\beta \hbar \omega}{2} \right).$$

We can insert  $\omega_{\text{pl}}$  from (4.4.6)

$$= \sum_c \frac{m_c}{\hbar q^3} \omega_{c,\text{pl}}^2 \sqrt{\frac{2\pi m_c}{k_B T}} \cdot e^{-\frac{\beta}{2} \left( \frac{m_c \omega^2}{q^2} - \frac{\hbar^2 q^2}{4m_c} \right)} \sinh \left( \frac{\beta \hbar \omega}{2} \right).$$

In the case of only one particle species, we can omit the species index  $c$ :

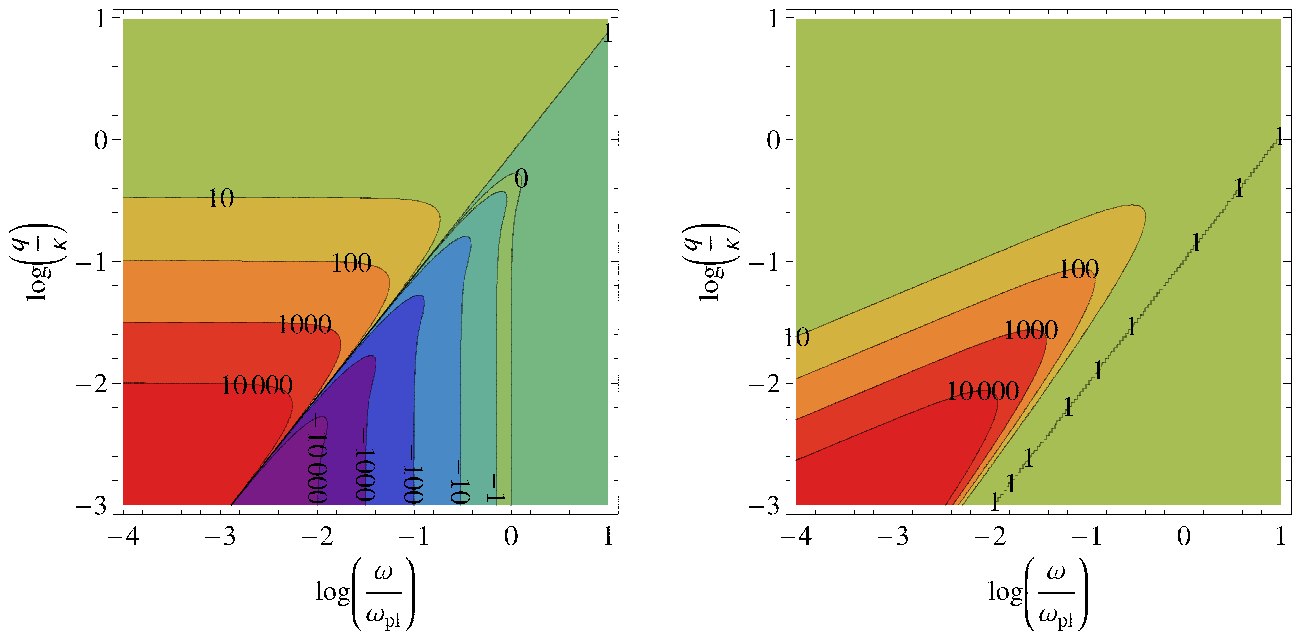
$$\begin{aligned} & \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar(\omega + i0)) \right\} \Big|_{e^{\beta\mu} \ll 1} \\ &= \frac{m}{\hbar q^3} \omega_{\text{pl}}^2 \sqrt{\frac{2\pi m}{k_B T}} \cdot e^{-\frac{\beta}{2} \left( \frac{m\omega^2}{q^2} - \frac{\hbar^2 q^2}{4m} \right)} \sinh \left( \frac{\beta \hbar \omega}{2} \right). \end{aligned}$$

It is important to mention, that the imaginary part of the dielectric function in RPA-approximation vanishes for low frequencies and long wavelengths:

$$\lim_{\omega \rightarrow 0} \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar\omega + i\eta) \right\} = 0 \quad (4.4.10)$$




$$\lim_{q \rightarrow 0} \text{Im} \left\{ \varepsilon^{\text{RPA}}(q, \hbar\omega + i\eta) \right\} \rightarrow 0. \quad (4.4.11)$$

Especially in the long-wavelength limit  $q \rightarrow 0$ , the plasmon resonance is not attenuated.



Real part (left) and imaginary part (right) of the dielectric function in RPA-approximation as a function of  $\frac{\omega}{\omega_{\text{pl}}}$  and  $\frac{q}{\kappa}$  for solar core conditions ( $T = 100$  Ryd,  $n = 8.9 \text{ a}_{\text{E}}^{-3}$ ). Obviously, there is a significant discontinuity at  $\varepsilon^{\text{RPA}}(q \rightarrow 0, \omega \rightarrow 0)$ . Additionally, we can see, that at  $\omega \approx \omega_{\text{pl}}$ , the real part of the dielectric function vanishes, while for certain parameter sets, the imaginary part becomes arbitrary small. Thus, undamped plasmon excitation is possible.

## 4.5 Vertex equation

In equation (4.3.6), we already saw a contribution of the type . Such graphs have not been under examination until now. Obviously, when taking into account higher orders of these graphs, diagram fragments of the form , , ... appear. These so-called vertex corrections can be collected in a new diagram element  $\Gamma = \text{img alt="A diagram showing a vertex with two outgoing lines and one incoming line." data-bbox="420 210 450 235"/>-, that can be defined through the self-consistent vertex equation$

$$\Gamma_1 \left( 1iz_{\nu_1}, 1'iz_{\nu_1'}; q, iz_{\mu} \right) = \Gamma_1^0 + KG_1G_1\Gamma_1 \quad (4.5.1)$$

$$\Leftrightarrow \text{img alt="A diagram showing a vertex with two outgoing lines and one incoming line." data-bbox="475 321 505 344"/>- = \text{img alt="A diagram showing a vertex with two outgoing lines and one incoming line." data-bbox="530 321 560 344"/>- + \text{img alt="A diagram showing a vertex with two outgoing lines and one incoming line, with a box labeled K on the incoming line." data-bbox="605 321 675 344"/>-, \quad (4.5.2)$$

where

$$\Gamma_1^0 \left( 1iz_{\nu_1}, 1'iz_{\nu_1'}; q, iz_{\mu} \right) = \text{img alt="A diagram showing a vertex with two outgoing lines and one incoming line, with a dot on the incoming line." data-bbox="215 424 245 453"/> = e_1 \delta_{p_1+q, p_1'} \delta_{z_{\nu_1}+z_{\mu}, z_{\nu_1'}} \delta_{c_1, c_1'} \delta_{\sigma_1 \sigma_1'} \quad (4.5.3)$$

is the single-particle vertex in lowest order. Note, that besides the quantum number conserving  $\delta$ -functions, it only contains a constant factor. Thus, when considering the  $\delta$ -functions separately, we can also write

$$\Gamma_1^0 \left( 1iz_{\nu_1}, 1'iz_{\nu_1'}; q, iz_{\mu} \right) = \Gamma_1^0 \delta_{p_1+q, p_1'} \delta_{z_{\nu_1}+z_{\mu}, z_{\nu_1'}} \delta_{c_1, c_1'} \delta_{\sigma_1 \sigma_1'} , \quad (4.5.4)$$

where the symbol  $\Gamma_1^0$  denotes the particle's charge.

Again the particle indices 1, 1' are used as a shorthand for respective single-particle properties, such as momentum  $p$ , species  $c$ , and spin  $\sigma$ . The effective interaction  $K(11', 22', iz_{\lambda})$  represents any irreducible particle-hole scattering contribution<sup>9</sup>.

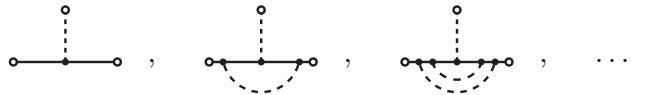
The integral form of the vertex equation is

$$\begin{aligned} \Gamma_1 \left( 1iz_{\nu_1}, 1'iz_{\nu_1'}; q, iz_{\mu} \right) &= \Gamma_1^0 \left( 1iz_{\nu_1}, 1'iz_{\nu_1'}; q, iz_{\mu} \right) + \sum_{\substack{22' \\ 33'}} K(11', 22', iz_{\lambda}) G_1(23, iz_{\nu} + iz_{\lambda}) \times \\ &\quad \times G_1(2'3', iz_{\nu'} - iz_{\lambda}) \Gamma_1(3iz_{\nu} + iz_{\lambda}, 3'iz_{\nu'} - iz_{\lambda}; q, iz_{\mu}) . \end{aligned} \quad (4.5.5)$$

<sup>9</sup>In very general, having four external momenta,  $K$  will carry up to three frequency arguments.

In a very simple approach, we could replace  $K \approx V$  and  $G \approx G^0$ . Then, the vertex equation has a similar structure as the screening equation (4.3.5). However, as long as the interaction is not separable, the vertex equation does not factorize. Thus, it cannot be solved directly as it was the case for the screening equation, where we could find an algebraic expression for the screened potential with the dielectric function  $\varepsilon$ .

The vertex-graphs, resulting from this approximation have a significant form:



They are called 'rainbow diagrams'. In quantum electrodynamics (QED), the contribution of those vertex corrections leads to a charge renormalization, i.e. the vertex charge is replaced  $e \rightarrow \tilde{e}$ .

## 4.6 Consistent approximation to the single-particle self-energy

Having defined the screened interaction in section 4.3, we can introduce the screened single-particle self-energy as a native generalization of the HARTREE-FOCK self-energy (see section 4.1):

$$\begin{aligned} \Sigma_1^{\text{MW}}(1, iz_\nu) &= \text{diagram} = \text{diagram} + \text{diagram} + \text{diagram} + \dots \\ &= \delta_{11'} \sum_{\substack{22' \\ q, iz_\lambda}} \Gamma_1^0(1iz_\nu, 2iz_\nu + iz_\lambda; q, iz_\lambda) G_1^0(22', iz_\nu + iz_\lambda) \times \\ &\quad \times \Gamma_1^0(2'iz_\nu + iz_\lambda, 1'iz_\nu; -q, -iz_\lambda) V^s(q, iz_\nu) . \end{aligned} \quad (4.6.1)$$

is the so-called MONTROLL-WARD approximation, that – due to homogeneity of space and time (energy and momentum conservation) – is diagonal in the single-particle quantum numbers  $1 = \{p c \sigma\}$ . Thus,  $1' = 1$  and we could omit one argument of the self-energy. This diagram describes the interaction of a particle with the DEBYE cloud. It has already been under intense examination for plasmas and semiconductors. It is possible to show, that in the nondegenerate limit  $\langle \Sigma_1^{\text{MW}} \rangle = -\frac{e^2 \kappa}{8\pi\epsilon}$ . This momentum-independent shift can be transformed into a shift of the the chemical potential  $\mu$ . This is the DEBYE approximation.<sup>10</sup>

However, it can be shown, that vertex corrections are of the same order of magnitude as self-energy contributions. The fundamental relation between the self-energy  $\Sigma_1$  and the vertex function  $\Gamma_1$  is the WARD-TAKAHASHI identity, that states, that the vertex function is given by<sup>11</sup>

$$\Gamma_1(1iz_{\nu_1}, 1'iz_{\nu_1'}; p, iz_\mu) = \left[ 1 - \frac{\partial \Sigma_1(p, z)}{\partial z} \right]_{z=iz_\mu} e_1 \delta_{p_1+q, p_1'} \delta_{z_{\nu_1}+z_\mu, z_{\nu_1'}} \delta_{c_1, c_1'} \delta_{\sigma_1, \sigma_1'} . \quad (4.6.2)$$

It is only valid in the limit of small transfer momentum  $q \rightarrow 0$ . N.B. (4.6.2) is the WARD-TAKAHASHI identity for scalar vertices  $\Gamma$ . For vectorial vertices, an analogous relation can be derived, but will not be discussed here, since during this lecture we will only need the scalar equation.

Since from (4.6.2), we see that vertex corrections and self-energy contributions are of the same importance, a consistent single-particle self-energy, that contains contributions beyond RPA is

$$\Sigma_1(1, iz_\nu) = \text{diagram} = \text{diagram} + \text{diagram} + \text{diagram} + \dots \quad (4.6.3)$$

with the screened interaction (wiggly line) given by the polarization function

$$\Pi(q, iz_\mu) = \text{diagram} = \text{diagram} + \text{diagram} + \text{diagram} + \dots \quad (4.6.4)$$

The evaluation of these diagrams leads to an infinite hierarchy of equations, that has to be truncated on a certain level for practical calculations. A very often used truncation rule is the so-called *GW*-approximation, where the vertex function is neglected and only the particle propagators and their

<sup>10</sup>Detailed calculations can be found in the monograph [KKER86], section 4.3 *Self-Energy in  $V^s$ -Approximation*.

<sup>11</sup>We will not make any further digression about this important relation, but due to its importance, we strongly recommend further literature, for example [Mah90], section 7.1.D: *Ward identities*, where a proof for (4.6.2) can be found.



respective self-energies are considered. The additional simplification that the polarization function is given in random phase approximation  $\Pi = \Pi^{\text{RPA}}$ , leads to the  $GW^{(0)}$  approximation.<sup>12</sup> These assumptions on the vertex function and the polarization function lead to analytically solvable equations, however, they violate the WARD-TAKAHASHI-identity. The inclusion of the vertex function in lowest order of the screened potential would be a further improvement to the  $GW$  approximation - the  $GWT$  approximation. The further consistent treatment leads to the so-called  $\Phi$ -derivable approximations.<sup>13</sup>

---

<sup>12</sup>For exemplary calculations and further references, see [FRW07].

<sup>13</sup>See for example [Bay62] for a very fundamental work on  $\Phi$ -derivable approximations.

## 4.7 Excursus: Dielectric function, index of refraction, absorption coefficient, and dynamic conductivity

The GREEN's functions technique can be used as a tool to investigate transport and optical properties of many-body-systems, in particular of plasmas. To relate optical observables such as the absorption coefficient  $\alpha(\omega)$  or the emission coefficient  $j(\omega)$  to the quantities already introduced in this lecture, we consider the propagation of a monochromatic plane wave in an absorbing medium. Note, that in thermal equilibrium,  $\alpha(\omega)$  and  $j(\omega)$  are linked by KIRCHHOFF's law. Thus, it is sufficient to study one of these quantities. Considering the long-wavelength limit  $q \rightarrow 0$ , we already dropped the explicit dependence of the quantities on the wave-number  $q$ . We start from MAXWELL's equations for the magnetic field  $\vec{H}$  and the electric field  $\vec{E}$  in frequency space

$$i\omega \mu(\omega)\vec{H} = c \operatorname{rot} \vec{E}, \quad (4.7.1)$$

$$i\omega \varepsilon(\omega)\vec{E} = -c \operatorname{rot} \vec{H}, \quad (4.7.2)$$

allowing for a frequency-dependent dielectric function  $\varepsilon(\omega)$  and magnetic susceptibility  $\mu(\omega)$ .

Eliminating the magnetic field results in the wave equation for  $\vec{E}$ ,

$$\Delta \vec{E} + \varepsilon(\omega)\mu(\omega)\frac{\omega^2}{c^2}\vec{E} = 0. \quad (4.7.3)$$

After applying FOURIER-transformation for a homogeneous system, we have

$$\left(k^2 - \varepsilon(\omega)\mu(\omega)\frac{\omega^2}{c^2}\right)\vec{E} = 0, \quad (4.7.4)$$

or

$$k^2 = \varepsilon(\omega)\mu(\omega)\frac{\omega^2}{c^2}. \quad (4.7.5)$$

Assuming, that we have an unmagnetized plasma,  $\mu = 1$ , this equation leads to a complex wave vector if  $\varepsilon(\omega)$  itself is complex or  $\varepsilon(\omega) < 0$ . For such a situation, we consider a complex representation  $\vec{k} = \operatorname{Re} \vec{k} + i \operatorname{Im} \vec{k}$ , implying a split of the plane wave

$$e^{i\vec{k}\cdot\vec{r}} = e^{i\operatorname{Re} \vec{k}\cdot\vec{r}} \cdot e^{-\operatorname{Im} \vec{k}\cdot\vec{r}} \quad (4.7.6)$$

into a phase factor and a part describing the damping of the wave by the medium. Note, that this effect was already studied in elementary electrodynamics in the context of propagation of electromagnetic waves in conducting media (telegrapher's equations).

