

Quantum Many-particle Systems (Note)

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1 Second Quantization and Coherent States

We define a state $|\vec{r}\sigma\tau\rangle$, which is a state of the particle localized at point \vec{r} , with a projection of the spin σ and isospin τ . These states span the Hilbert space of the particle:

$$\sum_{\sigma=\pm\frac{1}{2}} \sum_{\tau=\pm\frac{1}{2}} \int d^3r |\vec{r}\sigma\tau\rangle \langle\vec{r}\sigma\tau| = 1$$

where we suppose the particle has only two eigenvalues of isospin τ , like a proton or neutron.

Their overlap is given by:

$$\langle\vec{r}\sigma\tau|\vec{r}'\sigma'\tau'\rangle = \delta_{\sigma\sigma'}\delta_{\tau\tau'}\delta^3(\vec{r}-\vec{r}')$$

We order:

$$|x\rangle \equiv |\vec{r}\sigma\tau\rangle$$

and

$$\int dx = \sum_{\sigma=\pm\frac{1}{2}} \sum_{\tau=\pm\frac{1}{2}} \int d^3r;$$
$$\delta(x-x') = \delta_{\sigma\sigma'}\delta_{\tau\tau'}\delta^3(\vec{r}-\vec{r}')$$

Using this notation, we can write:

$$\int dx |x\rangle \langle x| = 1$$

and

$$\langle x|x'\rangle = \delta(x-x')$$

For describing a system with N particles, define Hilbert space \mathcal{H}_N :

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}$$

$$|\alpha_1 \dots \alpha_N\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_N\rangle$$

To distinguish Bosons and Fermions, and for convenience, we shall adopt the following unified notation:

$$\psi(\vec{r}_{P1}, \vec{r}_{P2}, \dots, \vec{r}_{PN}) = \zeta^P \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

A wave function belongs to the Hilbert space of N Bosons \mathcal{B}_N , or the Hilbert space of N Fermions \mathcal{F}_N , if ζ equals to +1 or -1.

The symmetrization operator \mathcal{P}_B and the antisymmetrization operator \mathcal{P}_F :

$$\mathcal{P}_{\{B\}} \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{1}{N!} \sum_P \zeta^P \psi(\vec{r}_{P1}, \vec{r}_{P2}, \dots, \vec{r}_{PN})$$

For Bosons:

$$\mathcal{P}_B \psi(\vec{r}_1, \vec{r}_2) = \frac{1}{2} [\psi(\vec{r}_1, \vec{r}_2) + \psi(\vec{r}_2, \vec{r}_1)];$$

and for Fermions:

$$\mathcal{P}_F \psi(\vec{r}_1, \vec{r}_2) = \frac{1}{2} [\psi(\vec{r}_1, \vec{r}_2) - \psi(\vec{r}_2, \vec{r}_1)]$$

The operator $\mathcal{P}_{\{B\}}$ may be shown to be a projector as follows:

$$\begin{aligned} \mathcal{P}_{\{B\}}^2 \psi(\vec{r}_1, \dots, \vec{r}_N) &= \frac{1}{N!} \frac{1}{N!} \sum_P \sum_{P'} \zeta^P \zeta^{P'} \psi(\vec{r}_{P'P1}, \vec{r}_{P'P2}, \dots, \vec{r}_{P'PN}) \\ &= \frac{1}{N!} \sum_P \left[\frac{1}{N!} \sum_Q \zeta^Q \psi(\vec{r}_{Q1}, \vec{r}_{Q2}, \dots, \vec{r}_{QN}) \right] \\ &= \frac{1}{N!} \sum_P \mathcal{P}_{\{B\}} \psi(\vec{r}_1, \dots, \vec{r}_N) \\ &= \mathcal{P}_{\{B\}} \psi(\vec{r}_1, \dots, \vec{r}_N) \end{aligned}$$

These operators project \mathcal{H}_N onto the Hilbert space of Bosons \mathcal{B}_N and the Hilbert space of Fermions \mathcal{F}_N :

$$\mathcal{B}_N = \mathcal{P}_B \mathcal{H}_N$$

$$\mathcal{F}_N = \mathcal{P}_F \mathcal{H}_N$$

Thus, a system of N Bosons or Fermions can be represented as follows:

$$\begin{aligned} |\alpha_1 \dots \alpha_N\rangle &= \sqrt{N!} \mathcal{P}_{\{B\}} |\alpha_1 \dots \alpha_N\rangle \\ &= \frac{1}{\sqrt{N!}} \sum_P \zeta^P |\alpha_{P1}\rangle \otimes \dots \otimes |\alpha_{PN}\rangle \end{aligned}$$

It follows that if $|\alpha_1 \dots \alpha_N\rangle$ is a basis of \mathcal{H}_N , then $\mathcal{P}_{\{F\}}|\alpha_1 \dots \alpha_N\rangle$ is a basis of \mathcal{B}_N or \mathcal{F}_N . The normalized states is written as $|\alpha_1 \dots \alpha_N\rangle$:

$$|\alpha_1 \dots \alpha_N\rangle = \frac{1}{\sqrt{\prod_{\alpha} n_{\alpha}!}} |\alpha_1 \dots \alpha_N\rangle$$

where n_{α} is the occupation number of each state.

Let \mathcal{O} be an arbitrary operator in \mathcal{B}_N or \mathcal{F}_N , For any states, and any permutation:

$$(\alpha_{P_1} \dots \alpha_{P_N} | \mathcal{O} | \alpha'_{P_1} \dots \alpha'_{P_N}) = (\alpha_1 \dots \alpha_N | \mathcal{O} | \alpha'_1 \dots \alpha'_N)$$

An operator \hat{U} is a one-body operator if:

$$\hat{U}|\alpha_1 \dots \alpha_N\rangle = \sum_{i=1}^N \hat{U}_i |\alpha_1 \dots \alpha_N\rangle$$

For example, the kinetic operator \hat{T} in the $\{\vec{p}\}$ basis acts as:

$$\hat{T}|\vec{p}_1 \dots \vec{p}_N\rangle = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} |\vec{p}_1 \dots \vec{p}_N\rangle$$

and a local potential operator \hat{W} in $\{x\}$ basis acts as:

$$\hat{W}|x_1 \dots x_N\rangle = \sum_{i=1}^N W(x_i) |x_1 \dots x_N\rangle$$

Similarly, an operator \hat{V} is a two-body operator if:

$$\hat{V}|\alpha_1 \dots \alpha_N\rangle = \sum_{1 \leq i < j \leq N} \hat{V}_{ij} |\alpha_1 \dots \alpha_N\rangle$$

A two-body interaction \hat{V} is said to be local, or to be velocity independent, when it is diagonal in configuration space (and spin and isospin, if appropriate).

$$(\vec{r}_1 \vec{r}_2 | \hat{V} | \vec{r}_3 \vec{r}_4) = \delta(\vec{r}_1 - \vec{r}_3) \delta(\vec{r}_2 - \vec{r}_4) v(\vec{r}_1 - \vec{r}_2)$$

Notice that $\hat{V}_{ij} = \hat{V}_{ji}$. In this case, we have

$$\hat{V}|\alpha_1 \dots \alpha_N\rangle = \frac{1}{2} \sum_{1 \leq i \neq j \leq N} v(\vec{r}_1 - \vec{r}_2) |\alpha_1 \dots \alpha_N\rangle$$

In general, we define an n-body operator \hat{R} which acts on $|\alpha_1 \dots \alpha_N\rangle$ as:

$$\hat{R}|\alpha_1 \dots \alpha_N\rangle = \frac{1}{n!} \sum_{1 \leq i_1 \neq i_2 \neq \dots \neq i_n \leq N} \hat{R}_{i_1 i_2 \dots i_n} |\alpha_1 \dots \alpha_N\rangle.$$

The creation operator: a_λ^\dagger

$$a_\lambda^\dagger |\lambda_1 \dots \lambda_N\rangle \equiv |\lambda \lambda_1 \dots \lambda_N\rangle$$

In order to allow the creation operator a_λ^\dagger and annihilation operator a_λ to operate within one space, we define the Fock space \mathcal{B} and \mathcal{F} as direct sum of Boson or Fermion spaces:

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \mathcal{B}_2 \oplus \dots = \oplus_{n=0}^{\infty} \mathcal{B}_n$$

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \dots = \oplus_{n=0}^{\infty} \mathcal{F}_n$$

Where by defination:

$$\mathcal{B}_0 = \mathcal{F}_0 = |0\rangle$$

$$\mathcal{B}_1 = \mathcal{F}_1 = \mathcal{H}$$

The closure relation in the Fock space may be written:

$$1 = |0\rangle \langle 0| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \dots \lambda_N} |\lambda_1 \dots \lambda_N\rangle \langle \lambda_1 \dots \lambda_N|$$

The annihilation operator a_λ . For Bosons:

$$a_\lambda |n_{\beta_1} n_{\beta_2} \dots n_\lambda \dots\rangle = \sqrt{n_\lambda} |n_{\beta_1} n_{\beta_2} \dots (n_\lambda - 1) \dots\rangle,$$

which is expressed in occupation number representation. For Fermions:

$$a_\lambda |\beta_1 \dots \beta_n\rangle = \begin{cases} (-1)^{i-1} |\beta_1 \dots \hat{\beta}_i \dots \beta_n\rangle, & \text{if } |\lambda\rangle \text{ is occupied} \\ 0, & \text{if } |\lambda\rangle \text{ is unoccupied.} \end{cases}$$

$$\begin{aligned} a_{\tilde{\alpha}}^\dagger |\alpha_1 \dots \alpha_n\rangle &= \sum_{\alpha} \langle \alpha | \tilde{\alpha} \rangle |\alpha \alpha_1 \dots \alpha_n\rangle \\ &= \sum_{\alpha} \langle \alpha | \tilde{\alpha} \rangle a_{\alpha}^\dagger |\alpha_1 \dots \alpha_n\rangle \end{aligned}$$

The creation operators satisfy the operator equation:

$$a_{\tilde{\alpha}}^\dagger = \sum_{\alpha} \langle \alpha | \tilde{\alpha} \rangle a_{\alpha}^\dagger$$

and the annihilation operators satisfy the adjoint equation:

$$a_{\tilde{\alpha}} = \sum_{\alpha} \langle \alpha | \tilde{\alpha} \rangle a_{\alpha}$$

To represent the operator in the diagonal basis, we define the numnber operator \hat{n}_α :

$$\hat{n}_\alpha = a_{\alpha}^\dagger a_{\alpha}$$

The operator \hat{N} counts the total number of particles in a state:

$$\hat{N} = \sum_{\alpha} \hat{n}_{\alpha} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$$

\hat{U} is a one-body operator, and is diagonal in the orthonormal basis $|\alpha\rangle$.

$$U_{\alpha} = \langle \alpha | U | \alpha \rangle$$

We can write:

$$\begin{aligned} \{\alpha'_1 \dots \alpha'_N | U | \alpha_1 \dots \alpha_N \} &= \sum_P \zeta^P \sum_{i=1}^N \prod_{k \neq i} \langle \alpha'_{Pk} | \alpha_k \rangle \langle \alpha'_{Pi} | U | \alpha_i \rangle \\ &= \left(\sum_{i=1}^N U_{\alpha_i} \right) \{\alpha'_1 \dots \alpha'_N | \alpha_1 \dots \alpha_N \} \\ &= \{\alpha'_1 \dots \alpha'_N | \sum_{\alpha} U_{\alpha} \hat{n}_{\alpha} | \alpha_1 \dots \alpha_N \} \end{aligned}$$

Since the equality holds for any states, we obtain the operator equation:

$$\hat{U} = \sum_{\alpha} U_{\alpha} \hat{n}_{\alpha} = \sum_{\alpha} \langle \alpha | U | \alpha \rangle a_{\alpha}^{\dagger} a_{\alpha}$$

\hat{V} is a diagonal two-body operator

$$V_{\alpha\beta} = \langle \alpha\beta | V | \alpha\beta \rangle$$

$\hat{P}_{\alpha\beta}$ is an operator which counts the number of pairs of particles in the states $|\alpha\rangle$ and $|\beta\rangle$. If $|\alpha\rangle$ and $|\beta\rangle$ are different, the number of pairs is $n_{\alpha}n_{\beta}$ whereas if $|\alpha\rangle = |\beta\rangle$, the number of pairs is $n_{\alpha}(n_{\beta} - 1)$. Hence, the operator which counts pairs may be written

$$\hat{P}_{\alpha\beta} = \hat{n}_{\alpha}\hat{n}_{\beta} - \delta_{\alpha\beta}\hat{n}_{\alpha}$$

Notice that

$$a_{\alpha}a_{\beta}^{\dagger} - \zeta a_{\beta}^{\dagger}a_{\alpha} = \delta_{\alpha\beta}$$

Thus $\hat{P}_{\alpha\beta}$ can be written in terms of creation and annihilation operators

$$\begin{aligned} \hat{P}_{\alpha\beta} &= a_{\alpha}^{\dagger}a_{\alpha}a_{\beta}^{\dagger}a_{\beta} - \delta_{\alpha\beta}a_{\alpha}^{\dagger}a_{\alpha} \\ &= a_{\alpha}^{\dagger}\zeta a_{\beta}^{\dagger}a_{\alpha}a_{\beta} + \delta_{\alpha\beta}a_{\alpha}^{\dagger}a_{\beta} - \delta_{\alpha\beta}a_{\alpha}^{\dagger}a_{\alpha} \\ &= a_{\alpha}^{\dagger}a_{\beta}^{\dagger}a_{\beta}a_{\alpha} \end{aligned}$$

Using this operator, the action of two-body operator \hat{V} can be written as:

$$\{\alpha'_1 \dots \alpha'_n | \hat{V} | \alpha_1 \dots \alpha_n \} = \{\alpha'_1 \dots \alpha'_n | \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} | \alpha_1 \dots \alpha_n \}$$

Hence we obtain the operator equation:

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta} V_{\alpha\beta} \hat{P}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta} (\alpha\beta | V | \alpha\beta) a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta} a_{\alpha}$$

The general expression for a two-body potential is

$$\hat{V} = \frac{1}{2} \sum_{\lambda\mu\nu\rho} (\lambda\mu | V | \nu\rho) a_{\lambda}^{\dagger} a_{\mu}^{\dagger} a_{\nu} a_{\rho}$$

The preceding derivations for one and two-body operators may be straightforwardly generalized to n-body operators, with the result:

$$\hat{R} = \frac{1}{n!} \sum_{\lambda_1 \dots \lambda_n} \sum_{\mu_1 \dots \mu_n} (\lambda_1 \dots \lambda_n | \hat{R} | \mu_1 \dots \mu_n) a_{\lambda_1}^{\dagger} \dots a_{\lambda_n}^{\dagger} a_{\mu_1} \dots a_{\mu_n}$$

Coherent States

Coherent states are defined as eigenstates of annihilation operators. For an arbitrary state $|\phi\rangle$ in Fock space, we can expand it as:

$$|\phi\rangle = \sum_{n=0}^{\infty} \sum_{\alpha_1 \dots \alpha_n} \phi_{\alpha_1 \dots \alpha_n} |\alpha_1 \dots \alpha_n\rangle$$

Assuming $|\phi\rangle$ is a eigenstate of the annihilation operators, then

$$a_{\alpha} |\phi\rangle = \phi_{\alpha} |\phi\rangle$$

The commutation and anticommutation relations of Bosons and Fermions imply the corresponding relations for the eigenvalues:

$$[\phi_{\alpha}, \phi_{\beta}]_{-\zeta} = 0$$

For Fermions, the eigenvalues anticommute, we will need to define anticommute variables called Grassmann numbers. However, for Bosons, the eigenvalues commute and we can just proceed straightforwardly using ordinary numbers.

