Imaginary-time or Matsubara formalism

Quantum field theory (QFT) describes interactions of elementary particles, like electrons and photons, and it is mostly focused on scattering processes of particles which occur in vacuum. An objective of statistical quantum field theory is to describe a many-body system, like that of many electrons and photons, in terms of quantum field theory of its constituents. However, elementary interaction processes, which are responsible for a behavior of many-body system, occur not in vacuum but in an environment of many particles. We will use the term 'vacuum QFT' as a counterpart of 'statistical QFT'.

There are two formulations of statistical QFT: the *imaginary-time* or *Matsubara formalism* and the *real-time* or *Keldysh-Schwinger formalism*. We start the introduction to statistical quantum field theory with the former one which is also called as *thermal field theory*. The method was discovered by Takeo Matsubara (1921-2014) in 1955.

Basic concepts

- As we remember, the partition function, which carries a complete information on a many-body system in equilibrium, is defined as

$$Z \equiv \mathrm{Tr}[e^{-\beta \hat{H}}] \equiv \sum_{\alpha} \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle, \tag{1}$$

  where $\beta \equiv T^{-1}$ is the inverse temperature, $\hat{H}$ is the system's Hamiltonian and the sum is performed over a complete set of states of the system under consideration. The hats are used to denote operators acting in the space of states.

- The basic idea of the Matsubara formalism is that the density matrix $\hat{\rho} = e^{-\beta \hat{H}}$, which enters the partition function (1), can be formally treated as a quantum evolution operator $e^{-i\hat{H}t}$ in imaginary time from $t = 0$ to $t = -i\beta$. It is important to note here that the full Hamiltonian $\hat{H}$ is assumed to be time independent.

- The main object of the Matsubara formalism is the temperature Green's function which is defined for the complex scalar field $\hat{\phi}$ in the following way

$$\Delta(\tau, \mathbf{x}) \equiv \langle \mathcal{T} \hat{\phi}(-i\tau, \mathbf{x})\, \hat{\phi}^{\dagger}(0, \mathbf{0}) \rangle, \tag{2}$$

  where the operation $\langle \dots \rangle$ is understood as

$$\langle \dots \rangle \equiv \frac{1}{Z}\, \mathrm{Tr}[e^{-\beta \hat{H}} \dots], \tag{3}$$

  and the symbol $\mathcal{T}$ represents ordering in the imaginary time that is

$$\begin{aligned} \mathcal{T} \hat{\phi}(-i\tau_1, \mathbf{x}_1)\, \hat{\phi}^{\dagger}(-i\tau_2, \mathbf{x}_2) &= \Theta(\tau_1 - \tau_2)\, \hat{\phi}(-i\tau_1, \mathbf{x}_1)\, \hat{\phi}^{\dagger}(-i\tau_2, \mathbf{x}_2) \\ &+ \Theta(\tau_2 - \tau_1)\, \hat{\phi}^{\dagger}(-i\tau_2, \mathbf{x}_2)\, \hat{\phi}(-i\tau_1, \mathbf{x}_1). \end{aligned} \tag{4}$$

  The definition (2) assumes that the system under consideration is translationally invariant.

- We have assumed that $0 < \tau < \beta$, but actually the function $\Delta(\tau, \mathbf{x})$ is periodic in τ with the period β. Indeed, one finds

$$\begin{aligned}\Delta(\tau,\mathbf{x}) &= \frac{1}{Z}\,\mathrm{Tr}[e^{-\beta\hat{H}}\mathcal{T}\hat{\phi}(-i\tau,\mathbf{x})\,\hat{\phi}^\dagger(0,\mathbf{0})] = \frac{1}{Z}\,\mathrm{Tr}[e^{-\beta\hat{H}}\hat{\phi}(-i\tau,\mathbf{x})\,\hat{\phi}^\dagger(0,\mathbf{0})] \\ &= \frac{1}{Z}\,\mathrm{Tr}[\hat{\phi}^\dagger(0,\mathbf{0})\,e^{-\beta\hat{H}}\hat{\phi}(-i\tau,\mathbf{x})] = \frac{1}{Z}\,\mathrm{Tr}[e^{-\beta\hat{H}}e^{\beta\hat{H}}\hat{\phi}^\dagger(0,\mathbf{0})\,e^{-\beta\hat{H}}\hat{\phi}(-i\tau,\mathbf{x})] \\ &= \frac{1}{Z}\,\mathrm{Tr}[e^{-\beta\hat{H}}\hat{\phi}^\dagger(-i\beta,\mathbf{0})\,\hat{\phi}(-i\tau,\mathbf{x})] = \frac{1}{Z}\,\mathrm{Tr}[e^{-\beta\hat{H}}\mathcal{T}\hat{\phi}(-i\tau,\mathbf{x})\hat{\phi}^\dagger(-i\beta,\mathbf{0})] \\ &= \Delta(\tau-\beta,\mathbf{x}). \qquad (5)\end{aligned}$$

Free temperature Green's function

We derive here an explicit form of the Green's function of noninteracting fields, applying the method which was used in Lecture II to get the partition function of free fields (see Eq. (7) of Lecture II).

Green's function in coordinate space

- Let us introduce the auxiliary functions $\Delta^>(\tau,\mathbf{x})$ and $\Delta^<(\tau,\mathbf{x})$ defined as

$$\Delta^>(\tau,\mathbf{x}) \equiv \langle\hat{\phi}(-i\tau,\mathbf{x})\,\hat{\phi}^\dagger(0,\mathbf{0})\rangle, \qquad (6)$$

$$\Delta^<(\tau,\mathbf{x}) \equiv \langle\hat{\phi}^\dagger(0,\mathbf{0})\hat{\phi}(-i\tau,\mathbf{x})\,\rangle. \qquad (7)$$

- We will first compute $\Delta^>(\tau,\mathbf{x})$ and $\Delta^<(\tau,\mathbf{x})$ and using the identity

$$\Delta(\tau,\mathbf{x}) = \Theta(\tau)\,\Delta^>(\tau,\mathbf{x}) + \Theta(-\tau)\,\Delta^<(\tau,\mathbf{x}), \qquad (8)$$

  we will find the function $\Delta(\tau,\mathbf{x})$.