Generalizing the convention from electrodynamics, we define

$$k = \left(n(\omega) + i\frac{c}{2\omega}\alpha(\omega)\right)\frac{\omega}{c} = \sqrt{\varepsilon(\omega)}\frac{\omega}{c}, \quad (4.7.7)$$

where  $n(\omega)$  is the index of refraction and  $\alpha(\omega)$  the absorption coefficient. Both quantities can be expressed in terms of  $\operatorname{Re} \varepsilon(\omega)$  and  $\operatorname{Im} \varepsilon(\omega)$ :

$$\alpha(\omega) = \frac{\omega}{cn(\omega)} \operatorname{Im} \varepsilon(\omega) \quad (4.7.8)$$

$$n(\omega) = \frac{1}{\sqrt{2}} \sqrt{\operatorname{Re} \varepsilon(\omega) + |\varepsilon(\omega)|} . \quad (4.7.9)$$

Equations (4.7.8) and (4.7.9) can be shown by simple algebraic conversion. Dropping the frequency parameter  $\omega$  for convenience, from (4.7.7), we have

$$\begin{aligned} \left(n + i \frac{c}{2\omega} \alpha\right)^2 &= \varepsilon = \operatorname{Re} \varepsilon + i \operatorname{Im} \varepsilon \\ n^2 - \frac{\alpha^2 c^2}{4\omega^2} + i \frac{cn\alpha}{\omega} &= \operatorname{Re} \varepsilon + i \operatorname{Im} \varepsilon . \end{aligned}$$

Comparing the real and imaginary part of the left and right hand side, we find (4.7.8)

$$\alpha = \frac{\omega}{cn} \operatorname{Im} \varepsilon$$

and

$$\begin{aligned} n^2 - \frac{(\operatorname{Im} \varepsilon)^2}{4n^2} &= \operatorname{Re} \varepsilon \\ n^4 - n^2 \operatorname{Re} \varepsilon - \frac{(\operatorname{Im} \varepsilon)^2}{4} &= 0 \\ n^2 &= \frac{1}{2} \operatorname{Re} \varepsilon + \sqrt{\frac{(\operatorname{Re} \varepsilon)^2 + (\operatorname{Im} \varepsilon)^2}{4}} \\ \Rightarrow n &= \frac{1}{\sqrt{2}} \sqrt{\operatorname{Re} \varepsilon + |\varepsilon|} , \end{aligned}$$

which is (4.7.9).

Thus, the knowledge of the dielectric function  $\varepsilon(\omega) = \lim_{q \rightarrow 0} \varepsilon(q, \omega)$  is essential to describe optical observables like  $\alpha(\omega)$  or  $n(\omega)$ .

In addition, the dynamic (frequency-dependent) conductivity  $\sigma(\omega)$ , is related to the dielectric function via the DRUDE relation:

$$\sigma(\omega) = i\omega\varepsilon_0 (\varepsilon(\omega) - 1) . \quad (4.7.10)$$

Its low-frequency limit, i.e. the static conductivity  $\sigma_0 = \lim_{\omega \rightarrow 0} \sigma(\omega)$  is also an important observable, that is experimentally accessible.

Note, that a first-principle treatment of photons propagating in a medium by a GREEN's functions theory should be done by introducing a photon propagator into the theory in addition to the COULOMB interaction. This can be done starting from quantum electrodynamics (QED). For a classical plasma ( $k_B T \ll mc^2$ ), a treatment within traditional quantum mechanics is possible, starting from the

nonrelativistic HAMILTONIAN

$$\begin{aligned}
 H = & \sum_a \frac{1}{2m_a} \int d^3\vec{r} \psi_a^+(\vec{r}, t) \left[ \frac{\hbar}{i} \nabla - \frac{e_a}{c} \vec{A}(\vec{r}, t) \right]^2 \psi_a(\vec{r}, t) \\
 & + \frac{1}{8\pi} \int d^3\vec{r} \left[ \vec{E}^2(\vec{r}, t) + \vec{B}^2(\vec{r}, t) \right] \\
 & + \frac{1}{2} \sum_{a,b} e_a e_b \int d^3\vec{r} \int d^3\vec{r}' \psi_a^+(\vec{r}, t) \psi_b^+(\vec{r}', t) \frac{1}{|\vec{r} - \vec{r}'|} \psi_b(\vec{r}', t) \psi_a(\vec{r}, t) , \quad (4.7.11)
 \end{aligned}$$

where  $a$  and  $b$  label the species,  $\vec{A}$  is the vector potential and the expression is given in COULOMB gauge  $\nabla \cdot \vec{A} = 0$ . In this treatment, the photon is connected to the GREEN's function of the vector potential<sup>14</sup>:

$$\hat{D}_{\mu\nu}(\vec{k}, \tau) = \frac{1}{c} \langle \text{T} [A_\mu(\vec{k}, \tau) A_\nu(-\vec{k}, 0)] \rangle \quad (4.7.12)$$

and can be related to the transverse current-current correlation function due to the minimal coupling between the particle current and the vector potential  $\vec{A}$ . Thus, a perturbation expansion of the COULOMB (longitudinal) and radiation (transversal) part is possible. Finally, the same relations as (4.7.8), (4.7.9) are obtained in the long-wavelength limit  $q \rightarrow 0$ .

---

<sup>14</sup>See [Mah90], section 3.2.: *Matsubara Green's Functions* for details.

## 4.8 Bound states

Because for a bound state at least two particles are needed, a closer look on two- and more-particle GREEN's functions has to be taken. For simplicity, we will only refer to the propagation of two particles and thus a correlation function of the form  $a_1^+ a_2^+ a_{2'} a_{1'}$  has to be examined, compare equation (2.1.6).

For non-interacting distinguishable particles (zeroth order in  $V$  and different particle species or spin, etc.), the two-particle GREEN's function results to

$$G_2^0(12, 1'2', i\omega_\lambda) = \begin{array}{c} \xrightarrow{k_2, i\omega_\lambda - iz_\nu} \\ \xrightarrow{k_1, iz_\nu} \end{array} = \frac{1 - f(\epsilon_1) - f(\epsilon_2)}{i\omega_\lambda - \epsilon_1 - \epsilon_2} \delta_{11'} \delta_{22'} . \quad (4.8.1)$$

with the BOSE MATSUBARA frequency  $\omega_\lambda$ .

The initial expression for  $G_2^0(12, i\omega_\lambda)$  can be found by applying the rules from section 3.2. Afterwards a partial fraction decomposition has to be performed to derive (4.8.1):

$$\begin{aligned} G_2^0(12, 1'2', i\omega_\lambda) &= -\frac{1}{\beta} \sum_{z_\nu} \frac{1}{iz_\nu - \epsilon_1} \frac{1}{i\omega_\lambda - iz_\nu - \epsilon_2} \delta_{11'} \delta_{22'} \\ &= -\frac{1}{i\omega_\lambda - \epsilon_1 - \epsilon_2} \cdot \left( \underbrace{\frac{1}{\beta} \sum_{z_\nu} \frac{1}{iz_\nu - \epsilon_1}}_{f(\epsilon_1)} + \underbrace{\frac{1}{\beta} \sum_{z_\nu} \frac{1}{i\omega_\lambda - iz_\nu - \epsilon_2}}_{-f(i\omega_\lambda - \epsilon_2)} \right) \delta_{11'} \delta_{22'} \\ &= \frac{f(i\omega_\lambda - \epsilon_2) - f(\epsilon_1)}{i\omega_\lambda - \epsilon_1 - \epsilon_2} \end{aligned}$$

Because of  $\omega_\lambda = \frac{\pi\lambda}{\beta}$  with  $\lambda = 0, \pm 2, \dots$  and thus  $e^{i\beta\omega_\lambda} = 1$ , we are able to write  $f(i\omega_\lambda - \epsilon_2) = \frac{1}{1 + e^{-\beta\epsilon_2}} = \frac{e^{\beta\epsilon_2 + 1} - 1}{e^{\beta\epsilon_2 + 1} + 1} = 1 - f(\epsilon_2)$

$$G_2^0(12, 1'2', i\omega_\lambda) = \frac{1 - f(\epsilon_1) - f(\epsilon_2)}{i\omega_\lambda - \epsilon_1 - \epsilon_2} \delta_{11'} \delta_{22'} .$$

If the two particles are indistinguishable, i.e. are of the same species, spin, etc., the respective exchange contribution has to be included in (4.8.1). For fermionic particles (antisymmetric wave function), the two-particle propagator takes the form

$$G_2^0(12, 1'2', i\omega_\lambda) = \begin{array}{c} \xrightarrow{\quad} \quad \xrightarrow{\quad} \\ \xrightarrow{\quad} \quad \xrightarrow{\quad} \end{array} - \begin{array}{c} \xrightarrow{\quad} \quad \xrightarrow{\quad} \\ \xrightarrow{\quad} \quad \xrightarrow{\quad} \end{array} = \frac{1 - f(\epsilon_1) - f(\epsilon_2)}{i\omega_\lambda - \epsilon_1 - \epsilon_2} (\delta_{11'} \delta_{22'} - \delta_{12'} \delta_{21'}) , \quad (4.8.2)$$

while for bosonic particles (symmetric wavefunction), the negative sign is replaced by a positive one and the FERMI functions by BOSE distributions. In the following, we will only concentrate on FERMI particles and thus use the two-particle propagator from (4.8.2).

Neglecting the FERMI functions, (4.8.2) describes the propagation of two non-interacting particles in the low-density limit: For  $n \rightarrow 0$ ,  $f(\epsilon) \ll 1$  holds and  $G_2^0$  formally has the same structure as  $G_1^0$ . Thus, the bound state can be treated as a new particle species in a chemical picture.

To include interaction, we apply the diagram representation of perturbation theory. Since we want to solve the two-particle problem, it is sufficient to examine such diagrams that only contain two fermionic propagators.

$$G_2(12, 1'2', i\omega_\lambda) =$$

$$+ \mathcal{O}(V^3), \quad (4.8.3)$$

where any diagram has to be taken in the correct multiplicity and the respective exchange terms have to be included. Due to the same reasons as for  $G_1(11', \tau)$  (see chapter 2.1), the two-particle GREEN'S function only depends on the three time differences instead of four times. In (4.8.1), we additionally assumed that both particles are entering and leaving the system at the same time:  $\tau_1 = \tau_2$  and  $\tau_{1'} = \tau_{2'}$ , respectively, and thus only the time difference  $\tau = \tau_1 - \tau_{1'}$  between these moments is an open parameter. Its conjugate variable  $i\omega_\lambda$  has been introduced via FOURIER transform.

Computing the infinite sum in (4.8.3) is rather exhaustive (or correctly said impossible). Fortunately, some approximations are possible. In the ladder approximation, only diagrams with direct interaction between the two particles are considered. Since all other graphs produce terms of higher order in the density  $n$ , the ladder approximation is applicable in the low-density limit. It produces all binary interacting systems and is a solution to the two body problem (two body SCHRÖDINGER equation). The structure of the ladder approximation is similar to the DYSON- and screening equations (4.2.5) and (4.3.5), respectively. It is called BETHE-SALPETER equation in ladder approximation:

$$G_2^{\text{ladd.}}(12, 1'2', i\omega_\lambda) = G_2^0(12, 1'2', i\omega_\lambda) + \sum_{\substack{34 \\ 3'4'}} G_2^0(12, 34, i\omega_\lambda) V(34, 3'4') G_2^{\text{ladd.}}(3'4', 1'2', i\omega_\lambda) \quad (4.8.4)$$

$$\Leftrightarrow \begin{array}{c} \text{1} \quad \text{1}' \\ \text{---} \text{---} \\ \text{2} \quad \text{2}' \end{array} G_2^{\text{ladd.}} = \begin{array}{c} \text{1} \quad \delta_{1'1'} \\ \text{---} \text{---} \\ \text{2} \quad \delta_{2'2'} \end{array} - \begin{array}{c} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array} + \begin{array}{c} \text{1} \quad \text{3} \quad \text{3}' \quad \text{1}' \\ \text{---} \text{---} \text{---} \text{---} \\ \text{2} \quad \text{4} \quad \text{4}' \quad \text{2}' \end{array} G_2^{\text{ladd.}} \quad (4.8.5)$$

$$= \begin{array}{c} \text{---} \\ \text{---} \end{array} - \begin{array}{c} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \\ \text{---} \text{---} \end{array} - \begin{array}{c} \text{---} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \\ \text{---} \text{---} \end{array} - \begin{array}{c} \text{---} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \text{---} \end{array} + \dots \quad (4.8.6)$$

The  $\delta$ -functions at the propagators in the first summand express that here incoming and outgoing particles are left unchanged, see (4.8.1) and (4.8.2).

Bound states cannot be derived in a finite order of perturbation theory. That is why we have to sum over an infinite number of diagrams.

For low densities and thus  $f(\epsilon) \ll 1$ , we can show that the BETHE-SALPETER equation is satisfied by

$$G_2^{\text{ladd.}}(12, 1'2', i\omega_\lambda) = \sum_{nP} \psi_{nP}(12) \frac{1}{i\omega_\lambda - E_{nP} + \mu_{12}} \psi_{nP}^*(1'2') \quad (4.8.7)$$

with the collective chemical potential  $\mu_{12} = \mu_1 + \mu_2$ , the antisymmetrized two-particle wave function

$$\psi_{nP}(12) = \frac{1}{\sqrt{2}} \left[ \Psi_{nP}(12) - \Psi_{nP}(21) \right] \quad (4.8.8)$$

and the energy of the two-particle state  $E_{nP}$  as a solution of the SCHRÖDINGER equation

$$(E_1 + E_2 - E_{nP}) \psi_{nP}(12) + \sum_{1'2'} V(12, 1'2') \psi_{nP}(1'2') = 0. \quad (4.8.9)$$

In (4.8.9)  $P = p_1 + p_1 = p_{1'} + p_{2'}$  is the total momentum. The internal quantum number  $n$  represents bound but also scattering states, where it has to be reinterpreted as an asymptotic value of the relative momentum  $p$ . The summation is running through all 2-particle states.

In the low density case  $f(\epsilon) \ll 1$ , the two-particle GREEN's function (4.8.2) yields

$$G_2^0(12, 1'2', i\omega_\lambda) = \frac{1}{i\omega_\lambda - \epsilon_1 - \epsilon_2} (\delta_{11'} \delta_{22'} - \delta_{12'} \delta_{21'})$$

We will now show that (4.8.5) is satisfied by (4.8.7) using the two-particle SCHRÖDINGER equation (4.8.9):

$$\begin{aligned} & \begin{array}{c} \xrightarrow{1} \delta_{11'} 1' \\ \xrightarrow{2} \delta_{22'} 2' \end{array} - \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} + \begin{array}{c} \xrightarrow{1} 3 \quad 3' \\ \xrightarrow{2} 4 \quad 4' \end{array} \left[ G_2^{\text{ladd.}} \right] \begin{array}{c} 1' \\ 2' \end{array} \\ &= G_2^0(12, 1'2', i\omega_\lambda) + \sum_{\substack{34 \\ 3'4'}} G_2^0(12, 34, i\omega_\lambda) V(34, 3'4') G_2^{\text{ladd.}}(3'4', 1'2', i\omega_\lambda) \\ &\stackrel{(4.8.7)}{=} G_2^0(12, 1'2', i\omega_\lambda) + \sum_{\substack{34 \\ nP}} G_2^0(12, 34, i\omega_\lambda) \underbrace{\sum_{3'4'} V(34, 3'4') \psi_{nP}(3'4')}_{\stackrel{(4.8.9)}{=} (E_3 + E_4 - E_{nP}) \psi_{nP}(34)} \\ &\quad \cdot \frac{1}{i\omega_\lambda - E_{nP} + \mu_{1'2'}} \psi_{nP}^*(1'2'). \end{aligned}$$

We can now make use of  $(E_3 + E_4 - E_{nP}) = (i\omega_\lambda - E_{nP} + \mu_{1'2'}) - (i\omega_\lambda - E_1 - E_2 + \mu_{1'2'})$  and  $\epsilon_{1/2} = E_{1/2} - \mu_{1/2}$  to write

$$\begin{aligned}
 &= G_2^0(12, 1'2', i\omega_\lambda) - \underbrace{\sum_{34} G_2^0(12, 34, i\omega_\lambda) \underbrace{\sum_{nP} \psi_{nP}(34) \psi_{nP}^*(1'2')}_{=\delta_{31'}\delta_{42'} - \delta_{41'}\delta_{32'} \text{ (completeness)}}}_{G_2^0(12, 1'2', i\omega_\lambda)} \\
 &\quad \underbrace{\sum_{nP} \sum_{34} \delta_{13}\delta_{24} \frac{i\omega_\lambda - E_3 - E_4 + \mu_{1'2'}}{i\omega_\lambda - \epsilon_1 - \epsilon_2} \psi_{nP}(34)}_{=1 \cdot \psi_{nP}(12)} \cdot \frac{1}{i\omega_\lambda - E_{nP} + \mu_{1'2'}} \psi_{nP}^*(1'2') \\
 (4.8.7) \quad \underline{\underline{G_2^{\text{ladd.}}}}(12, 1'2', i\omega_\lambda) &= \underline{\underline{\frac{1}{2} \left[ \underline{\underline{G_2^{\text{ladd.}}}} \right]_{2'}^{1'}}}
 \end{aligned}$$

As we will see in the following section, we can interpret parts of (4.8.7) as an operator in a basis-free representation. This will lead to an equal treatment of single-particle and bound states. In fact, the bound state can be identified and treated as a new particle species.

Equation (4.8.7) has been shown to fulfill the BETHE-SALPETER and SCHRÖDINGER's equation in the low-density case and thus represents a correct limit here. At higher densities, effects of the surrounding medium on the single-particle properties and the characteristics of the bound states (clusters) become evident, but were not treated here. Compared to a more phenomenological approach, here the GREEN's functions technique offers a systematic way to treat bound states in dense matter. Some elements of this way will be shown in section 5.1.