We shall start with Bosons coherent states. A Boson coherent state can be expanded in occupation number representation as

$$|\phi\rangle = \sum_{n_{\alpha_1} \dots n_{\alpha_p}} \phi_{n_{\alpha_1} \dots n_{\alpha_p}} |n_{\alpha_1} \dots n_{\alpha_p}\rangle$$

According to the eigenequation, the relations on coefficients for all $\{n_\alpha\}$ is

$$\sqrt{n_{\alpha_i}} \phi_{n_{\alpha_1} \dots n_{\alpha_i} \dots} = \phi_{\alpha_i} \phi_{n_{\alpha_1} \dots (n_{\alpha_i}-1) \dots}$$

By recursion, we obtain

$$\begin{aligned} \phi_{n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i}} &= \frac{\phi_{\alpha_1}^{n_{\alpha_1}} \phi_{\alpha_2}^{n_{\alpha_2}} \dots \phi_{\alpha_i}^{n_{\alpha_i}} \dots}{\sqrt{n_{\alpha_1}!} \sqrt{n_{\alpha_2}!} \dots \sqrt{n_{\alpha_i}!} \dots} \\ |n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_p} \dots\rangle &= \frac{(a_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{(a_{\alpha_2}^\dagger)^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \dots \frac{(a_{\alpha_p}^\dagger)^{n_{\alpha_p}}}{\sqrt{n_{\alpha_p}!}} \dots |0\rangle \end{aligned}$$

Hence we finally obtain:

$$\begin{aligned} |\phi\rangle &= \sum_{n_{\alpha_1}, n_{\alpha_2} \dots n_{\alpha_p}} \frac{(\phi_{\alpha_1} a_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{n_{\alpha_1}!} \frac{(\phi_{\alpha_2} a_{\alpha_2}^\dagger)^{n_{\alpha_2}}}{n_{\alpha_2}!} \dots \frac{(\phi_{\alpha_p} a_{\alpha_p}^\dagger)^{n_{\alpha_p}}}{n_{\alpha_p}!} |0\rangle \\ &= \exp \left[\sum_{\alpha} \phi_{\alpha} a_{\alpha}^\dagger \right] |0\rangle \\ \langle\phi| &= \langle 0| \exp \left[\sum_{\alpha} \phi_{\alpha}^* a_{\alpha} \right] \end{aligned}$$

The action of a creation operator on a coherent state is given by

$$a_{\alpha}^\dagger |\phi\rangle = a_{\alpha}^\dagger \exp \left[\sum_{\alpha} \phi_{\alpha} a_{\alpha}^\dagger \right] |0\rangle = \frac{\partial}{\partial \phi_{\alpha}} |\phi\rangle$$

with the adjoint relation:

$$\langle\phi| a_{\alpha} = \frac{\partial}{\partial \phi_{\alpha}^*} \langle\phi|$$

The overlap of two coherents is given by

$$\langle\phi|\phi'\rangle = \exp \left[\sum_{\alpha} \phi_{\alpha}^* \phi'_{\alpha} \right]$$

Coherent states are overcomplete in Fock space. Any state $|\psi\rangle$ can be represented as:

$$|\psi\rangle = \int \prod_{\alpha} \frac{d\phi_{\alpha}^* d\phi_{\alpha}}{2\pi i} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} \psi(\phi^*) \cdot |\phi\rangle$$

where

$$\frac{d\phi_{\alpha}^* d\phi_{\alpha}}{2\pi i} = \frac{d(\text{Re}\phi_{\alpha}) d(\text{Im}\phi_{\alpha})}{\pi}$$

and

$$\psi(\phi^*) = \langle\phi|\psi\rangle$$

is the coherent state representation of the state $|\psi\rangle$. According to equations above, we find:

$$\langle\phi|a_\alpha|f\rangle = \frac{\partial}{\partial\phi_\alpha^*}f(\phi^*)$$

$$\langle\phi|a_\alpha^\dagger|f\rangle = \phi_\alpha^*f(\phi^*)$$

Hence we can write the annihilation and creation operator in coherent state representation:

$$a_\alpha = \frac{\partial}{\partial\phi_\alpha^*}$$

$$a_\alpha^\dagger = \phi_\alpha^*$$

which is consistent with the Boson commutation rules:

$$[\phi_\alpha^*, \phi_\beta^*] = \left[\frac{\partial}{\partial\phi_\alpha^*}, \frac{\partial}{\partial\phi_\beta^*} \right] = 0$$

$$\left[\frac{\partial}{\partial\phi_\alpha^*}, \phi_\beta^* \right] = \delta_{\alpha\beta}$$

The projection of the schrodinger equation:

$$H(\phi_\alpha^*, \frac{\partial}{\partial\phi_\alpha^*})\psi(\phi^*) = E\psi(\phi^*)$$

For a standart Hamiltonian eith one and two-body operators, it reads:

$$\left(\sum_{\alpha,\beta} T_{\alpha\beta} \phi_\alpha^* \frac{\partial}{\partial\phi_\beta^*} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|\gamma\delta) \phi_\alpha^* \phi_\beta^* \frac{\partial}{\partial\phi_\gamma^*} \frac{\partial}{\partial\phi_\delta^*} \right) \psi(\phi^*) = E\psi(\phi^*)$$

Grassmann Algebra

Algebras of anticommuting numbers are called Grassmann algebras. A Grassmann algebra is defined by a set of generators $\{\xi_\alpha\}$, $\alpha = 1, \dots, n$. These generators anticommute:

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0$$

Thus $\xi_\alpha^2 = 0$. The basis of the Grassmann algebra is made of all distinct products of the generators. Thus, a number in Grassmann algebra is a linear combination with complex coefficients of the numbers $\{1, \xi_{\alpha_1}, \xi_{\alpha_1}\xi_{\alpha_2}, \dots, \xi_{\alpha_1}\xi_{\alpha_2} \dots \xi_{\alpha_n}\}$. The dimension of a Grassmann algebra with n generators is 2^n .

Conjugation in a Grassmann algebra:

$$(\xi_\alpha)^* = \xi_\alpha^*$$

$$(\xi_\alpha^*)^* = \xi_\alpha$$

If λ is a complex number,

$$(\lambda \xi_\alpha)^* = \lambda^* \xi_\alpha^*$$

and for any product of generators,

$$(\xi_{\alpha_1} \xi_{\alpha_2} \cdots \xi_{\alpha_n})^* = \xi_{\alpha_n}^* \xi_{\alpha_{n-1}}^* \cdots \xi_{\alpha_1}^* \quad (1)$$

Consider a Grassmann algebra with two generators ξ and ξ^* , and is generated by the four numbers: $\{1, \xi, \xi^*, \xi^* \xi\}$. Because of it's property, any function f defined on this algebra is a linear function.

$$f(\xi) = f_0 + f_1 \xi$$

The coherent state representation of an operator in the Grassmann algebra will be a function and must have the form:

$$A(\xi^*, \xi) = a_0 + a_1 \xi + \bar{a}_1 \xi^* + a_{12} \xi^* \xi$$

As for ordinary complex functions, a derivative operator can be defined for Grassmann variable functions.

$$\frac{\partial}{\partial \xi} (\xi^* \xi) = \frac{\partial}{\partial \xi} (-\xi \xi^*) = -\xi^*$$

Notice that

$$\frac{\partial}{\partial \xi} \frac{\partial}{\partial \xi^*} A(\xi^*, \xi) = -\frac{\partial}{\partial \xi^*} \frac{\partial}{\partial \xi} A(\xi^*, \xi)$$

Thus the operators $\frac{\partial}{\partial \xi}$ and $\frac{\partial}{\partial \xi^*}$ anticommute.

We define integration over Grassmann variables as a linear mapping which has fundamental property of ordinary integrals over functions vanishing at infinity that the integral of an exact differential form is zero.

$$\begin{aligned} \int d\xi 1 &= 0 \\ \int d\xi \xi &= 1 \end{aligned}$$

We can then define delta function in Grassmann algebra:

$$\begin{aligned} \delta(\xi, \xi') &= \int d\eta e^{-\eta(\xi - \xi')} \\ &= \int d\eta [1 - \eta(\xi - \xi')] \\ &= -(\xi - \xi') \end{aligned}$$

$$\begin{aligned}
\int d\xi' \delta(\xi, \xi') f(\xi') &= - \int d\xi' (\xi - \xi') (f_0 + f_1 \xi') \\
&= \int d\xi' (-f_0 \xi + f_1 \xi' \xi + f_0 \xi') \\
&= f_0 + f_1 \xi = f(\xi)
\end{aligned}$$

We then define a scalar product of Grassmann functions by:

$$\langle f|g \rangle = \int d\xi^* d\xi e^{-\xi^* \xi} f^*(\xi) g(\xi^*)$$

With this definition, we see that:

$$\begin{aligned}
\langle f|g \rangle &= \int d\xi^* d\xi (1 - \xi^* \xi) (f_0^* + f_1^* \xi) (g_0 + g_1 \xi^*) \\
&= f_0^* g_0 + f_1^* g_1
\end{aligned}$$

Grassmann functions have the structure of a Hilbert space. The coefficients of a Fermion coherent state must be Grassmann numbers. In order to construct Fermion coherent states, we need enlarge the Fermion Fock space.

\mathcal{G} is a Grassmann algebra with generators ξ_α for each annihilation operators a_α and ξ_α^* for each creation operators a_α^\dagger . We then construct the generalized Fock space as the set of linear combinations of states in Fock space \mathcal{F} with the coefficients in the Grassmann algebra \mathcal{G} . Any vector $|\psi\rangle$ in the generalized Fock space can be expanded as:

$$|\psi\rangle = \sum_{\alpha} \chi_{\alpha} |\phi_{\alpha}\rangle$$

where χ_{α} are Grassmann numbers and $|\phi_{\alpha}\rangle$ are vectors in Fock space \mathcal{F} . We require that:

$$\{\tilde{\xi}, \tilde{a}\} = 0$$

and

$$(\tilde{\xi} \tilde{a})^\dagger = \tilde{a}^\dagger \tilde{\xi}^*$$

We now define a Fermion coherent state $|\xi\rangle$ analogous to Boson coherent state:

$$\begin{aligned}
|\xi\rangle &= \exp \left[- \sum_{\alpha} \xi_{\alpha} a_{\alpha}^\dagger \right] |0\rangle \\
&= \prod_{\alpha} (1 - \xi_{\alpha} a_{\alpha}^\dagger) |0\rangle
\end{aligned}$$

$$\begin{aligned}
a_{\alpha} (1 - \xi_{\alpha} a_{\alpha}^\dagger) |0\rangle &= \xi_{\alpha} |0\rangle \\
&= \xi_{\alpha} (1 - \xi_{\alpha} a_{\alpha}^\dagger) |0\rangle
\end{aligned}$$

Thus

$$\begin{aligned} a_\alpha |\xi\rangle &= a_\alpha \prod_\alpha (1 - \xi_\alpha a_\alpha^\dagger) |0\rangle \\ &= \xi_\alpha |\xi\rangle \end{aligned}$$

Similarly, the adjoint of the coherent state is

$$\langle \xi| = \langle 0| \exp \left[- \sum_\alpha a_\alpha \xi_\alpha^* \right] = \langle 0| \exp \left[\sum_\alpha \xi_\alpha^* a_\alpha \right]$$

and

$$\begin{aligned} \langle \xi| a_\alpha^\dagger &= \langle \xi| \xi_\alpha^* \\ a_\alpha^\dagger |\xi\rangle &= -\frac{\partial}{\partial \xi_\alpha} |\xi\rangle \\ \langle \xi| a_\alpha &= \frac{\partial}{\partial \xi_\alpha^*} \langle \xi| \end{aligned}$$

The overlap of two coherent states is calculated as:

$$\begin{aligned} \langle \xi|\xi'\rangle &= \langle 0| \prod_\alpha (1 + \xi_\alpha^* a_\alpha) (1 - \xi_\alpha a_\alpha^\dagger) |0\rangle \\ &= \prod_\alpha (1 + \xi_\alpha^* \xi_\alpha) \\ &= \exp \left[\sum_\alpha \xi_\alpha^* \xi_\alpha \right] \end{aligned}$$

The closure relation can be written:

$$\int \prod_\alpha d\xi_\alpha^* d\xi_\alpha e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} |\xi\rangle \langle \xi| = 1$$

$\{|n\rangle\}$ is a complete set of states in Fock space. The trace of operator A can be written:

$$\begin{aligned} \text{Tr } A &= \sum_n \langle n| A |n\rangle \\ &= \int \prod_\alpha d\xi_\alpha^* d\xi_\alpha e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \sum_n \langle n|\xi\rangle \langle \xi| A |n\rangle \\ &= \int \prod_\alpha d\xi_\alpha^* d\xi_\alpha e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle -\xi| A \sum_n |n\rangle \langle n|\xi\rangle \\ &= \int \prod_\alpha d\xi_\alpha^* d\xi_\alpha e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle -\xi| A |\xi\rangle \end{aligned}$$

We can define a Grassmann coherent state representation analogous to the coherent state representation for Bosons.

$$|\psi\rangle = \int \prod_\alpha d\xi_\alpha^* d\xi_\alpha e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \psi(\xi^*) |\xi\rangle$$

Where

$$\psi(\xi^*) = \langle \xi | \psi \rangle$$

analogous to Boson case:

$$\langle \xi | a_\alpha | \psi \rangle = \frac{\partial}{\partial \xi_\alpha^*} \psi(\xi^*)$$

$$\langle \xi | a_\alpha^\dagger | \psi \rangle = \xi_\alpha^* \psi(\xi^*)$$

The operators a_α and a_α^\dagger are represented as $\frac{\partial}{\partial \xi_\alpha^*}$ and ξ_α^* in the coherent states representation.

