Functional Integral Formalism of Many-Particle Systems

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Outline

Motivation: One-Particle-Propagator could be written as an integral over the eigenvalues of the operators inside the Hamiltonian.

$$G(x_f, t_f; x_i, t_i) \;=\; \int_{(x_i, t_i)}^{(x_f, t_f)} D[x(t)]\, D[p(t)]\, e^{iS(x(t), p(t), t)}$$

Many-particle physics: One is interested in calculating expectation values of observables, for instance

$$\langle A \rangle \;=\; \mathrm{tr}\,(\rho A) \qquad \rho \;=\; \frac{e^{-\beta H}}{\mathrm{tr}\,(e^{-\beta H})}$$

Question: Is it possible to express the trace in a similar manner as the propagator in the one-particle case?

A typical many-particle Hamiltonian H consists of **creation** and **annihilation operators**, for instance

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} a^\dagger_{k\sigma} a_{k\sigma} + \sum_{\substack{klmn \\ \sigma\sigma'\tau\tau'}} V^{\sigma\sigma'\tau\tau'}_{klmn} a^\dagger_{k\sigma} a^\dagger_{l\sigma'} a_{n\tau'} a_{m\tau}$$

We have to construct eigenstates of the annihilation operators:
coherent states $a|\phi\rangle = \phi|\phi\rangle$

Bosonic case: In occupation number representation $|\phi\rangle$ must consist of a linear combination of states of every occupation number n. Ansatz:

$$|\phi\rangle = \sum_{n_{\alpha_1}, n_{\alpha_2}, \ldots}^{\infty} \phi_{n_{\alpha_1} n_{\alpha_2} \ldots} |n_{\alpha_1}, n_{\alpha_2}, \ldots\rangle \qquad , \phi_{n_{\alpha_1} n_{\alpha_2} \ldots} \in \mathbb{C}$$

$|n_{\alpha_1}, n_{\alpha_2}, \ldots\rangle$ normalized state with n_{α_1} particles in state α_1, ...

Let a act on this state:

$$
\begin{aligned}
a_{\alpha_i}|\phi\rangle &= \sum_{n_{\alpha_1},n_{\alpha_2},\dots}^{\infty} \phi_{n_{\alpha_1}n_{\alpha_2}\dots}\, a_{\alpha_i}|n_{\alpha_1},n_{\alpha_2},\dots\rangle \\
&= \sum_{n_{\alpha_1},n_{\alpha_2},\dots}^{\infty} \phi_{n_{\alpha_1}n_{\alpha_2}\dots}\, \sqrt{n_{\alpha_i}}\cdot|n_{\alpha_1},n_{\alpha_2},\dots,n_{\alpha_i}-1,\dots\rangle \\
&= \sum_{n_{\alpha_1},n_{\alpha_2},\dots}^{\infty} \phi_{n_{\alpha_1}n_{\alpha_2}\dots n_{\alpha_i}+1\dots}\, \sqrt{n_{\alpha_i}+1}\cdot|n_{\alpha_1},n_{\alpha_2},\dots\rangle \\
&\overset{!}{=} \phi_{\alpha_i} \sum_{n_{\alpha_1},n_{\alpha_2},\dots}^{\infty} \phi_{n_{\alpha_1}n_{\alpha_2}\dots}\, |n_{\alpha_1},n_{\alpha_2},\dots\rangle
\end{aligned}
$$

$$
\rightarrow \quad \phi_{n_{\alpha_1}n_{\alpha_2}\dots n_{\alpha_i}+1\dots} \overset{!}{=} \frac{\phi_{\alpha_i}}{\sqrt{n_{\alpha_i}+1}}\cdot\phi_{n_{\alpha_1}n_{\alpha_2}\dots n_{\alpha_i}\dots}
$$

Iteration of this relation yields

$$\phi_{n_{\alpha_1} n_{\alpha_2} \ldots} = \frac{(\phi_{\alpha_1})^{n_{\alpha_1}} \cdot (\phi_{\alpha_2})^{n_{\alpha_2}} \cdot \ldots}{\sqrt{n_{\alpha_1}!} \cdot \sqrt{n_{\alpha_2}!} \cdot \ldots} \cdot \phi_{000\ldots}$$

Usual convention: $\phi_{000\ldots} \equiv 1$

$$\rightarrow \quad |\phi\rangle = \sum_{n_{\alpha_1}, n_{\alpha_2}, \ldots}^{\infty} \frac{\phi_{\alpha_1}^{n_{\alpha_1}} \cdot \phi_{\alpha_2}^{n_{\alpha_2}} \cdot \ldots}{\sqrt{n_{\alpha_1}! \cdot n_{\alpha_2}! \cdot \ldots}} |n_{\alpha_1}, n_{\alpha_2}, \ldots\rangle \qquad \phi_{\alpha_i} \in \mathbb{C}$$