## 4.9 Abstract algebraic representation

When interpreting the single particle GREEN's function as a matrix element:

$$G_1^0(11', iz_\nu) = \text{---} = \delta_{11'} \frac{1}{iz_\nu - E_1 + \mu_1} = \langle 1 | \hat{G}_1 | 1' \rangle, \quad (4.9.1)$$

we can identify

$$\hat{G}_1^0(iz_\nu) = \sum_k |k\rangle \frac{1}{iz_\nu - E_k + \mu_k} \langle k| \quad (4.9.2)$$

as the single particle's propagation operator.

For the two-particle GREEN's function in the low density ladder approximation, a similar treatment is possible

$$\hat{G}_2^{\text{ladd.}}(i\omega_\lambda) = \sum_{nP} |nP\rangle \frac{1}{i\omega_\lambda - E_{nP} + \mu_{12}} \langle nP|. \quad (4.9.3)$$

In this case we can obtain our earlier results as matrix elements in the two-particle space, compare (4.8.7):

$$\langle 12 | \hat{G}_2^{\text{ladd.}} | 1'2' \rangle = \sum_{nP} \overbrace{\psi_{nP}(12)}^{\langle 12 | nP \rangle} \frac{1}{i\omega_\lambda - E_{nP} + \mu_{12}} \overbrace{\psi_{nP}^*(1'2')}^{\langle nP | 1'2' \rangle} = G_2^{\text{ladd.}}(12, 1'2', i\omega_\lambda) \quad (4.9.4)$$

as well as in the space of a cluster state:

$$\langle nP | \hat{G}_2^{\text{ladd.}} | n'P' \rangle = \delta_{nn'} \delta_{PP'} \frac{1}{i\omega_\lambda - E_{nP} + \mu_{12}} = G_2^{\text{ladd.}}(nP, n'P', i\omega_\lambda) = \text{---} \quad (4.9.5)$$

Now it is obvious that in the low-density limit, single-particle and bound states can be treated in an absolutely equivalent way as a mixture of free particles and bound states, since their propagation operators are subject to the same algebra. As an example, we refer to the mass action law (see section 5.2, which treats bound states as new particles, allowing for reactions to reach equilibrium).

## 4.10 Excursus: Solution to the two-particle Schrödinger equation with a separable potential

In general, for local interactions  $V(12, 1'2') = V(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_1 - \vec{r}'_1) \delta(\vec{r}_2 - \vec{r}'_2) \delta_{\sigma_1, \sigma'_1} \delta_{\sigma_2, \sigma'_2}$  there is no algebraic solution to the ladder sum. In momentum space, it leads to an integral equation, in coordinate space to a differential equation, that cannot be solved algebraically, as it was the case with the self-energy  $\Sigma$  or the polarization  $\Pi$ . However, there are other forms of potentials, that allow for a factorization of the equations. These interactions are non-local in coordinate space and factorize in momentum space.

With the ansatz (the internal variables like spin are omitted)

$$V(p_1 p_2, p_1' p_2') = -\frac{\lambda}{\Omega} w(\hbar p) w(\hbar p') \delta_{P, P'} , \quad (4.10.1)$$

the two-particle SCHRÖDINGER equation is solvable and the scattering phase shifts  $\delta_0(E)$  can analytically be calculated. The solution includes scattering states as well as bound states. The potential is constructed as the product of the form factor  $w(\hbar p)$ , that depends on the relative momentum

$$\hbar \vec{p} = \frac{\hbar(m_1 \vec{p}_2 - m_2 \vec{p}_1)}{m_1 + m_2} \quad \text{and} \quad \hbar \vec{p}' = \frac{\hbar(m_1 \vec{p}_2' - m_2 \vec{p}_1')}{m_1 + m_2} \quad (4.10.2)$$

of the incoming and outgoing particles, respectively. The collective momentum is  $\hbar \vec{P} = \hbar(\vec{p}_1 + \vec{p}_2)$ . For simplicity, the species- and spin-indices have been omitted and in the following we will consider two particles of equal mass, i.e.  $m_1 = m_2 \equiv m$ .

It can be shown that every potential can be decomposed into a sum of separable potentials. In particular, this can be a sum of potentials, acting in different channels of angular momentum  $l$ . We only consider  $l = 0$ .

Separable potentials are for example applied for modelling of interaction effects in superconductivity and nuclear and atomic physics.

An example for such a potential is the so-called YAMAGUCHI interaction<sup>15</sup> with

$$w(\hbar p) = \frac{1}{p^2/\gamma^2 + 1} , \quad (4.10.3)$$

that is constructed as a kind of factorized screened potential with the screening parameter  $\gamma$  (compare the DEBYE potential).

When inserting such a separable potential into the time-independent SCHRÖDINGER equation and separating the kinetic energy for the center-of-mass motion  $E_{nP} = E_n + \frac{\hbar^2 P^2}{4m}$ , we can calculate the energy eigenvalues of the two particles via

$$1 = \lambda \int \frac{d^3 p'}{(2\pi)^3} \frac{w(\hbar p')^2}{\frac{\hbar^2 p'^2}{m} - E_n} . \quad (4.10.4)$$

<sup>15</sup>See [Yam54] and [YY54], respectively.

For a bound state  $E_n < 0$ , since  $\lambda > 0$ .

Since the total momentum  $\hbar\vec{P} = \hbar(\vec{p}_1 + \vec{p}_2)$  of the two-particle cluster is conserved (no external potential), we can examine the SCHRÖDINGER equation in the representation for the relative momentum  $\hbar p$ :

$$\sum_{p'} \hat{H}(p, p') \psi_n(p') = E_n \psi_n(p)$$

with the wave function

$$\psi_{nP}(p_1 p_2) = \psi_n(p) \delta_{P, p_1 + p_2}$$

and the HAMILTONIAN

$$\hat{H}(p, p') = \frac{\hbar^2 p^2}{2\mu} \delta_{p, p'} + V(p, p') .$$

The quantum number  $n$  is a placeholder for any internal excitation of the system. For example in the case of a hydrogen-like atom, this would be  $n = n l m m_s$ . For  $m_1 = m_2 \equiv m$ , the reduced mass is  $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m}{2}$ :

$$\sum_{p'} \frac{\hbar^2 p^2}{m} \delta_{p, p'} \psi_n(p') + \sum_{p'} V(p, p') \psi_n(p') = E_n \psi_n(p) .$$

By summing over all outgoing states  $p'$ , we find

$$\begin{aligned} \frac{\hbar^2 p^2}{m} \psi_n(p) - \sum_{p'} \frac{\lambda}{\Omega} w(\hbar p) w(\hbar p') \psi_n(p') &= E_n \psi_n(p) \\ \frac{\hbar^2 p^2}{m} \psi_n(p) - \frac{\lambda}{\Omega} w(\hbar p) \underbrace{\sum_{p'} w(\hbar p') \psi_n(p')}_{=: c_n} &= E_n \psi_n(p) \\ \longrightarrow \psi_n(p) &= \frac{\lambda w(\hbar p) c_n}{\Omega \left( \frac{\hbar^2 p^2}{m} - E_n \right)} . \end{aligned}$$

Thus, for  $c_n$  we have

$$c_n = \sum_{p'} w(\hbar p') \psi_n(p') = \sum_{p'} w(\hbar p') \frac{\lambda w(\hbar p') c_n}{\Omega \left( \frac{\hbar^2 p'^2}{m} - E_n \right)} ,$$

so that

$$1 = \sum_{p'} \frac{\lambda w^2(\hbar p')}{\Omega \left( \frac{\hbar^2 p'^2}{m} - E_n \right)} ,$$

or in integral representation

$$1 = \lambda \int \frac{\Omega d^3 p'}{(2\pi)^3} \frac{w^2(\hbar p')}{\Omega \left( \frac{\hbar^2 p'^2}{m} - E_n \right)} .$$

In the case of the YAMAGUCHI interaction (4.10.3), the integral equation can be solved analytically and the binding energy results to

$$E^{(0)} = -\frac{\hbar^2 \gamma^2}{m} \left( \sqrt{\frac{\lambda m \gamma}{8\pi \hbar^2}} - 1 \right)^2. \quad (4.10.5)$$

We insert (4.10.3) into (4.10.4):

$$1 = \lambda \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{\left(\frac{p'^2}{\gamma^2} + 1\right)^2} \frac{1}{\left(\frac{\hbar^2 p'^2}{m} - E^{(0)}\right)},$$

transform to spherical coordinates:

$$1 = \frac{4\pi\lambda}{(2\pi)^3} \int_0^\infty \frac{p'^2 dp'}{\left(\frac{p'^2}{\gamma^2} + 1\right)^2 \left(\frac{\hbar^2 p'^2}{m} - E^{(0)}\right)}$$

and substitute  $x := \frac{p'}{\gamma}$ :

$$1 = \frac{4\pi\lambda}{(2\pi)^3} \frac{m\gamma}{\hbar^2} \int_0^\infty \frac{x^2 dx}{(x^2 + 1)^2 \left(x^2 - \frac{E^{(0)}m}{\hbar^2 \gamma^2}\right)}.$$

We can now make use of the integral  $\int_0^\infty \frac{x^2 dx}{(x^2+1)^2(x^2+y)} = \frac{\pi}{4(1+\sqrt{y})^2}$  with  $y = -\frac{E^{(0)}m}{\hbar^2 \gamma^2}$ :

$$\begin{aligned} 1 &= \frac{\pi^2 \lambda}{(2\pi)^3} \frac{m\gamma}{\hbar^2} \frac{1}{\left(1 + \sqrt{-\frac{E^{(0)}m}{\hbar^2 \gamma^2}}\right)^2} \\ \rightarrow E^{(0)} &= -\frac{\hbar^2 \gamma^2}{m} \left( \sqrt{\frac{\lambda m \gamma}{8\pi \hbar^2}} - 1 \right)^2. \end{aligned}$$

Usually, we would use equation (4.10.5) to fit the interaction parameter  $\lambda$  to some experimental value of the binding energy  $E^{(0)}$ . Then, the scattering phase shifts  $\delta_l(E)$  can be evaluated. Again, we only consider  $s$ -wave scattering, i.e.  $l = 0$  and find

$$\delta_0(\tilde{E}) = \arctan \frac{2\sqrt{\tilde{E}}}{\frac{8\pi}{\lambda} \frac{\hbar^2}{\mu\gamma} (1 + \tilde{E})^2 - (1 - \tilde{E})} \quad (4.10.6)$$

with the reduced scattering state energy  $\tilde{E} = \frac{\mu}{\hbar^2 \gamma^2} E > 0$ .

We start from the BETHE-SALPETER equation (4.8.5) in ladder approximation (for convenience, we omit the exchange terms):

$$T(12, 1'2', z) = V(12, 1'2') + \sum_{1''2''} V(12, 1''2'') G_2^0(1''2'', z) T(1''2'', 1'2', z)$$

with the two-particle propagator

$$G_2^0(1''2'', z) \stackrel{(4.8.1)}{=} \frac{1 - f(1'') - f(2'')}{z - \epsilon_{1''} - \epsilon_{2''}}$$

and a separable potential

$$V(12, 1'2') = -\frac{\lambda}{\Omega} w(12)w(1'2')$$

as well as a separable approach for the  $T$ -matrix:

$$T(12, 1'2', z) = w(12)w(1'2')t(P, z),$$

introducing the relative and center-of-mass momenta (N.B. conservation of momentum)

$$p = \frac{p_{1''} - p_{2''}}{2} \quad P = p_{1''} + p_{2''} = p_1 + p_2,$$

to find

$$t(P, z) = -\frac{\lambda}{\Omega} \left[ 1 + \frac{\lambda}{\Omega} \sum_p w^2(p) \frac{1 - f(p + P/2) - f(p - P/2)}{z - \epsilon_{p+P/2} - \epsilon_{p-P/2}} \right]^{-1}.$$

Since we analyze the low density case, we omit the FERMI functions, i.e.  $f \ll 1$ . Thus, after transforming to the center-of-mass system  $P = 0$ , we find:

$$t(0, z) = -\frac{\lambda}{\Omega} \left[ 1 + \frac{\lambda}{\Omega} \sum_p \frac{w^2(p)}{z - 2\epsilon_p} \right]^{-1}$$

and

$$T(12, 1'2', z) = -\frac{\lambda}{\Omega} w(12)w(1'2') \cdot \frac{1}{1 + \frac{\lambda}{\Omega} \int \frac{\Omega d^3p}{(2\pi)^3} \frac{w^2(p)}{z - 2\epsilon_p}}.$$

Since the integrand only depends on the length of  $p$ , the integral in the denominator can be simplified in spherical coordinates:

$$I(z) = \lambda \int \frac{d^3p}{(2\pi)^3} \frac{w^2(p)}{z - 2\epsilon_p} = \frac{\lambda}{2\pi^2} \int_0^\infty dp \frac{p^2 w^2(p)}{z - \frac{\hbar^2 p^2}{\mu}}.$$

For selecting the scattering case, we set  $z = E > 0$  and after inserting the YAMAGUCHI form factor (4.10.3), we have

$$I(E) = \frac{\lambda}{2\pi^2} \int_0^\infty dp \frac{p^2}{(p^2/\gamma^2 + 1)^2} \cdot \frac{1}{E - \frac{\hbar^2 p^2}{\mu}}$$

Substitution of  $x = p/\gamma$  and insertion of the reduced energy  $\tilde{E} = \frac{\mu}{\hbar^2 \gamma^2} E > 0$  leads to the integral that we already considered in our previous calculation:

$$\begin{aligned} I(E) &= -\frac{\lambda}{2\pi^2} \frac{\mu\gamma}{\hbar^2} \int_0^\infty dx \frac{x^2}{(x^2 + 1)^2 (x^2 + (-\tilde{E}))} \\ &= -\frac{\lambda}{2\pi^2} \frac{\mu\gamma}{\hbar^2} \frac{\pi}{4(1 + \sqrt{-\tilde{E}})^2} \\ &= -\frac{\lambda}{8\pi} \frac{\mu\gamma}{\hbar^2} \frac{1}{4(1 + i\sqrt{\tilde{E}})^2}. \end{aligned}$$

We separate for real and imaginary part:

$$= -\frac{\lambda}{8\pi} \frac{\mu\gamma}{\hbar^2} \frac{1}{(1 + \tilde{E})^2} \cdot \left[ (1 - \tilde{E}) + i(-2\sqrt{\tilde{E}}) \right].$$

Insertion of the real and imaginary part of the integral into the  $T$ -matrix leads to

$$\begin{aligned} T(12, 1'2', \tilde{E}) &= \frac{-\frac{\lambda}{\Omega} w(12)w(1'2')}{(1 + \text{Re}\{I(\tilde{E})\}) + i(\text{Im}\{I(\tilde{E})\})} \\ &= -\frac{\lambda}{\Omega} w(12)w(1'2') \cdot \frac{(1 + \text{Re}\{I(\tilde{E})\}) - i(\text{Im}\{I(\tilde{E})\})}{(1 + \text{Re}\{I(\tilde{E})\})^2 + (\text{Im}\{I(\tilde{E})\})^2}. \end{aligned}$$

Since the form factors  $w(p)$  and the parameter  $\lambda$  are real-valued, we can now calculate the scattering phase-shift:

$$\tan(\delta_0(\tilde{E})) = \frac{\text{Im}\{T(12, 1'2', \tilde{E})\}}{\text{Re}\{T(12, 1'2', \tilde{E})\}} = \frac{-\text{Im}\{I(\tilde{E})\}}{1 + \text{Re}\{I(\tilde{E})\}} = \frac{2\sqrt{\tilde{E}}}{\frac{8\pi}{\lambda} \frac{\hbar^2}{\mu\gamma} (1 + \tilde{E})^2 - (1 - \tilde{E})}$$

According to the relation

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2}r_0k^2 - \dots \quad (4.10.7)$$

with  $E = \frac{\hbar^2k^2}{2\mu}$ , the scattering length  $a$  and the effective range  $r_0$  can be calculated from expression (4.10.6)<sup>16</sup>:

$$a = \left(1 - \frac{8\pi\hbar^2}{\lambda\mu\gamma}\right)^{-1} \frac{\sqrt{2}}{\gamma} \quad (4.10.8)$$

$$r_0 = \left(1 + 2 \cdot \frac{8\pi\hbar^2}{\lambda\mu\gamma}\right) \frac{1}{\sqrt{2}\gamma}. \quad (4.10.9)$$

The reduced energy is

$$\tilde{E} = \frac{\mu}{\hbar^2\gamma^2} E = \frac{\mu}{\hbar^2\gamma^2} \frac{\hbar^2k^2}{2\mu} = \frac{k^2}{2\gamma^2},$$

so that from (4.10.6), we find

$$\begin{aligned} k \cot \delta_0(k^2) &= k \cdot \frac{\frac{8\pi}{\lambda} \frac{\hbar^2}{\mu\gamma} \left(1 + \frac{k^2}{2\gamma^2}\right)^2 - \left(1 - \frac{k^2}{2\gamma^2}\right)}{\sqrt{2} \frac{k}{\gamma}} \\ &= \frac{\gamma}{\sqrt{2}} \left( \frac{8\pi}{\lambda} \frac{\hbar^2}{\mu\gamma} \left(1 + \frac{k^2}{\gamma^2} + \frac{k^4}{4\gamma^4}\right) - \left(1 - \frac{k^2}{2\gamma^2}\right) \right) \\ &= -\underbrace{\frac{\gamma}{\sqrt{2}} \left(1 - \frac{8\pi\hbar^2}{\lambda\mu\gamma}\right)}_{1/a} + \underbrace{\frac{1}{\sqrt{2}\gamma} \left(1 + 2 \cdot \frac{8\pi\hbar^2}{\lambda\mu\gamma}\right)}_{r_0} \cdot \frac{k^2}{2} + \mathcal{O}(k^4). \end{aligned}$$

<sup>16</sup>See equation (20) in [Yam54].