The anticommutation relation is written:

$$\left\{ \frac{\partial}{\partial \xi_\alpha^*}, \xi_\beta^* \right\} = \delta_{\alpha\beta}$$

However, different from Boson, the expectation value of the number operator is not a real number. And it is meaningless to talk about the average number of particles in a Fermion coherent state.

$$\frac{\langle \xi | N | \xi \rangle}{\langle \xi | \xi \rangle} = \sum_\alpha \xi_\alpha^* \xi_\alpha$$

Guassian Integrals

$$\begin{aligned} \int \frac{dx_1 \dots dx_n}{(2\pi)^{\frac{n}{2}}} e^{-\frac{1}{2} x_i A_{ij} x_j + x_i J_i} &= [\det A]^{-\frac{1}{2}} e^{\frac{1}{2} J_i A_{ij}^{-1} J_j} \\ \int \prod_{i=1}^n \frac{dx_i^* dx_i}{2\pi i} e^{-x_i^* H_{ij} x_j + J_i^* x_i + J_i x_i^*} &= [\det A]^{-1} e^{J_i^* H_{ij}^{-1} J_j} \\ \int d\xi^* d\xi e^{-\xi^* a \xi} &= \int d\xi^* d\xi (1 - \xi^* a \xi) = a \end{aligned}$$

2 General Formalism at Finite Temperature

Functional Integral Formulation

Consider a Matrix element of the evolution operator for a particle governed by Hamiltonian $\hat{H}(\hat{p}, \hat{x})$

$$\mathcal{U}(x_f t_f, x_i t_i) = \langle x_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | x_i \rangle$$

Let the time interval $t_f - t_i$ be divided into M equal steps of size ϵ :

$$\epsilon = \frac{t_f - t_i}{M}$$

with intermediate times denoted:

$$t_n = t_i + n\epsilon$$

with this notation:

$$t_0 \equiv t_i \quad \text{and} \quad t_M \equiv t_f$$

Use the same convention for coordinates:

$$x_0 \equiv x_i \quad \text{and} \quad x_M \equiv x_f$$

$$\begin{aligned} \mathcal{U} &= \langle x_f | e^{-\frac{i}{\hbar} \hat{H}(t_f - t_i)} | x_i \rangle \\ &= \int \prod_{k=1}^{M-1} dx_k \langle x_f | e^{-i \frac{\epsilon}{\hbar} \hat{H}} | x_{M-1} \rangle \langle x_{M-1} | e^{-i \frac{\epsilon}{\hbar} \hat{H}} | x_{M-2} \rangle \\ &\quad \langle x_{M-2} | \dots e^{-i \frac{\epsilon}{\hbar} \hat{H}} | x_1 \rangle \langle x_1 | e^{-i \frac{\epsilon}{\hbar} \hat{H}} | x_i \rangle \end{aligned}$$

The infinitesimal evolution operator is written:

$$\langle x_n | e^{-i \frac{\epsilon}{\hbar} \hat{H}(\hat{p}, \hat{x})} | x_{n-1} \rangle = \int d^3 p_n \langle x_n | p_n \rangle \langle p_n | e^{-i \frac{\epsilon}{\hbar} \hat{H}(\hat{p}, \hat{x})} | x_{n-1} \rangle$$

The Hamiltonian for a single particle in a potential:

$$H_v(\hat{p}, \hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

We define an operator to be in normal form if all the \hat{p} 's appear to the left of all the \hat{x} 's. The result of reordering an operator $\mathcal{O}(\hat{p}, \hat{x})$ into normal form is denoted as $:\mathcal{O}(\hat{p}, \hat{x}):$.

$$: e^{-i \frac{\epsilon}{\hbar} H_v(\hat{p}, \hat{x})} := \sum_{n=0}^{\infty} \left(-i \frac{\epsilon}{\hbar}\right)^n \sum_{k=0}^n \frac{1}{k!(n-k)!} \left(\frac{\hat{p}^2}{2m}\right)^k (V(\hat{x}))^{n-k}$$

For any $\hat{H}(\hat{p}, \hat{x})$ in normal form,

$$e^{-i \frac{\epsilon}{\hbar} H_v(\hat{p}, \hat{x})} =: e^{-i \frac{\epsilon}{\hbar} H_v(\hat{p}, \hat{x})} : + \left(-i \frac{\epsilon}{\hbar}\right)^2 \sum_{n=0}^{\infty} \frac{\left(-i \frac{\epsilon}{\hbar}\right)^n}{(n+2)!} ([H(\hat{p}, \hat{x})]^{n+2} - :[H(\hat{p}, \hat{x})]^{n+2}:)$$

For the special case: $H_v(\hat{p}, \hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$, the leading correction is

$$-\frac{\epsilon^2}{2\hbar^2} \left[V, \frac{\hat{p}^2}{2m} \right] = -\frac{\epsilon^2}{4m\hbar^2} (V'' + 2iV'\hat{p})$$

If the infinitesimal evolution operator is approximated by the normal-ordered evolution operator, the error is ϵ^2 times an operator which may be expressed in terms of multiple commutators of the operators comprising the Hamiltonian. So that in limit $\epsilon \rightarrow 0$, we are assured

that $: e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} :$ yields the correct evolution of the wave function.

$$\begin{aligned}\langle x_n | : e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} : | x_{n-1} \rangle &= \int d^3 p_n \langle x_n | p_n \rangle \langle p_n | : e^{-i\frac{\epsilon}{\hbar}H(\hat{p},\hat{x})} : | x_{n-1} \rangle \\ &= \int \frac{d^3 p_n}{(2\pi\hbar)^3} e^{ip_n(x_n - x_{n-1})} e^{-i\frac{\epsilon}{\hbar}H(p_n, x_{n-1})}\end{aligned}$$

According to Gaussian integral, we have

$$\begin{aligned}\langle x_n | e^{-i\frac{\epsilon}{\hbar}(\frac{p^2}{2m} + V(\hat{x}))} | x_{n-1} \rangle &= \langle x_n | : e^{-i\frac{\epsilon}{\hbar}(\frac{p^2}{2m} + V(\hat{x}))} : | x_{n-1} \rangle + \mathcal{O}(\epsilon^2) \\ &= \int \frac{d^3 p}{(2\pi\hbar)^3} e^{ip(x_n - x_{n-1}) - i\frac{\epsilon}{\hbar}\frac{p^2}{2m} - i\frac{\epsilon}{\hbar}V(x_{n-1})} + \mathcal{O}(\epsilon^2) \\ &= \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\left(\frac{m}{2\epsilon}(x_n - x_{n-1})^2 - \epsilon V(x_{n-1})\right)} + \mathcal{O}(\epsilon^2)\end{aligned}$$

Thus, the matrix element of the evolution operator may be written:

$$\mathcal{U}(x_i t_f, x_i t_i) = \lim_{M \rightarrow \infty} \int \prod_{k=1}^{M-1} dx_k \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3M}{2}} e^{\frac{i}{\hbar}\epsilon \sum_{k=1}^M \left(\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right)}$$

The set of points $\{x_0, x_1, \dots, x_M\}$ defines a trajectory. After changing the sum of discrete points into cotinuous integral:

$$\begin{aligned}\epsilon \sum_{k=1}^M \frac{m}{2} \left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 &\rightarrow \int_{t_i}^{t_f} dt \frac{m}{2} \left(\frac{dx}{dt}\right)^2 \\ \epsilon \sum_{k=1}^M V(x_{k-1}) &\rightarrow \int_{t_i}^{t_f} dt V(x(t))\end{aligned}$$

The Feynman path integral, which is defined as $M \rightarrow \infty$, is denoted:

$$\begin{aligned}\mathcal{U}(x_f t_f, x_i t_i) &= \int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left(\frac{m}{2} \left(\frac{dx}{dt}\right)^2 - dt V(x(t))\right)} \\ &= \int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \mathcal{S}[x(t)]}\end{aligned}$$

where

$$\int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] = \lim_{M \rightarrow \infty} \int \prod_{k=1}^{M-1} dx_k \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{3M}{2}}$$

the action $\mathcal{S}[x(t)]$ is

$$\mathcal{S}[x(t)] = \int_{t_i}^{t_f} \mathcal{L}[x(t)]$$

and the Lagrangian $\mathcal{L}[x(t)]$ is

$$\mathcal{L}[x(t)] = \frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x(t))$$

Thus the element of evolution operator between the states $|x_i\rangle$ and $|x_f\rangle$ is written. The superposition principle, which may be written at any time t in the form:

$$\mathcal{U}(x_f t_f, x_i t_i) = \int dx \mathcal{U}(x_f t_f, xt) \mathcal{U}(xt, x_i t_i)$$

is expressed in terms of path integrals as:

$$\begin{aligned} \int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt' \mathcal{L}[x(t')]} &= \int dx \left\{ \int_{(x, t)}^{(x_f, t_f)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \int_t^{t_f} dt' \mathcal{L}[x(t')]} \right. \\ &\quad \times \left. \int_{(x_i, t_i)}^{(x, t)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} \int_{t_i}^t dt' \mathcal{L}[x(t')]} \right\} \end{aligned}$$

The functional integral may be normalized by solutions of analytically solvable reference problem. For example, when the potential is set to zero, the transition amplitude is:

$$\mathcal{U}_0(x_f t_f, x_i t_i) = \left[\frac{m}{2\pi i \hbar (t_f - t_i)} \right]^{\frac{3}{2}} e^{i \frac{m}{2\hbar} \frac{(x_f - x_i)^2}{t_f - t_i}}$$

The functional integral above is called the Lagrangian form and requires the Hamiltonian have quadratic dependence of momentum. The Hamiltonian form of functional integral is:

$$\begin{aligned} \mathcal{U}(x_f t_f, x_i t_i) &= \lim_{M \rightarrow \infty} \int \prod_{k=1}^{M-1} dx_k \prod_{k=1}^M \frac{dp_k}{(2\pi \hbar)^3} e^{\frac{i}{\hbar} \sum_{k=1}^M [p_k(x_k - x_{k-1}) - \epsilon \frac{p_k^2}{2m} - \epsilon V(x_{k-1})]} \\ &\rightarrow \int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] \mathcal{D}[p(t)] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt [p(t) \frac{\partial}{\partial t} x(t) - H(p(t), x(t))]} \end{aligned}$$

The trajectories $x(t)$ obey the same boundary conditions as in the Lagrangian form, and trajectories $p(t)$ have no boundary conditions. The path integral automatically represent time-ordered product:

$$\begin{aligned} \langle x_f | T \mathcal{O}_1(\hat{x}, t_1) \mathcal{O}_2(\hat{x}, t_2) e^{-\frac{i}{\hbar} \int_{t_i}^{t_f} dt \hat{H}(t)} | x_i \rangle \\ = \int_{(x_i, t_i)}^{(x_f, t_f)} \mathcal{D}[x(t)] \mathcal{O}_1(\hat{x}, t_1) \mathcal{O}_2(\hat{x}, t_2) e^{-\frac{i}{\hbar} \int_{t_i}^{t_f} dt \mathcal{L}[x(t)]} \end{aligned}$$

Imaginary-time Path Integral and the Partition Function

The partition function for a single particle may be written:

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}} \\ &= \int dx \langle x | e^{-\beta \hat{H}} | x \rangle \end{aligned}$$

and may be thought of as the sum over diagonal matrix elements of the imaginary time evolution operator

$$\mathcal{U}(x_f t_f, x_i t_i) = \langle x_f | e^{-(\tau_f - \tau_i) \frac{\hat{H}}{\hbar}} | x_i \rangle$$

where the imaginary time interval $(\tau_f - \tau_i) = \beta \hbar$. We require $\epsilon = (\tau_f - \tau_i)/M$, and in this case

$$\begin{aligned} \mathcal{U}(x_f t_f, x_i t_i) &= \lim_{M \rightarrow \infty} \int \prod_{k=1}^{M-1} d^3 x_k \prod_{k=1}^M \langle x_k | e^{-\frac{\epsilon}{\hbar} H(\hat{p}, \hat{x})} | x_{k-1} \rangle \\ &= \int_{(x_i, \tau_i)}^{(x_f, \tau_f)} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} \int_{\tau_i}^{\tau_f} d\tau \left(\frac{m}{2} \left(\frac{dx(\tau)}{d\tau} \right)^2 + V(x(\tau)) \right)} \\ &= \int_{(x_i, \tau_i)}^{(x_f, \tau_f)} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} \int_{\tau_i}^{\tau_f} d\tau H[x(\tau)]} \end{aligned}$$

An alternative derivation showing how the Lagrangian in the real time case is transformed into the Hamiltonian in the imaginary case, is to perform an analytic continuation of the functional integral of Lagrangian form. This continuation is known as a Wick rotation:

$$t = -i\tau$$

Thus

$$\frac{dx}{d\tau} = \frac{dt}{d\tau} \frac{dx}{dt} = -i \frac{dx}{dt}$$

and the Lagrangian in the real time case is then transformed into Hamiltonian. According to the equations above, the partition function can be written as:

$$\begin{aligned} Z &= \int dx \int_{x(0)=x}^{x(\beta\hbar)=x} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left(\frac{m}{2} \left(\frac{dx(\tau)}{d\tau} \right)^2 + V(x(\tau)) \right)} \\ &= \int_{x(0)=x(\beta\hbar)} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau H[x(\tau)]} \end{aligned}$$

The partition function is thus a sum over all periodic trajectories with period $\beta \hbar$. It's convenient to use units in which $\hbar = 1$ except we concerned the classical limit in which $\hbar \rightarrow 0$.

