

IV. QUANTUM FIELD THEORY, GREEN'S FUNCTION, AND PERTURBATION THEORY

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I will give a short introduction into field theoretical methods used for quantum many-body problems, the perturbative expansion of the partition function and of the (single particle) Green's function. We sketch and use some useful methods like Wick's theorem and the linked cluster expansion. Diagrams for finite temperature perturbation theory are conveniently written in Fourier space using Matsubara-frequencies. I will show how simple series of particular diagrams can be resummed by self-consistent equations, Hartree-Fock, T-matrix, RPA. They cure different problems concerning expansions in bare parameters. A rearrangement in terms of "renormalized" parameters leads to better behaved expansions.

A. Field theoretical methods for the partition function, perturbative expansions

The grand partition function of a many body system at temperature $T = 1/\beta$ is the basic object which contains all its thermodynamic information

$$Z = \text{Tr} e^{-\beta(H - \mu N)} \quad (1)$$

where H is the Hamiltonian and μ the chemical potential. In the limit of large volumes Ω the grand partition function is related to the pressure P via

$$Z_g = e^{\beta P \Omega} \quad (2)$$

In general, we will not be able to find an exact solution for an interacting N -body Hamiltonian, but for a simpler reference-system H_0 , and we have

$$H = H_0 + V \quad (3)$$

and naturally, we try a perturbation expansion in power of V .

Quantum Mechanical Perturbation Theory. Straightforward perturbation theory for the energy eigenvalue E_n in terms of the unperturbed values $E_n^{(0)}$ and the matrix elements $V_{nm} = \langle E_n^{(0)} | V | E_m^{(0)} \rangle$ gives

$$E_n = E_n^{(0)} + V_{nn} + \sum_{m \neq n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} + \dots \quad (4)$$

and the canonical free-energy expansion therefore writes

$$\begin{aligned} F &= -T \log \sum_n e^{-\beta E_n} \\ &= F_0 + \sum_n V_{nn} e^{-\beta(E_n^{(0)} - F_0)} + \frac{1}{2} \sum_{m,n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} \left(e^{-\beta(E_n^{(0)} - F_0)} - e^{-\beta(E_m^{(0)} - F_0)} \right) + \frac{\beta}{2} \left[\sum_n V_{nn} e^{-\beta(E_n^{(0)} - F_0)} \right]^2 + \dots \end{aligned} \quad (5)$$

This straightforward expansions is rather limited for general N -body systems.

- The perturbative expansion assumes non-degenerate energy eigenstates $E_n^{(0)}$. However, in an extended quantum systems many energy eigenstates are degenerate or nearly degenerate in the limit of infinite system size. The thermodynamic limit must be taken with particular care.

- Only adiabatic changes can be obtained, where E_n has a one-to-one correspondence to $E_n^{(0)}$. What about new (bound) states which do not exist for the reference system?
- Higher order contributions are not only difficult to calculate, but already difficult to write down. Structural analysis of the perturbation expansion is not easy.

We are therefore faced to reformulate perturbation theory for the many-body problem, in order to perform a general perturbation analysis.

Interaction Representation. Analogous to quantum field theory we can introduce the interaction representation with “time”-dependant operators, O

$$O(\tau) = e^{\tau(H_0 - \mu N)} O e^{-\tau(H_0 - \mu N)} \quad (7)$$

where $O \equiv O(\tau = 0)$. We further introduce a matrix $\mathcal{A}(\tau)$ defined via

$$\begin{aligned} e^{-\tau(H - \mu N)} &= e^{-\tau(H_0 - \mu N)} \mathcal{A}(\tau) \\ e^{\tau(H - \mu N)} &= \mathcal{A}^{-1}(\tau) e^{\tau(H_0 - \mu N)} \end{aligned} \quad (8)$$

which plays the role of the S-matrix. We can obtain an explicit representation of \mathcal{A} differentiating the first equation with respect to τ

$$-(H - \mu N) e^{-\tau(H - \mu N)} = -(H_0 - \mu N) e^{-\tau(H_0 - \mu N)} \mathcal{A}(\tau) + e^{-\tau(H_0 - \mu N)} \frac{d\mathcal{A}(\tau)}{d\tau} \quad (9)$$

or

$$e^{-\tau(H_0 - \mu N)} \frac{d\mathcal{A}(\tau)}{d\tau} = (H_0 - H) e^{-\tau(H_0 - \mu N)} \mathcal{A}(\tau) \quad (10)$$

Multiplying both sides with $e^{\tau(H_0 - \mu N)}$ and introducing the perturbation in the interaction representation, $V(\tau) = e^{\tau(H_0 - \mu N)} (H - H_0) e^{-\tau(H_0 - \mu N)}$, we get

$$\frac{d\mathcal{A}(\tau)}{d\tau} = -V(\tau) \mathcal{A}(\tau) \quad (11)$$

The formal solution of this differential equation satisfying the initial value $\mathcal{A}(\tau = 0) = 1$ has the form

$$\mathcal{A}(\tau) = T_\tau \exp \left\{ - \int_0^\tau V(\tau') d\tau' \right\} \quad (12)$$

where the “time-ordering” operator T_τ means that all operators must be arranged from the left to the right in order of decreasing τ , including a factor -1 for fermions.