# 5 Diagram technique and Cluster decompositions

## 5.1 Elements of the diagram technique and the chemical picture

The GREEN's functions technique is a very powerful tool for calculating physical properties of many-particle systems: After evaluating the GREEN's function of a certain system, we can calculate the spectral function and correlation functions. Therefrom, the physical characteristics, we are interested in, such as density, pressure, or the dielectric function, can be derived (see section 2.2).

The GREEN's function itself can be deduced from the diagram technique as a visual representation of perturbation theory, which allows to select relevant contributions to perform partial summations.

Some fundamental components of this technique are

- free fermion propagator

$$G_1^0(1, iz_\nu) = \text{---} \overrightarrow{1, iz_\nu} \text{---} = \frac{1}{iz_\nu - \epsilon_1}$$

- interaction, e.g. COULOMB interaction

$$V^0(q, iz_\mu) = \text{---} \overrightarrow{q, iz_\mu} \text{---} = \frac{1}{\Omega \epsilon_0 q^2}$$

- vertex for COULOMB systems

$$\Gamma_1^0(1z_{\nu_1}, 2iz_{\nu_2}; q, iz_\lambda) = \text{---} \overrightarrow{q, iz_\lambda} \text{---} = e_1 \delta_{c_1, c_2} \delta_{p_1+q, p_2} \delta_{z_1+z_\lambda, z_2} \delta_{\sigma_1 \sigma_2} .$$

In our notation, the superscript index 0 denotes the respective quantities for free particles, i.e. the zero density limit.

However, this picture contains some open questions, that have to be answered in the framework of a quantum statistical approach.

One important concept is elementary for the statistical description: the idea of 'particles' and their interaction. Although historically, the elementary particles of statistical physics and thermodynamics are molecules, that are treated as simple particles, we know that they consist of atoms which again contain smaller constituents. While especially the inneratomic structure of electrons and nucleons and finally quarks and gluons can only be excited with the high energies of elementary particle physics experiments, the molecular structure can be resolved with low excitation energies that are sufficient to stimulate vibration and rotation of the molecules.

Therefore, it is a question of temperature (and also density), whether the internal degrees of freedom of a composed particle can be excited. If this is not the case, it can be treated as an 'elementary' particle.

A closed and consistent description of all these structural features with the GREEN's functions technique and its diagram representation is possible in the so-called 'chemical picture'. There, the bound states that are sufficiently stable, are interpreted as a new sort of particles. The many-particle system

is then described as consisting of the primary unbound particles and the new bound species that are compounds of at least two primary particles.<sup>1</sup>

At sufficiently low densities and temperatures (below MOTT criterion), bound states are evident. Here, the treatment in a chemical picture leads to the formulation of a mass-action-law and the chemical equilibrium.

To describe the propagation of particle clusters, in section 4.8 we have introduced the ladder approximation as a new diagram element that satisfies the BETHE-SALPETER equation. In the following, we will not consider the exchange terms:

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} G_2^{\text{ladd}} = \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} G_2^{\text{ladd}} = \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \quad (5.1.1)$$

It can be represented in two-particle space  $|nP\rangle$  by

$$G_2^{\text{ladd.}}(nP, n'P', iz_\mu) = \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = \frac{\delta_{PP'} \delta_{nn'}}{iz_\mu - E_{nP} - \mu_{12}} \equiv G_2^{\text{ladd.}}(nP, iz_\mu), \quad (5.1.2)$$

when considering the low density limit. As we already saw in section 4.9, with this formalism, a completely analogous treatment of single-particle and binary bound states is possible.

Consequently, we can introduce a two-particle vertex as an interaction with each of the two bound particles similar to (4.5.3):

$$\Gamma_2^0(nP, iz_\mu, n'P + q, iz_\mu + iz_\lambda) = \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + \begin{array}{c} \text{---} \text{---} \text{---} \\ | \quad | \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \quad (5.1.3)$$

$$= \sum_{\substack{12 \\ 1'2'}} \psi_{nP}^* (12) \left( e_1 \delta_{p_1, p'_1+q} \delta_{p_2, p'_2} + e_2 \delta_{p_1, p'_1} \delta_{p_2, p'_2+q} \right) \psi_{n'P'} (1'2') \delta_{z_\mu+z_\lambda, z'_\mu} \delta_{P+q, P'} \quad (5.1.4)$$

In the long wavelength limit  $q \rightarrow 0$  for a hydrogen-like cluster  $e_2 = -e_1$ , the two particle vertex can describe the coupling of an atom to the electric field through its dipole matrix element:

$$\Gamma_2^0(nP, iz_\mu, n'P + q, iz_\mu + iz_\lambda) \xrightarrow{q \rightarrow 0} \Gamma_2^0(nn', q \rightarrow 0) = ie\vec{q} \vec{d}_{nn'} \delta_{P+q, P'} \delta_{z_\mu+z_\lambda, z'_\mu}. \quad (5.1.5)$$

with the dipole matrix element

$$\vec{d}_{nn'} = \int d^3\vec{r} \psi_n^*(\vec{r}) \vec{r} \psi_{n'}(\vec{r}). \quad (5.1.6)$$

Starting from (5.1.4), we can introduce the particle's collective momentum  $\vec{P} = \vec{p}_1 + \vec{p}_2$  and the relative momentum

$$\vec{p}_{\text{rel}} = \frac{m_2 \vec{p}_1 - m_1 \vec{p}_2}{m_1 + m_2},$$

<sup>1</sup>See the monograph [KKER86] for further details.

which in the case of interaction with particle 1 (first summand in brackets) yields

$$\vec{p}'_{\text{rel}} = \frac{m_2 (\vec{p}_1 - \vec{q}) - m_1 \vec{p}_2}{m_1 + m_2} = \vec{p}_{\text{rel}} - \frac{m_2}{m_1 + m_2} \vec{q}$$

and in the other case

$$\vec{p}'_{\text{rel}} = \vec{p}_{\text{rel}} + \frac{m_1}{m_1 + m_2} \vec{q}.$$

After transforming the wave functions to relative momentum representation:  $\psi_{nP}(12) = \psi_n(\vec{p}_{\text{rel}}) \delta_{P, p_1 + p_2}$ , we have

$$\begin{aligned} & \Gamma_2^0(nP, iz_\mu, n'P + q, iz_\mu + iz_\lambda) \\ &= \delta_{P+q, P'} \delta_{z_\mu + z_\lambda, z'_\mu} \int \frac{\Omega d^3 \vec{p}_{\text{rel}}}{(2\pi)^3} \psi_n^*(\vec{p}_{\text{rel}}) \\ & \cdot \left[ e_1 \psi_{n'} \left( \vec{p}_{\text{rel}} - \frac{m_2}{m_1 + m_2} \vec{q} \right) + e_2 \psi_{n'} \left( \vec{p}_{\text{rel}} + \frac{m_1}{m_1 + m_2} \vec{q} \right) \right]. \end{aligned}$$

For simplicity we assume that particle 1 is a proton while particle 2 is an electron. Thus we can use  $e \equiv e_2 = -e_1$  and  $m_2 \ll m_1 \rightarrow m_2 \approx 0$ :

$$\approx -e \delta_{P+q, P'} \delta_{z_\mu + z_\lambda, z'_\mu} \int \frac{\Omega d^3 \vec{p}_{\text{rel}}}{(2\pi)^3} \psi_n^*(\vec{p}_{\text{rel}}) [\psi_{n'}(\vec{p}_{\text{rel}}) - \psi_{n'}(\vec{p}_{\text{rel}} + \vec{q})].$$

Now we can transform the wave-functions into coordinate space via  $\psi_n(\vec{p}) = \frac{1}{\sqrt{\Omega}} \int d^3 \vec{r} \psi_n(\vec{r}) e^{i\vec{p}\vec{r}}$ :

$$\begin{aligned} &= -e \delta_{P+q, P'} \delta_{z_\mu + z_\lambda, z'_\mu} \int d^3 \vec{r}_1 \int d^3 \vec{r}_2 \int \frac{d^3 \vec{p}_{\text{rel}}}{(2\pi)^3} \psi_n^*(\vec{r}_1) e^{-i\vec{p}_{\text{rel}} \vec{r}_1} \\ & \cdot \left[ \psi_{n'}(\vec{r}_2) e^{i\vec{p}_{\text{rel}} \vec{r}_2} - \psi_{n'}(\vec{r}_2) e^{i(\vec{p}_{\text{rel}} + \vec{q}) \vec{r}_2} \right] \\ &= e \delta_{P+q, P'} \delta_{z_\mu + z_\lambda, z'_\mu} \int d^3 \vec{r}_1 \int d^3 \vec{r}_2 \int \frac{d^3 \vec{p}_{\text{rel}}}{(2\pi)^3} \underbrace{e^{i\vec{p}_{\text{rel}}(\vec{r}_2 - \vec{r}_1)}}_{\delta^3(\vec{r}_2 - \vec{r}_1)} \\ & \cdot \psi_n^*(\vec{r}_1) \left[ e^{i\vec{q}\vec{r}_2} - 1 \right] \psi_{n'}(\vec{r}_2) \\ &= e \delta_{P+q, P'} \delta_{z_\mu + z_\lambda, z'_\mu} \int d^3 \vec{r}_1 \psi_n^*(\vec{r}_1) \left[ e^{i\vec{q}\vec{r}_1} - 1 \right] \psi_{n'}(\vec{r}_1). \end{aligned}$$

After expanding the exponential function for  $\vec{q} \rightarrow 0$  and renaming  $\vec{r}_1 \rightarrow \vec{r}$ , we reach

$$\begin{aligned} &= e \delta_{P+q, P'} \int d^3 \vec{r} \delta_{z_\mu + z_\lambda, z'_\mu} \psi_n^*(\vec{r}) \left[ i\vec{q}\vec{r} - \frac{1}{2} (\vec{q}\vec{r})(\vec{q}\vec{r}) + \dots \right] \psi_{n'}(\vec{r}) \\ &\approx i e \delta_{P, P'+q} \delta_{z_\mu + z_\lambda, z'_\mu} \vec{q} \int d^3 \vec{r} \psi_n^*(\vec{r}) \vec{r} \psi_{n'}(\vec{r}), \end{aligned}$$

which is the same as (5.1.5) with the dipole matrix element

$$\vec{d}_{nn'} = \int d^3 \vec{r} \psi_n^*(\vec{r}) \vec{r} \psi_{n'}(\vec{r}).$$

Obviously, the final three free parameters of  $\Gamma_2^0$  in the long-wavelength limit are the internal quantum numbers  $nn'$  and the transfer momentum  $q$ .

Note, that for an instantaneous interaction, the interaction and thus also the vertex function becomes

independent of the frequency and we can write

$$\Gamma_2^0(nP, iz_\mu, n'P + q, iz_\mu + iz_\lambda) \equiv \Gamma_2^0(nP, n'P + q) . \quad (5.1.7)$$

A generalization to clusters with  $A > 2$  constituents is possible by adding graphs, where the single-particle propagators are replaced with  $A$ -particle propagators, that represent the bound contributions.




Within the perturbation theory, the diagrams must be counted correctly (i.e. spin degeneration, ...) and special care has to be taken to avoid double counting throughout the different diagram classes. This is becoming even more complicated when considering a mixture of free and bound states, since often divergent or double-counted graphs are not obvious.

For example, when calculating the single-particle self-energy  $\Sigma_1$  in a screened ladder approximation

$$\Sigma = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots$$

with contributions of the polarization function  $\Pi$  in the screened interaction

$$\Pi = \text{[diagram 5]}$$

the diagram  will appear in  as well as in .

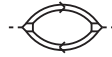
Thus, in the lower orders the corresponding diagrams have to be subtracted, what leads to the so-called 'parquet approximations'.


For instance


$$\Sigma = \underbrace{\text{[diagram 7]}}_{\text{binary collisions (T-matrix)}} + \underbrace{\text{[diagram 8]}}_{\text{screened dielectric function}} - \underbrace{\text{[diagram 9]}}_{\text{BORN contribution subtracted because of double counting}} - \dots$$

is the GOULD-DEWITT approximation.

An analogous problem for example arises when examining contributions to the polarization function of the type



as we will do in section 5.3. Here, also a vacuum diverging graph of the form  and

the unintentionally double-counted graph  (that is reducible) appear.

Thus whenever working with the diagram technique, special care has to be taken to avoid inconsistencies with real physics and nonanalytical behavior in mathematics.

In section 4.4 we found an approximation for the single-particle's polarization function  $\Pi \approx \Pi^{\text{RPA}}$  as in (4.4.1). With the screening equation (4.3.5) it is now possible to find expressions for the screened

potential  $V^s$  and thus appropriate contributions to the self-energy to calculate the equation of state or the optical and transport properties:

- The MONTROLL-WARD approximation

$$\Sigma_1^{\text{MW}}(p, iz_\mu) = \text{diagram} \quad (5.1.8)$$

has already been under consideration as the the single-particle screened self-energy, compare section 4.6.

- The screened two-particle self-energy

$$\begin{aligned} \Sigma_2(nn', P, iz_\mu) &= \text{diagram} \\ &= \delta_{P, P'} \delta_{z_\mu, z'_\mu} \sum_{n_1, q, iz_\lambda} \Gamma_2^0(nP, iz_\mu; n_1, P + q, iz_\mu + iz_\lambda) G_2^{\text{ladd.}}(n_1, P + q, iz_\mu + iz_\lambda) \\ &\quad \Gamma_2^0(n_1, P + q, iz_\mu + iz_\lambda; n, P, iz_\mu) V^s(q, iz_\lambda) \end{aligned} \quad (5.1.9)$$

would be an appropriate generalization to two-particle GREEN's functions<sup>2</sup>. It describes the interaction of the cluster's dipole moment with the environmental polarization. This approach for example allows us, to calculate the spectral line shape (see section 5.4). However, its evaluation is not straightforward. For example, in general it is not diagonal in the internal quantum number  $n$  in contrast to  $P$  and  $iz_\mu$  for homogeneous systems.

A solution for  $\Sigma_2$  can be derived by solving an effective wave-equation with an additional potential term that describes the (dynamic) coupling to the environment (dielectric function). It contains the contribution of the dynamic self-energy to the single-particle energy as well as the dynamic screening of the interaction<sup>3</sup>.

<sup>2</sup>The screened self-energy including dynamical screening has for example been investigated in [ZKK<sup>+</sup>78].

<sup>3</sup>Since a complete evaluation of this diagram would go beyond this lecture, we again refer to the book [KKER86], section 8.2.1 *Explicit expression for shift and broadening*, where with equation (8.36) a closed expression for  $\Sigma_2$  is derived.

## 5.2 Cluster expansion for the single-particle self-energy and equation of state

For computation of the single-particle GREEN's function  $G_1$ , the self-energy  $\Sigma_1$  is needed. If we want to describe a system with bound states we have to perform a cluster expansion for  $\Sigma_1$  in terms of the  $T$ -matrix<sup>4</sup>:

$$\Sigma_1 = \begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} T_{\text{ladd.}}^{(2)} + \begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} T_{\text{ladd.}}^{(3)} + \dots \quad (5.2.1)$$

Thus, for example the density of the bound state is incorporated into the equation of state  $n(T, \mu)$  (mass action law).

The calculation of the  $T$ -matrices is performed via a BETHE-SALPETER equation

$$G_A = G_A^0 + G_A^0 T^{(A)} G_A^0 \quad (5.2.2)$$

$$\begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} T_{\text{ladd.}}^{(A)} = \begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} V^{(A)} + \begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} V^{(A)} \begin{array}{c} \text{---} \circ \text{---} \\ \updownarrow \\ \text{---} \circ \text{---} \\ \text{---} \end{array} T_{\text{ladd.}}^{(A)} \quad (5.2.3)$$

$$T^{(A)} = V^{(A)} + V^{(A)} G_A^0 V^{(A)} \quad (5.2.4)$$

$$V^{(A)} = \sum_{i < j} V(ij, i'j') \delta_{kk'} \quad (5.2.5)$$

in analogy to the  $A$ -particle propagators, compare equation (4.8.5). When inserting (5.2.3) into (5.2.1), the respective double-counted contributions have to be subtracted correctly.

Environmental effects for clusters, especially interaction with other clusters and exchange contributions, can be described by respective terms for the cluster self-energy.