The Feynman path integral can be generalized to many-particle systems. according to the symmetry of each basis in state $|x_1 \dots x_n\rangle$, the partition function of N-particle systems

is written:

$$\begin{aligned} Z &= \frac{1}{N!} \int \prod_{k=1}^N dx_k \{x_1 \dots x_n | e^{-\beta \hat{H}} | x_1 \dots x_n \} \\ &= \frac{1}{N!} \sum_P \zeta^p \int \prod_{k=1}^N dx_k (x_{p1} \dots x_{pN} | e^{-\beta \hat{H}} | x_1 \dots x_n) \end{aligned}$$

The Hamiltonian of an N-particle system is

$$H = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} + \sum_{i < j} v(\hat{x}_i - \hat{x}_j)$$

The partition function can be written:

$$Z = \frac{1}{N!} \int_{x_k(\beta)=x_{pk}(0)} \mathcal{D}[x_1(\tau)] \dots \mathcal{D}[x_N(\tau)] e^{-\int_0^\beta d\tau \left[\sum_{i=1}^N \frac{m}{2} \left(\frac{dx_i(\tau)}{d\tau} \right)^2 + \sum_{i < j} v(x_i(\tau) - x_j(\tau)) \right]}$$

Coherent State Functional Integral

For a many-particle Hamiltonian expressed in a second quantized form, a general functional integral for a many-particle evolution operator may be obtained using coherent states $|\phi\rangle$, instead of position and momentum eigenstates. We will evaluate the matrix element of evolution operators between an initial state $|\phi_i\rangle$ with coefficients $\phi_{\alpha,i}$ and a final state $\langle\phi_f|$ with coefficients $\phi_{\alpha,f}^*$. As before, the time interval $[t_i, t_f]$ is divided into M times steps.

$$\begin{aligned} \phi_{\alpha,0} &\equiv \phi_{\alpha,1} \\ \phi_{\alpha,M}^* &\equiv \phi_{\alpha,f}^* \end{aligned}$$

As for the Hamiltonian expressed in second quantization form, the normal order is to write the creation operators to the left side and the annihilation operators to the right side. As in the path integral case:

$$e^{\epsilon H(a_\alpha^\dagger, a_\alpha)} =: e^{\epsilon H(a_\alpha^\dagger, a_\alpha)} : + \mathcal{O}(\epsilon^2)$$

The matrix element of the evolution operator may be written:

$$\begin{aligned} \mathcal{U}(\phi_{\alpha,f}^* t_f, \phi_{\alpha,i} t_i) &= \lim_{M \rightarrow \infty} \int \prod_{k=1}^M \prod_{\alpha} \frac{1}{\mathcal{N}} d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_{k=1}^{M-1} \sum_{\alpha} \phi_{\alpha,k}^* \phi_{\alpha,k}} \\ &\quad \times \prod_{k=1}^M \langle \phi_k | : e^{-i\epsilon H(a_\alpha^\dagger, a_\alpha)} : + \mathcal{O}(\epsilon^2) | x_{k-1} \rangle \\ &= \lim_{M \rightarrow \infty} \int \prod_{k=1}^M \prod_{\alpha} \frac{1}{\mathcal{N}} d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_{k=1}^{M-1} \sum_{\alpha} \phi_{\alpha,k}^* \phi_{\alpha,k}} \\ &\quad \times e^{\sum_{k=1}^M \left(\sum_{\alpha} \phi_{\alpha,k}^* \phi_{\alpha,k-1} - i\epsilon H(\phi_{\alpha,k}^*, \phi_{\alpha,k-1}) \right)} \end{aligned} \tag{2}$$

notice that the first term on the exponent in the last line comes from

$$\langle \phi_k | \phi_{k-1} \rangle = e^{\sum_{\alpha} \phi_{\alpha,k}^* \phi_{\alpha,k-1}}$$

As in the case of path integral, it is convenient to introduce a trajectory $\phi_{\alpha}(t)$ to replace the set $\{\phi_{\alpha,1}, \phi_{\alpha,2} \dots \phi_{\alpha,M}\}$. Notice that

$$\phi_{\alpha,k}^* \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} \equiv \phi_{\alpha}^*(t) \frac{\partial}{\partial t} \phi_{\alpha}(t)$$

and

$$H(\phi_{\alpha,k}^*, \phi_{\alpha,k-1}) \equiv H(\phi_{\alpha}^*(t), \phi_{\alpha}(t))$$

In which case the exponent of Eq.(2) may be written as

$$\begin{aligned} & \sum_{\alpha} \phi_{\alpha,M}^* \phi_{\alpha,M-1} - i\epsilon H(\phi_{\alpha,M}^*, \phi_{\alpha,M-1}) + i\epsilon \sum_{k=1}^{M-1} \left(\sum_{\alpha} i\phi_{\alpha,k}^* \left(\frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} \right) - H(\phi_{\alpha,k}^*, \phi_{\alpha,k-1}) \right) \\ &= \sum_{\alpha} \phi_{\alpha}^*(t_f) \phi_{\alpha}(t_f) + i \int_{t_i}^{t_f} dt \left[\sum_{\alpha} i\phi_{\alpha}^*(t) \frac{\partial}{\partial t} \phi_{\alpha}(t) - H(\phi_{\alpha}^*(t), \phi_{\alpha}(t)) \right] \\ &= \sum_{\alpha} \phi_{\alpha}^*(t_f) \phi_{\alpha}(t_f) + i \int_{t_i}^{t_f} dt \mathcal{L}[\phi_{\alpha}^*(t), \phi_{\alpha}(t)] \end{aligned}$$

Hence we can write the integral

$$\mathcal{U}(\phi_{\alpha,f}^* t_f, \phi_{\alpha,i} t_i) = \int_{(\phi_{\alpha,i}, t_i)}^{(\phi_{\alpha,f}, t_f)} \mathcal{D}[\phi_{\alpha}^*(t) \phi_{\alpha}(t)] e^{\sum_{\alpha} \phi_{\alpha}^*(t_f) \phi_{\alpha}(t_f)} e^{i \int_{t_i}^{t_f} dt \mathcal{L}[\phi_{\alpha}^*(t), \phi_{\alpha}(t)]}$$

where

$$\int_{(\phi_{\alpha,i}, t_i)}^{(\phi_{\alpha,f}, t_f)} \mathcal{D}[\phi_{\alpha}^*(t) \phi_{\alpha}(t)] = \lim_{M \rightarrow \infty} \int \prod_{k=1}^M \prod_{\alpha} \frac{1}{\mathcal{N}} d\phi_{\alpha,k}^* d\phi_{\alpha,k}$$

The Partition Function for Many-particle Systems

The partition function for many-particle system may be written:

$$\begin{aligned} Z &= \text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})} \\ &= \int \prod_{\alpha} d\phi_{\alpha}^* d\phi_{\alpha} e^{-\sum_{\alpha} \phi_{\alpha}^* \phi_{\alpha}} \langle \zeta \phi | e^{-\beta(\hat{H} - \mu \hat{N})} | \phi \rangle \end{aligned}$$

Operate the continuation to imaginary time, the trajectory imposes periodic or antiperiodic boundary conditions:

$$\begin{aligned} \phi_{\alpha,0} &\equiv \phi_{\alpha} \\ \phi_{\alpha,M}^* &\equiv \zeta \phi_{\alpha}^* \end{aligned}$$

The resulting partition function is

$$Z = \lim_{M \rightarrow \infty} \int \prod_{k=1}^M \prod_{\alpha} \frac{1}{\mathcal{N}} d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\mathcal{S}(\phi^*, \phi)}$$

where the action $\mathcal{S}(\phi^*, \phi)$ is

$$\mathcal{S}(\phi^*, \phi) = e^{-\epsilon \sum_{k=1}^M \left[\sum_{\alpha} \phi_{\alpha,k}^* \left(\frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} - \mu \phi_{\alpha,k-1} \right) + H(\phi_{\alpha,k}^*, \phi_{\alpha,k-1}) \right]}$$

Using the trajectory notation, and notice the periodicity of the trajectory

$$Z = \int_{\phi(\beta) = \zeta \phi(0)} \prod_{\alpha} \frac{1}{\mathcal{N}} \mathcal{D}[\phi_{\alpha}^*(\tau), \phi_{\alpha}(\tau)] e^{-\int_0^{\beta} d\tau \left[\sum_{\alpha} \phi_{\alpha}^*(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) \phi_{\alpha}(\tau) + H(\phi_{\alpha}^*(\tau), \phi_{\alpha}(\tau)) \right]}$$

We write thermal, or imaginary-time Green's function as follows:

$$\begin{aligned} & \mathcal{G}^{(n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n | \alpha_{2n} \tau_{2n}, \dots, \alpha_{n+1} \tau_{n+1}) \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta(\hat{H} - \mu \hat{N})} T a_{\alpha_1}^{(H)}(\tau_1) \dots a_{\alpha_n}^{(H)}(\tau_n) a_{\alpha_{n+1}}^{(H)\dagger}(\tau_{n+1}) \dots a_{\alpha_{2n}}^{(H)\dagger}(\tau_{2n}) \right] \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta(\hat{H} - \mu \hat{N})} \zeta^P \tilde{a}_{\alpha_{P1}}^{(H)}(\tau_{P1}) \tilde{a}_{\alpha_{P2}}^{(H)}(\tau_{P2}) \dots \tilde{a}_{\alpha_{P2N}}^{(H)}(\tau_{P2N}) \right] \end{aligned}$$

Where the permutation P arranges the times in chronological order and \tilde{a}_{α_i} is an annihilation operator for $i \leq n$ and a creation operator for $i > n$. The Green's function may be written as follows:

$$\begin{aligned} & \mathcal{G}^{(n)}(\alpha_1 \tau_1, \dots, \alpha_n \tau_n | \alpha_{2n} \tau_{2n}, \dots, \alpha_{n+1} \tau_{n+1}) \\ &= \frac{1}{Z} \int \mathcal{D}[\phi_{\alpha}^*(\tau), \phi_{\alpha}(\tau)] \left[e^{-\int_0^{\beta} d\tau \left[\sum_{\alpha} \phi_{\alpha}^*(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) \phi_{\alpha}(\tau) + H(\phi_{\alpha}^*(\tau), \phi_{\alpha}(\tau)) \right]} \right. \\ & \quad \times \phi_{\alpha_1}(\tau_1) \dots \phi_{\alpha_n}(\tau_n) \phi_{\alpha_{n+1}}^*(\tau_{n+1}) \dots \phi_{\alpha_{2n}}^*(\tau_{2n}) \left. \right] \end{aligned}$$

For convenience, we choose a base in which H_0 is diagonal:

$$H_0 = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$$

The discrete expression of the partition function may be written:

$$\begin{aligned} Z_0 &= \lim_{M \rightarrow \infty} \prod_{\alpha} \left[\prod_{k=1}^n \int d\phi_k^* d\phi_k \frac{1}{\mathcal{N}} e^{-\sum_{i,j=1}^M \phi_i^* \mathcal{S}_{ij}^{(\alpha)} \phi_j} \right] \\ &= \lim_{M \rightarrow \infty} \prod_{\alpha} [\det \mathcal{S}^{(\alpha)}]^{-\zeta} \end{aligned}$$

Where the matrix $\mathcal{S}^{(\alpha)}$ is written:

$$\mathcal{S}^{(\alpha)} = \begin{bmatrix} 1 & 0 & \dots & 0 & -\zeta a \\ -a & 1 & 0 & & 0 \\ 0 & -a & 1 & \ddots & \vdots \\ & 0 & -a & \ddots & 0 \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & \dots & -a & 1 \end{bmatrix} \quad \phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_M \end{bmatrix}$$

Where

$$a = 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)$$

The determinant of $\mathcal{S}^{(\alpha)}$ can be evaluated:

$$\begin{aligned} \lim_{M \rightarrow \infty} \det \mathcal{S}^{(\alpha)} &= \lim_{M \rightarrow \infty} [1 + (-1)^{M-1} \zeta (-a)^M] \\ &= \lim_{M \rightarrow \infty} \left[1 - \zeta \left(1 - \frac{\beta}{M}(\epsilon_\alpha - \mu) \right) \right] \\ &= 1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)} \end{aligned}$$

Thus the partition function for non-interaction particles can be written as:

$$Z_0 = \prod_{\alpha} \left[1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)} \right]^{-\zeta}$$

The single particle Green's function for non-interacting particles is

$$\begin{aligned} \mathcal{G}_0(\alpha\tau_q | \gamma\tau_r) &= \frac{1}{Z_0} \text{Tr} \left[T e^{-\int_0^\beta d\tau (H_0 - \mu N)} a_\alpha(\tau_q) a_\gamma^\dagger(\tau_r) \right] \\ &= \delta_{\alpha\gamma} \mathcal{S}_{qr}^{(\alpha)-1} \end{aligned}$$

Using the result we got before, and after calculating, we obtain:

$$\begin{aligned} \mathcal{G}_0(\alpha\tau | \alpha'\tau') &= \langle T a_\alpha(\tau) a_{\alpha'}^\dagger(\tau') \rangle \\ &= \delta_{\alpha\alpha'} e^{-(\epsilon_\alpha - \mu)(\tau - \tau')} \{ \theta(\tau - \tau' - \eta)(1 + \zeta n_\alpha) + \zeta \theta(\tau' - \tau + \eta) n_\alpha \} \\ &= \delta_{\alpha\alpha'} g_\alpha(\tau - \tau' - \eta) \end{aligned}$$

Where the infinitesimal η serves as a reminder that the second term contributes at equal times.

Perturbation Theory

We consider the case of a Hamiltonian which has been decomposed into the sum of a one-body Hamiltonian H_0 and the residual Hamiltonian V . We'll develop a systematic perturbation expansion in powers of V .