$$T_\tau [\Psi(\mathbf{r}, \tau) \Psi^\dagger(\mathbf{r}', \tau')] = \begin{cases} \Psi(\mathbf{r}, \tau) \Psi^\dagger(\mathbf{r}', \tau') & \text{for } \tau > \tau' \\ \pm \Psi(\mathbf{r}', \tau') \Psi^\dagger(\mathbf{r}, \tau) & \text{for } \tau < \tau' \end{cases} \quad (13)$$

We can verify this solution by direct differentiation.

We have now a different starting point for doing perturbation theory writing

$$Z = \text{Tr} \left\{ e^{-\beta(H_0 - \mu N)} T_\tau \exp \left[- \int_0^\beta V(\tau') d\tau' \right] \right\} \quad (14)$$

Expanding the exponential on the rhs we obtain the perturbation series in power of V

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n \langle T_\tau [V(\tau_1) V(\tau_2) \dots V(\tau_n)] \rangle_0 \quad (15)$$

where $\langle \dots \rangle_0$ is the average corresponding to the reference Hamiltonian H_0 and partition function Z_0 . Now, for almost all real problems, the reference Hamiltonian is a quadratic form in the field operator

$$H_0 - \mu N = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[-\frac{\nabla^2}{2m} + u(\mathbf{r}) - \mu \right] \Psi(\mathbf{r}) \quad (16)$$

where we have used that

$$N = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) \quad (17)$$

Since H_0 commutes with itself, and also with N , $H_0 - \mu N$ is time-independent in the interaction representation. The interaction, V , contains some powers of field operators. Concretely, we limit the discussion to a two-body interaction

$$V(\tau) = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \Psi^\dagger(\mathbf{r}\tau) \Psi^\dagger(\mathbf{r}'\tau) v(|\mathbf{r} - \mathbf{r}'|) \Psi(\mathbf{r}'\tau) \Psi(\mathbf{r}\tau) \quad (18)$$

Note that we use the convention that

$$\Psi(\mathbf{r}\tau) \equiv e^{\tau(H_0 - \mu N)} \Psi(\mathbf{r}) e^{-\tau(H_0 - \mu N)} \quad (19)$$

$$\Psi^\dagger(\mathbf{r}\tau) \equiv e^{\tau(H_0 - \mu N)} \Psi^\dagger(\mathbf{r}) e^{-\tau(H_0 - \mu N)} \quad (20)$$

so that $\Psi^\dagger(\mathbf{r}\tau)$ is not the hermitian operator of $\Psi(\mathbf{r}\tau)$ (however, the analytic continuations of the operators, $\Psi(\mathbf{r}t)$ and $\Psi^\dagger(\mathbf{r}t)$, to “real time” t , $\tau \rightarrow it$, are hermitian).

Wick’s theorem. A typical term in the perturbative expansion of the partition function will involve expectation values over a certain number of time-ordered field operators like for example

$$\langle T_\tau [\Psi^\dagger(\mathbf{r}_1, \tau_1) \Psi^\dagger(\mathbf{r}_2, \tau_2) \Psi(\mathbf{r}_3, \tau_3) \Psi(\mathbf{r}_4, \tau_4)] \rangle_0 \quad (21)$$

Expressions like this can be simplified using Wick’s theorem, which can be written as

$$\begin{aligned} & \langle T_\tau [\Psi(\mathbf{r}_{i_1}, \tau_{i_1}) \Psi(\mathbf{r}_{i_2}, \tau_{i_2}) \dots \Psi(\mathbf{r}_{i_N}, \tau_{i_N}) \Psi^\dagger(\mathbf{r}_{j_N}, \tau_{j_N}) \Psi^\dagger(\mathbf{r}_{j_{N-1}}, \tau_{j_{N-1}}) \dots \Psi^\dagger(\mathbf{r}_{j_1}, \tau_{j_1})] \rangle_0 \\ &= \sum_P (\pm 1)^P \langle T_\tau [\Psi(\mathbf{r}_{i_1}, \tau_{i_1}) \Psi^\dagger(\mathbf{r}_{j_1}, \tau_{j_P(1)})] \rangle_0 \langle T_\tau [\Psi(\mathbf{r}_{i_2}, \tau_{i_2}) \Psi^\dagger(\mathbf{r}_{j_P(2)}, \tau_{j_P(2)})] \rangle_0 \dots \langle T_\tau [\Psi(\mathbf{r}_{i_N}, \tau_{i_N}) \Psi^\dagger(\mathbf{r}_{j_P(N)}, \tau_{j_P(N)})] \rangle_0 \end{aligned} \quad (22)$$

where $+$ -sign ($-$ -sign) must be used for bosons (fermions). Expressions which do not contain the same number of creation and annihilation operators do not conserve the total number of particles and vanish identically. Note that the time-ordering operator always allows us to change the ordering in expressions like Eq. (21) to bring it into the form of Wick’s theorem, Eq. (22), changing the sign each time two fermion-operators are commuted.