Similar to the equation of state  $n^{(0)}(\beta, \mu) = (2s + 1) \int \frac{d^3 p}{(2\pi)^3} f_1(E_p)$  of an ideal quantum gas, we will derive the mass action law as an equation of state for an interacting system that forms a mixture of free particles and  $A$ -particle clusters.

---

<sup>4</sup>For a more detailed discussion of the cluster expansion for the self-energy and the ladder  $T$ -matrix approximation, we recommend considering the publication [RMS82].

As we already introduced earlier in this lecture, we express the particle density  $n$  in terms of the spectral function  $A$ :

$$n(\beta, \mu) = \frac{1}{\Omega} \sum_1 \langle a_1^\dagger a_1 \rangle = \frac{1}{\Omega} \sum_1 \int \frac{d\omega}{2\pi} f(\omega) A(1, \omega) \quad (\underline{\text{A}})$$

$$\begin{aligned} A(1, \omega) &\stackrel{(2.2.10)}{=} 2\text{Im} \{G_1(1, \omega - i\varepsilon)\} \\ &\stackrel{(4.2.4)}{=} 2\text{Im} \left\{ \frac{1}{\omega - E_1 - \Sigma(1, \omega - i\varepsilon) - i\varepsilon} \right\} \\ &= \frac{2\text{Im} \{\Sigma(1, \omega - i\varepsilon)\}}{[\omega - E_1 - \text{Re} \{\Sigma(1, \omega)\}]^2 + [\text{Im} \{\Sigma(1, \omega - i\varepsilon)\}]^2} . \end{aligned}$$

Thus, the spectral function takes the form

$$\equiv \frac{2\Delta(\omega)}{f^2(\omega) + \Delta^2(\omega)} = 2\pi\delta^\Delta(f(\omega)) ,$$

that in the limit  $\Delta \rightarrow 0$  is the  $\delta$  distribution:

$$\lim_{\Delta(\omega) \rightarrow 0} \delta^\Delta(f(\omega)) = \delta(f(\omega)) .$$

We assume, the imaginary part of the self-energy and thus  $\Delta(\omega)$  to be small and perform a TAYLOR expansion

$$\delta^\Delta(f(\omega)) = \delta(f(\omega)) + \Delta \left. \frac{d}{d\Delta} \delta^\Delta(f(\omega)) \right|_{\Delta=0} ,$$

and use the connection between the delta distribution and the principal value distribution for small  $\Delta$ <sup>5</sup>

$$\lim_{\Delta \rightarrow 0} \frac{d}{d\Delta} \delta^\Delta(E) = - \lim_{\Delta \rightarrow 0} \frac{1}{\pi} \frac{d}{dE} \frac{\mathcal{P}}{E}$$

to derive

$$\begin{aligned} A(1, \omega) &= 2\pi\delta\left(\omega - \underbrace{(E_1 + \text{Re} \{\Sigma(1, \omega)\})}_{E_1^{\text{qu.}}}\right) \\ &\quad - 2\pi\text{Im} \{\Sigma(1, \omega - i\varepsilon)\} \frac{1}{\pi} \frac{d}{d\omega} \frac{\mathcal{P}}{\omega - E_1 - \text{Re} \{\Sigma(1, \omega)\}} \\ &= 2\pi\delta(\omega - E_1^{\text{qu.}}) - \frac{2\text{Im} \{\Sigma(1, \omega - i\varepsilon)\}}{[\omega - E_1^{\text{qu.}}]^2} \end{aligned}$$

Thus, when considering the self-energy corrections (especially the imaginary part) as to be small compared to the single-particle energy  $\Sigma \ll E$ , the spectral function is:

$$A(1, \omega) = 2\pi\delta(\omega - E_1) + \frac{2\text{Im} \{\Sigma(1, \omega)\}}{[\omega - E_1]^2} , \quad (\underline{\text{B}})$$

<sup>5</sup>For a further discussion of these calculations, we recommend the publication [KKL84].

where the first summand is the well-known quasi-particle contribution with the quasi-particle energy  $E_1^{\text{qu.}} = E_1 + \text{Re}\{\Sigma_a(1, \omega)\}|_{\omega=E_1^{\text{qu.}}}$ .

We will evaluate (A) in the low-density limit  $n \rightarrow 0$  with the cluster decomposition of the self-energy

$$\Sigma = \Sigma^{(2)} + \Sigma^{(3)} + \dots = \text{diag}_{\text{ladd.}}^{(2)} + \text{diag}_{\text{ladd.}}^{(3)} + \dots,$$

where the contribution of interaction with  $(A-1)$ -particle clusters is given by

$$\Sigma^{(A)} = T^{(A)} G_{A-1}^0 = \text{diag}_{\text{ladd.}}^{(A)} G_0^{(A-1)}. \quad (\text{C})$$

In the low-density case  $n \rightarrow 0$ , we know the following expression for the free  $(A-1)$ -particle propagator, compare (4.8.7):

$$G_{A-1}^0(2 \dots A, 2' \dots A', iz_\nu) = \frac{\delta_{22'} \dots \delta_{AA'}}{iz_\nu - E_{2 \dots A}}. \quad (\text{D})$$

Here and in the following, we have to take care of the collective spin of the cluster, i.e. if  $(A-1)$  is even, the propagator describes a bosonic particle and  $iz_\nu$  corresponds to an even MATSUBARA frequency. For odd  $(A-1)$ , we have fermionic character and thus odd MATSUBARA frequencies. This also determines the character of the frequency argument of the  $T$ -matrix.

The  $T$ -matrix can be written in bilinear decomposition<sup>6</sup> as

$$\begin{aligned} T^{(A)}(1 \dots A, 1' \dots A', iz_\mu) \\ = \sum_{nP} (E_{A,nP} - E_{1 \dots A}) \frac{\psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1' \dots A')}{iz_\mu - E_{A,nP}} (iz_\mu - E_{1' \dots A'}) \end{aligned}$$

and after using  $(iz_\mu - E_{1' \dots A'}) = (iz_\mu - E_{A,nP} + E_{A,nP} - E_{1' \dots A'})$ , we have

$$= \sum_{nP} (E_{A,nP} - E_{1 \dots A}) \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1' \dots A') \left[ 1 - \frac{E_{A,nP} - E_{1' \dots A'}}{E_{A,nP} - iz_\mu} \right]. \quad (\text{E})$$

We can now insert (D) and (E) into (C) and find

$$\begin{aligned} \Sigma^{(A)}(11', iz_\lambda) \\ = \frac{1}{\beta} \sum_{\substack{z_\mu \\ 2 \dots A, 2' \dots A'}} T^{(A)}(1 \dots A, 1' \dots A', iz_\mu) G_{A-1}^0(2 \dots A, 2' \dots A', iz_\mu - iz_\lambda) \\ = \frac{1}{\beta} \sum_{\substack{z_\mu \\ 2 \dots A, 2' \dots A'}} \sum_{nP} (E_{A,nP} - E_{1 \dots A}) \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1' \dots A') \\ \cdot \left[ 1 - \frac{E_{A,nP} - E_{1' \dots A'}}{E_{A,nP} - iz_\mu} \right] \frac{\delta_{22'} \dots \delta_{AA'}}{iz_\mu - iz_\lambda - E_{2 \dots A}}. \end{aligned}$$

<sup>6</sup>This expression has been derived for a more general case for example in [SZ79].



Due to the  $\delta$  functions, the sums over  $2' \dots i'$  can be executed. After some reordering, we find

$$= \sum_{\substack{nP \\ 2 \dots A}} (E_{A,nP} - E_{1 \dots A}) \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1 \dots A) \\ \cdot \frac{1}{\beta} \sum_{z_\mu} \left[ 1 - \frac{E_{A,nP} - E_{1 \dots A}}{E_{A,nP} - iz_\mu} \right] \frac{1}{iz_\mu - iz_\lambda - E_{2 \dots A}}$$

and after a partial fraction decomposition in the second summand

$$= \sum_{\substack{nP \\ 2 \dots A}} (E_{A,nP} - E_{1 \dots A}) \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1 \dots A) \\ \cdot \frac{1}{\beta} \sum_{z_\mu} \left[ \frac{1}{iz_\mu - iz_\lambda - E_{2 \dots A}} + \frac{E_{A,nP} - E_{1 \dots A}}{iz_\lambda - E_{A,nP} + E_{2 \dots A}} \left( \frac{1}{iz_\mu - iz_\lambda - E_{2 \dots A}} - \frac{1}{iz_\mu - E_{A,nP}} \right) \right].$$

Using expression (3.3.2), the frequency sum can be performed:

$$= \sum_{\substack{nP \\ 2 \dots A}} (E_{A,nP} - E_{1 \dots A}) \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1 \dots A) \\ \cdot \left[ f_A(iz_\lambda + E_{2 \dots A}) + \frac{E_{A,nP} - E_{1 \dots A}}{iz_\lambda - E_{A,nP} + E_{2 \dots A}} (f_A(iz_\lambda + E_{2 \dots A}) - f_A(E_{A,nP})) \right].$$

Here, the distribution function  $f_A$  is a generalization of the FERMI and BOSE distribution to  $A$ -particle clusters:

$$f_A(E) = \frac{1}{e^{\beta(E-A\mu)} - (-1)^A}.$$

Since it results from some HARTREE-FOCK contributions, we will omit the first summand in the following. Additionally, we know that the external frequency  $iz_\lambda$  corresponds to odd (fermionic) MATSUBARA frequencies and thus  $f_A(iz_\lambda + E) = -f_{A-1}(E)$ . Now we have a compact expression for the  $A$ -particle self-energy:

$$\Sigma^{(A)}(1, iz_\lambda) = - \sum_{\substack{nP \\ 2 \dots A}} (E_{A,nP} - E_{1 \dots A})^2 \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1 \dots A) \\ \cdot \frac{f_{A-1}(E_{2 \dots A}) + f_A(E_{A,nP})}{iz_\lambda - E_{A,nP} + E_{2 \dots A}} \\ \Sigma(1, iz_\lambda) = \sum_A \Sigma^{(A)}(1, iz_\lambda).$$

This result can be inserted into (B). Since we assume the energy correction due to self-energy effects to be small compared to the single-particle free energy  $E_1$ , we can omit the respective terms in the denominator of (B). The imaginary part of  $\Sigma^{(A)}(11', \omega - i\varepsilon)$  can be calculated with the DIRAC identity (2.2.8) and altogether we find

$$A(1, \omega) = 2\pi \delta(\omega - E_1) + 2\pi \sum_A \sum_{\substack{nP \\ 2 \dots A}} \frac{(E_{A,nP} - E_{1 \dots A})^2}{(\omega - E_1)^2} \psi_{nP}^{(A)}(1 \dots A) \psi_{nP}^{(A)*}(1 \dots A) \\ \cdot (f_{A-1}(E_{2 \dots A}) + f_A(E_{A,nP})) \delta(\omega - E_{A,nP} + E_{2 \dots A}),$$

what in (A) results to

$$\begin{aligned}
 n(\beta, \mu) &= \frac{1}{\Omega} \sum_1 \int \frac{d\omega}{2\pi} f_1(\omega) A(1, \omega) \\
 &= \frac{1}{\Omega} \sum_A \sum_{1\dots A} \sum_{nP} \frac{(E_{A,nP} - E_{1\dots A})^2}{(E_{A,nP} - \underbrace{(E_{2\dots A} + E_1)}_{E_{1\dots A}})^2} \psi_{nP}^{(A)}(1\dots A) \psi_{nP}^{(A)*}(1\dots A) \\
 &\quad \cdot f_1(E_{A,nP} - E_{2\dots A}) (f_{A-1}(E_{2\dots A}) + f_A(E_{A,nP})) \\
 &= \frac{1}{\Omega} \sum_A \sum_{\substack{1\dots A \\ nP}} \psi_{nP}^{(A)}(1\dots A) \psi_{nP}^{(A)*}(1\dots A) f_1(E_{A,nP} - E_{2\dots A}) \\
 &\quad \cdot (f_{A-1}(E_{2\dots A}) - f_A(E_{A,nP})) .
 \end{aligned}$$

Being only interested in the self-energy corrections, we omitted the quasi-particle contribution  $2\pi\delta(\omega - E_1)$  in the spectral function  $A(1, \omega)$ .

While the argument of the first distribution function in the last factor contains contributions of  $(A-1)$  particles and thus includes  $(A-1) \cdot \mu$ , the argument of the second function covers  $A$  particles and thus  $A \cdot \mu$ . Every factor  $e^{\beta\mu} \propto n\Lambda^3$  contributes one order in the density  $n$ . That is why, in the low-density case  $n \rightarrow 0$ , we can neglect the second summand in comparison to the first one.

Additionally, we can also expect non-degeneracy in the low-density limit with finite temperature, and thus replace the BOSE and FERMI functions by MAXWELL distributions:

$$\begin{aligned}
 n(\beta, \mu) &= \frac{1}{\Omega} \sum_A \sum_{\substack{1\dots A \\ nP}} \psi_{nP}^{(A)}(1\dots A) \psi_{nP}^{(A)*}(1\dots A) \\
 &\quad \cdot e^{-\beta(E_{A,nP} - E_{2\dots A} - \mu)} \cdot e^{-\beta(E_{2\dots A} - (A-1)\mu)} \\
 &= \frac{1}{\Omega} \sum_A \sum_{\substack{1\dots A \\ nP}} \psi_{nP}^{(A)}(1\dots A) \psi_{nP}^{(A)*}(1\dots A) e^{-\beta(E_{A,nP} - A\mu)} .
 \end{aligned}$$

Up to now, we only considered the  $T$ -matrix with one definite incoming and outgoing particle. In fact, the  $A$ -particle  $T$ -matrix has  $A$  such particles, so that we cannot determine a certain external one. Thus, we have to introduce a factor  $A$ , that obeys the free choice of the incoming particle:

$$= \frac{1}{\Omega} \sum_A \sum_{nP} A \cdot e^{-\beta(E_{A,nP} - A\mu)} .$$

Since in equilibrium all primary particles experience the same chemical potential  $\mu$  and thus an  $A$ -particle cluster has the chemical potential  $A \cdot \mu$ , we have found an explicit expression for any partial density in a system of primary particles and  $A$ -particle clusters and the total density as their sum:

$$n(\beta, \mu) = \frac{1}{\Omega} \sum_A \sum_{nP} A \cdot e^{-\beta(E_{A,nP} - A\mu)} . \quad (5.2.6)$$

with the clusters kinetic energy  $E_{A,nP}$ , that contains the center-off-mass movement (collective momentum  $P$ ) and internal excitation (internal quantum number  $n$ ).

With  $\frac{1}{\Omega} \sum_P = \int \frac{d^3P}{(2\pi)^3}$ , we can evaluate the momentum and spin summation in  $P$  and find

$$n(\beta, \mu) = \sum_A (2s_A + 1) A \cdot \Lambda_A^{-3} e^{A\beta\mu} \cdot \sum_n e^{-\beta E_n^{\text{int.}}}, \quad (5.2.7)$$

where  $E_n^{\text{int.}}$  is the energy of any internal degree of freedom  $E_n^{\text{int.}} = E_{A,nP} - \frac{\hbar^2 P^2}{2M_A}$  and  $\Lambda_A$  the respective thermal wavelength.

The equation of state for the many-particle system (5.2.6) is the mass action law. For example in the case of  $A = 2$ , it describes the chemical reaction electron+ion  $\rightleftharpoons$  atom.

The equation of state for the bound system can be further improved by several approaches:

- The inclusion of scattering states leads to the BETH-UHLENBECK formula <sup>7</sup>:

$$\Omega \cdot n^{(2)} = \sum_P \left[ \sum_n^{\text{bound}} e^{\beta(E_{nP}^{\text{bound}} - 2\mu)} + \sum_l (2l + 1) \int^{\text{scatt.}} \frac{dE}{2\pi} g_2(E) \frac{d}{dE} \delta_l(E) \right] \quad (5.2.8)$$

with the scattering phase shifts  $\delta_l(E)$ . It is interesting to mention, that, since the exponential term in the first sum also results from a BOSE distribution  $g_2(E)$ , the BETH-UHLENBECK-expression formally can contain two singularities. They describe BOSE-EINSTEIN-condensation of atoms (first summand) and the formation of COOPER-pairs (second summand).

- The inclusion of an improved  $(N - 1)$ -particle propagator in  $T_{\text{ladd.}}^N$  instead of  $N$  single-particle propagators, i.e.



$$(5.2.9)$$

enables us to describe cluster-cluster-interaction, what leads to the VAN-DER-WAALS interaction.

- The interaction itself can be improved by accounting for media effects by replacing the bare COULOMB potential by a screened one.

<sup>7</sup>A very detailed derivation can be found in [Hua87], section 10.3: *The second virial coefficient*.

### 5.3 Cluster-RPA for the polarization function

In section 4.4, we evaluated the polarization function of a single particle in random phase approximation. Obviously, an isolated particle can neither show any spectral lines nor other features of a plasmas emission spectrum, e.g. DOPPLER- and pressure broadening, etc. Especially spectral lines result from internal transitions of bound particle systems. When describing their impact on the dielectric function by calculating a bound states polarization function, we can model the optical properties of a plasma from fundamental principles.