The basis is chosen to diagonalize $H_0 = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$, and the normal-ordered many-body part is written as $V(a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \dots a_{\gamma} a_{\delta} \dots)$. The operator form of the partition function is written:

$$\begin{aligned} Z &= \text{Tr} \left[T e^{-\int_0^{\beta} d\tau \sum_{\alpha} (\epsilon_{\alpha} - \mu) a_{\alpha}^{\dagger}(\tau) a_{\alpha}(\tau) + V(a_{\alpha}^{\dagger}(\tau) a_{\beta}^{\dagger}(\tau) \dots a_{\gamma}(\tau) a_{\delta}(\tau))} \right] \\ &= Z_0 \langle e^{-\int_0^{\beta} d\tau V(a_{\alpha}^{\dagger}(\tau) a_{\beta}^{\dagger}(\tau) \dots a_{\gamma}(\tau) a_{\delta}(\tau))} \rangle_0 \end{aligned}$$

Where the thermal average of an operator F is written:

$$\begin{aligned} &\langle F(a_{\alpha}^{\dagger}(\tau_i) a_{\beta}^{\dagger}(\tau_j) \dots a_{\gamma}(\tau_k) a_{\delta}(\tau_l) \dots) \rangle_0 \\ &= \frac{1}{Z_0} \text{Tr} \left[e^{-\int_0^{\beta} d\tau \sum_{\alpha} (\epsilon_{\alpha} - \mu) a_{\alpha}^{\dagger}(\tau) a_{\alpha}(\tau)} F(a_{\alpha}^{\dagger}(\tau_i) a_{\beta}^{\dagger}(\tau_j) \dots a_{\gamma}(\tau_k) a_{\delta}(\tau_l) \dots) \right] \end{aligned}$$

In terms of functional integrals, the partition function may be written:

$$\begin{aligned} Z &= \int_{\psi(\beta)=\zeta\psi(0)} \mathcal{D}[\psi_{\alpha}^*(\tau) \psi_{\alpha}(\tau)] e^{-\int_0^{\beta} d\tau \left(\sum_{\alpha} \psi_{\alpha}^*(\tau) (\partial_{\tau} + \epsilon_{\alpha} - \mu) \psi_{\alpha}(\tau) + V(\psi_{\alpha}^*(\tau), \psi_{\beta}^*(\tau), \dots, \psi_{\gamma}(\tau), \psi_{\delta}(\tau), \dots) \right)} \\ &= Z_0 \langle e^{-\int_0^{\beta} d\tau V(\psi_{\alpha}^*(\tau), \psi_{\beta}^*(\tau), \dots, \psi_{\gamma}(\tau), \psi_{\delta}(\tau), \dots)} \rangle_0 \end{aligned} \quad (3)$$

where the thermal average of operator F is defined:

$$\begin{aligned} &\langle F(\psi_{\alpha}^*(\tau_i), \psi_{\beta}^*(\tau_j), \dots, \psi_{\gamma}(\tau_k), \psi_{\delta}(\tau_l)) \rangle_0 \\ &= \frac{1}{Z_0} \int_{\psi(\beta)=\zeta\psi(0)} \mathcal{D}[\psi_{\alpha}^*(\tau) \psi_{\alpha}(\tau)] e^{-\int_0^{\beta} d\tau \left(\sum_{\alpha} \psi_{\alpha}^*(\tau) (\partial_{\tau} + \epsilon_{\alpha} - \mu) \psi_{\alpha}(\tau) \right)} \\ &\quad \times F(\psi_{\alpha}^*(\tau_i), \psi_{\beta}^*(\tau_j), \dots, \psi_{\gamma}(\tau_k), \psi_{\delta}(\tau_l)) \end{aligned}$$

The partition function of the non-interacting system, Z_0 , may be written:

$$\begin{aligned} Z_0 &= \text{Tr} \left[T e^{-\int_0^{\beta} d\tau \left(\sum_{\alpha} (\epsilon_{\alpha} - \mu) a_{\alpha}^{\dagger}(\tau) a_{\alpha}(\tau) \right)} \right] \\ &= \int_{\psi(\beta)=\zeta\psi(0)} \mathcal{D}[\psi_{\alpha}^*(\tau) \psi_{\alpha}(\tau)] e^{-\int_0^{\beta} d\tau \left(\sum_{\alpha} \psi_{\alpha}^*(\tau) (\partial_{\tau} + \epsilon_{\alpha} - \mu) \psi_{\alpha}(\tau) \right)} \end{aligned}$$

The perturbation expansion is obtained by expanding Eq.(3) in a power series

$$\begin{aligned} \frac{Z}{Z_0} &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \dots d\tau_n \\ &\quad \langle V(\psi_{\alpha}^*(\tau_1) \dots, \psi_{\gamma}(\tau_1) \dots) \dots V(\psi_{\alpha}^*(\tau_n) \dots, \psi_{\gamma}(\tau_n) \dots) \rangle_0 \end{aligned}$$

For simplicity, we will consider the special case in which the interaction V is a two-body interaction:

$$V(\psi^*(\tau), \psi(\tau)) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | v | \gamma\delta \rangle \psi_{\alpha}^*(\tau) \psi_{\beta}^*(\tau) \psi_{\gamma}(\tau) \psi_{\delta}(\tau)$$

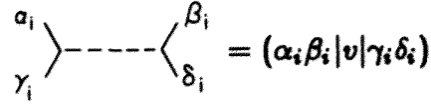
the term of order n in V of $\frac{Z}{Z_0}$ in this case is:

$$\left(\frac{Z}{Z_0}\right)_n = \frac{(-1)^n}{n!2^n} \sum_{\alpha_1\beta_1\gamma_1\delta_1} \cdots \sum_{\alpha_n\beta_n\gamma_n\delta_n} \langle \alpha_1\beta_1 | v | \gamma_1\delta_1 \rangle \langle \alpha_n\beta_n | v | \gamma_n\delta_n \rangle \int_0^\beta d\tau_1 \dots d\tau_n \quad (4)$$

$$\times \langle \psi_{\alpha_1}^*(\tau_1) \psi_{\beta_1}^*(\tau_1) \psi_{\gamma_1}(\tau_1) \psi_{\delta_1}(\tau_1) \dots \psi_{\alpha_n}^*(\tau_n) \psi_{\beta_n}^*(\tau_n) \psi_{\gamma_n}(\tau_n) \psi_{\delta_n}(\tau_n) \rangle_0$$

Labeled Feynman Diagrams

a representation of all the complete sets of contractions contributing to $(\frac{Z}{Z_0})_n$ is given by labeled diagrams defined to reproduce each of the contributions to Eq.(4). According to Wick theorem, the thermal average equals to the sum of all arrangements of contractions. Each contraction will join some $\psi_{\eta_i}^*(\tau_i)$ to some $\psi_{\eta_j}(\tau_j)$. yielding a propagator $\delta_{\eta_i\eta_j} g_{\eta_i}(\tau_i - \tau_j)$ which will be represented by a directed line originating at $\psi_{\eta_i}^*(\tau_i)$ and terminating at $\psi_{\eta_j}(\tau_j)$. each interaction will yield a vertex having two incoming lines corresponding to $\psi_{\delta_i}(\tau_i)$ and $\psi_{\gamma_i}(\tau_i)$, and two outgoing lines corresponding to $\psi_{\alpha_i}^*(\tau_i)$ and $\psi_{\beta_i}^*(\tau_i)$.



$$\begin{array}{c} \alpha_i \\ \gamma_i \end{array} \rangle \text{---} \langle \begin{array}{c} \beta_i \\ \delta_i \end{array} = (\alpha_i \beta_i | v | \gamma_i \delta_i)$$

Fig.1



$$\begin{array}{c} \alpha \\ \gamma \end{array} \rangle \text{---} \tau \text{---} \langle \begin{array}{c} \beta \\ \delta \end{array} = \begin{array}{c} \rangle_L \text{---} \tau \text{---} \langle_R$$

Fig.2

We derive the rules for constructing labeled diagrams which give a faithful representation of the complete set of contractions contributing to the n^{th} perturbation expansion of $\frac{Z}{Z_0}$.

- Draw all distinct labeled diagrams composed of n vertices connected by directed lines. Two diagrams are distinct if they can't be deformed so as to coincide completely, including all times labels τ_i , left-right labels $L - R$ and the direction of arrows on propagators.
- assign a single-particle index to each directed line and include the corresponding factor:

$$\int_{\tau'}^{\tau} g_a = g_a(\tau - \tau') = e^{-(\epsilon_a - \mu)(\tau - \tau')} [(1 + \zeta n_a) \theta(\tau - \tau' - \eta) + \zeta n_a \theta(\tau' - \tau + \eta)]$$

- For each vertex, include the following factor:

$$\begin{array}{c} \alpha_i \\ \gamma_i \end{array} \rangle \text{-----} \langle \begin{array}{c} \beta_i \\ \delta_i \end{array} = (\alpha_i \beta_i | v | \gamma_i \delta_i)$$

- Sum over all single-particle indices and integrate over all times over the interval $[0, \beta]$.
- Multiply the result by the factor $\frac{(-1)^n}{n! 2^n} \zeta^{n_L}$, where n_L is the number of closed loops in the diagram.

Labeled Feynman Diagrams

For a general interaction which has no special properties other than the symmetry

$$(\alpha \beta | v | \gamma \delta) = (\beta \alpha | v | \delta \gamma)$$

There are two types of transformations leaving the value of a diagram invariant. One is permutation of times labels $\tau_1 \tau_2 \dots \tau_n$, cause all times labels are integrated over $[0, \beta]$. the other is the exchange of extremities of each vertex, according to the symmetry of the interaction matrix.

The most general transformation leaving the value of a diagram invariant is the combination of a permutation of times labels and an exchange of vertex extremities. This kind of transformations of an n^{th} order diagram is a group, denoted by G . Consider the action of this group of transformations, G , on a labeled diagram Γ . Some set of transformations G_Γ will transform Γ into a deformation of itself, while the rest of transformations will yield diagrams which are distinct from Γ . G_Γ defined in this way is a subgroup of G .

We define S as the number of deformations of Γ generated by the action of G . S is the number of elements of G_Γ . since G_Γ is a subgroup of G , S is a divisor of $2^n n!$. consider a diagram Γ' which is distinct from Γ and is generated from Γ by a transformation of

G . Cause Γ' corresponds to some permutation of τ and L – R labels on Γ , it transforms into deformation of itself under G_Γ . (G is an Abelian group.) Thus Γ' has S deformations of itself. And the $2^n n!$ diagrams generated by action of G on Γ can be grouped into $\frac{2^n n!}{S}$ sets of S diagrams, S.t. diagrams in the same set are deformation of each other and diagrams in different sets are distinct. All distinct diagrams will thus be counted correctly if we multiply the value of one diagram by the factor $\frac{2^n n!}{S}$.

An unlabeled diagram is obtained by removing times and L – R labels on vertices from a labeled diagram. It is composed of completely unlabeled vertices connected by directed lines. The rules of drawing the n^{th} order contribution to the perturbation expansion of $\frac{Z}{Z_0}$ are summarized.

- Draw all distinct unlabeled diagrams composed of n vertices connected by directed lines. Two diagrams are distinct if they cannot be deformed so as to coincide completely including the direction of arrows on propagators.
- Calculate the symmetry factor S for the diagram.
- Assign a time label τ_i to each vertex, and a single-particle index to each directed line. For each directed line include the factor.

$$\begin{array}{c} \tau \\ \nearrow \\ \alpha \end{array} = g_\alpha(\tau - \tau') = e^{-(\epsilon_\alpha - \mu)(\tau - \tau')} [(1 + \zeta n_\alpha) \theta(\tau - \tau' - \eta) + \zeta n_\alpha \theta(\tau' - \tau + \eta)]$$

- For each vertex, include the factor

$$\begin{array}{c} \alpha_i \\ \nearrow \\ \gamma_i \end{array} \text{---} \begin{array}{c} \beta_i \\ \nwarrow \\ \delta_i \end{array} = (\alpha_i \beta_i | v | \gamma_i \delta_i)$$

- Sum over all single-particle index and integrate all times labels over the interval $[0, \beta]$.
- Multiply the result by the factor $\frac{(-1)^n}{S} \zeta^{n_L}$.

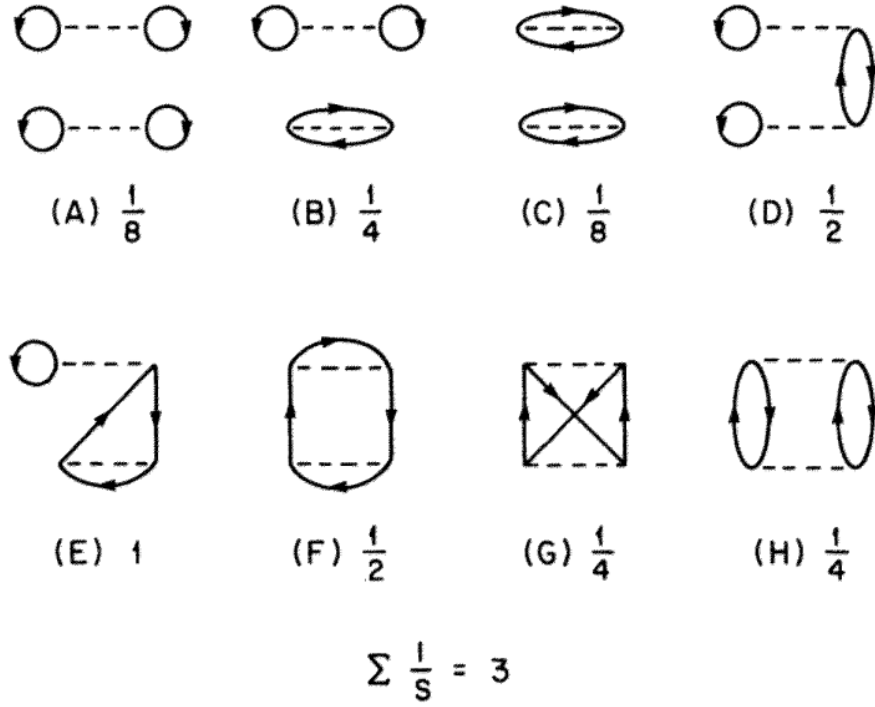


Fig.3 Second order unlabeled Feynman diagrams with symmetry factor $\frac{1}{s}$

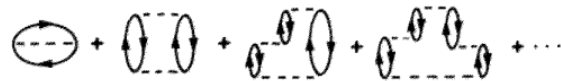
If we regard the product of an interaction and two propagators as a matrix in the time and single-particle labels:

$$\begin{array}{c} \alpha' \\ \gamma \end{array} \begin{array}{c} \tau' \\ \tau \end{array} \begin{array}{c} \gamma' \\ \gamma \end{array} = [vgg]_{\alpha\gamma\tau,\alpha'\gamma'\tau'} = (\alpha\alpha'|v|\gamma\gamma')g_{\alpha'}(\tau'-\tau)g_{\gamma'}(\tau-\tau')$$

Then the sum of first order diagrams and all direct ring diagrams is

$$\sum_{n=1}^{\infty} \frac{(-\zeta)^n}{2n} \text{Tr}[vgg]^n$$

that is



In the n^{th} order contribution, there is totally $(2n)!$ labeled diagrams. And for each transformation group G , the number of distinct diagrams corresponding to a unlabeled diagram is $\frac{2^n n!}{S}$. Hence


$$\sum \frac{2^n n!}{S} = (2n)!$$

$$\sum \frac{1}{S} = \frac{(2n)!}{2^n n!} = (2n-1)!!$$

For the second order case, all the eight unlabeled diagrams and their symmetry factors are shown in Fig.(3). And it indeed satisfy the equation above.