- As we remember, the free field can decomposed in plane waves as

$$\hat{\phi}(x) = \int\frac{d^3k}{(2\pi)^3\sqrt{2\omega_k}}\Big(\hat{a}(\mathbf{k})e^{-ikx} + \hat{a}^\dagger(\mathbf{k})e^{ikx}\Big), \qquad (9)$$

  where $k^\mu = (\omega_\mathbf{k},\mathbf{k})$ and $\omega_\mathbf{k} \equiv \sqrt{\mathbf{k}^2+m^2}$. The discrete version of the plane-wave decomposition is

$$\hat{\phi}(x) = \sqrt{\Delta_\mathbf{k}}\sum_i\frac{1}{\sqrt{2\omega_i}}\Big(\hat{a}_i e^{-ik_ix} + \hat{a}_i^\dagger e^{ik_ix}\Big), \qquad (10)$$

  with $\Delta_\mathbf{k}$ being the volume of a momentum-space cell and $\hat{a}_i \equiv \sqrt{\Delta_\mathbf{k}}\hat{a}(\mathbf{k}_i)$ and $\hat{a}_i^\dagger \equiv \sqrt{\Delta_\mathbf{k}}\hat{a}^\dagger(\mathbf{k}_i)$.

- The discrete operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ are dimensionless and satisfy the following commutation relations

$$\big[\hat{a}_i,\hat{a}_j^\dagger\big] = \delta^{ij}, \qquad \big[\hat{a}_i,\hat{a}_j\big] = 0, \qquad \big[\hat{a}_i^\dagger,\hat{a}_j^\dagger\big] = 0. \qquad (11)$$

- The discrete normally ordered Hamiltonian is

$$\hat{H} = \sum_i\omega_i\hat{a}_i^\dagger\hat{a}_i = \sum_i\omega_i\hat{n}_i, \qquad (12)$$

  where $\hat{n}_i \equiv \hat{a}_i^\dagger\hat{a}_i$.

- As discussed in Lecture I, the Fock space is built of the mutually orthogonal energy eigenstates $|n_1, n_2, n_3, \dots\rangle$, and the action of the annihilation and creation operators is defined in the following way

$$\hat{a}_i|n_1, n_2, \dots, n_i, \dots\rangle = \sqrt{n_i}\,|n_1, n_2, \dots, n_i - 1, \dots\rangle, \tag{13}$$

$$\hat{a}_i^\dagger|n_1, n_2, \dots, n_i, \dots\rangle = \sqrt{n_i + 1}\,|n_1, n_2, \dots, n_i + 1, \dots\rangle. \tag{14}$$

- Keeping in mind that the Green's function $\Delta^>(\tau, \mathbf{x})$ equals

$$\begin{aligned}\Delta^>(\tau, \mathbf{x}) = Z^{-1} \int \frac{d^3k\, d^3p}{2(2\pi)^3\sqrt{\omega_k\omega_p}} \sum_{n_1}\sum_{n_2}\sum_{n_3}\dots \\ \times\big\langle n_1, n_2, \dots \big| \exp(-\beta\hat{H})\Big(\hat{a}(\mathbf{k})e^{-ikx} + \hat{a}^\dagger(\mathbf{k})e^{ikx}\Big) \\ \times\Big(\hat{a}(\mathbf{p}) + \hat{a}^\dagger(\mathbf{p})\Big)\big|n_1, n_2, \dots\big\rangle,\end{aligned} \tag{15}$$

the discrete version is written as

$$\begin{aligned}\Delta^>(\tau, \mathbf{x}) = Z^{-1}\Delta_{\mathbf{k}} \sum_{n_1}\sum_{n_2}\sum_{n_3}\dots e^{-\beta\omega_1 n_1}e^{-\beta\omega_2 n_2}e^{-\beta\omega_3 n_3}\dots\sum_i\sum_j \frac{1}{2\sqrt{\omega_i\omega_j}} \\ \times\Big[e^{-ik_ix}\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i\hat{a}_j\big|n_1, \dots, n_j, \dots\big\rangle \\ +e^{-ik_ix}\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i\hat{a}_j^\dagger\big|n_1, \dots, n_j, \dots\big\rangle \\ +e^{ik_ix}\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i^\dagger\hat{a}_j\big|n_1, \dots, n_j, \dots\big\rangle \\ +e^{ik_ix}\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i^\dagger\hat{a}_j^\dagger\big|n_1, \dots, n_j, \dots\big\rangle\Big],\end{aligned} \tag{16}$$

where $x^\mu = (-i\tau, \mathbf{x})$, $k_i^\mu = (\omega_i, \mathbf{k}_i)$ and $p_i^\mu = (\omega_i, \mathbf{p}_i)$.

- Computing

$$\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i\hat{a}_j\big|n_1, \dots, n_j, \dots\big\rangle = 0, \tag{17}$$

$$\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i^\dagger\hat{a}_j^\dagger\big|n_1, \dots, n_j, \dots\big\rangle = 0, \tag{18}$$

$$\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i\hat{a}_j^\dagger\big|n_1, \dots, n_j, \dots\big\rangle = \sqrt{(n_i+1)(n_j+1)}\;\delta^{ij}, \tag{19}$$

$$\big\langle n_1, \dots, n_i, \dots\big|\hat{a}_i^\dagger\hat{a}_j\big|n_1, \dots, n_j, \dots\big\rangle = \sqrt{n_i n_j}\;\delta^{ij}, \tag{20}$$

one finds

$$\begin{aligned}\Delta^>(\tau, \mathbf{x}) = Z^{-1}\Delta_{\mathbf{k}} \sum_{n_1}\sum_{n_2}\sum_{n_3}\dots e^{-\beta\omega_1 n_1}e^{-\beta\omega_2 n_2}e^{-\beta\omega_3 n_3}\dots \\ \times\sum_i \frac{1}{2\omega_i}\Big[n_i\Big(e^{-ik_ix} + e^{ik_ix}\Big) + e^{-ik_ix}\Big].\end{aligned} \tag{21}$$

- Using the formulas

$$\sum_{n=0}^{\infty} q^n = \frac{1}{1-q}, \qquad \sum_{n=0}^{\infty} nq^n = \frac{q}{(1-q)^2}, \tag{22}$$

one obtains

$$\Delta^{>}(x) = \Delta_{\mathbf{k}} \sum_i \frac{1}{2\omega_i} \left[\frac{e^{-\beta\omega_i}}{1 - e^{-\beta\omega_i}} \left(e^{-ik_i x} + e^{ik_i x} \right) + e^{-ik_i x} \right], \tag{23}$$

where the partition function Z (given by Eq. (17) of Lecture II) cancels out.