Wick’s theorem can be demonstrated using an expansion of the field operator in eigenstates of the unperturbed system, $\varphi_n(\mathbf{r})$ with corresponding energies ε_n

$$\Psi(\mathbf{r}) = \sum_n \varphi_n(\mathbf{r}) a_n \quad (23)$$

which diagonalizes the unperturbed Hamiltonian

$$H_0 = \sum_n \varepsilon_n a_n^\dagger a_n \quad (24)$$

Expanding also the field operators in the the perturbative expansion, e.g. Eq. (21), we get

$$\sum_{n_1, n_2, n_3, n_4} \varphi_{n_1}^*(\mathbf{r}_1) \varphi_{n_2}^*(\mathbf{r}_2) \varphi_{n_3}(\mathbf{r}_3) \varphi_{n_4}(\mathbf{r}_4) \langle T_\tau [a_{n_1}^\dagger(\tau_1) a_{n_2}^\dagger(\tau_2) a_{n_3}(\tau_3) a_{n_4}(\tau_4)] \rangle_0 \quad (25)$$

Since the time-evolution of the operators in the eigenmodes is rather trivial,

$$a_n(\tau) = e^{-\tau(\varepsilon_n - \mu)} a_n(0) \quad (26)$$

$$a_n^\dagger(\tau) = e^{\tau(\varepsilon_n - \mu)} a_n^\dagger(0) \quad (27)$$

the expression (25) reduces to a static average over annihilation/ creation operators in a thermal state. The time-ordering operator fixes only the order of the operators involved.

For any thermal state the only non-zero terms contributing in the summation in the expression (25) are $n_1 = n_3$, $n_2 = n_4$ or $n_1 = n_4$, $n_2 = n_3$. Summation over all $n_1 \neq n_2$ we recover the result of Wick’s theorem. For a thermal state, the mean occupation of each mode is of order N^{-1} , and we can therefore neglect the contribution $n_1 = n_2 = n_3 = n_4$ in the summation in expression (25) for large systems. Note that we explicitly exclude phenomena

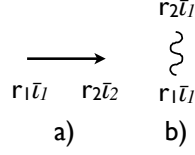


FIG. 1: a) Basic propagator representing $G_0(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2)$, and b) interaction vertex $v(\mathbf{r}_1 - \mathbf{r}_2)$.

like Bose condensation, where one mode is macroscopically occupied. If we want to apply Wick's system to Bose condensed systems, we have to separate the condensate mode first.

We have demonstrated Wick's theorem for the case of four operators, the general case can be shown by induction. Using a path integral representation for the quantum field, Wick's theorem reduces to the properties of a gaussian statistics, where all moments can be expressed in terms of the second moment.

Feynman diagrams. Inserting the potential in the interaction representation in the perturbative expression for the partition function, Eq. (15), we can apply Wick's theorem and obtain a systematic expansion which we can summarize using Feynman diagrams. Basic elements are the unperturbed propagator, G_0 ,

$$G_0(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) = -\langle T_\tau [\Psi(\mathbf{r}_1, \tau_1) \Psi^\dagger(\mathbf{r}_2, \tau_2)] \rangle_0 \quad (28)$$

and the bare interaction $v(|\mathbf{r}_1 - \mathbf{r}_2|)$ which is instantaneous in time τ . Both are graphically represented by an arrow or a wavy line (see Fig. (1)). We have achieved the first goal: using Feynman diagrams the perturbation theories can be systematically represented up to very high orders.

Linked Cluster Theorem. This theorem states that only connected diagrams contribute to the logarithm of the partition function

$$\log \frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n \langle T_\tau [V(\tau_1) V(\tau_2) \dots V(\tau_n)] \rangle_{0,c} \quad (29)$$

For a first demonstration we decompose all graphs with n interaction vertices into groups of connected graphs. We will have m_1 connected graphs with 1 vertex, m_2 connected graphs with 2 vertices, etc., so that $n = \sum_i m_i i$. We denote Ξ_m the connected diagram of order m ,

$$\Xi_m = \frac{(-1)^m}{m!} \int d\tau_1 \int d\tau_2 \dots \int d\tau_m \langle T_\tau [V(\tau_1) V(\tau_2) \dots V(\tau_m)] \rangle_{0,c} \quad (30)$$

where we have divided by the number of possibilities $m!$ for different labels of the interaction vertices. The n th order of the perturbation expansion, Eq. (15), now writes

$$\frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n \langle T_\tau [V(\tau_1) V(\tau_2) \dots V(\tau_n)] \rangle_0 = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \dots \sum_{m_n=0}^{\infty} \delta_{\sum_i i m_i, n} \prod_i \frac{1}{m_i!} \Xi_i^{m_i} \quad (31)$$

where we have used that the number of different labels of the interaction vertices is given by

$$n! \prod_i \frac{1}{m_i! (i!)^{m_i}} \quad (32)$$

The factor $i!$ as well as the sign stemming from $(-1)^n = \prod (-1)^{i m_i}$ has been absorbed in our definition of Ξ_i , Eq. (30).