At first, we have to formulate the dielectric function in a way, that absorption and emission of photons by bound states, e.g. atoms, can be easily handled. A cluster decomposition of the dielectric function, utilizing the chemical picture, offers such a possibility:

$$\Pi_{\text{cl}}^{\text{RPA}}(q, i\omega_\lambda) = \Pi_1^{\text{RPA}}(q, i\omega_\lambda) + \Pi_2^{\text{RPA}}(q, i\omega_\lambda) + \dots \quad (5.3.1)$$

with

$$\Pi_1^{\text{RPA}}(\vec{q}, i\omega_\lambda) \stackrel{(4.4.1)}{=} \vec{q}, iz_\nu \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \vec{q}, iz_\nu = \sum_p \frac{f(\epsilon_p) - f(\epsilon_{p-q})}{i\omega_\lambda - (\epsilon_p - \epsilon_{p-q})} \quad (5.3.2)$$

$$\Pi_2^{\text{RPA}}(\vec{q}, i\omega_\lambda) = \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} = \sum_{nn'P} |\Gamma_2^0(n, P; n', P-q)|^2 \frac{g(\epsilon_{n,P}) - g(\epsilon_{n',P-q})}{i\omega_\lambda - (\epsilon_{n,P} - \epsilon_{n',P-q})} \quad (5.3.3)$$

See equation (5.1.7) and remarks there for arguments, why the vertex function's frequency parameter has been omitted.

With the bosonic equivalent to (3.3.2), the proof for (5.3.3) is short:

$$\begin{aligned} & \begin{array}{c} G_2(i\Omega_\lambda; n, \vec{P}) \\ \Gamma_2, \vec{q}, i\omega_\lambda \rightarrow \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \rightarrow \Gamma_2, \vec{q}, i\omega_\lambda \\ G_2(i\Omega_\lambda - i\omega_\lambda; n', \vec{P} - \vec{q}) \end{array} \\ &= \sum_{nn', P, \Omega_\lambda} -\Gamma_2(n, P; n', P-q) \cdot \frac{1}{i\Omega_\lambda - \epsilon_{n,P}} \cdot \frac{1}{i\Omega_\lambda - i\omega_\lambda - \epsilon_{n',P-q}} \cdot \Gamma_2(n', P-q; n, P) \\ &= \sum_{nn'P} |\Gamma_2^0(nP, n'P-q)|^2 \frac{1}{i\omega_\lambda - (\epsilon_{n,P} - \epsilon_{n',P-q})} \left[ \frac{1}{i\Omega_\lambda - \epsilon_{n,P}} - \frac{1}{i\Omega_\lambda - i\omega_\lambda - \epsilon_{n',P-q}} \right] \\ &= \sum_{nn'P} |\Gamma_2^0(nP, n'P-q)|^2 \frac{g(\epsilon_{n,P}) - g(\epsilon_{n',P-q})}{i\omega_\lambda - (\epsilon_{n,P} - \epsilon_{n',P-q})}. \end{aligned}$$

We perform an analytic continuation  $i\omega_\lambda \rightarrow \hbar\omega + i\eta$ :

$$\Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega) = \sum_{nn'P} |\Gamma_2^0(n, P; n', P-q)|^2 \frac{g(\epsilon_{n,P}) - g(\epsilon_{n',P-q})}{\hbar\omega + i\eta - (\epsilon_{n,P} - \epsilon_{n',P-q})}. \quad (5.3.4)$$

In many applications, it is sufficient to approximate the index of refraction as  $n(\omega) \approx 1$ , reducing our task of calculating  $\alpha(\omega)$  to finding  $\text{Im} \varepsilon(\omega)$ , compare section 4.7. Using  $\varepsilon(\omega) = 1 - V(q)\Pi(q, \omega)$ , compare (4.3.9), this can be accomplished by determining  $\text{Im} \Pi_2$ :

$$\text{Im} \Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega) \stackrel{(2.2.8)}{=} -\pi \sum_{nn'P} |\Gamma_2^0(n, P; n', P - q)|^2 \cdot (g(\epsilon_{n,P}) - g(\epsilon_{n',P-q})) \cdot \delta(\hbar\omega - (\epsilon_{n,P} - \epsilon_{n',P-q})) . \quad (5.3.5)$$

In the long-wavelength limit  $q \rightarrow 0$ , we can analyze this expression in more detail. Let us consider a classical plasma  $n\Lambda^3 \ll 1$ , where the BOSE-function of the atoms can be replaced by a MAXWELLIAN distribution

$$g_{\text{atomic}}(E_{n,P}) \approx \frac{1}{4} n(E_n) \Lambda_{ei}^3 e^{-\beta \frac{\hbar^2 P^2}{2M}} \quad (5.3.6)$$

with the thermal wavelength  $\Lambda_{ei} = \sqrt{\frac{2\pi\hbar^2}{Mk_B T}}$ . Here,  $n(E_n) = e^{-\beta E_n}$  is the BOLTZMANN distribution for the bound states and the total energy  $E_{n,P} = E_n + \frac{\hbar^2 P^2}{2M}$  also contains the kinetic energy from the center of mass motion. With  $\Gamma_2^0 \xrightarrow{q \rightarrow 0} ie\vec{q} \vec{d}_{nn'} \delta_{P,P'+q}$ , cf. (5.1.5), we obtain the clusters polarization function in random phase approximation, 'cluster-RPA':

$$\text{Im} \Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega) = -\frac{1}{2(2\pi)^{\frac{3}{2}}} \frac{(M\beta)^{\frac{1}{2}}}{\hbar q} \sum_{nn'} \left| \Gamma_2^0\left(n, P + \frac{q}{2}; n', P - \frac{q}{2}\right) \right|^2 \cdot [n(E_n) - n(E_{n'})] \cdot e^{-\beta \frac{Mc^2}{2\omega^2} (\omega - \omega_{nn'})^2} \quad (5.3.7)$$

Note, that the expression is written in terms of the relative momenta as it is often usual. With the transformation  $P \rightarrow P + \frac{q}{2}$ , we can simply recast it to the form, that has been introduced in section 5.1.

To verify this expression, we perform a variable substitution  $P \rightarrow P + \frac{q}{2}$  in (5.3.5) and choose the  $z$ -axis of the  $\vec{P}$ -integration along the direction of  $\vec{q}$ . Note, that  $\delta_{P+\frac{q}{2}, P'-\frac{q}{2}}$  holds due to the long-wavelength limit, cf. (5.1.5). Thus:

$$\begin{aligned} 0 &\stackrel{!}{=} \hbar\omega - (\epsilon_{n, P+\frac{q}{2}} - \epsilon_{n', P-\frac{q}{2}}) = \hbar\omega - (E_n - E_{n'}) - \frac{\hbar^2 \vec{P}\vec{q}}{M} \frac{1}{2} - \frac{\hbar^2 \vec{P}\vec{q}}{M} \frac{1}{2} \\ &= \hbar\omega - (E_n - E_{n'}) - \frac{\hbar^2}{M} P_z q \\ &\Rightarrow P_z = \frac{M}{\hbar^2 q} (\hbar\omega - (E_n - E_{n'})) \\ &= \frac{M}{\hbar q} (\omega - \omega_{nn'}) , \end{aligned}$$

defining the transition frequency  $\omega_{nn'} = \frac{1}{\hbar} (E_n - E_{n'})$ .

Using cylindrical coordinates, the perpendicular part can be integrated:

$$\begin{aligned} \text{Im } \Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega) &= -\frac{\pi}{4} \frac{1}{(2\pi)^3} \left( \frac{2M}{\hbar^2 \beta} \right) \Lambda_{ei}^3 \sum_{nn'} \left| \Gamma_2^0 \left( n, P + \frac{q}{2}; n', P - \frac{q}{2} \right) \right|^2 \\ &\quad \cdot [n(E_n) - n(E_{n'})] e^{-\beta \frac{\hbar^2 P^2}{2M}} \cdot \delta \left( \hbar\omega - \left( E_n - E_{n'} - \frac{\hbar^2}{M} P_z q \right) \right) \\ &= -\frac{\pi}{4} \frac{1}{(2\pi)^3} \left( \frac{2M}{\hbar^2 \beta} \right) \Lambda_{ei}^3 \frac{M}{\hbar^2 q} \sum_{nn'} \left| \Gamma_2^0 \left( n, P + \frac{q}{2}; n', P - \frac{q}{2} \right) \right|^2 e^{-\beta \frac{M}{2q^2} (\omega - \omega_{nn'})^2} \end{aligned}$$

Finally, taking  $q = \frac{\omega}{c}$ , we arrive at eq. (5.3.7).

Having found an expression for  $\text{Im } \Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega)$ , we can use (4.3.11) to calculate the imaginary part of the dielectric function  $\text{Im } \varepsilon^{\text{RPA}}(\vec{q}, \hbar\omega)$  and finally, with (4.7.8) the absorption coefficient  $\alpha(\omega)$ :

$$\text{Im } \Pi_2^{\text{RPA}}(\vec{q}, \hbar\omega) \stackrel{(4.3.11)}{\longleftrightarrow} \text{Im } \varepsilon^{\text{RPA}}(\vec{q}, \hbar\omega) \stackrel{(4.7.8)}{\longleftrightarrow} \alpha(\omega) . \quad (5.3.8)$$

Note, that eq. (5.3.7) has an interesting interpretation. First of all, it is a GAUSSIAN distribution with respect to the frequency, having a maximum at

$$\omega = \omega_{nn'} = \frac{1}{\hbar} (E_n - E_{n'}) . \quad (5.3.9)$$

Thus, we indeed obtain spectral lines, where the maximum position is given by the allowed transition frequencies between two bound states  $n$  and  $n'$ . Note also, that the dipole matrix element  $\vec{d}_{nn'}$  enters the expression via  $|\Gamma_2^0|^2$ . In this way, the traditional selection rules for dipole radiation are established in eq. (5.3.7).

However, the spectral lines are broadened due to the motion of the bound states (in the form of a MAXWELLIAN distribution). Thus, we describe the DOPPLER broadening of spectral lines due to the thermal motion of absorbers and emitters in a plasma. The same result is derived in plasma theory by averaging the DOPPLER shift for a velocity  $v$  over a MAXWELLIAN distribution.

Obviously, this approximation is important for describing a partially ionized plasma in the limit of low densities. While  $\Pi_1^{\text{RPA}}$  only results in contributions to the continuum,  $\Pi_2^{\text{RPA}}$  already describes DOPPLER broadened atomic transitions.<sup>8</sup> Now it is possible to treat strongly correlated state contributions (bound states) for calculating the dielectric function as well as density-correlation functions (dynamic structure coefficient).

<sup>8</sup>For further details and more sophisticated calculations, see [RD79].

## 5.4 Consistent approximations for the cluster self-energy

In section 5.3, we have shown, that a cluster decomposition of  $\Pi_2$  can be used to investigate optical properties of a plasma. By calculating  $\text{Im}\Pi_2^{\text{RPA}}$ , DOPPLER broadening can be described accounting for the thermal motion of absorbers and emitters. However, there are additional effects leading also to a broadening of spectral lines. They are due to the perturbation of the emitting and absorbing atoms by the surrounding medium, in our case by a plasma. Having free charges around the atom, the bound states are modified by the STARK effect. Since the motion of the plasma particles is random, the atom is subject to a fluctuating electric field both in magnitude and direction. Of course, these changes will be the more pronounced, the higher the density/pressure in the system. Therefore, this kind of broadening is referred to as pressure-broadening.

The obvious way to account for medium modifications within the GREEN's functions technique is an approximative treatment of the self-energy which contains all corrections to the atom propagator beyond the isolated, unperturbed one.

Thus, we consider:

$$\begin{array}{c} \Rightarrow \\ \Rightarrow \end{array} = \begin{array}{c} \Rightarrow \\ \Rightarrow \end{array} + \begin{array}{c} \Rightarrow \\ \Rightarrow \end{array} \overset{\Sigma_2}{\text{---}} \begin{array}{c} \Rightarrow \\ \Rightarrow \end{array} \quad (5.4.1)$$

In order to describe the collision of a plasma electron with the radiating atom, we start from the screened two-particle self-energy:

$$\Sigma_2(n, P; iz_\mu) = \begin{array}{c} q, iz_\nu \\ \text{---} \\ n, P, iz_\mu \end{array} \begin{array}{c} \Rightarrow \\ \Rightarrow \end{array} \begin{array}{c} n, P, iz_\mu \\ n', P' \\ iz_\mu + iz_\nu \end{array} \quad (5.4.2)$$

Here,  $n$  labels the bound state,  $P$  the center of mass movement and  $z_\mu$  is a bosonic MATSUBARA frequency.

This diagram has already been considered in section 5.1:

$$\begin{aligned} \Sigma_2(n, P; iz_\mu) &= \sum_{n', q, iz_\nu} \Gamma_2^0(n, P; n', P + q; iz_\mu + iz_\nu) \\ &\quad \cdot G_2^{\text{ladd.}}(n', P + q; iz_\mu + iz_\nu) \\ &\quad \cdot \Gamma_2^0(n', P + q; n, P; iz_\mu + iz_\nu) V^s(q, iz_\nu) \end{aligned}$$

and can be further evaluated using (5.1.2):

$$G_2^{\text{ladd.}}(n', P + q; iz_\mu + iz_\nu) = \frac{1}{iz_\mu + iz_\nu - \epsilon_{n', P+q} - \mu_{12}}$$

and the spectral representation of the dynamically screened interaction (4.3.12)

$$V^s(q, iz_\nu) = V(q) \left[ 1 + \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \text{Im} \{ \epsilon^{-1}(q, \omega - i\eta) \} \cdot \frac{1}{iz_\nu - \omega} \right].$$

Performing the MATSUBARA sum with respect to  $z_\nu$  and neglecting a FERMI function for  $n\Lambda^3 \ll 1$ , we obtain

$$\langle n | \Sigma (iz_\mu) | n \rangle = -\frac{1}{e^2} \int \frac{d^3q}{(2\pi)^3} V(q) \sum_{n'} |\Gamma_2^0(n, P; n', P+q)| \cdot \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (1 + n_B(\omega)) \frac{\text{Im} \epsilon_{\text{RPA}}^{-1}(\omega, q - i\eta)}{iz_\mu - \epsilon_{n', P+q} - \hbar\omega} \quad (\underline{A})$$

Here,  $n_B(\omega) = (e^{\beta\hbar\omega} - 1)^{-1}$  is the BOSE function,  $\epsilon_{\text{RPA}}$  is the dielectric function in Random Phase Approximation as discussed in section 4.4. The integrals in (A) can usually only be evaluated numerically.

Having the complex two-particle self-energy at our disposal, we can now generalize the polarization function by using medium-modified atom-propagators:

$$\Pi_2^{(S)} = \text{Diagram} \quad (5.4.3)$$

In this way, self-energy corrections (S) are included. This diagram can be evaluated using the two-particle spectral function  $A_2$  given by

$$G_2(n, P; iz_\nu) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_2(\omega)}{iz_\nu - \omega} \quad (5.4.4)$$

In dilute systems, it is appropriate to approximate  $A_2$  by a LORENTZIAN profile,

$$A_2(\omega) = \frac{2\Gamma_1}{(\hbar\omega - E_1 - \Delta_1)^2 + \Gamma_1^2}, \quad (5.4.5)$$

where  $\Delta_1$  is connected to  $\text{Re} \Sigma_2$  and  $\Gamma_1$  to  $\text{Im} \Sigma_2$  just as discussed in the context of the single-particle GREEN's function, cf. (4.2.6)-(4.2.9).

Inserting (5.4.4) and proceeding as in the proof of (5.3.3) results in

$$\Pi_2^{(S)}(q, i\omega_\lambda) = \sum_{nn'P} \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} A_2(\omega_1) A_2(\omega_2) \frac{g(\omega_1) - g(\omega_2)}{i\omega_\lambda - (\omega_1 - \omega_2)} |\Gamma_2^0|^2 \quad (5.4.6)$$

If we assume sharply peaked LORENTZians for  $A_2$ , the double integration can be performed and  $\Pi_2^{(S)}$  reads

$$\Pi_2^{(S)}(q, i\omega_\lambda) = \sum_{nn'P} \frac{[g(\epsilon_{n,P}) - g(\epsilon_{n',P+q})] |\Gamma_2^0|^2}{i\omega_\lambda - (\epsilon_{n,P} + \Delta_1 - \epsilon_{n',P+q} - \Delta_2) + i(\Gamma_1 + \Gamma_2)}, \quad (5.4.7)$$

where  $\Delta_1$ ,  $\Delta_2$  and  $\Gamma_1$ ,  $\Gamma_2$  are the LORENTZian parameters for the upper and lower two-particle GREEN's function, respectively.

We do not venture into a further calculation of this expression but comment on its structure as compared to (5.3.3).  $\Delta_1$  and  $\Delta_2$  lead to a shift of the unperturbed transition frequency  $\omega_{nn'}$ . Thus,



the real part of the self-energy is connected to a shift in the transition frequency. On the other hand, the imaginary part of  $\Sigma_2$ , which enters via  $\Gamma_1$  and  $\Gamma_2$ , shows up as an additional imaginary contribution in the denominator, implying a broadening as compared to (5.3.3). In particular, in this approximation, the broadening is of LORENTZIAN type. This reflects a result from traditional spectral line theory, where the total profile is a convolution of a GAUSSIAN DOPPLER broadening and a LORENTZIAN pressure broadening, leading in total to a VOIGT profile.