- In the final step we change a discrete momentum space into a continuous one and we get

$$\boxed{\Delta^{>}(\tau, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_{\mathbf{k}}} \left[\big(f(\omega_{\mathbf{k}}) + 1\big) e^{-\omega_{\mathbf{k}}\tau} e^{i\mathbf{k}\cdot\mathbf{x}} + f(\omega_{\mathbf{k}}) e^{\omega_{\mathbf{k}}\tau} e^{-i\mathbf{k}\cdot\mathbf{x}} \right],} \tag{24}$$

where the boson distribution function equals

$$f(\omega_{\mathbf{k}}) \equiv \frac{1}{e^{\beta\omega_{\mathbf{k}}} - 1}. \tag{25}$$

- Repeating the same steps as in case of $\Delta^{>}$, we find $\Delta^{<}$ as

$$\boxed{\Delta^{<}(\tau, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_{\mathbf{k}}} \left[f(\omega_{\mathbf{k}}) e^{-\omega_{\mathbf{k}}\tau} e^{i\mathbf{k}\cdot\mathbf{x}} + \big(f(\omega_{\mathbf{k}}) + 1\big) e^{\omega_{\mathbf{k}}\tau} e^{-i\mathbf{k}\cdot\mathbf{x}} \right].} \tag{26}$$

Exercise: Derive the formula (26).

- Due to the identity (8) we have

$$\Delta(\tau, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{f(\omega_{\mathbf{k}})}{2\omega_{\mathbf{k}}} \left[e^{-\omega_{\mathbf{k}}\tau} e^{i\mathbf{k}\cdot\mathbf{x}} + e^{\omega_{\mathbf{k}}\tau} e^{-i\mathbf{k}\cdot\mathbf{x}} \right] \tag{27}$$

$$+ \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_{\mathbf{k}}} \left[\Theta(\tau) e^{-\omega_{\mathbf{k}}\tau} e^{i\mathbf{k}\cdot\mathbf{x}} + \Theta(-\tau) e^{\omega_{\mathbf{k}}\tau} e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \tag{28}$$

Green's function in momentum space

- Since the function $\Delta(\tau, \mathbf{x})$ is periodic in τ with the period equal to β, the Fourier transformation of $\Delta(\tau, \mathbf{x})$ is

$$\Delta(\omega_n, \mathbf{p}) \equiv \int_0^\beta d\tau \int d^3x \; e^{i(\omega_n\tau - \mathbf{p}\cdot\mathbf{x})} \Delta(\tau, \mathbf{x}) \tag{29}$$

and its inverse equals

$$\Delta(\tau, \mathbf{x}) = T \sum_{n=-\infty}^{\infty} \int \frac{d^3p}{(2\pi)^3} \; e^{-i(\omega_n\tau - \mathbf{p}\cdot\mathbf{x})} \Delta(\omega_n, \mathbf{p}), \tag{30}$$

where

$$\omega_n \equiv 2\pi T \, n. \tag{31}$$

The frequencies ω_n are known as the Matsubara frequencies.

- Using the formulas

$$\int_0^\beta d\tau\, e^{a\tau} = \frac{e^{a\beta}-1}{a}, \qquad \int d^3x\, e^{\pm i\mathbf{q}\cdot\mathbf{x}} = (2\pi)^3\delta^{(3)}(\mathbf{q}), \tag{32}$$

one performs the Fourier transformation (29) of the function (27) and obtains

$$\Delta(\omega_n,\mathbf{p}) = \frac{1}{2\omega_\mathbf{p}}\Big[\big(f(\omega_\mathbf{p})+1\big)\frac{e^{(i\omega_n-\omega_\mathbf{p})\beta}-1}{i\omega_n-\omega_\mathbf{p}} + f(\omega_\mathbf{p})\frac{e^{(i\omega_n+\omega_\mathbf{p})\beta}-1}{i\omega_n+\omega_\mathbf{p}}\Big]. \tag{33}$$

- Keeping in mind that $e^{i\omega_n\beta} = e^{2\pi n i} = 1$, the formula (33) becomes

$$\Delta(\omega_n,\mathbf{p}) = \frac{1}{2\omega_\mathbf{p}}\Big[\big(f(\omega_\mathbf{p})+1\big)\,\frac{e^{-\beta\omega_\mathbf{p}}-1}{i\omega_n-\omega_\mathbf{p}} + f(\omega_\mathbf{p})\,\frac{e^{\beta\omega_\mathbf{p}}-1}{i\omega_n+\omega_\mathbf{p}}\Big]. \tag{34}$$

- Since $f(\omega_\mathbf{p}) = (e^{\beta\omega_\mathbf{p}}-1)^{-1}$, one finally finds

$$\boxed{\Delta(\omega_n,\mathbf{p}) = \frac{1}{\omega_n^2+\omega_\mathbf{p}^2}.} \tag{35}$$

Perturbative expansion

An objective of the perturbive expansion, which plays a crucially important role in quantum field theory, is to express quantities characterizing a system of interacting fields through those of noninteracting ones. The procedure assumes a weakness of the interaction.

- The key observation, which allows one to obtain the perturbative expansion in QFT, is that an operator $\hat{\mathcal{O}}_\mathrm{H}(t)$ in the Heisenberg picture can be written through the operator $\hat{\mathcal{O}}_\mathrm{int}(t)$ in the interaction picture as

$$\hat{\mathcal{O}}_\mathrm{H}(t) = \hat{U}_\mathrm{int}(0,t)\,\hat{\mathcal{O}}_\mathrm{int}(t)\,\hat{U}_\mathrm{int}(t,0), \tag{36}$$

where $\hat{U}_\mathrm{int}(t,0)$ is the evolution operator in the interaction picture which is

$$\begin{aligned}\hat{U}_\mathrm{int}(t,0) &= Te^{-i\int_0^t dt'\,\hat{H}^I_\mathrm{int}(t')} \\ &= 1 - i\int_0^t dt'\,\hat{H}^I_\mathrm{int}(t') + \frac{(-i)^2}{2!}\int_0^t dt_1\int_0^t dt_2\,T\hat{H}^I_\mathrm{int}(t_1)\,\hat{H}^I_\mathrm{int}(t_2) + \dots\end{aligned} \tag{37}$$

T denotes "left later" ordering and $\hat{H}^I_\mathrm{int}$ is the interaction Hamiltonian in the interaction picture.