Adding all contributions from all orders in n , the constraint of the discrete delta of each order in n , e.g. in the rhs of Eq. (31), becomes irrelevant, and we can write the perturbation expansion of Eq. (15) in the following way

$$\frac{Z}{Z_0} = \sum_{m_1=0}^{\infty} \frac{\Xi_1^{m_1}}{m_1!} \sum_{m_2=0}^{\infty} \frac{\Xi_2^{m_2}}{m_2!} \dots \sum_{m_n=0}^{\infty} \frac{\Xi_n^{m_n}}{m_n!} = \exp \left[\sum_{m=1}^{\infty} \Xi_m \right] \quad (33)$$

and we directly obtain Eq. (15). We see that the disconnected graphs actually do not contribute to the logarithm of the partition function. In contrast to disconnected diagrams, connected diagrams are all proportional to the total number of particles and the linked cluster theorem ensures therefore the extensivity of the free energy. We have

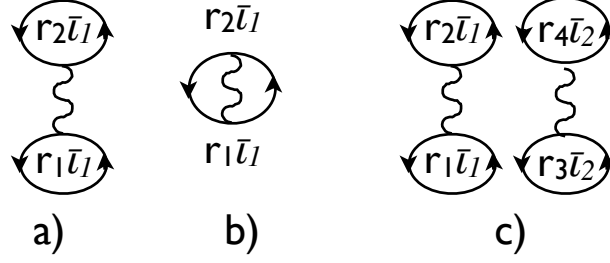


FIG. 2: First order diagrams contributing to the free energy a) direkt diagram, b) exchange diagram. A disconnected diagram of the partition function is shown in c)

managed to arrange perturbation theory in order to obtain a meaningful expansion of the free energy in the sense that its extensivity is guaranteed in each order in perturbation theory, considering only connected graphs of order n .

Replica trick. A different way to obtain the linked cluster theorem is to use the replica trick, where we look at

$$\log \frac{Z}{Z_0} = \lim_{n \rightarrow 0} \frac{(Z/Z_0)^n - 1}{n} \quad (34)$$

where we used that $x^n = e^{n \log x}$. Now, Z^n can be written also as a single partition function with n different systems, the replicas. Each particle in one of the systems is interacting with all other particles in the same system, but not with the ones of the other replicas. Therefore, each connected graph in the perturbative expansion of Eq. (34) can occur independently for each replica, therefore it can only occur in the combination n times the value of the connected graph for one replica. Disconnected graphs of the perturbative expansion are then at least of order n^2 . We can analytically continue the series given for integer positive n to obtain a function of n , where we can take the limit of $n \rightarrow 0$ in Eq. (34). We recover the linked cluster theorem, since only terms proportional to n in the perturbative expansion of the replicas survive corresponding to connected graphs only.

Feynman rules for Ξ_n . Explicitly, we obtain the n th order of the perturbation expansion, Eq. (29), by drawing all connected, closed diagrams using m interaction vertices, and $2m$ propagators G_0 . In general, all topological equivalent diagrams will contribute with the same value. We obtain all topological equivalent diagrams by fixing one of the n vertices V and by permuting the $(n-1)$ remaining vertices. Considering only one of the topological diagrams we have to multiply its value with $(n-1)!/n! = 1/n$ considering the $1/n!$ of the definition of Ξ_n . Further we have to include the sign $(-1)^n$ and integrate over all coordinates and times. Note that any propagator with vanishing time corresponds to the limit

$$G_0(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_1) \equiv \lim_{\tau \rightarrow 0^+} G_0(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_1 + \tau) \quad (35)$$

since equal time ordering has to reproduce the normal order of the interaction, Eq. (18). If we are looking at fermions, we have to multiply the expression with $(-1)^F$ where F is the number of fermion loops. We obtain the last sign by considering that the original ordering of the operators in expression (18) for m vertices corresponds to $2m$ fermion loops contracting the two operators from the same interaction which gives rise to a positive term separately for each interaction (the direct term). Any exchange which changes the number of loops by one is associated with an odd number of operator-permutations and obtains an additional minus sign.