Finally, we have to discuss one further extension of our approach. So far, we have discussed self-energy corrections to the polarization function, see eq. (5.4.3). It can be shown, that vertex corrections, for example of the type

$$\text{Diagram} = \text{Diagram} + \text{Diagram}, \quad (5.4.8)$$

tend to be as important as self-energy corrections. The underlying general theorem is known as the WARD-TAKAHASHI identity and is often used in QED, see also section 4.6.

Our final ansatz for the polarization function therefore reads

$$\Pi_2(q, i\omega_\lambda) = \text{Diagram} = \text{Diagram} + \text{Diagram}. \quad (5.4.9)$$

In total, the polarization function is then given by

$$\begin{aligned} \Pi_2(q, \omega) = n\Lambda_{ei}^3 (1 - e^{-\beta\hbar\omega}) \sum_{n, n_2} \sum_{n'_1, n'_2} \sum_P \Gamma_{n_1, n_2}^0(q) \Gamma_{n_2, n'_1}^{0*}(q) e^{-\beta E_{n_1, P}^0} \\ \cdot \langle n'_2 | \langle n_1 | (L(\Delta\omega) + i\Gamma^\nu)^{-1} | n'_1 \rangle | n_2 \rangle \end{aligned} \quad (5.4.10)$$

and

$$\begin{aligned} L(\Delta\omega) = \Delta\omega - \frac{\vec{P}\vec{k}}{M} - \frac{k^2}{2M} - \text{Re}\{\Sigma_i(\Delta\omega) - \Sigma_f(\Delta\omega)\} \\ + i\text{Im}\{\Sigma_i(\Delta\omega) + \Sigma_f(\Delta\omega)\}, \end{aligned} \quad (5.4.11)$$

where  $\Gamma^\nu$  is the vertex function introduced in (5.4.9) as the filled vertex.

In real calculations, the effect of perturbing ions has to be considered as well. While electron collisions can be treated perturbatively, the effect of ions is hard to be accounted for within perturbation theory. Especially for stationary ions, a number of neighboring ions will influence the radiating atoms at a given instant in time. Therefore, models for the ionic microfield are usually taken from outside of a GREEN's functions approach. In particular, for uncorrelated ions, the ionic microfield distribution is given by the famous HOLTZMARK distribution. Correlation effects among ions have been included by BARANGER and MOZER, HOOPER, and IGLESIAS et al. (APEX), to name but the most important approaches.

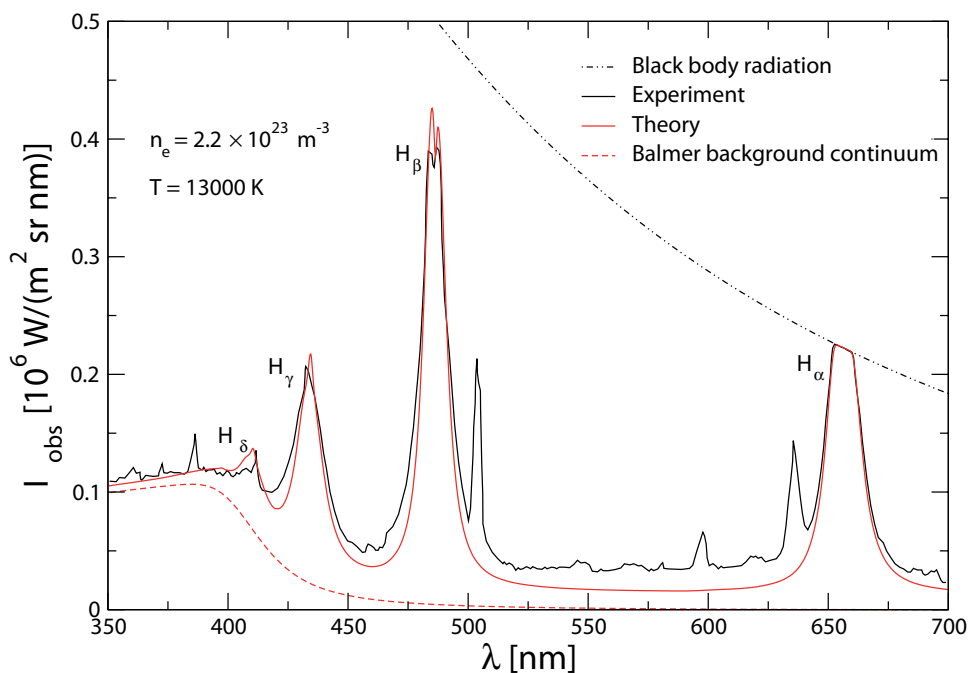
We will briefly summarize a few applications of this theoretical approach to real systems. The shift and width of the  $H_\alpha$  line of hydrogen (BALMER- $\alpha$ ) in dense plasmas has been discussed by S. BÖDDEKER, S. GÜNTER, A. KÖNIES, L. HITZSCHKE and H.J. KUNZE in [BGK<sup>+</sup>93], see figure 3.

TABLE II. Experimental and theoretical shift of the  $H_\alpha$  line.

$N_e$ ( $10^{18} \text{ cm}^{-3}$ )	$T_e$ (eV)	$\Delta\lambda_{\text{expt}}$ ( $\text{\AA}$ )	$\Delta\lambda_{\text{theor,Günter}}$ ( $\text{\AA}$ )	$\Delta\lambda_{\text{theor,Griem}}$ ( $\text{\AA}$ )
0.88	5.6	$4.20 \pm 0.38$	4.69	6.07
1.00	5.7	$5.33 \pm 0.30$	5.35	6.79
1.30	6.0	$6.73 \pm 0.72$	7.00	8.50
1.39	6.1	$7.25 \pm 0.51$	7.49	8.99
1.90	6.4	$9.41 \pm 1.20$	10.27	11.82
2.34	7.0	$11.24 \pm 1.76$	12.59	13.9
3.05	7.8	$15.49 \pm 3.22$	16.16	17.11
4.00	8.5	$19.66 \pm 4.91$	20.63	20.96
5.47	9.2	$20.11 \pm 5.58$	26.99	26.84
6.88	9.8	$22.99 \pm 5.46$	32.74	31.89
8.33	10.2	$27.16 \pm 6.88$	38.76	36.78
9.76	10.4	$35.43 \pm 8.81$	44.62	41.48

FIGURE 3: Shift of the  $H_\alpha$  line in a plasma with electron density  $N_e$  and temperature  $T_e$ , from [BGK<sup>+</sup>93].

The BALMER spectrum has also been measured at smaller densities and temperatures in a well-stabilized arc plasma. In figure 4, a complete synthetic spectrum as obtained from the GREEN's functions approach is compared to the experimental results, see B. OMAR et al., [OWGR07].

FIGURE 4: Experimentally measured and theoretically calculated spectra of hydrogen for  $N_e = 2.2 \times 10^{23} \text{ m}^{-3}$  and  $T = 13000 \text{ K}$ , from [OWGR07]. Self absorption is taken into account by truncation at the black body radiation spectrum.

Investigations have also been carried out for laser-produced plasmas. In particular, hydrogen-like carbon spectra measured by WILHEIM et al. have been analyzed. Figure 5 shows again experimental results compared to synthetic spectra based on the GREEN's functions approach including self-absorption for optical thick media. The results can be found in S. SORGE et al. [SWR<sup>+</sup>00].

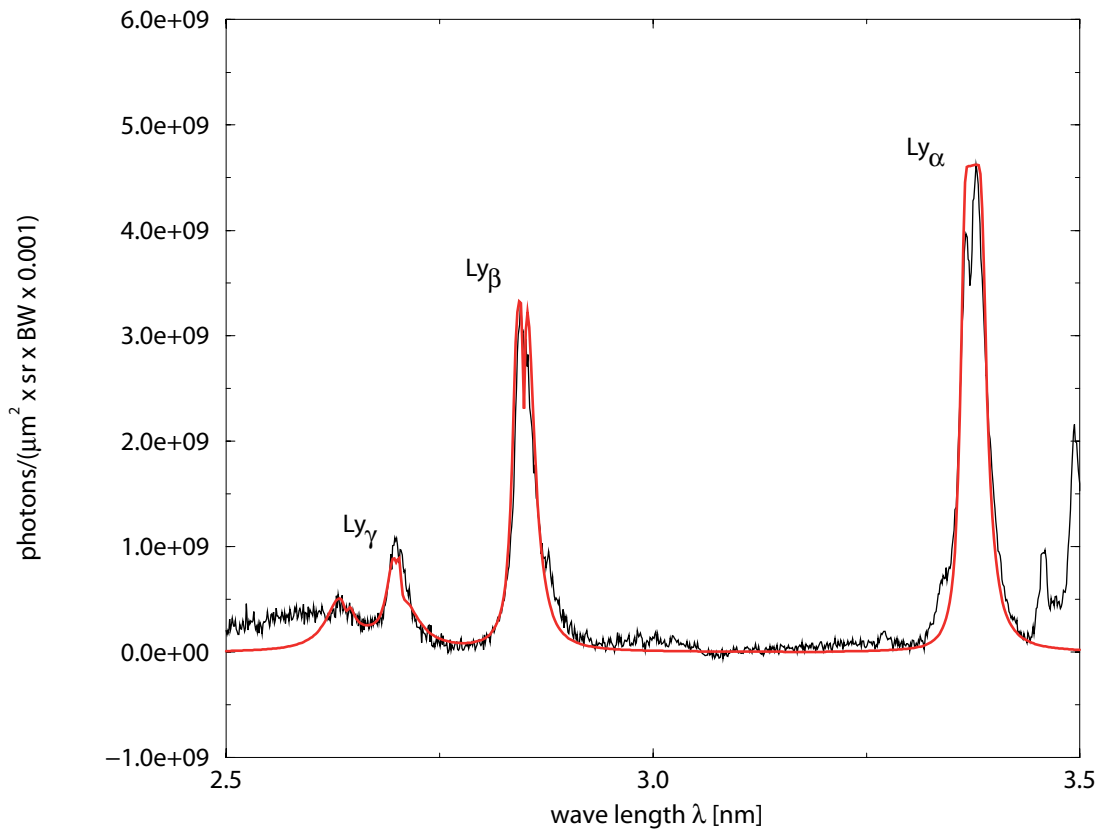


FIGURE 5: Synthetic and measured spectra of a laser-produced carbon plasma, from [SWR<sup>+</sup>00].



## 6 Synopsis / Outlook

During this lecture, we constructed an apparatus for perturbatively treating real (interacting) quantum systems with the HAMILTONIAN

$$H = T + V \quad (6.1.1)$$

in thermal equilibrium. We considered the grand canonical ensemble, modelling the contact with a bath via the temperature  $T$  and the chemical potential  $\mu$ . The ensemble is described by the statistical operator  $\rho_{\text{eq}} = e^{-S}$  with the normalization  $\text{Tr}\{\rho_{\text{eq}}\} = 1$  and given mean values  $\text{Tr}\{\rho_{\text{eq}} H\} = U$ ,  $\text{Tr}\{\rho_{\text{eq}} N\} = \Omega n$ .

The maximum of the mean entropy  $\text{Tr}\{\rho_{\text{eq}} S\}$  at given average energy and particle number is found as the grand-canonical GIBBS ensemble with

$$S = \ln Z(T, \Omega, \mu) + \frac{H}{k_B T} - \mu \frac{N}{k_B T} = S^{(0)} + S^{(1)} + S^{(2)}, \quad (6.1.2)$$

where we used a systematic cluster decomposition with the c-number  $S^{(0)} = \ln Z(T, \Omega, \mu)$  (note, that  $-k_B T \ln Z(T, \Omega, \mu)$  is the grand canonical potential  $J = -p\Omega$ ), the single particle contribution  $S^{(1)} = \sum_{k,k'} s_{kk'}^{(1)} c_k^+ c_{k'}$ , that contains the kinetic energy and the chemical potential, and a two-particle contribution  $S^{(2)}$ , which contains the interaction.

The entropy is an observable and therefore HERMITEAN. The single-particle contribution  $S^{(1)}$  can be diagonalized, e.g. by using momentum eigenstates if the system is homogeneous (no external potential). For this special form of the ideal entropy, all correlation functions can be calculated using WICKS theorem. The higher order contributions (two-particle  $S^{(2)}$  and possibly higher) to the entropy can be treated by perturbation theory. This way, higher order correlation functions appear, which can also be calculated using WICKS theorem. Note, that in the case of an external potential, where  $S^{(1)}$  is not diagonal in momentum representation, we can also diagonalize the single-particle contribution  $S^{(1)}$  by using the solution of the corresponding single-particle Schrödinger equation.

We showed, how the unperturbed higher-order correlation functions that appear in the perturbation expansion can be evaluated using the GREEN's functions technique and its diagrammatic representation. An open problem using perturbative expansions is the convergence. To avoid divergences or non-analytic behavior, we had to perform partial summations of the different diagram classes.

A significant part of correlation effects is already accounted for in the quasi-particle picture, which is a single-pole approximation to the spectral function. Due to the influence of the background mean-field and the resulting self-energy contributions, the interacting particles could be treated as ideal particles with renormalized energies. However, bound particles cannot be described in a mean-field view. We are able to develop a formalism which considers bound states as new entities on the same level as the “elementary” particles, the so-called chemical picture, by considering ladder diagrams. This way, we obtain the correct low-density behavior described by a mass action law.

Although we already included bound states into our method corresponding to a chemical picture, where they were treated as new additional particle species, the inclusion of the cluster formation process and the correct treatment of their internal structure from fundamental principles can only be done in our physical picture, that accounts for the composites' substructure. There, the formation of bound particles at low densities and their dissolution at high densities and temperatures because of screening and PAULI blocking can be described in a systematic way. Selecting out special diagram classes, one has to take care for consistency. For instance, since the impact of self-energy contributions and vertex corrections are of the same magnitude, both have to be considered simultaneously.

With the GREEN's functions technique, a very detailed description of many-particle-systems in thermal equilibrium can be performed. Of course, other approaches, such as numerical simulations can be used to overcome problems of convergence of the perturbation expansion, but numerical solutions have other shortcomings, such as the finiteness of the simulated system and the impossibility to find analytical expressions in limiting cases.

Some further extensions of the GREEN's functions approach given here, are possible and will be briefly discussed:

- The approach, shown in this lecture is restricted to systems, that do not show any phase transition. A perturbative or virial expansion into the region of a phase transition is impossible, because the thermodynamic properties exhibit discontinuities, that cannot be removed. We have to allow for inhomogeneous solutions to find the minimum of the free energy. Note, that the grand canonical ensemble is not equivalent to the canonical one at phase transitions, because the fluctuations of the particle number density are no longer small, and we have to define the ensemble appropriately. For the general investigation of phase transitions, we refer to special courses in this field.
- The description in thermodynamic grand-canonical equilibrium may also become inappropriate in other cases. For example, BOSE-EINSTEIN-condensation cannot be modelled, since  $T$  and  $\mu$  will not fix the number  $N_{\text{condensate}}$  of particles in the condensate. Due to the pole in the BOSE distribution, the ground state is macroscopically occupied. In addition to  $T$  and  $\mu$  ( $\neq 0$ ), we have to fix the total number of particles.

A related problem is the occurrence of quantum condensates in Fermi systems. By introducing a generalized GIBBS ensemble, for example via

$$S^{(1)} = \sum_{11'} s_{11'}^{(1)} a_{1'}^{\dagger} a_1 + \sum_{11'} F_{11'}^{(1)} a_{1'}^{\dagger} a_{\bar{1}}^{\dagger} + \sum_{11'} F_{11'}^{(1)*} a_{\bar{1}} a_{1'} , \quad (6.1.3)$$

where  $\bar{1} = (-p_1, -\sigma_1)$  denotes contributions of the 'conjugate' momentum, it is possible, to account for violated conservation of the particle number. Instead, a 'phase' of the quantum condensate appears and in addition to  $\langle H \rangle$  and  $\langle N \rangle$ , the new order parameter  $\langle a_{1'}^{\dagger} a_{\bar{1}}^{\dagger} \rangle$  and further LANGRANGE multipliers  $F_{11'}^{(1)}$  besides  $T$  and  $\mu$  are implemented.

The additional anomalous terms ( $F_{11'}^{(1)} a_{1'}^{\dagger} a_{\bar{1}}^{\dagger} + \text{c.c.}$ ) in  $S^{(1)}$  can be removed with a BOGOLIUBOV-transform, which has the structure

$$b^{\dagger} = u a^{\dagger} + v a \quad b = u^* a + v^* a^{\dagger} \quad (6.1.4)$$

$$\langle b^{\dagger} b^{\dagger} \rangle = 0 \quad \langle b b \rangle = 0 \quad (6.1.5)$$

with appropriate  $u$  and  $v$ , so that  $S^{(1)}$  is diagonal in  $b$  and only contains contributions  $\propto b^+b$ . Thus, an application of the WICK theorem and the diagram technique is possible again. Some keywords for further studies are: BARDEEN-COOPER-SCHRIEFFER theory, gap-equation, superconductivity, superfluidity, generalized GIBBS-ensemble. It can be shown that below a critical temperature, stationary solutions are possible for  $S$  with non-vanishing pair amplitude  $F_{11'}^{(1)}$ , describing the formation of a quantum condensate.