<u>Exercise</u>: Discus and prove the equality (36).

- Introducing the imaginary time $\tau = it$ such that $0 < \tau < \beta$, one writes

$$\mathrm{Tr}\big[e^{-\beta\hat{H}}\hat{\mathcal{O}}_\mathrm{H}(-i\tau)\big] = \mathrm{Tr}\big[e^{-\beta\hat{H}}\hat{U}_\mathrm{int}(0,-i\tau)\,\hat{\mathcal{O}}_\mathrm{int}(-i\tau)\,\hat{U}_\mathrm{int}(-i\tau,0)\big]. \tag{38}$$

- Using the equation (36), one finds the relation

$$\begin{aligned} e^{-\beta\hat{H}} &= \hat{U}_{\rm int}(0,-i\beta)\, e^{-\beta\hat{H}_{\rm int}}\, \hat{U}_{\rm int}(-i\beta,0) \\ &= \mathcal{T}\big[e^{-\int_\beta^0 d\tau'\, \hat{H}^I_{\rm int}(-i\tau')}\big]\, e^{-\beta\hat{H}_{\rm int}}\, \hat{U}_{\rm int}(-i\beta,0) = e^{-\beta\hat{H}^0_{\rm int}}\, \hat{U}_{\rm int}(-i\beta,0), \end{aligned} \tag{39}$$

  which substituted into the formula (38) gives

$$\begin{aligned} {\rm Tr}\big[e^{-\beta\hat{H}}\hat{\mathcal{O}}_{\rm H}(-i\tau)\big] &= {\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\, \hat{U}_{\rm int}(-i\beta,0)\hat{U}_{\rm int}(0,-i\tau)\, \hat{\mathcal{O}}_{\rm int}(-i\tau)\, \hat{U}_{\rm int}(-i\tau,0)\big] \\ &= {\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\, \hat{U}_{\rm int}(-i\beta,-i\tau)\, \hat{\mathcal{O}}_{\rm int}(-i\tau)\, \hat{U}_{\rm int}(-i\tau,0)\big] \\ &= {\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\, \mathcal{T}[\hat{U}_{\rm int}(-i\beta,0)\, \hat{\mathcal{O}}_{\rm int}(-i\tau)]\big] \\ &= {\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\, \mathcal{T}[e^{-\int_0^\beta d\tau'\, \hat{H}^I_{\rm int}(-i\tau')}\, \hat{\mathcal{O}}_{\rm int}(-i\tau)]\big]. \end{aligned} \tag{40}$$

- We temporarily define the expectation value of an operator as

$$\langle\hat{\mathcal{O}}_{\rm H}(-i\tau)\rangle \equiv \frac{{\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\mathcal{T}[e^{-\int_0^\beta d\tau'\, \hat{H}^I_{\rm int}(-i\tau')}\hat{\mathcal{O}}_{\rm int}(-i\tau)]\big]}{{\rm Tr}\big[e^{-\beta\hat{H}^0_{\rm int}}\big]}. \tag{41}$$

  As we will show later on, the free Hamiltonian from the denominator in Eq. (41) should be replaced by the full Hamiltonian. In this way contributions corresponding to the so-called disconnected Feynman diagrams are eliminated.

- Generalizing the formula (41), the temperature Green's function (2) is written as

$$i\Delta(\tau,\mathbf{x}) = \Big\langle \mathcal{T}\big[e^{-\int_0^\beta d\tau\, \hat{H}^I_{\rm int}(-i\tau')}\, \hat{\phi}_{\rm int}(-i\tau,\mathbf{x})\, \hat{\phi}^\dagger_{\rm int}(0,\mathbf{0})\big]\Big\rangle. \tag{42}$$

- Expanding the exponential function in the formula (42) as in Eq. (37), we get the perturbative expansion of temperature Green's function.
- One may worry that the operators in Eq. (42) are in the interaction picture while the states are in the Heisenberg picture. However, when the exponential function is expanded and the Wick theorem, which is discussed further on, is applied, the Green's function (42) is expressed as a sum of products of free Green's functions. And when we deal with free fields the Heisenberg and interaction pictures coincide with each other.
- The problem to be solved is how to calculate the expressions which originate from the perturbative expansion of the formula (42) which are of the form

$$\Big\langle \mathcal{T}\big[\hat{H}^I_{\rm int}(-i\tau_1)\, \hat{H}^I_{\rm int}(-i\tau_2)\, \dots \hat{H}^I_{\rm int}(-i\tau_n)\, \hat{\phi}_{\rm int}(-i\tau_x,\mathbf{x})\, \hat{\phi}^\dagger_{\rm int}(-i\tau_y,\mathbf{y})\big]\Big\rangle, \tag{43}$$

  where n numerates the terms in the expansion (37).
- Further on, we suppress the subscript 'int'.
- The Lagrangian density of interacting fields includes, except the terms quadratic in fields, the term or terms of higher power. As an example, we consider the interacting scalar complex field of the Lagrangian density

$$\hat{\mathcal{L}}(x) = \partial^\mu\hat{\phi}(x)\partial_\mu\hat{\phi}^\dagger(x) - m^2\hat{\phi}(x)\hat{\phi}^\dagger(x) - \frac{\lambda}{2!\,2!}\big(\hat{\phi}(x)\hat{\phi}^\dagger(x)\big)^2, \tag{44}$$

  where the last quartic term represents the interaction and λ is the coupling constant which is assumed to be a small number.

- There is a conserved charge in the theory described by the Lagrangian (44) and there are positively and negatively charged particles.
- The interaction Hamiltonian equals

$$\hat{H}^I(t) = \frac{\lambda}{2!\,2!}\int d^3x\,\big(\hat{\phi}(x)\hat{\phi}^\dagger(x)\big)^2, \tag{45}$$

where $x = (t, \mathbf{x})$.