In Fig. 2, the first order diagrams are drawn. They correspond to the expressions

$$\Xi_1^{(a)} = - \int d\mathbf{r}_1 \int d\mathbf{r}_2 \int_0^\beta d\tau G_0(\mathbf{r}_1 \tau; \mathbf{r}_1 \tau + 0^+) v(|\mathbf{r}_1 - \mathbf{r}_2|) G_0(\mathbf{r}_2 \tau; \mathbf{r}_2 \tau + 0^+) \quad (36)$$

$$\Xi_1^{(b)} = \mp \int d\mathbf{r}_1 \int d\mathbf{r}_2 \int_0^\beta d\tau G_0(\mathbf{r}_1 \tau; \mathbf{r}_2 \tau + 0^+) v(|\mathbf{r}_1 - \mathbf{r}_2|) G_0(\mathbf{r}_2 \tau; \mathbf{r}_1 \tau + 0^+) \quad (37)$$

The minus sign in the second equation corresponds to bosons, the plus sign to fermions, since the graph in Fig. 2b) contains only one fermion loop.

B. Finite-temperature Green's function

Up to now, we have derived a perturbation expansion of the free energy, which we can analyze graphically using Feynman's diagram; each diagram corresponds to a precise expression with fixed rules. In general, perturbative series of interacting systems, are not absolutely convergent, but have only asymptotic character. Strictly speaking, the range of validity of asymptotic series is zero, unless an exact resummation of all terms can be performed. Nevertheless, restricted to the first few terms, they can give precise results for small parameter. However, increasing the order of the terms involved, the precision can get worse. Roughly speaking, one encounters frequently situations where the first order expressions are not too bad, but no improvement is found considering further the second or third order in perturbation theory.

Proper resummation can cure this problem of asymptotic series, however, in order to control this method, one needs more information concerning the analytic structure of the series. A convenient tool for that is the one-particle Green's function at finite temperature defined by

$$\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \tau) = \begin{cases} -\langle e^{\tau(H-\mu N)} \Psi(\mathbf{r}_1, 0) e^{-\tau(H-\mu N)} \Psi^\dagger(\mathbf{r}_2, 0) \rangle, & \text{for } \tau > 0 \\ \mp \langle e^{-\tau(H-\mu N)} \Psi^\dagger(\mathbf{r}_2, 0) e^{\tau(H-\mu N)} \Psi(\mathbf{r}_1, 0) \rangle, & \text{for } \tau < 0 \end{cases} \quad (38)$$

where the lower sign is again for fermions.

Perturbative Expansion. As before, we will derive the perturbative expansion in the interaction representation. Using Eqs. (8), and noting that

$$\mathcal{A}(\beta) \mathcal{A}^{-1}(\tau) = T_\tau \left[\exp \left(- \int_\tau^\beta V(\tau') d\tau' \right) \right] \quad (39)$$

we get

$$\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \tau) = - \frac{\left\langle T_\tau \left[\exp \left(- \int_\tau^\beta V(\tau') d\tau' \right) \Psi(\mathbf{r}_1, \tau) \exp \left(- \int_0^\tau V(\tau') d\tau' \right) \Psi^\dagger(\mathbf{r}_2, 0) \right] \right\rangle_0}{\left\langle T_\tau \exp \left(- \int_0^\beta V(\tau') d\tau' \right) \right\rangle_0} \quad (40)$$

$$= - \frac{\left\langle T_\tau \left[\exp \left(- \int_0^\beta V(\tau') d\tau' \right) \Psi(\mathbf{r}_1, \tau) \Psi^\dagger(\mathbf{r}_2, 0) \right] \right\rangle_0}{\left\langle T_\tau \exp \left(- \int_0^\beta V(\tau') d\tau' \right) \right\rangle_0} \quad (41)$$

We obtain the Green's function from a generalized partition function

$$\frac{\tilde{Z}}{Z_0} = \left\langle T_\tau \exp \left[- \int_0^\beta \tilde{V}(\tau') d\tau' \right] \right\rangle_0 \quad (42)$$

including an additional source term

$$\tilde{V}(\tau) = V(\tau) + \int [J(\mathbf{r}, \tau) \Psi^\dagger(\mathbf{r}, \tau) + J^*(\mathbf{r}, \tau) \Psi(\mathbf{r}, \tau)] \quad (43)$$

The generalized partition function \tilde{Z} is a functional of $J(\mathbf{r}, \tau)$ and $J^*(\mathbf{r}, \tau)$, and its logarithm serves as generating functional for \mathcal{G}

$$\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2, \tau) = \begin{cases} - \frac{\delta^2 \log \tilde{Z} / Z_0}{\delta J(\mathbf{r}_2, 0) \delta J^*(\mathbf{r}_1, \tau)} \Big|_{J=J^*=0}, & \text{for } \tau > 0 \\ \mp \frac{\delta^2 \log \tilde{Z} / Z_0}{\delta J(\mathbf{r}_2, 0) \delta J^*(\mathbf{r}_1, \tau)} \Big|_{J=J^*=0}, & \text{for } \tau < 0 \end{cases} \quad (44)$$

We can easily write down the rules for the perturbative expansion of \mathcal{G} . The n th order term is obtained by variation of the $n+1$ th order of \tilde{Z} , and we obtain $n+1$ equal valued connected diagrams with n interacting vertices and $2n+2$ propagators connecting (\mathbf{r}_1, τ) to $(\mathbf{r}_2, 0)$. We see that the Feynman rules for \mathcal{G} are the same as for $\log Z$ with the only exception that we do not need to include a factor of $1/n$ for the n th order term of \mathcal{G} .