Hugenholtz Diagrams

For many purposes it is convenient to combine the unlabeled Feynman diagrams in a single symmetrized or antisymmetrized matrix element. The resulting diagram is called Hugenholtz diagram. We again consider the case of a two-body potential. Since we no longer wish to distinguish direct and exchange diagrams, the vertex will now be represented by a dot with two incoming and outgoing lines:



$$= \{\alpha\beta|v|\gamma\delta\}$$

The rules for calculating n^{th} order contribution to the perturbation expansion of $\frac{Z}{Z_0}$ using Hugenholtz diagrams:

- Draw all distinct labeled diagrams composed of n vertices connected by directed lines. Two diagrams are distinct if they can't be deformed so as to coincide completely, including the direction of arrows on propagators.
- Calculate the symmetry factor S for the diagram. Add times labels to each vertex, and S is the number of time permutations which transform the diagrams to a deformation of itself.
- Assign a time label τ_i to each vertex and a single-particle index to each directed line. For each directed line include the factor:

$$\frac{\tau}{\tau'} \Big|_a = g_a(\tau - \tau') = e^{-(\epsilon_a - \mu)(\tau - \tau')} [(1 + \zeta n_a) \theta(\tau - \tau' - \eta) + \zeta n_a \theta(\tau' - \tau + \eta)]$$

- For each vertex, include the factor:

$$\begin{array}{c} \alpha \\ \swarrow \\ \bullet \\ \searrow \\ \gamma \end{array} \begin{array}{c} \beta \\ \swarrow \\ \bullet \\ \searrow \\ \delta \end{array} = \{\alpha\beta|v|\gamma\delta\} = (\alpha\beta|v|\gamma\delta) + \zeta(\alpha\beta|v|\delta\gamma)$$

- Sum over all single-particle index and integrate all times over the interval $[0, \beta]$
- Multiply the result by the factor $\frac{(-1)^n \zeta^{n_L}}{2^{n_e} S}$, where n_e is the number of pairs of lines beginning at the same vertex, terminating at the same end, and oriented in the same direction.

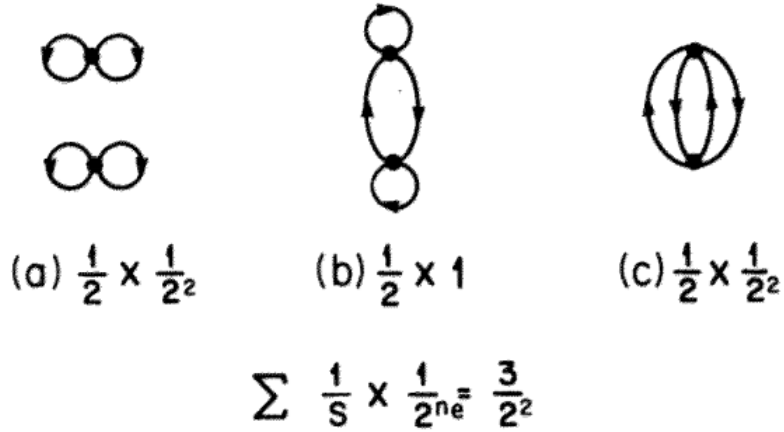


Fig.4 Second order Hugenholtz diagrams with symmetry factors

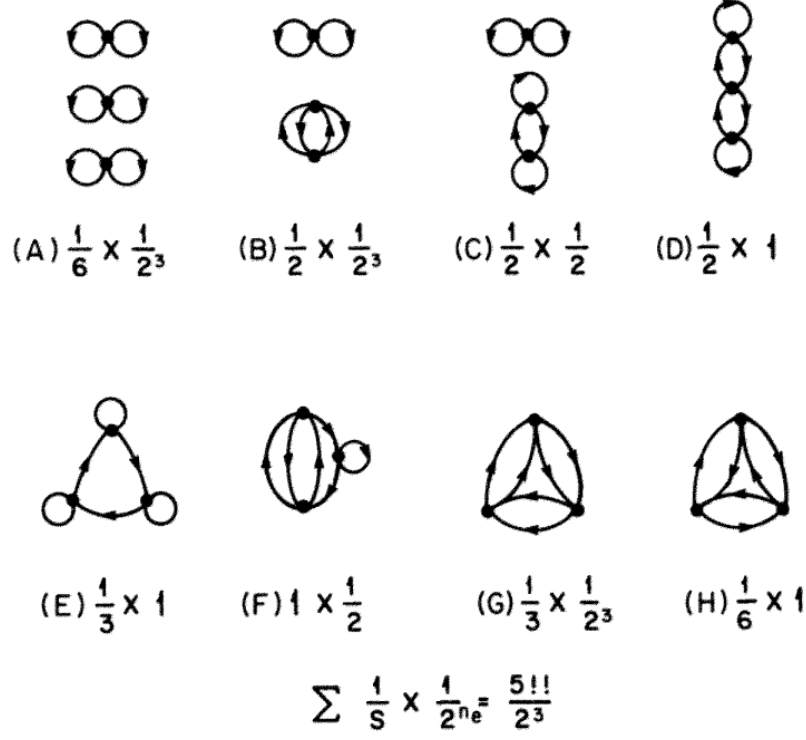


Fig.5 Third order Hugenholtz diagrams with symmetry factors

Frequency and Momentum Representation

For problems which are homogeneous in time, it is useful to Fourier transform from time to frequency.

For a function of time $g(\tau)$ which is periodic or antiperiodic in the interval $[0, \beta]$, we write the Fourier series as:

$$\tilde{g}(\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} g(\tau)$$

$$g(\tau) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau} \tilde{g}(\omega_n)$$

Where for the periodic functions

$$\omega_n = \frac{2n\pi}{\beta}$$

while for the antiperiodic functions

$$\omega_n = \frac{2(n+1)\pi}{\beta}$$

Denoting the discrete momentum $\vec{k}_n \equiv (k_{n_x}^x, k_{n_y}^y, k_{n_z}^z)$, and the volume $\mathcal{V} = L_x L_y L_z$. The matrix element of potential v evaluated with the normalized eigenstates is:

$$\begin{aligned} (\vec{k}_{n_1} \vec{k}_{n_2} | v | \vec{k}_{n_3} \vec{k}_{n_4}) &= \int \frac{d^3 x_1 d^3 x_2}{\mathcal{V}^2} v(\vec{x}_1 - \vec{x}_2) e^{i[(\vec{k}_1 - \vec{k}_3) \cdot \vec{x}_1 + (\vec{k}_2 - \vec{k}_4) \cdot \vec{x}_2]} \\ &= \int \frac{d^3 r d^3 R}{\mathcal{V}^2} v(\vec{r}) e^{i\vec{R}(\vec{k}_{n_1} + \vec{k}_{n_2} - \vec{k}_{n_3} - \vec{k}_{n_4}) + \frac{i\vec{r}}{2}(\vec{k}_{n_1} - \vec{k}_{n_3} + \vec{k}_{n_4} - \vec{k}_{n_2})} \\ &= \frac{1}{\mathcal{V}} \delta_{\vec{k}_{n_1} + \vec{k}_{n_2}, \vec{k}_{n_3} + \vec{k}_{n_4}} v(\vec{k}_{n_1} - \vec{k}_{n_3}) \end{aligned}$$

Thus, each interaction conserves momentum. Every diagram can be decomposed into several connected parts. In fig.5, diagram A has three connected parts, diagrams B and C have two connected parts and diagrams D through H has only one connected part.

Fourier transformation from τ to ω for a problem which is homogeneous in time: (notice that $\omega = \frac{2n\pi}{\beta}$ for Bosons and $\omega = \frac{(2n+1)\pi}{\beta}$ for Fermions, and $e^{i\beta\omega_n} = \zeta$.)

$$\begin{aligned} \tilde{g}_\alpha &= \int_0^\beta d\tau e^{(i\omega_n - (\epsilon_\alpha - \mu))\tau} [\theta(\tau)(1 + \zeta n_\alpha) + \zeta \theta(-\tau)n_\alpha] \\ &= \int_0^\beta d\tau e^{(i\omega_n - (\epsilon_\alpha - \mu))\tau} (1 + \zeta n_\alpha) \end{aligned}$$

Notice that

$$n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} - \zeta}$$

thus we obtain:

$$\begin{aligned} \tilde{g}_\alpha &= \frac{\zeta e^{\beta(\epsilon_\alpha - \mu)} - 1}{i\omega_n - (\epsilon_\alpha - \mu)} \frac{e^{\beta(\epsilon_\alpha - \mu)}}{e^{\beta(\epsilon_\alpha - \mu)} - \zeta} \\ &= \frac{\zeta - e^{\beta(\epsilon_\alpha - \mu)}}{[i\omega_n - (\epsilon_\alpha - \mu)](e^{\beta(\epsilon_\alpha - \mu)} - \zeta)} \\ &= -\frac{1}{i\omega_n - (\epsilon_\alpha - \mu)} \end{aligned}$$

And hence

$$g_\alpha(\tau) = -\sum_{\omega_n} \frac{1}{\beta} e^{-i\omega_n \tau} \frac{1}{i\omega_n - (\epsilon_\alpha - \mu)}$$

In order to invoke the proper θ -function in the case where the propagator begins and ends at the same vertex, the argument is always shifted by an infinitesimal η to $g_\alpha(\tau - \eta)$. This same result may be obtained by multiplying $\tilde{g}_\alpha(\omega_n)$ by the factor $e^{i\omega_n \eta}$, in which case:

$$\begin{aligned} \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n(\tau - \eta)} \tilde{g}_\alpha(\omega_n) &= -\frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n(\tau - \eta)} \frac{1}{i\omega_n - (\epsilon_\alpha - \mu)} \\ &= g_\alpha(\tau - \eta) \end{aligned}$$

According to calculation, the contribution of an n^{th} order diagram is proportional to β^{-n} , then the diagram rules presented previously are modified as follows in frequency representation.

- Assign frequency labels to each directed line as follows. Within each connected part containing m interactions, select $m+1$ propagators to label independently and use frequency conservation at each vertex to label remaining propagators. Assign single-particle indices as before. For each directed line include the factor:

$$\nearrow_{\alpha, \omega_n} = \tilde{g}_{\alpha}(\omega_n) = \frac{-1}{i\omega_n - (\epsilon_{\alpha} - \mu)}$$

图 1

For propagators beginning and ending at the same vertex, include an additional factor $e^{i\omega_n\eta}$.

- Sum over all single-particle indices, and sum over all frequencies ω_n .
- Multiply the factor defined previously by $\frac{1}{\beta^m}$, where m is the number of interactions.

The generalization of these rules using momentum and frequency representation to n -body interactions is straightforward. It is often convenient to use momentum and frequency representation simultaneously in which case one associates with each propagator with a four-momentum (ω_n, k) , which is conserved at each vertex.

The expansion of Z contains all power of the volume \mathcal{V} , with an individual diagram with n_c connected parts being proportional to \mathcal{V}^{n_c} . Thus it is not an extensive quantity. In contrast, the ground potential $\Omega = -\frac{1}{\beta} \ln Z = -P\mathcal{V}$ is an extensive quantity. So it must be possible to find an extensive expansion of Ω . The linked cluster theorem states that $\ln Z$ is in fact given by the sum of all connected diagrams.

We will derive this theorem using replica technique. The basic idea of replica method is to evaluate Z^n for integer n by replicating the system n times and expand the result as follows:

$$Z^n = e^{n \ln Z} = 1 + n \ln Z + \sum_{m=2}^{\infty} \frac{(n \ln Z)^m}{m!}$$

in which $\ln Z$ is given by the coefficients of terms proportional to n . A more general statement of this method is to calculate Z^n , and continue the function to $n = 0$:

$$\begin{aligned} \lim_{n \rightarrow 0} \frac{d}{dn} Z^n &= \lim_{n \rightarrow 0} \frac{d}{dn} (e^{n \ln Z}) \\ &= \ln Z \end{aligned}$$

We first evaluate Z^n for integer n by perturbation. $\ln Z$ will be given by the coefficient of graphs proportional to n . Remember that

$$Z = \int_{\psi_\alpha(\beta)=\zeta\psi_\alpha(0)} \mathcal{D}(\psi_\alpha^*(\tau), \psi_\alpha(\tau)) e^{-\int_0^\beta d\tau [\sum_\alpha \psi_\alpha^*(\tau)(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha(\tau) + V(\psi_\alpha^*(\tau), \psi_\alpha(\tau))]}$$

We may write Z^n as a function integral over n sets of fields $\psi_\alpha^{\sigma*}(\tau), \psi_\alpha^\sigma(\tau)$

$$\begin{aligned} \left(\frac{Z}{Z_0}\right)^n &= \frac{1}{Z_0^n} \int_{\psi_\alpha^\sigma(\beta)=\zeta\psi_\alpha^\sigma(0)} \prod_{\sigma=1}^n \mathcal{D}(\psi_\alpha^{\sigma*}(\tau), \psi_\alpha^\sigma(\tau)) \\ &\quad \times e^{-\int_0^\beta d\tau \sum_{\sigma=1}^n [\sum_\alpha \psi_\alpha^{\sigma*}(\tau)(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha^\sigma(\tau) + V(\psi_\alpha^{\sigma*}, \psi_\alpha^\sigma)]} \end{aligned}$$

Now, all propagators leaving or entering a given vertex have the same index σ , and all σ 's are summed from 1 to n . It is evident that each connected part of a diagram must carry a single index σ , which when summed from 1 to n , yields a factor n . Thus, a graph with n_c connected parts is proportional to n_c and graphs proportional to n are those with only one connected part, that is connected graphs. As a consequence, we obtain the linked cluster theorem:

$$\Omega - \Omega_0 = \frac{1}{\beta} \sum (\text{all connected graphs})$$

Where Ω_0 is the grand potential of the unperturbed system

$$\Omega_0 = \frac{\zeta}{\beta} \sum_\alpha \ln(1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)})$$

Calculations Of Observables And Greens Function

The expectation value of operator R can be written as

$$\begin{aligned} \langle R \rangle &= \frac{\int \mathcal{D}(\psi_\alpha^*, \psi_\alpha) \left[e^{-\int_0^\beta d\tau \sum_\alpha \psi_\alpha^*(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha + V(\psi_\alpha^*, \psi_\alpha)} R(\psi_\alpha^*(0), \psi_\alpha(0)) \right]}{\int \mathcal{D}(\psi_\alpha^*, \psi_\alpha) e^{-\int_0^\beta d\tau \sum_\alpha \psi_\alpha^*(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha + V(\psi_\alpha^*, \psi_\alpha)}} \\ &= \frac{\left\langle e^{-\int_0^\beta d\tau V(\psi_\alpha^*, \psi_\alpha)} R(\psi_\alpha^*(0), \psi_\alpha(0)) \right\rangle_0}{\left\langle e^{-\int_0^\beta d\tau V(\psi_\alpha^*, \psi_\alpha)} \right\rangle_0} \end{aligned}$$