- The perturbative expansion is constructed out of non-interacting fields which obey Klein-Gordon equations. Therefore, the fields are expressed as superpositions of plane waves

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3\sqrt{2\omega_{\mathbf{k}}}}\big[e^{-ikx}\hat{a}(\mathbf{k}) + e^{ikx}\,\hat{b}^\dagger(\mathbf{k})\big], \tag{46}$$

$$\hat{\phi}^\dagger(x) = \int \frac{d^3k}{(2\pi)^3\sqrt{2\omega_{\mathbf{k}}}}\big[e^{-ikx}\,\hat{b}(\mathbf{k}) + e^{ikx}\hat{a}^\dagger(\mathbf{k})\big]. \tag{47}$$

where $k^\mu = (\omega_{\mathbf{k}}, \mathbf{k})$ with $\omega_{\mathbf{k}} \equiv \sqrt{m^2 + \mathbf{k}^2}$, and $\hat{a}^\dagger(\mathbf{k})$, $\hat{b}^\dagger(\mathbf{k})$ are creation operators of positively and negatively charged particles, respectively, and $\hat{a}(\mathbf{k})$, $\hat{b}(\mathbf{k})$ are annihilation operators.

- We see that the expression (43) is the expectation value of a product of field operators ordered in imaginary time. The fields are expressed through the creation and annihilation operators due to Eqs. (46, 47). So, the expression to be computed is

$$\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle, \tag{48}$$

where α_i is either the annihilation or creation operator.

Wick's theorem

- The Wick's theorem shows that the expectation value $\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle$ can be expressed as a sum of products of $\langle \hat{\alpha}_i\hat{\alpha}_j\rangle$.
- We are going to compute $\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle$. Since the trace is taken over the eigenstates of particle number operator, the numbers of creation and annihilation operators of a given particle species must be the same in $\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle$. So, the number m must be even. Otherwise the expectation value vanishes.
- We manipulate the expression $\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle$ moving the operator $\hat{\alpha}_1$ from left to right. In the first step we get

$$\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle = \langle [\hat{\alpha}_1, \hat{\alpha}_2]\hat{\alpha}_3\ldots\hat{\alpha}_m\rangle + \langle \hat{\alpha}_2\hat{\alpha}_1\hat{\alpha}_3\ldots\hat{\alpha}_m\rangle, \tag{49}$$

where $[\hat{\alpha}_1, \hat{\alpha}_2]$ is the commutator of $\hat{\alpha}_1$ and $\hat{\alpha}_2$ which is assumed to be a $c-$number. Therefore, it can be pull-out of the expectation value. So, we have

$$\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle = [\hat{\alpha}_1, \hat{\alpha}_2]\langle \hat{\alpha}_3\ldots\hat{\alpha}_m\rangle + \langle \hat{\alpha}_2\hat{\alpha}_1\hat{\alpha}_3\ldots\hat{\alpha}_m\rangle. \tag{50}$$

- Moving α_1 further to the right we commute it with α_3, α_4, etc. Thus, we obtain

$$\begin{aligned}\langle \hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle &= [\hat{\alpha}_1, \hat{\alpha}_2]\langle \hat{\alpha}_3\ldots\hat{\alpha}_m\rangle + [\hat{\alpha}_1, \hat{\alpha}_3]\langle \hat{\alpha}_2\ldots\hat{\alpha}_m\rangle + \cdots + [\hat{\alpha}_1, \hat{\alpha}_m]\langle \hat{\alpha}_2\ldots\hat{\alpha}_{m-1}\rangle \\ &\quad + \langle \hat{\alpha}_2\hat{\alpha}_3\ldots\hat{\alpha}_m\hat{\alpha}_1\rangle.\end{aligned} \tag{51}$$

- Now, we write down the last term explicitly and use the cyclic property of trace

$$\langle\hat{\alpha}_2\hat{\alpha}_3\ldots\hat{\alpha}_m\hat{\alpha}_1\rangle \equiv \frac{\mathrm{Tr}[\hat{\rho}\,\hat{\alpha}_2\hat{\alpha}_3\ldots\hat{\alpha}_m\hat{\alpha}_1]}{\mathrm{Tr}[\hat{\rho}]} = \frac{\mathrm{Tr}[\hat{\alpha}_1\hat{\rho}\,\hat{\alpha}_2\hat{\alpha}_3\ldots\hat{\alpha}_m]}{\mathrm{Tr}[\hat{\rho}]}. \tag{52}$$

- In the next step, we make an important assumption about the density matrix $\hat{\rho}$. Specifically, we assume that

$$\hat{\alpha}_i\hat{\rho} = \hat{\rho}\,\hat{\alpha}_i\,\eta_i \tag{53}$$

where η^i is a $c-$number. The assumption (53) limits a class of states which allow for the Wick's decomposition. As we will see, it is satisfied by the equilibrium density matrix $\hat{\rho} = e^{-\beta\hat{H}^0}$.

- Using the equality (53), Eq. (52) provides

$$\langle\hat{\alpha}_2\hat{\alpha}_3\ldots\hat{\alpha}_m\hat{\alpha}_1\rangle = \eta_1\langle\hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle. \tag{54}$$

- Substituting the result (54) into Eq. (51), we get

$$\langle\hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle = \frac{[\hat{\alpha}_1,\hat{\alpha}_2]}{1-\eta_1}\langle\hat{\alpha}_3\ldots\hat{\alpha}_m\rangle + \frac{[\hat{\alpha}_1,\hat{\alpha}_3]}{1-\eta_1}\langle\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle + \cdots + \frac{[\hat{\alpha}_1,\hat{\alpha}_m]}{1-\eta_1}\langle\hat{\alpha}_2\ldots\hat{\alpha}_{m-1}\rangle. \tag{55}$$

- In the l.h.s. of Eq. (55) there is the expectation value of the product of m operators while in the r.h.s. of the equation there is a sum of the expectation values of the products of $(m-2)$ operators. Applying repeatedly the same procedure to every expectation value from Eq. (55), we finally obtain

$$\langle\hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle = \sum_{\text{permutations}} \frac{[\hat{\alpha}_1,\hat{\alpha}_2]}{1-\eta_1}\frac{[\hat{\alpha}_3,\hat{\alpha}_4]}{1-\eta_3}\cdots\frac{[\hat{\alpha}_{m-1},\hat{\alpha}_m]}{1-\eta_{m-1}}, \tag{56}$$

where the sum is over all permutations of pairs (contractions) of the operators $\hat{\alpha}_i$ and $\hat{\alpha}_j$.