Dyson equation. The small simplification of the Feynman rules for \mathcal{G} (no explicit factor of $1/n$) simplifies the diagrammatic analysis. As one can see from Fig. (3) we can basically iterate simple structures and build self-consistent equations for the Green's function. In general, we can write

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G} \quad (45)$$

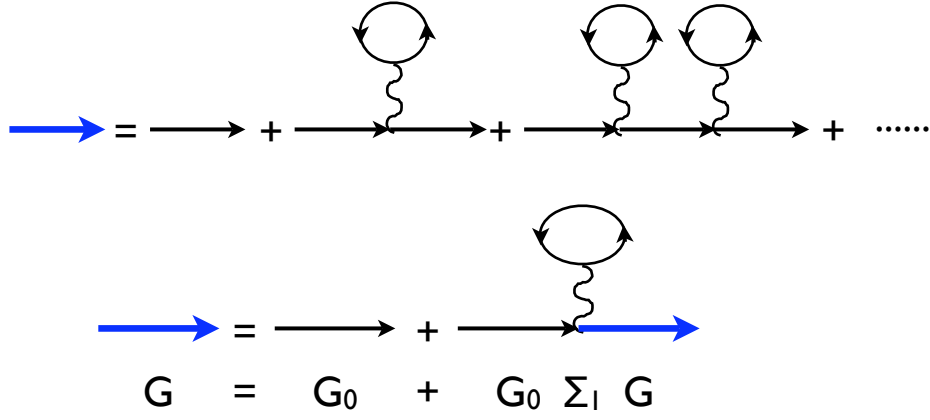


FIG. 3: Example of a first order self energy.

which defines the self energy Σ . The self energy diagrams can be obtained from a diagram for the Green's function by cutting the first and last non-interacting propagators \mathcal{G}_0 . The exact self energy is given by all irreducible diagrams, that means, diagrams which do not disconnect if a single propagator line is cut. It is convenient to write Dyson's equation for the inverse of the operators

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma \quad (46)$$

Note that Dyson's equation, Eq. (45), is a matrix notation and in the space-time representation it writes

$$\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \tau) = \mathcal{G}_0(\mathbf{r}_1, \mathbf{r}_2; \tau) + \int d\mathbf{r}' \int d\mathbf{r}'' \int d\tau' \int d\tau'' \mathcal{G}_0(\mathbf{r}_1, \mathbf{r}'; \tau') \Sigma(\mathbf{r}', \mathbf{r}'', \tau'' - \tau') \mathcal{G}(\mathbf{r}'', \mathbf{r}_2; \tau - \tau'') \quad (47)$$

The equation simplifies if we chose the diagonal representation. For homogeneous system, the spatial part is diagonalized in momentum space, taking the Fourier transform

$$\begin{aligned} \mathcal{G}(\mathbf{r}) &= \mathcal{G}(\mathbf{r}_1, \mathbf{r}_1 + \mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p} \cdot \mathbf{r}} \mathcal{G}(\mathbf{p}) \\ \mathcal{G}(\mathbf{p}) &= \int d\mathbf{r} e^{-i\mathbf{p} \cdot \mathbf{r}} \mathcal{G}(\mathbf{r}) \end{aligned} \quad (48)$$

The equivalent of the Fourier-transform in energy-time space is given by the representation using Matsubara frequencies.

Matsubara frequencies. Note that the Green's function, $\mathcal{G}(\tau)$, is a function of τ defined for $-\beta \leq \tau \leq \beta$, so that we can expand it in a Fourier series

$$\mathcal{G}(\tau) = T \sum_n e^{-i\omega_n \tau} \mathcal{G}(\omega_n) \quad (49)$$

$$\mathcal{G}(\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} e^{i\omega_n \tau} \mathcal{G}(\tau) d\tau, \quad \omega_n = n\pi T \quad (50)$$

However, we can see from the definition of the Green's function, Eq. (38), that $\mathcal{G}(\tau < 0)$ is related to $\mathcal{G}(\tau > 0)$ via

$$\mathcal{G}(\tau < 0) = \pm \mathcal{G}(\tau + \beta) \quad (51)$$

We therefore get

$$\mathcal{G}(\omega_n) = \frac{1}{2} \int_0^{\beta} e^{i\omega_n \tau} \mathcal{G}(\tau) d\tau \pm \int_{-\beta}^0 e^{i\omega_n \tau} \mathcal{G}(\tau + \beta) d\tau \quad (52)$$

$$= \frac{1}{2} [1 \pm e^{-i\omega_n \beta}] \int_0^{\beta} e^{i\omega_n \tau} \mathcal{G}(\tau) d\tau \quad (53)$$