- Time dependent fluctuations in equilibrium have not been covered until now. As an example, the propagator

$$\langle a_{1'}^+(t'_1) a_1(t_1) \rangle = \text{Tr} \left\{ \varrho_{\text{eq.}} e^{\frac{i}{\hbar} H t'_1} a_{1'}^+ e^{-\frac{i}{\hbar} H (t'_1 - t_1)} a_1 e^{-\frac{i}{\hbar} H t_1} \right\} \quad (6.1.6)$$

$$= \sum_{mn} \int d\omega \frac{e^{-\beta \epsilon_n}}{Z} e^{\frac{i}{\hbar} \omega (t'_1 - t_1)} \langle n | a_{1'}^+ | m \rangle \langle n | a_1 | n \rangle \delta(\epsilon_n - \epsilon_m - \omega) \quad (6.1.7)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{\frac{i}{\hbar} \omega (t'_1 - t_1)} I_1(11', \omega) \quad (6.1.8)$$

is related to the same spectral function introduced for the MATSUBARA GREEN's function above. Thus it is the analytical continuation of  $\langle a_{1'}^+ a_1(\tau) \rangle$  via  $(-\tau) \rightarrow \frac{i}{\hbar}(t'_1 - t_1)$ . An important example are density-density fluctuations  $\langle \varrho n(\vec{r}_1, t_1) n(\vec{r}_2, t_2) \rangle$  with  $n(\vec{r}) = a^+(\vec{r}) a(\vec{r})$ , that are related to the dynamical structure factor. They are evaluated after transformation to momentum representation and evaluating the corresponding spectral function or MATSUBARA GREEN's function (polarization function). Such correlation functions are of interest in transport theory (linear response theory). One can formulate a microscopic approach of the dynamical structure factor, the (longitudinal) dielectric function and the absorption coefficient. The time evolution of equilibrium fluctuations are related to dissipation (keyword: Fluctuation-Dissipation-Theorem).

- A general treatment of the nonequilibrium is possible by extending the approach to equilibrium sketched above via supplementing the set of relevant observables  $\{B_n\}$  with known averages

$$\langle B_n \rangle = \text{Tr} \{ \varrho_{\text{rel}}(t) B_n \} . \quad (6.1.9)$$

The relevant statistical operator is obtained from the maximum of entropy

$$S = -k_B \langle \ln \varrho_{\text{rel}} \rangle \quad (6.1.10)$$

with fixed mean values (constraints) taken into account by LAGRANGE multipliers  $\lambda_n(t)$ . This leads to the generalized Gibbs ensemble

$$\varrho_{\text{rel}}(t) = \frac{1}{Z_{\text{rel}}(t)} e^{-\sum_n \lambda_n(t) B_n} . \quad (6.1.11)$$

The statistical operator is given by ABELS theorem

$$\varrho(t) = \epsilon \int_{-\infty}^t dt' e^{\epsilon(t-t')} e^{-\frac{i}{\hbar} H(t-t')} \varrho_{\text{rel}}(t') e^{\frac{i}{\hbar} H(t-t')} . \quad (6.1.12)$$

For further details, we recommend the special course on nonequilibrium statistical physics. Here, we only mention that in the nonequilibrium case, we have exponents containing the interaction part of the HAMILTONian, which can also be treated using the methods given here.

- Finally, we would like to emphasize, that in addition to many particle physics, the diagram technique has found its application in many other fields of physics. As the original example, we will only mention quantum electrodynamics (QED), where the HAMILTONIAN  $H = \int d^3r \mathcal{H}$  is replaced by the HAMILTON density  $\mathcal{H}$ ,

$$\begin{aligned}
 \mathcal{H} = & \sum_c \bar{\phi}_c(\vec{r}, t) \left( -i\hbar c \vec{\gamma} \cdot \nabla + m_c c^2 \right) \phi_c(\vec{r}, t) \\
 & + \left[ \frac{1}{2\epsilon_0} \vec{P}_{\text{transv}}^2(\vec{r}, t) + \frac{\epsilon_0 c^2}{2} \left( \vec{\nabla} \times \vec{A}(\vec{r}, t) \right)^2 \right] \\
 & + \sum_c \bar{\phi}_c(\vec{r}, t) \left( -e_c c \vec{\gamma} \cdot \vec{A}(\vec{r}, t) \right) \phi_c(\vec{r}, t) \\
 & + \frac{1}{2} \sum_{c,d} \int d^3\vec{r}' \phi_c^\dagger(\vec{r}, t) \phi_d^\dagger(\vec{r}', t) \frac{e_c e_d}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} \phi_d(\vec{r}', t) \phi_c(\vec{r}, t)
 \end{aligned} \tag{6.1.13}$$

or, respectively,

$$\mathcal{H} = \underbrace{\mathcal{H}_{\text{DIRAC}}}_{\text{Electron / Positron}} + \underbrace{\mathcal{H}_{\text{MAXWELL}}}_{\text{(transversal) Photon}} + \underbrace{\mathcal{H}_{\text{Radiation}}}_{\text{Photon}} + \underbrace{\mathcal{H}_{\text{COULOMB}}}_{\text{Coulomb}} \tag{6.1.14}$$

The COULOMB part as well as the radiation part can be treated using perturbation theory. The FEYNMAN diagrams, that are subject to very similar rules as the diagrams given above, have originally been introduced for this purpose: While during this lecture, we only concentrated on the COULOMB contribution in a many-body system, an analogous approach is also possible for the radiation part. However, due to the spinor-character of the wave functions or operators, respectively, the algebra is much more complicated. Therefore, we recommend a special course on quantum electrodynamics for further studies in this field.

Although many attempts have been made, a unification of quantum many-body theory and quantum electrodynamics remains open and is subject of current intense research.



# Bibliography

- [AB84] Nestor R. Arista and Werner Brandt. Dielectric response of quantum plasmas in thermal equilibrium. *Physical Review A*, 29(3):1471–, March 1984.
- [Bay62] Gordon Baym. Self-Consistent Approximations in Many-Body Systems. *Physical Review*, 127(4):1391–, August 1962.
- [BGK<sup>+</sup>93] St. Böddeker, S. Günter, A. Könies, L. Hitzschke, and H.-J. Kunze. Shift and width of the  $H_\alpha$  line of hydrogen in dense plasmas. *Physical Review E*, 47(4):2785–, April 1993.
- [For08] Carsten Fortmann. Self-consistent spectral function for non-degenerate Coulomb systems and analytic scaling behaviour. *Journal of Physics A: Mathematical and Theoretical*, 41(44):445501–, 2008.
- [For09] C. Fortmann. Single-particle spectral function for the classical one-component plasma. *Physical Review E*, 79(1):016404–11, January 2009.
- [FRW07] C. Fortmann, G. Röpke, and A. Wierling. Optical Properties and One-Particle Spectral Function in Non-Ideal Plasmas. *Contributions to Plasma Physics*, 47(4-5):297–308, 2007.
- [FW71] A. L. Fetter and J. D. Walecka. *Quantum Theory of Many-Particle Systems*. International Series in Pure and Applied Physics. McGraw-Hill, Inc., 1971.
- [Hua87] K. Huang. *Statistical Mechanics*. John Wiley & Sons, 2nd edition, 1987.
- [KB62] L. P. Kadanoff and G. Baym. *Quantum Statistical Mechanics*. Advanced Book Classics. Addison-Wesley Publishing Company Inc., 1989, originally published in 1962.
- [KKER86] W. D. Kraeft, D. Kremp, W. Ebeling, and G. Röpke. *Quantum Statistics of Charged Particle Systems*. Akademie-Verlag, Berlin, 1986.
- [KKL84] D. Kremp, W. D. Kraeft, and A. J. D. Lambert. Equation of state and ionization equilibrium for nonideal plasmas. *Physica A: Statistical and Theoretical Physics*, 127(1-2):72–86, August 1984.
- [LPL84] L. D. Landau, L. P. Pitaevskii, and E. M. Lifshitz. *Electrodynamics of Continuous Media*, volume 8 of *Course of Theoretical Physics*. Butterworth-Heinemann, 2nd edition, 1984.
- [Mah90] G. D. Mahan. *Many-Particle Physics*. Physics of Solids and Liquids. Plenum Press, New York and London, 2nd edition, 1990.
- [Nol03] W. Nolting. *Quantenmechanik*, volume 5/2 of *Grundkurs theoretische Physik*. Springer-Verlag GmbH, 5th edition, 2003.
- [OWGR07] B. Omar, A. Wierling, S. Günter, and G. Röpke. Hydrogen Balmer Spectrum from a High-Pressure Arc Discharge: Revisited. *Contributions to Plasma Physics*, 47(4-5):315–323, 2007.
- [RD79] G. Röpke and R. Der. The influence of two-particle states (excitons) on the dielectric function of the electron-hole plasma. *Physica Status Solidi (b)*, 92(2):501–510, 1979.
- [Ric81] G. Rickayzen. *Green's Functions and Condensed Matter*. Techniques of Physics. Academic Press, 1981.

- [RMS82] G. Röpke, L. Münchow, and H. Schulz. Particle clustering and Mott transitions in nuclear matter at finite temperature : (I). Method and general aspects. *Nuclear Physics A*, 379(3):536–552, May 1982.
- [SR93] H. Stein and G. Röpke. Greensfunktions-Technik für statistische Gesamtheiten. Lecture notes, August 1993.
- [SWR<sup>+</sup>00] S. Sorge, A. Wierling, G. Röpke, W. Theobald, R. Sauerbrey, and T. Wilhein. Diagnostics of a laser-induced dense plasma by hydrogen-like carbon spectra. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 33(16):2983–3000, 2000.
- [SZ79] H. Stolz and R. Zimmermann. Correlated pairs and a mass action law in two-component Fermi systems excitons in an electron-hole plasma. *Physica Status Solidi (b)*, 94(1):135–146, 1979.
- [Yam54] Yoshio Yamaguchi. Two-Nucleon Problem When the Potential Is Nonlocal but Separable. I. *Physical Review*, 95(6):1628–, September 1954.
- [YY54] Yoshio Yamaguchi and Yoriko Yamaguchi. Two-Nucleon Problem When the Potential Is Nonlocal but Separable. II. *Physical Review*, 95(6):1635–, September 1954.
- [ZKK<sup>+</sup>78] R. Zimmermann, K. Kilimann, W. D. Kraeft, D. Kremp, and G. Röpke. Dynamical screening and self-energy of excitons in the electron-hole plasma. *Physica Status Solidi (b)*, 90(1):175–187, 1978.

# Index

## A

Absorption coefficient ..... 72  
Annihilation operator ..... 5

## B

BETH-UHLENBECK formula ..... 97  
BETHE-SALPETER eq. .... 76, 88, 92  
BOGOLIUBOV transform..... 108  
BOSE distribution ..... 7  
BOSE-EINSTEIN condensation ..... 97, 108  
Bound states ..... 75, 88, 92

## C

Chemical picture ..... 75, 87, 98  
Cluster  
    multi-particle ..... 92  
    random phase approximation..... 98  
    self-energy ..... 101  
Conductivity ..... 73  
Contraction ..... 12  
    creator & annihilator ..... 13  
Convergence factor ..... 40  
COOPER pairs..... 97  
Correlation function  
    high-order ..... 12  
COULOMB interaction ..... 38, 54  
Creation operator ..... 5

## D

Debye approximation ..... 70  
Density matrix ..... 21  
    connection to  $G_1^{\lessgtr}$  ..... 23  
Diagram rules ..... 39  
    HARTREE-FOCK approximation ..... 44  
Diagram technique, elements of ..... 87  
Dielectric function ..... 55, 72  
    absorption coefficient ..... 72  
    cluster decomposition ..... 98  
    index of refraction ..... 72

    LANDAU damping ..... 64 ff.  
    long wavelength limit ..... 62  
    random phase approx. .... 60, 67  
    static limit ..... 61  
Dipole matrix element ..... 88  
DIRAC identity ..... 29  
DOPPLER broadening ..... 100, 103  
DRUDE relation ..... 73  
DYSON  
    equation ..... 51  
    series ..... 9

## E

Effective mass ..... 51  
Electromagnetic waves ..... 72  
Energy conservation ..... 17, 40  
Ensemble, grand-canonical ..... 6  
Entropy operator ..... 6  
    cluster decomposition ..... 6  
EOS ..... *see* equation of state  
Equation of state  
    ideal FERMI gas ..... 33  
    many-particle system ..... 97  
Exchange term ..... 75

## F

FERMI distribution ..... 7  
FEYNMAN diagrams ..... 36, 110  
Fluctuations, time dependent ..... 109  
FOCK diagram ..... 46  
Form factor ..... 80  
FOURIER  
    expansion of Green's function ..... 25  
    transform of  $G_1^<$  ..... 27

## G

GOULD-DEWITT approximation ..... 90  
GREEN's function ..... 21  
    ideal FERMI gas ..... 31

- perturbation theory ..... 35  
 scheme of application ..... 30  
 GW-approximation ..... 70  
 GW<sup>(0)</sup>-approximation ..... 71  
 GWT-approximation ..... 71
- H**
- HAMILTON
- density ..... 110  
 operator  
   general ..... 6  
   ideal quantum gas ..... 5  
   ideal FERMI gas ..... 31
- HARTREE diagram ..... 46
- HARTREE-FOCK
- approximation ..... 15, 44  
 energy shift ..... 19  
 equation of state ..... 15, 49  
 occupation number ..... 18  
 self-energy ..... 47 f.  
 spectral function ..... 49
- HEAVISIDE step-function ..... 22
- HEISENBERG picture ..... 21
- I**
- Ideal FERMI gas ..... 31  
 Index of refraction ..... 72  
 Interaction picture ..... 35  
 Interaction, properties ..... 37  
 Ionic microfield ..... 103
- J**
- JORDAN's lemma ..... 42
- K**
- KIRCHHOFF's law ..... 72  
 KUBO-MARTIN-SCHWINGER cond. .... 23
- L**
- Ladder approximation ..... 76  
 LANDAU damping ..... 64 ff.
- M**
- Magnetic susceptibility ..... 72  
 MAL ..... *see* mass action law
- Mass action law ..... 92, 97  
 MATSUBARA  
   frequency ..... 25  
   frequency summation ..... 41  
   GREEN's function ..... 25  
 MAXWELL's equations ..... 72  
 Momentum conservation ..... 40  
 MONTROLL-WARD approximation ..... 70, 91
- N**
- Non-equilibrium ..... 109
- P**
- Parquet approximation ..... 90  
 Partial summation ..... 47  
 Perturbation theory ..... 9  
   diagrammatic representation ..... 37  
   GREEN's function ..... 35  
   time-dependent ..... 36  
 Phase transition ..... 108  
 Plasmon resonance ..... 60, 67  
 Polarization function ..... 53 f.  
   cluster decomposition ..... 98, 101 ff.  
   random phase approx. .... 59  
 Pressure broadening ..... 101, 103  
 Propagator  
   algebraic representation ..... 79  
   photon ..... 53 f.  
   single-particle  
     full ..... 50  
     single-particle, free ..... 33  
   two-particle  
     free ..... 75  
     ladder approximation ..... 77, 88
- Q**
- Quantum condensate ..... 108  
 Quantum electrodynamics ..... 110  
 Quasi particle concept ..... 47
- R**
- Rainbow diagrams ..... 69  
 Random phase approximation  
   dielectric function ..... 60  
   polarization function ..... 59  
 Reduced distribution function ..... 21

- 
- Renormalization, charge.....69  
Residue theorem.....42  
RPA..... *see* random phase approx.
- S**
- Scattering  
    length.....85  
    phase-shift.....82  
SCHRÖDINGER eq., two-particle.....77, 80  
Screened interaction.....54 f.  
    spectral representation.....58  
Screening  
    DEBYE.....61  
    effect.....58  
    equation.....53 f.  
Self-energy  
    cluster, consistent approx.....101  
    single-particle.....50  
    cluster expansion.....92  
    HARTREE-FOCK.....47 f.  
    screened.....70, 91  
    shift.....51  
    spectral function.....52  
    two-particle, screened.....91  
Separable potential.....80  
Spectral  
    density.....27 f.  
    function.....29  
    lines.....100  
Statistical operator.....6  
    ideal FERMI gas.....31  
Summation  
    MATSUBARA frequency.....41  
    wave-number.....7
- T**
- $T$ -matrix.....92  
Thomas-Fermi approximation.....60  
Time ordering operator.....22  
Topological equivalence.....39  
Two-particle problem.....76
- V**
- VAN-DER-WAALS interaction.....97  
Vertex.....40, 53 f.  
    equation.....68  
    single-particle.....68  
    two-particle.....88  
VOIGT profile.....103
- W**
- WARD-TAKAHASHI identity.....70, 103  
Wave equation.....72  
WICK's theorem.....12
- Y**
- YAMAGUCHI interaction.....80  
    binding energy.....81