- Since

$$\langle\hat{\alpha}_i\hat{\alpha}_j\rangle = \frac{[\hat{\alpha}_i,\hat{\alpha}_j]}{1-\eta_i}, \tag{57}$$

we see that the equality (56) can be rewritten as

$$\langle\hat{\alpha}_1\hat{\alpha}_2\ldots\hat{\alpha}_m\rangle = \sum_{\text{permutations}} \langle\hat{\alpha}_1\hat{\alpha}_2\rangle\langle\hat{\alpha}_3\hat{\alpha}_4\rangle\langle\hat{\alpha}_{m-1}\hat{\alpha}_m\rangle, \tag{58}$$

which shows that the expectation value of the product of m operators ($m > 2$) can be expressed as a sum of products of expectation values of products of two operators. This is the statement of Wick's theorem.

- We note that a big part of terms in Eq. (58), which are obtained by permutation of the operators $\hat{\alpha}_1,\ \hat{\alpha}_2,\ldots\hat{\alpha}_m$ vanish. A non-zero contribution is provided only by the terms where all two-operator expectation values include one creation and one annihilation operator of the same particle species.

Simple examples

- To see how the Wick's theorem works, let us first consider the expectation value $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$, where $\hat{a}_i^\dagger$ and $\hat{a}_j$ are the creation and annihilation operators of the discretized model of real scalar field which is discussed in detail in Lecture I. The field is in thermodynamic equilibrium and the density matrix is $\hat{\rho} = e^{-\beta \hat{H}^0}$. So, we are going to consider the following expression

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \frac{\mathrm{Tr}[e^{-\beta \hat{H}^0} \hat{a}_i^\dagger \hat{a}_j]}{\mathrm{Tr}[e^{-\beta \hat{H}^0}]}. \tag{59}$$

- Since the trace is computed with the eigenstates of the particle number operator $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$, one immediately realizes that the expression (59) is nonzero only for $i = j$. Then, one finds

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \delta^{ij} \frac{\mathrm{Tr}[e^{-\beta \hat{H}^0} \hat{n}_i]}{\mathrm{Tr}[e^{-\beta \hat{H}^0}]} = \delta^{ij} n_i. \tag{60}$$

- On the other hand Eq. (57) tell us that

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \frac{[\hat{a}_i^\dagger, \hat{a}_j]}{1 - \eta_i}. \tag{61}$$

- We are going to show that the r.h.s of Eq. (59) equals the the r.h.s of Eq. (61).
- Since the annihilation and creation operators satisfy the commutation relation

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta^{ij}, \tag{62}$$

see Lecture I, Eq. (61) becomes

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \frac{\delta^{ij}}{\eta_i - 1}. \tag{63}$$

- So, we have to find η_i which is defined through Eq. (53). For $\alpha_i = \hat{a}_i^\dagger$ and $\hat{\rho} = e^{-\beta \hat{H}^0}$, Eq. (53) is

$$\hat{a}_i^\dagger e^{-\beta \hat{H}^0} = e^{-\beta \hat{H}^0} \hat{a}_i^\dagger \eta_i, \tag{64}$$

where $\hat{H}^0 = \sum_j \omega_j \hat{a}_j^\dagger \hat{a}_j$.

- Expanding the exponential function, one commutes $\hat{a}_i^\dagger$ with $\hat{\rho}$ and finds after a rather tedious analysis that

$$\hat{a}_i^\dagger e^{-\beta \hat{H}^0} = e^{-\beta \hat{H}^0} \hat{a}_i^\dagger + e^{-\beta \hat{H}^0} \big(e^{\beta \omega_i} - 1\big) \hat{a}_i^\dagger = e^{-\beta \hat{H}^0} \hat{a}_i^\dagger \, e^{\beta \omega_i}. \tag{65}$$

Therefore,

$$\eta_i = e^{\beta \omega_i} = \frac{n_i + 1}{n_i}, \tag{66}$$

where

$$n_i = \frac{1}{e^{\beta \omega_i} - 1}. \tag{67}$$

<u>Exercise</u>: Prove the equality (64) with $\eta_i = e^{\beta \omega_i}$.

- Substituting the result (66) into Eq. (63), we reproduce Eq. (60).

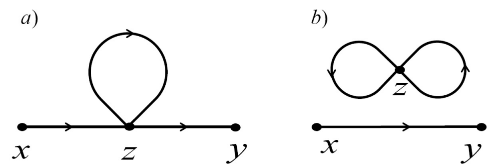

Figure 1: The first order contributions to the Green's function

- Let us now consider $\langle \hat{a}_i \hat{a}_j^\dagger \rangle$. Analogously to Eq. (60), one finds

$$\langle \hat{a}_i \hat{a}_j^\dagger \rangle = \frac{\mathrm{Tr}[e^{-\beta \hat{H}^0}(\delta^{ij} + \delta^{ij}\hat{n}_i)]}{\mathrm{Tr}[e^{-\beta \hat{H}^0}]} = \delta^{ij}(n_i + 1). \tag{68}$$

- The analog of Eq. (63) is

$$\langle \hat{a}_i \hat{a}_j^\dagger \rangle = \frac{\delta^{ij}}{1 - \eta_i}, \tag{69}$$

  and η_i in this case equals

$$\eta_i = e^{-\beta\omega_i} = \frac{n_i}{n_i + 1}. \tag{70}$$

  Exercise: Derive Eq. (70) from Eq. (53) for $\alpha_i = \hat{a}_i$ and $\hat{\rho} = e^{-\beta \hat{H}^0}$.

Feynman rules

A calculation of successive terms of perturbative expansion of the temperature Green's function can be changed into an algorithmic procedure with a set of mnemonic rules analogous to the Feynman rules of the vacuum QFT. The key element of the procedure are the Feynman diagrams. We are not going to elaborate the Feynman rule which depend on the field theory under consideration. Since the Feynman rules of the Matsubara formalism are rather similar to those of the vacuum QFT, we discuss here only the differences.