From the last equation we conclude that we always have

$$\mathcal{G}(\omega_n) = \int_0^\beta e^{i\omega_n \tau} \mathcal{G}(\tau) d\tau \quad (54)$$

where

$$\omega_n = 2n\pi T, \quad \text{for bosons} \quad (55)$$

$$\omega_n = (2n+1)\pi T, \quad \text{for fermions} \quad (56)$$

with $n = 0, \pm 1, \pm 2, \dots$

For a homogeneous system, we have $\Psi(\mathbf{r}) = (2\pi)^{-3} \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}} a_{\mathbf{p}}$, and $\varepsilon_{\mathbf{p}} = p^2/2m$, and we get

$$\mathcal{G}_0(\mathbf{r}, \tau > 0) = -\langle \Psi(\mathbf{r}, \tau) \Psi^\dagger(0, 0) \rangle_0 \quad (57)$$

$$\mathcal{G}_0(\mathbf{p}, \tau > 0) = -\langle e^{-\tau(\varepsilon_p - \mu)} a_{\mathbf{p}} a_{\mathbf{p}}^\dagger \rangle_0 = -[1 \pm f(\varepsilon_p)] e^{-\tau(\varepsilon_p - \mu)} \quad (58)$$

with the Bose/ Fermi function

$$f(\omega) = \frac{1}{e^{\beta(\omega - \mu)} \mp 1} \quad (59)$$

We therefore obtain

$$\mathcal{G}_0(\mathbf{p}, \omega_n) = -\frac{1 \pm f(\varepsilon_p)}{i\omega_n - \varepsilon_p + \mu} [e^{\beta(i\omega_n - \varepsilon_p + \mu)} - 1] = \frac{1 \pm f(\varepsilon_p)}{i\omega_n - \varepsilon_p + \mu} [1 \mp e^{-\beta(\varepsilon_p - \mu)}] \quad (60)$$

Now $1 \pm f(\omega) = e^{\beta(\omega - \mu)} f(\omega)$ and we simply get

$$\mathcal{G}_0^{-1}(\mathbf{p}, \omega_n) = \pm [i\omega_n + \mu - \varepsilon_p] \quad (61)$$

Feynman's rules in momentum/ frequency space are rather simple, since the interaction vertex conserves the total momentum/ energy, so that the sum of all in-coming momenta/ Matsubara-frequencies must equal the sum of all out-coming momenta/ Matsubara-frequencies.

C. Hartree-Fock, T-matrix, RPA

There are certain classes of diagrams which can be summed up easily. We will see that it is quite often necessary to treat the diagrams inside these classes consistently in order to obtain a better behaved perturbation expansion in renormalized parameter space. In the following we will consider Bose systems, however, most of the analysis can be extended to Fermions.

Hartree-Fock. The mean-field Hartree-Fock equations are obtained by the following approximation for the self-energy

$$\Sigma_{HF}(\mathbf{k}) = -T \sum_{n'} \int \frac{d\mathbf{p}}{(2\pi)^3} [v(0) \mathcal{G}_{HF}(p, \omega'_n) + v(|\mathbf{p} - \mathbf{k}|) \mathcal{G}_{HF}(p, \omega'_n)] \quad (62)$$

where \mathcal{G}_{HF} is the full propagator within this approximation

$$\mathcal{G}_{HF}^{-1} = G_0^{-1} - \Sigma_{HF} \quad (63)$$

Note that the self-energy is independent of ω_n in this approximation. Let us for the moment consider a system where the interaction potential is sufficiently weak, and does not depend on momentum (at least in the energy-region considered), $v(p) \simeq v(0) \equiv g$. In that case the self-energy is also momentum independent and is proportional to the density

$$\Sigma_{HF} = 2gn_{HF} \quad (64)$$

$$n_{HF} = -T \sum_n \int \frac{d\mathbf{p}}{(2\pi)^3} \mathcal{G}_{HF}(p, \omega_n) \quad (65)$$

$$= \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon_p + \Sigma_{HF} - \mu)} - 1} \quad (66)$$

$$= \lambda^{-3} g_{3/2} \left(e^{\beta(\mu - \Sigma_{HF})} \right) \quad (67)$$

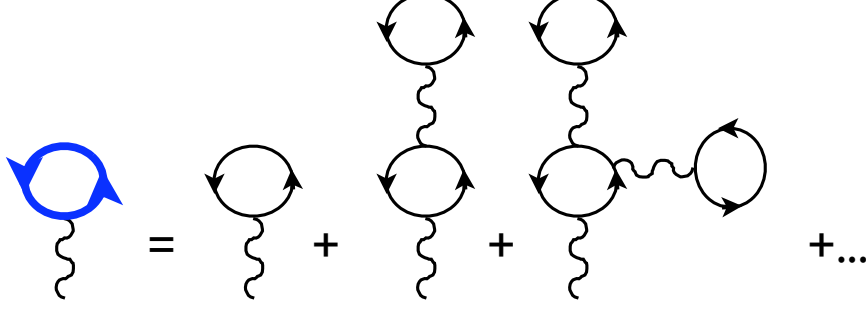


FIG. 4: The direct term of the self-energy in the Hartree-Fock approximation and its expansion in bare propagators.