Use the replica technique again. introduce n fields $\psi_\alpha^{\sigma*}, \psi_\alpha^\sigma$ where σ runs from 1 to n

$$\begin{aligned} R_n &= Z_0^{-n} \int \mathcal{D}(\psi_\alpha^{\sigma*}, \psi_\alpha^\sigma) R(\psi_\alpha^{1*}(0), \psi_\alpha^1(0)) \\ &\quad \times e^{-\int_0^\beta d\tau \sum_{\sigma=1}^n [V(\psi_\alpha^{\sigma*}, \psi_\alpha^\sigma) + \sum_\alpha \psi_\alpha^{\sigma*}(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha^\sigma]} \end{aligned}$$

Note that the operator R is calculated with the field $\psi_\alpha^{1*}, \psi_\alpha^1$ associated with $\sigma = 1$ and is evaluated at $\tau = 0$. By separating the $\sigma = 1$ component from the $n - 1$ other components, we obtain

$$R_n = \left\langle e^{-\int_0^\beta d\tau V(\psi_\alpha^*, \psi_\alpha)} R(\psi_\alpha^*(0), \psi_\alpha(0)) \right\rangle_0 \left\langle e^{-\int_0^\beta d\tau V(\psi_\alpha^*, \psi_\alpha)} \right\rangle_0^{n-1}$$

thus the expectation value of R is obtained when $n = 0$:

$$\langle R \rangle = R_0$$

The perturbation expansion of R_n is

$$R_n = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!} \sum_{\sigma_1=1}^n \cdots \sum_{\sigma_m=1}^n \int_0^\beta d\tau_1 \dots d\tau_m \\ \times \langle V(\psi_\alpha^{*\sigma_1}(\tau_1), \psi_\alpha^{\sigma_1}(\tau_1)) \dots V(\psi_\alpha^{*\sigma_p}(\tau_p), \psi_\alpha^{\sigma_p}(\tau_p)) R(\psi_\alpha^{*1}(0), \psi_\alpha^1(0)) \rangle_0$$

Since R is constrained to carry $\sigma = 1$, σ must be 1 everywhere in the portion of the diagram linked to R . In the additional disconnected parts, there is at least one summation over σ leading to an overall factor of at least one power of n . Hence all diagrams with disconnected parts will vanish when n is set equal to 0, and $\langle R \rangle$ is given by all connected diagrams linked to R .

The symmetry factor S of such diagrams containing an operator labeled R is 1 or 2. Only S of a diagram which are symmetric on both side of R is 2, in which case a permutation of times τ_i perform a deformation of the diagram. Thus we can summarize the rules for calculating the p^{th} order contribution to the perturbation expansion of the expectation value of a two-body operator $\langle R \rangle$ using unlabeled Feynman diagrams:

- Draw all distinct unlabeled connected diagrams composed of one R -vertex and p v -vertices connected by directed lines. Two diagrams are distinct if they can't be deformed so as to coincide completely including the directions on propagators. For each distinct diagram, evaluate the contribution as follows.
- Calculate the symmetry factor S for the diagram. If the exchange of the extremities of R with some permutations of times and exchanges of extremities of interactions yields a deformation of itself, $S = 2$. Otherwise, $S = 1$.
- Assign a time label τ_i to each v -vertex, associate $\tau = 0$ with the R -vertex, and assign a single-particle index to each directed line. For each directed line include the factor:

$$\tau \diagup \alpha = g_\alpha(\tau - \tau') = e^{-(\epsilon_\alpha - \mu)(\tau - \tau')} [(1 + \zeta n_\alpha) \theta(\tau - \tau' - \eta) + \zeta n_\alpha \theta(\tau' - \tau + \eta)]$$

- For each v -vertex include the factor

$$\begin{array}{c} \alpha \\ \swarrow \\ \gamma \end{array} \text{---} \begin{array}{c} \beta \\ \swarrow \\ \delta \end{array} = (\alpha\beta|v|\gamma\delta)$$

- For each R -vertex include the factor

$$\begin{array}{c} \alpha \\ \swarrow \\ \gamma \end{array} \text{---} \begin{array}{c} \beta \\ \swarrow \\ \delta \end{array} = (\alpha\beta|R|\gamma\delta)$$

- Sum over all single-particle indices and integrate p times over the interval $[0, \beta]$.
- Multiply the result by the factor $\frac{(-1)^p}{S} \zeta^{n_L}$, where n_L is the number of closed loops and S is the symmetry number.

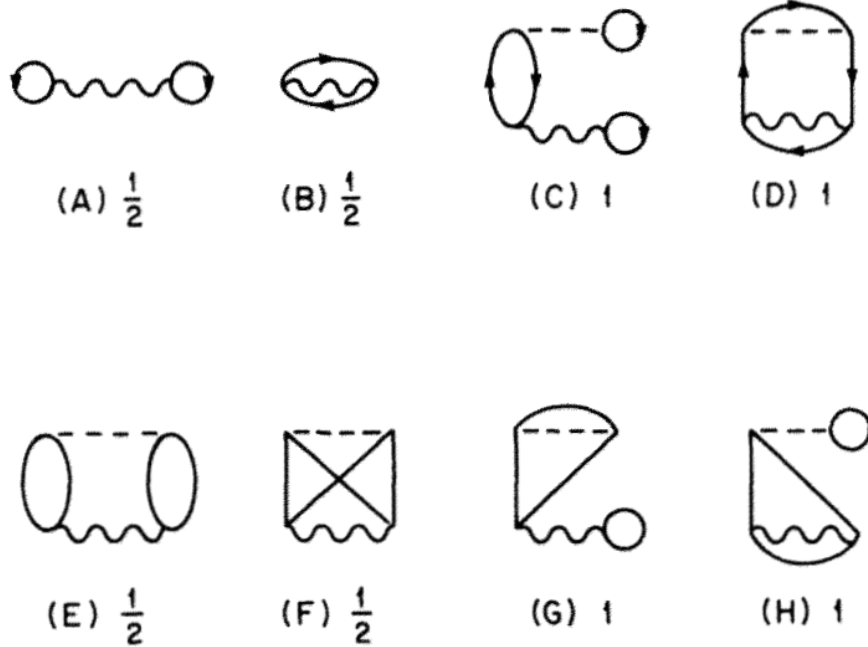


Fig.6 Unlabeled Feynman diagrams for $\langle R \rangle$ with factor $\frac{1}{S}$

The eight unlabeled diagrams contributing to $\langle R \rangle$ in orders $p = 0$ and $p = 1$ are shown in Fig.6, together with the factors $\frac{1}{\zeta}$. The contribution at order 0 is given by diagrams A and B.

$$\langle R \rangle^{(0)} = \frac{1}{2} \sum_{\alpha, \beta} [(\alpha\beta|R|\alpha\beta) + \zeta(\alpha\beta|R|\beta\alpha)] n_\alpha n_\beta$$

and a typical contribution at order 1 is that of diagram E

$$\langle R \rangle^{(E)} = -\frac{1}{2} \sum_{\alpha\beta\gamma\delta} \int_0^\beta d\tau (\alpha\beta|R|\gamma\delta)(\gamma\delta|v|\alpha\beta) g_\alpha(-\tau) g_\beta(-\tau) g_\gamma(\tau) g_\delta(\tau)$$

The derivation of the diagrammatic expansion for the imaginary-time Green's function

$$\begin{aligned} & \mathcal{G}^{(n)}(\alpha_1\beta_1, \dots, \alpha_n\beta_n | \alpha'_1\beta'_1, \dots, \alpha'_n\beta'_n) \\ &= \frac{\langle e^{-\int d\tau V(\psi_\alpha^*(\tau), \psi_\alpha(\tau))} \psi_{\alpha_1}(\beta_1) \dots \psi_{\alpha_n}(\beta_n) \psi_{\alpha'_n}^*(\beta'_n) \dots \psi_{\alpha'_1}^*(\beta'_1) \rangle_0}{\langle e^{-\int d\tau V(\psi_\alpha^*(\tau), \psi_\alpha(\tau))} \rangle_0} \end{aligned}$$

is analogous to that for the expectation value $\langle R \rangle$ with the operator $R(\psi_\alpha^*(0), \psi_\alpha(0))$ replaced by $\psi_{\alpha_1}(\beta_1) \dots \psi_{\alpha_n}(\beta_n) \psi_{\alpha'_n}^*(\beta'_n) \dots \psi_{\alpha'_1}^*(\beta'_1)$. The symmetry factor of a Green's function is 1. The rules for calculating the r^{th} order contribution to the expansion of Green's function $\mathcal{G}^{(n)}(\alpha_1\beta_1, \dots, \alpha_n\beta_n | \alpha'_1\beta'_1, \dots, \alpha'_n\beta'_n)$ using unlabeled Feynman diagrams are as follows:

- Draw all distinct unlabeled connected diagrams composed of n external points $\psi_{\alpha_i}(\beta_i)$, n external points $\psi_{\alpha'_i}^*(\beta'_i)$, and r interaction vertices connected by directed lines.
- Each external point correspond to a specified state α_i and time β_i . Assign a internal time label τ_i to each of the r interaction vertices and for any propagator which is not connected to an external point assign an internal single-particle index. For each directed line include the factor

$$\begin{aligned} & \begin{array}{c} \nearrow \tau, \alpha \\ \nwarrow \tau', \alpha' \end{array} = \delta_{\alpha'\alpha} g_\alpha(\tau - \tau') \\ &= \delta_{\alpha'\alpha} e^{-(\epsilon_\alpha - \mu)(\tau - \tau')} [(1 + \zeta n_\alpha) \theta(\tau - \tau' - \eta) + \zeta n_\alpha \theta(\tau' - \tau + \eta)] \end{aligned}$$

- For each interaction vertex include the factor

$$\begin{array}{c} \alpha \quad \beta \\ \swarrow \quad \nwarrow \\ \gamma \quad \delta \end{array} \text{---} = (\alpha\beta|v|\gamma\delta)$$

- Sum over all single-particle indices and integrate r times τ_i over the interval $[0, \beta]$.
- Multiply the result by the factor $(-1)^r \zeta^P \zeta^{n_L}$ where n_L is the number of closed loops and ζ^P is the sign of the permutation P such that each propagator line originating at the external point $\psi_{\alpha'_m}^*(\beta'_m)$ terminates at the external point $\psi_{\alpha_{Pm}}^*(\beta_{Pm})$

$$\begin{aligned}
G_1^{(I)}(\alpha_1, \beta_1 | \alpha'_1, \beta'_1) &= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} \\
G_2^{(I)}(\alpha_1, \beta_1; \alpha_2, \beta_2 | \alpha'_1, \beta'_1; \alpha'_2, \beta'_2) &= \text{Diagram 6} + \text{Diagram 7} + \text{Diagram 8} + \text{Diagram 9} + \text{Diagram 10}
\end{aligned}$$

Fig.7 Diagrams contributing to one- and two-particle Green's functions with overall sign factors.

Examples of graphs of contributing to the one- and two-particle Green's functions, together with the overall sign factor are given in Fig.(7)

The Effective Potential

In the presence of sources, the operators $\{a_\alpha^\dagger(\tau), a_\alpha(\tau)\}$ acquire non-zero expectation values. We define the average field

$$\begin{aligned}
\phi_\alpha &= \langle a_\alpha \rangle_{J^*, J} = \langle \psi_\alpha \rangle_{J^*, J} \\
&= \frac{\int \mathcal{D}[\psi_\alpha^* \psi_\alpha] \psi_\alpha e^{-\int_0^\beta d\tau [\sum_\alpha \psi_\alpha^* (\partial_\tau - \mu) \psi_\alpha + H[\psi_\alpha^* \psi_\alpha] + \sum_\alpha [J_\alpha^* \psi_\alpha + \psi_\alpha^* J_\alpha]]}}{\int \mathcal{D}[\psi_\alpha^* \psi_\alpha] e^{-\int_0^\beta d\tau [\sum_\alpha \psi_\alpha^* (\partial_\tau - \mu) \psi_\alpha + H[\psi_\alpha^* \psi_\alpha] + \sum_\alpha [J_\alpha^* \psi_\alpha + \psi_\alpha^* J_\alpha]]}} \\
&= -\frac{\delta}{\delta J_\alpha^*(\tau)} W[J_\alpha^*(\tau), J_\alpha(\tau)]
\end{aligned}$$

and its complex conjugate field

$$\begin{aligned}\phi_\alpha^*(\tau) &= \langle a_\alpha^\dagger(\tau) \rangle_{J^*, J} \\ &= -\zeta \frac{\delta}{\delta J_\alpha(\tau)} W[J_\alpha^*(\tau), J_\alpha(\tau)]\end{aligned}$$

$\langle \rangle_{J^*, J}$ denotes a thermal average with respect to H plus the source term. Instead of dealing with the generating function W as a function of the sources J^*, J , it is useful to perform a Legendre transformation to obtain a function of the fields ϕ^*, ϕ . Consider a familiar example of a spin system in a magnetic field. Denoting the Hamiltonian of the spin variable as $\mathcal{H}(s)$, the free energy as a function of an external magnetic field \vec{H} is given by

$$\text{Tr} e^{-\beta(\mathcal{H}(s) - \vec{H} \cdot \sum_i \vec{s}_i)} = e^{-\beta F(H)}$$

From which it follows that the magnetization is given by

$$M = -\frac{\partial F(H)}{\partial H} \quad (5)$$

A state function which depends upon the magnetization instead of external magnetic field is obtained by inverting the relation (5) to obtain $H(M)$ and defining the Legendre transform

$$G(M) = F(H(M)) + MH(M)$$

it follows that G satisfies the reciprocity relation

$$\frac{\partial G}{\partial M} = \frac{\partial F}{\partial H} \frac{\partial H}{\partial M} + H + M \frac{\partial H}{\partial M} = H$$

Whereas both $F(H)$ and $G(M)$ contain the same physical information.