- In the vacuum QFT this is the Feynman, or time-ordered, propagator which is perturbatively expanded. In the Matsubara formalism the temperature Green's function ordered in imaginary time is expanded. Instead of the real time integration from $-\infty$ to ∞, we integrate over the imaginary time from 0 to β.
- The next difference is a role the tadpoles *i.e.* the loops formed by single lines as that one shown in Fig. 1. A tadpole corresponds to the Green's function of vanishing space-time argument $\Delta(0)$. The tadpoles do not appear in the vacuum QFT as long the field vacuum expectation values vanish. In the operator formalism they are effectively eliminated by the operator normal ordering of the interaction Hamiltonian H^I. Then, $\langle 0| : \hat{\phi}(x)\, \hat{\phi}^\dagger(x) : |0\rangle = 0$. In the path-integral formulation the tadpoles, which are actually infinite, show up but are canceled by properly chosen counterterms.
- In statistical QFT the tadpoles play an important physical role. They appear due finite system's density. Since the function $\Delta(0)$ is ill defined (the ordering does not work), the tadpole is represented by $\Delta^>(0)$.

- The perturbative expansion in momentum space in thermal QFT is analogous to that in vacuum QFT. However, the frequencies are discrete and coincide with the Matsubara frequencies (31). Consequently, instead of integrations over energies there are sums of Matsubara frequencies.

The differences will be illustrated with a few examples discussed in the following lectures.

First-order contributions to Δ

- Let us now discuss the first-order correction to the Green's function in a theory of self-interacting complex scalar field described by the Lagrangian (44). The expression to be computed is

$$\Delta^{(1)}(x-y) = -\frac{\lambda}{2!\,2!}\int_0^\beta d^4z \langle \mathcal{T}\big[\big(\hat{\phi}(z)\hat{\phi}^\dagger(z)\big)^2\hat{\phi}(x)\hat{\phi}^\dagger(y)\big]\rangle, \tag{71}$$

where we use the notation

$$\int_0^\beta d^4x = \int_0^\beta d\tau \int d^3x \tag{72}$$

and the expectation value is temporarily defined as

$$\langle \dots \rangle = \frac{\mathrm{Tr}\big[e^{-\beta \hat{H}^0}\mathcal{T}[e^{-\int_0^\beta d\tau'\,\hat{H}^I_{\rm int}(-i\tau')}\dots]\big]}{\mathrm{Tr}\big[e^{-\beta\hat{H}^0}\big]}, \tag{73}$$

that is the free partition function is in the denominator. The four-positions like x are $x = (\tau_x, \mathbf{x})$ and the integration over $z_0 = \tau_z$ is performed from 0 to β. When x is the argument of the field operator $\hat{\phi}(x)$ it should be understood as $\hat{\phi}(-i\tau_x, \mathbf{x})$.

- The plane-wave decompositions (46, 47) show that the expectation values like $\langle\mathcal{T}\hat{\phi}(z)\hat{\phi}(x)\rangle$ and $\langle\mathcal{T}\hat{\phi}(z)^\dagger\hat{\phi}^\dagger(y)\rangle$ vanish. So, one realizes that there are two contributions

$$\Delta^{(1)}_a(x-y) = -\lambda\int_0^\beta d^4z\langle\mathcal{T}[\hat{\phi}(z)\hat{\phi}^\dagger(y)]\rangle\langle\mathcal{T}[\hat{\phi}(z)\hat{\phi}^\dagger(z)]\rangle\langle\mathcal{T}[\hat{\phi}^\dagger(z)\hat{\phi}(x)]\rangle, \tag{74}$$

$$\Delta^{(1)}_b(x-y) = -\frac{\lambda}{2}\langle\mathcal{T}[\hat{\phi}(x)\hat{\phi}^\dagger(y)]\rangle\int_0^\beta d^4z\langle\mathcal{T}[\hat{\phi}(z)\hat{\phi}^\dagger(z)]\rangle\langle\mathcal{T}[\hat{\phi}(z)\hat{\phi}^\dagger(z)]\rangle. \tag{75}$$

In case of the contribution a, there are two operators $\hat{\phi}(z)$ to be paired with $\hat{\phi}^\dagger(y)$ and two operators $\hat{\phi}^\dagger(z)$ to be paired with $\hat{\phi}(z)$, the combinatorial factor of 4 is included in the formula (74). In case of the contribution b, the combinatorial factor equals 2.

- The results (74, 75) can be written as

$$\Delta^{(1)}_a(x-y) = -\lambda\int_0^\beta d^4z\,\Delta(x-z)\,\Delta(0)\,\Delta(z-y), \tag{76}$$

$$\Delta^{(1)}_b(x-y) = -\frac{\lambda}{2}\Delta(x-y)\int_0^\beta d^4z\,\big(\Delta(0)\big)^2. \tag{77}$$

The two contributions are represented graphically by two diagrams shown in Fig. 1.

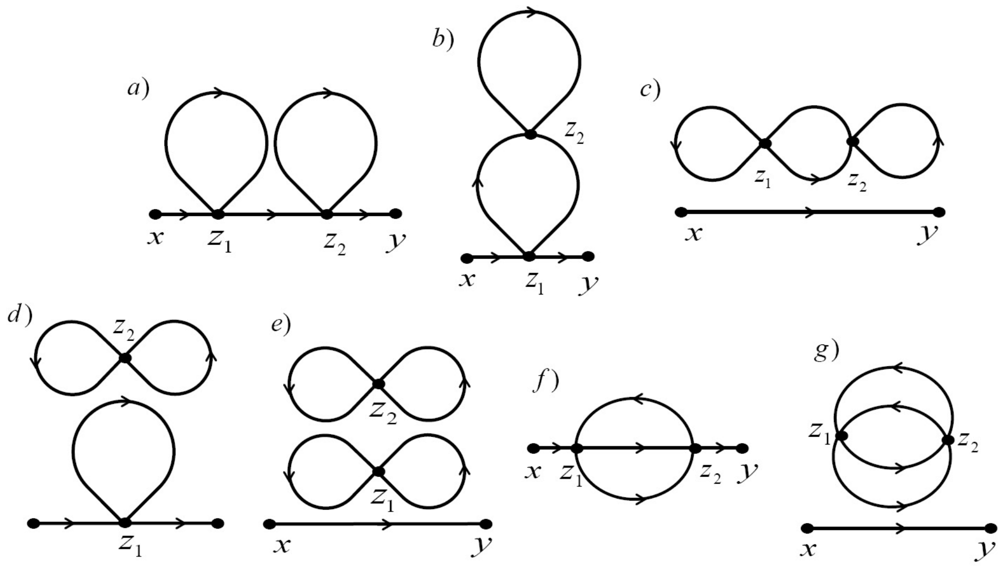

Figure 2: The second order contributions to the Green's function

Second-order contributions to Δ

- The expression to be computed is

$$\Delta^{(2)}(x-y) = \frac{\lambda^2}{(2!\,2!)^2 2!}\int_0^\beta d^4z_1 \int_0^\beta d^4z_2 \big\langle \mathcal{T}\big[\big(\hat\phi(z_1)\hat\phi^\dagger(z_1)\big)^2\big(\hat\phi(z_2)\hat\phi^\dagger(z_2)\big)^2\hat\phi(x)\hat\phi^\dagger(y)\big]\big\rangle. \quad (78)$$