Bose-Einstein condensation is reached in this approximation when $\mu = \Sigma_{HF}$, which is a selfconsistent equation for μ . Let us approach the phase transition, setting $\Sigma_{HF} - \mu \rightarrow 0^+$. We have $g_{3/2}(e^x) \simeq 2.61 - 3.54\sqrt{-x}$, $n_{HF} \sim \mathcal{O}(1)$, and therefore $\Sigma_{HF} \sim \mathcal{O}(g)$ is linear in the coupling constant of the interaction. However, due to the non-analytic behavior of the $g_{3/2}$, the region of validity of any Taylor expansion around $\Sigma_{HF} - \mu = 0$ is zero.

What do we get if we would have started with the strict (not self-consistent) perturbation expansion? The first and second order terms included by the Hartree-Fock analysis are

$$\Sigma_{HF}^{(2)} = -2g \sum_n \int \frac{d\mathbf{p}}{(2\pi)^3} \mathcal{G}_0(\mathbf{p}, n) \left\{ 1 - gT \sum_{n'} \int \frac{d\mathbf{p}'}{(2\pi)^3} [\mathcal{G}_0(\mathbf{p}', n')]^2 \right\} \quad (68)$$

Now the second term inside the bracket on the rhs behaves roughly like the derivative of the bare density with respect to μ , and we see that the mean-field actually contains a summation of a series in $g/|\beta\mu|^{1/2}$. If we want to approach the point of $|\mu| \rightarrow 0$ higher orders in the perturbation theory diverge even more strongly. In our case, these problems occur do to so-called ‘infrared divergencies’: in the limit of $\mu \rightarrow 0$, $\mathcal{G}(k, 0) \sim \mu - k^{-2}/2m$. The Green’s function approach allows us to estimate by simple dimensional analysis the effect of these infrared divergencies looking at the stricture of the integrals. We can see that the simple Hartree-Fock resummation cures the most diverging part, however, as soon as $\beta(\mu - \Sigma) \sim g^2$ additional diagrams have to be considered. Therefore, mean-field can be trusted outside this “critical region”.

Infrared problems are typical for phase-transitions, the renormalization group methods have developped powerful tools to “control” these problems. However, they all rely on basic assumptions of the (perturbative) analytic structure of the propagators.

T-matrix. A different series which can be treated and which is potentially divergent for short range potentials (particularly hard-core), is related to the two-particle scattering problem. Let us consider particle-particle scattering. In terms of Green’s function this is most easily done in terms of the two-particle Green’s function $\mathcal{G}_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; \tau)$, defined as the average over two annihilation and two creation operators. Repeated particle-particle scattering can be written as a self-consistent equation for \mathcal{G}_2 in a matrix notation (numbers occuring twice are integrated over)

$$\mathcal{G}_2(1, 2; 1', 2') = \mathcal{G}(1, 1')\mathcal{G}(2, 2') + \mathcal{G}(1, 2'; \tau)\mathcal{G}(2, 1') + \mathcal{G}(1, \bar{1})\mathcal{G}(2, \bar{2}, 4)V(\bar{1}, \bar{2})\mathcal{G}_2(\bar{1}, \bar{2}; 1', 2') \quad (69)$$

In the limit of $\beta\mu \rightarrow -\infty$ the system is dilute and the equation will include only two-particles scattering which each other. The two-body problem is solved by the complex T-matrix. For a dilute system \mathcal{G}_2 can be replaced by the two-body T-matrix which includes already repeated particle-particle scattering events. The on-shell T-matrix can be expressed in terms of the phase shifts, and in particular at low energies it reduces to a constant $4\pi\hbar^2 a/m$ where a is the scattering length.

RPA-approximation. The so-called RPA-approximation introduces another class of diagrams which are conveniently expressed by an effective interaction V_{eff} which includes the effect of repeated density-fluctuations

$$V_{eff}(1, 2; 1', 2') = v(1 - 2) + v(1 - 2)\mathcal{G}(1, \bar{1})\mathcal{G}(2, \bar{2})v_{eff}(\bar{1}, \bar{2}; 1', 2') \quad (70)$$

The corresponding diagrams are particularly important for long-range (Coulomb) interactions where they lead to an effective screened potential. A rearrangement of the perturbation theory in terms of the effective screened potential

is possible and gives finite results in the dilute limit, for example in the electron-gas.

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- [1] A.A. Abrikosov, L.P. Gorkov, and I.E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*.
 - [2] L. P. Kadanoff and G. Baym, *Green's Function Methods in Equilibrium and Nonequilibrium Problems*
 - [3] A. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems*.
 - [4] J.W. Negele and H. Orland, *Quantum Many-Particle Systems*.