In the case of the generating function $W[J_\alpha^*(\tau), J_\alpha(\tau)]$, the equations for $\phi_\alpha(J_\alpha^*, J_\alpha)$ and $\phi_\alpha^*(J_\alpha^*, J_\alpha)$ are inverted to obtain the sources as functions of the fields $J_\alpha^*(\phi_\alpha^*, \phi_\alpha)$ and $J_\alpha(\phi_\alpha^*, \phi_\alpha)$ and the effective potential (effective action) is defined as the Legendre transform

$$\Gamma[\phi_\alpha^*(\tau), \phi_\alpha(\tau)] = -W[J_\alpha^*(\tau), J_\alpha(\tau)] - \sum_\gamma \int_0^\beta d\tau' [\phi_\gamma^*(\tau') J_\gamma(\tau') + J_\gamma^*(\tau') \phi_\gamma(\tau')]$$

As in the example $G(M)$, the effective potential satisfies the reciprocity relation

$$\begin{aligned}\frac{\partial}{\partial \phi_\alpha^*(\tau)} \Gamma[\phi_\alpha^*(\tau), \phi_\alpha(\tau)] &= - \sum_\gamma \int_0^\beta d\tau' \left[\frac{\partial W}{\partial J_\gamma^*(\tau')} \frac{\partial J_\gamma^*(\tau')}{\partial \phi_\alpha^*(\tau)} + \frac{\partial W}{\partial J_\gamma(\tau')} \frac{\partial J_\gamma(\tau')}{\partial \phi_\alpha^*(\tau)} \right. \\ &\quad \left. + \delta_{\gamma\alpha} \delta(\tau - \tau') J_\gamma(\tau') + \zeta \phi_\gamma^*(\tau') \frac{\partial J_\gamma(\tau')}{\partial \phi_\alpha^*(\tau)} + \frac{\partial J_\gamma^*(\tau')}{\partial \phi_\alpha^*(\tau) \phi_\gamma(\tau')} \right] \\ &= -J_\alpha(\tau)\end{aligned}$$

and the companion equation

$$\frac{\partial}{\partial \phi_\alpha(\tau)} \Gamma[\phi_\alpha^*(\tau), \phi_\alpha(\tau)] = -\zeta J_\alpha^*(\tau)$$

When the sources are set equal to zero, the effective potential is stationary

$$\frac{\delta \Gamma(\tilde{\phi}_\alpha^*(\tau), \tilde{\phi}_\alpha(\tau))}{\delta \tilde{\phi}_\alpha^*(\tau)} = \frac{\delta \Gamma(\tilde{\phi}_\alpha^*(\tau), \tilde{\phi}_\alpha(\tau))}{\delta \tilde{\phi}_\alpha(\tau)} = 0$$

Where $\tilde{\phi}_\alpha^*(\tau)$ and $\tilde{\phi}_\alpha(\tau)$ are denoted for the fields in the absence of sources. The effective potential is a generating function for vertex functions. Vertex functions are generated by differentiating the effective potential $\Gamma[\phi_\alpha^*(\tau)\phi_\alpha(\tau)]$ just as connected Green's functions generated from W :

$$\begin{aligned} & \Gamma_{m\phi^*, n\phi}(\alpha_1\tau_1, \dots, \alpha_m\tau_m | \alpha'_1\tau'_1, \dots, \alpha'_n\tau'_n) \\ &= \frac{\delta^{m=n}}{\delta \phi_{\alpha_1}^*(\tau_1) \dots \delta \phi_{\alpha_m}^*(\tau_m) \delta \phi_{\alpha'_n}(\tau'_n) \dots \delta \phi_{\alpha'_1}(\tau'_1)} \Gamma[\phi_\alpha^*(\tau), \phi_\alpha(\tau)] \Bigg|_{J_\alpha^*=J_\alpha=0} \end{aligned}$$

Note that evaluate at $J_\alpha^* = J_\alpha = 0$ is equivalent to evaluation at the stationary solutions $\tilde{\phi}_\alpha^*, \tilde{\phi}_\alpha$.

The Self-energy And Dyson's Equation

Before proceeding to the general case, it is useful to study the vertex function $\Gamma_{\phi^*\phi}$. The derivatives of a function F can be written

$$\begin{aligned} \frac{\delta F(J^*, J)}{\delta \phi_{\alpha_1}(\tau_1)} &= \sum_{\alpha_2} \int_0^\beta d\tau_2 \left[\frac{\delta F}{\delta J_{\alpha_2}^*(\tau_2)} \frac{\delta J_{\alpha_2}^*(\tau_2)}{\delta \phi_{\alpha_1}(\tau_1)} + \frac{\delta F}{\delta J_{\alpha_2}(\tau_2)} \frac{\delta J_{\alpha_2}(\tau_2)}{\delta \phi_{\alpha_1}(\tau_1)} \right] \\ &= \sum_{\alpha_2} \int_0^\beta d\tau_2 \left[-\zeta \frac{\delta F}{\delta J_{\alpha_2}^*(\tau_2)} \frac{\delta^2 F}{\delta \phi_{\alpha_1}(\tau_1) \delta \phi_{\alpha_2}(\tau_2)} - \frac{\delta F}{\delta J_{\alpha_2}(\tau_2)} \frac{\delta^2 F}{\delta \phi_{\alpha_1}(\tau_1) \delta \phi_{\alpha_2}^*(\tau_2)} \right] \end{aligned}$$

and similarly

$$\frac{\delta F(J^*, J)}{\delta \phi_{\alpha_1}^*(\tau_1)} = \sum_{\alpha_2} \int_0^\beta d\tau_2 \left[-\zeta \frac{\delta F}{\delta J_{\alpha_2}^*(\tau_2)} \frac{\delta^2 F}{\delta \phi_{\alpha_1}^*(\tau_1) \delta \phi_{\alpha_2}(\tau_2)} - \frac{\delta F}{\delta J_{\alpha_2}(\tau_2)} \frac{\delta^2 F}{\delta \phi_{\alpha_1}^*(\tau_1) \delta \phi_{\alpha_2}^*(\tau_2)} \right]$$

The lowest order equation, a general matrix of Dyson's equation, is obtained by differentiating each of the quantites $\phi_{\alpha_3}(\tau_3)$ and $\phi_{\alpha_3}^*(\tau_3)$ with respect to $\phi_{\alpha_1}(\tau_1)$ and $\phi_{\alpha_1}^*(\tau_1)$. Calculating $\frac{\delta \phi_{\alpha_3}(\tau_3)}{\delta \phi_{\alpha_1}(\tau_1)}$ in detail, we obtain:

$$\delta_{\alpha_3\alpha_1} \delta(\tau_3, \tau_1) = \frac{\delta \phi_{\alpha_3}(\tau_3)}{\delta \phi_{\alpha_1}(\tau_1)}$$

It can be rewritten as

$$\delta(31) = \int d2 \left[\zeta \frac{\delta^2 W}{\delta J^*(2) \delta J^*(3)} \frac{\delta^2 F}{\delta \phi(1) \delta \phi(2)} + \frac{\delta^2 W}{\delta J(2) \delta J^*(3)} \frac{\delta^2 F}{\delta \phi(1) \delta \phi^*(2)} \right]$$

where 1 denotes the variables α_1, τ_1 and $\int d2$ means a sum over α_2 and an integral over τ_2 .

The remaining three derivatives yield

$$\begin{aligned} \delta(31) &= \frac{\delta \phi^*(3)}{\delta \phi^*(1)} \\ &= \int d2 \left[\frac{\delta^2 W}{\delta J^*(2) \delta J(3)} \frac{\delta^2 F}{\delta \phi^*(1) \delta \phi(2)} + \zeta \frac{\delta^2 W}{\delta J(2) \delta J(3)} \frac{\delta^2 F}{\delta \phi^*(1) \delta \phi^*(2)} \right] \\ 0 &= \frac{\delta \phi(3)}{\delta \phi^*(1)} \\ &= \int d2 \left[\frac{\delta^2 W}{\delta J^*(2) \delta J^*(3)} \frac{\delta^2 F}{\delta \phi^*(1) \delta \phi(2)} + \zeta \frac{\delta^2 W}{\delta J(2) \delta J^*(3)} \frac{\delta^2 F}{\delta \phi^*(1) \delta \phi^*(2)} \right] \\ 0 &= \frac{\delta \phi^*(3)}{\delta \phi(1)} \\ &= \int d2 \left[\frac{\delta^2 W}{\delta J^*(2) \delta J(3)} \frac{\delta^2 F}{\delta \phi(1) \delta \phi(2)} + \zeta \frac{\delta^2 W}{\delta J(2) \delta J(3)} \frac{\delta^2 F}{\delta \phi(1) \delta \phi^*(2)} \right] \end{aligned}$$

For a non-interacting system,

$$\sum_{\alpha_2} \left(\delta_{\alpha_1 \alpha_2} \left(\frac{\partial}{\partial \tau_1} - \mu \right) + \langle \alpha_1 | H_0 | \alpha_2 \rangle \right) \mathcal{G}_{0,c}^{(1)}(\alpha_2, \tau_1 | \alpha_3, \tau_3) = \delta_{\alpha_1 \alpha_3} \delta(\tau_1 - \tau_3)$$

Where H_0 is the single-particle Hamiltonian. Thus, for a non-interacting system

$$\begin{aligned} \Gamma_{\phi^* \phi}^{(0)}(\alpha_1, \tau_1 | \alpha_2, \tau_2) &= [\mathcal{G}_{0,c}^{(1)}]^{-1}(\alpha_1 \tau_1 | \alpha_2 \tau_2) \\ &= \left(\delta_{\alpha_1 \alpha_2} \left(\frac{\partial}{\partial \tau_1} - \mu \right) + \langle \alpha_1 | H_0 | \alpha_2 \rangle \right) \delta(\tau_1 - \tau_2) \end{aligned}$$

Define the self energy Σ as the difference between the vertex function for the interacting and non-interacting systems:

$$\Gamma_{\phi^* \phi}(1, 2) \equiv \Gamma_{\phi^* \phi}^{(0)}(1, 2) + \Sigma(1, 2)$$

Simplify the notation, the equation above may be rewritten as

$$\mathcal{G}^{-1} = [\mathcal{G}_0]^{-1} + \Sigma$$

which can yield the Dyson equation

$$\begin{aligned} \mathcal{G} &= \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G} \\ &= \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}_0 \Sigma \mathcal{G}_0 + \dots \end{aligned}$$

or, exhibiting the explicit α, τ dependence.

$$\begin{aligned} \mathcal{G}_c^{(1)}(\alpha_1 \tau_1 | \alpha_4 \tau_4) &= \mathcal{G}_{0,c}^{(1)}(\alpha_1, \tau_1 | \alpha_4, \tau_4) \\ &+ \sum_{\alpha_2 \alpha_3} \int_0^\beta d\tau_2 d\tau_3 \mathcal{G}_{0,c}^{(1)}(\alpha_1, \tau_1 | \alpha_2 \tau_2) \Sigma(\alpha_2 \tau_2, \alpha_3 \tau_3) \mathcal{G}_c^{(1)}(\alpha_3, \tau_3 | \alpha_4, \tau_4) \end{aligned}$$

The graphical expansion of the self-energy Σ is evident from expressing the Dyson equation and its series expansion in the diagrams

$$\begin{aligned} \text{Dyson equation: } \text{fermion line} &= \text{bare fermion line} - \text{fermion line with } \Sigma \\ \text{Series expansion: } \Sigma &= \text{bare fermion line} - \text{fermion line with } \Sigma + \text{fermion line with } 2 \Sigma - \text{fermion line with } 3 \Sigma + \dots \end{aligned}$$

Higher-order Vertex Functions

We introduce an economical graphical representation for differentiations

$$\text{Diagram } G \equiv \zeta^n \frac{\delta^{m+n} W(J^*, J)}{\delta J^*(1) \delta J^*(2) \dots \delta J^*(m) \delta J(n') \dots \delta J(2') \delta J(1')}$$

and

$$\text{Diagram } \Gamma \equiv \frac{\delta^{m+n} \Gamma(\phi^*, \phi)}{\delta \phi^*(1) \delta \phi(2) \dots \delta \phi^*(m) \delta \phi(n') \dots \delta \phi(2') \delta \phi(1')}$$

With this notation, we can write:

$$\zeta \xrightarrow{3} \textcircled{\text{G}} \xrightarrow{2} \textcircled{\Gamma} \xrightarrow{1} + \xrightarrow{3} \textcircled{\text{G}} \xrightarrow{2} \textcircled{\Gamma} \xrightarrow{1} = \delta_{(1,3)}$$

To simplify, disregard the direction of the arrows. let $\frac{\delta}{\delta\phi}$ represent either $\frac{\delta}{\delta\phi(i)}$ or $\frac{\delta}{\delta\phi^*(i)}$ and let $\frac{\delta}{\delta J}$ represent either $\frac{\delta}{\delta J(i)}$ or $\frac{\delta}{\delta J^*(i)}$. Then a functional derivative $\frac{\delta}{\delta\phi}$ applied to $\frac{\delta^n}{\delta\phi^n}\Gamma$ increases the number of legs by one:

$$\frac{\delta}{\delta\phi} \textcircled{\Gamma} \begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix} = - \textcircled{\Gamma} \begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix}$$

Using the chain rule $\frac{\delta}{\delta\phi} = \frac{\delta J}{\delta\phi} \frac{\delta}{\delta J}$, the functional derivative $\frac{\delta}{\delta\phi}$ applied to $\frac{\delta^n}{\delta J^n}W$ adds a leg containing $\frac{\delta J}{\delta\phi} = \frac{\delta^2\Gamma}{\delta\phi^2}$:

$$\frac{\delta}{\delta\phi} \textcircled{\text{G}} \begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix} = - \textcircled{\Gamma} - \textcircled{\text{G}} \begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix}$$

where notice that

$$-J_\alpha(\tau) = \frac{\partial}{\partial\phi_\alpha^*(\tau)} \Gamma[\phi_\alpha^*(\tau), \phi_\alpha(\tau)]$$

With this compact notation, evaluation of $\frac{\delta^n}{\delta\phi^n}[\phi] = \frac{\delta^n}{\delta\phi^n}[\frac{\partial W}{\partial J}]$ for successive values of n yields the desired hierarchy of equations. For $n = 1$, we get

$$- \textcircled{\Gamma} - \textcircled{\text{G}} = \delta$$

Stationary-Phase Approximation and Loop Expansion

The stationary-phase approximation, also referred to as the saddle point approximation or method of steepest descent, is a method for developing an asymptotic expansion in powers

of $\frac{1}{\downarrow}$ for an integral of the form

$$I(\downarrow) = \int_{-\infty}^{\infty} dt e^{-\downarrow f(t)}$$

where \downarrow is a real parameter and in general $f(t)$ is an analytic function in the complex t -plane.