- There are seven second-order contributions

$$\Delta_a^{(2)}(x-y) = \#\lambda^2\int_0^\beta d^4z_1\int_0^\beta d^4z_2\,\Delta(x-z_1)\,\Delta(0)\,\Delta(z_1-z_2)\,\Delta(0)\,\Delta(z_2-y), (79)$$

$$\Delta_b^{(2)}(x-y) = \#\lambda^2\int_0^\beta d^4z_1\int_0^\beta d^4z_2\,\Delta(x-z_1)\,\Delta(z_1-z_2)\,\Delta(z_2-z_1)\,\Delta(0)\,\Delta(z_1-y), (80)$$

$$\Delta_c^{(2)}(x-y) = \#\lambda^2\Delta(x-y)\int_0^\beta d^4z_1\int_0^\beta d^4z_2\Delta(0)\,\Delta(z_1-z_2)\,\Delta(z_2-z_1)\,\Delta(0), (81)$$

$$\Delta_d^{(2)}(x-y) = \#\lambda^2\int_0^\beta d^4z_1\,\Delta(x-z_1)\,\Delta(0)\,\Delta(z_1-y)\int_0^\beta d^4z_2\,\Delta(0)\,\Delta(0), (82)$$

$$\Delta_e^{(2)}(x-y) = \#\lambda^2\Delta(x-y)\int_0^\beta d^4z_1\,\Delta(0)\,\Delta(0)\int_0^\beta d^4z_2\,\Delta(0)\,\Delta(0), (83)$$

$$\Delta_f^{(2)}(x-y) = \#\lambda^2\int_0^\beta d^4z_1\int_0^\beta d^4z_2\,\Delta(x-z_1)\,\Delta(z_1-z_2)\,\Delta(z_1-z_2)\,\Delta(z_2-z_1)\,\Delta(z_2-y), (84)$$

$$\Delta_g^{(2)}(x-y) = \#\lambda^2\Delta(x-y)\int_0^\beta d^4z_1\int_0^\beta d^4z_2\,\Delta(z_1-z_2)\,\Delta(z_1-z_2)\,\Delta(z_2-z_1)\,\Delta(z_2-z_1), (85)$$

where # denotes a numerical coefficient. The contributions are represented by the diagrams shown in Fig. 2.

Exercise: Derive the numerical factors in Eqs. (79 - 85).

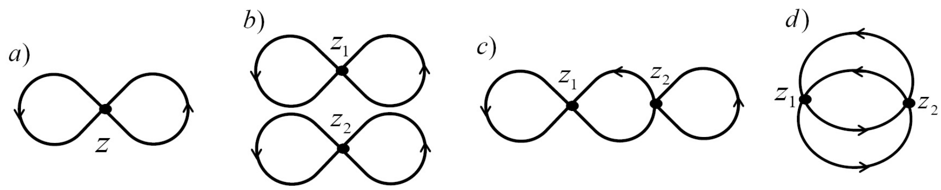

Figure 3: The first and second order contributions to the quantity (86)

Connected and disconnected diagrams

- The diagram b) in Fig. 1 and the diagrams c), d) and e) in Fig. 2 can be split each into two diagrams not cutting any line. These are the disconnected diagrams.
- One observes that the perturbative expansion of the quantity

$$\frac{\mathrm{Tr}\big[e^{-\beta \hat{H}^0_{\mathrm{int}}}\mathcal{T}\big[e^{-\int_0^\beta d\tau\, \hat{H}^I_{\mathrm{int}}(-i\tau)}\big]\big]}{\mathrm{Tr}\big[e^{-\beta \hat{H}^0_{\mathrm{int}}}\big]} \tag{86}$$

  gives unity in the zeroth order, the diagram a) from Fig. 3 in the first order and the diagrams b), c) and d) from Fig. 3 in the second order.
- It is also not difficult to observe that the perturbative expansion of the temperature Green's function can be expressed in a way which is shown graphically in Fig. 4.
- Combing the observation, one finds that the disconnected diagrams are eliminated from the perturbative expansion of Green's function is defined as

$$\Delta(x-y) \equiv \frac{\mathrm{Tr}\big[e^{-\beta \hat{H}^0_{\mathrm{int}}}\mathcal{T}\big[e^{-\int_0^\beta d\tau\, \hat{H}^I_{\mathrm{int}}(-i\tau)}\,\hat{\phi}_{\mathrm{int}}(x)\,\hat{\phi}^\dagger_{\mathrm{int}}(y)\big]\big]}{\mathrm{Tr}\big[e^{-\beta \hat{H}^0_{\mathrm{int}}}\mathcal{T}\big[e^{-\int_0^\beta d\tau\, \hat{H}^I_{\mathrm{int}}(-i\tau)}\big]\big]}, \tag{87}$$

  that is the partition function in the denominator is not free but the interacting one, as in the original definition (2).
- Further on, we will use the definition (87).

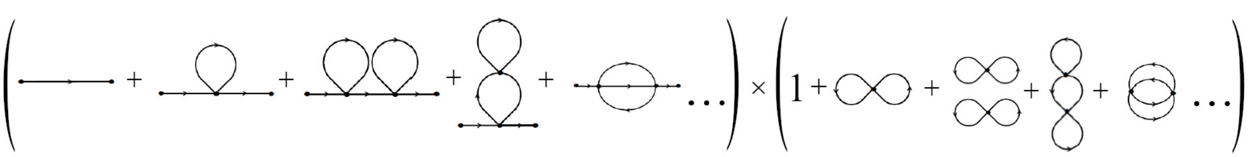

Figure 4: The perturbative expansion of the Green's function