As a last step one can insert

$$|n_{\alpha_1}, n_{\alpha_2}, \ldots\rangle = \frac{\left(a_{\alpha_1}^{\dagger}\right)^{n_{\alpha_1}} \cdot \left(a_{\alpha_2}^{\dagger}\right)^{n_{\alpha_2}} \cdot \ldots}{\sqrt{n_{\alpha_1}! \cdot n_{\alpha_2}! \cdot \ldots}} |0\rangle$$

Bosonic Coherent States have got the following representation:

$$|\phi\rangle = \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots}^{\infty} \frac{\left(\phi_{\alpha_1} a_{\alpha_1}^{\dagger}\right)^{n_{\alpha_1}} \cdot \left(\phi_{\alpha_2} a_{\alpha_2}^{\dagger}\right)^{n_{\alpha_2}} \cdot \dots}{n_{\alpha_1}! \cdot n_{\alpha_2}! \cdot \dots} |0\rangle$$

$$= \prod_i \sum_{n_{\alpha_i}=0}^{\infty} \frac{\left(\phi_{\alpha_i} a_{\alpha_i}^{\dagger}\right)^{n_{\alpha_i}}}{n_{\alpha_i}!} |0\rangle = \prod_i e^{\phi_{\alpha_i} a_{\alpha_i}^{\dagger}} |0\rangle$$

Remark: This last relation could also be deduced from canonical commutation relation

$$\left[a_{\alpha_i}, a_{\alpha_i}^{\dagger}\right] = 1 = [\hat{x}, i \cdot \hat{p}]$$

In the case of **fermions** the creation and annihilation operator **anticommute**. Suppose $|\psi\rangle$ denotes a fermionic coherent state now. Then:

$$a_1 a_2|\psi\rangle = -a_2 a_1|\psi\rangle \quad \rightarrow \quad \psi_1\psi_2 \overset{!}{=} -\psi_2\psi_1$$

The eigenvalues of the fermionic annihilation operator must be **Grassmann variables (Grassmann numbers)**

Grassmann Algebra (Exterior Algebra): Let V be a complex vector space with basis $\{\psi_1, ..., \psi_n, \bar{\psi}_1, ..., \bar{\psi}_n\}$. Then the Grassmann algebra is defined as:

$$\mathcal{G} := \oplus_k \Lambda^k V$$

Multiplication is defined by using the wedge product:

$$\psi \cdot \psi' \equiv \psi \wedge \psi'$$

$$\psi_i \cdot \psi_j \equiv \psi_i \wedge \psi_j = -\psi_i \wedge \psi_j \equiv -\psi_j \cdot \psi_i$$

Since $\psi_i^2 = -\psi_i^2 = 0$ all Grassmann variables (i.e. elements from the Grassmann algebra) are **monomials** of the $\psi_i, \bar{\psi}_i$, for example:

$$\psi = a + b \cdot \psi_2 + c \cdot \psi_3 \psi_5 \bar{\psi}_1 \quad a, b, c \in \mathbb{C}$$

We finish this section with the definition of **derivatives** and **integrals** with respect to Grassmann variables:

$$\frac{\partial \psi_j}{\partial \psi_i} = \frac{\partial \bar{\psi}_j}{\partial \bar{\psi}_i} = \delta_{ij} \qquad \frac{\partial \bar{\psi}_j}{\partial \psi_i} = \frac{\partial \psi_j}{\partial \bar{\psi}_i} = 0$$

$$\frac{\partial}{\partial \psi_i} \psi_{i_1} \dots \psi_{i_n} = \sum_{m=1}^{n} (-1)^{m-1} \psi_{i_1} \dots \psi_{i_{m-1}} \left(\frac{\partial \psi_{i_m}}{\partial \psi_i} \right) \psi_{i_{m+1}} \dots \psi_{i_n}$$

The integral is defined as the same mapping, i.e.

$$\int d\psi_i \equiv \frac{\partial}{\partial \psi_i}$$

Now extend usual Fock space by allowing coefficients from the Grassmann algebra. Furthermore:

$$\{a_\alpha, \psi_i\} = \{a_\alpha, \bar{\psi}_i\} = \{a^\dagger_\alpha, \psi_i\} = \{a^\dagger_\alpha, \bar{\psi}_i\} = 0$$
$$(\psi_i a_\alpha)^\dagger = a^\dagger_\alpha \bar{\psi}_i \qquad (\psi_i a^\dagger_\alpha)^\dagger = a_\alpha \bar{\psi}_i$$

Fermionic Coherent States have got the following representation:

$$|\psi\rangle = \prod_i e^{-\psi_{\alpha_i} a^\dagger_{\alpha_i}} |0\rangle = \prod_i \left(1 - \psi_{\alpha_i} a^\dagger_{\alpha_i}\right) |0\rangle$$

Proof:

$$\begin{aligned} a_{\alpha_i}|\psi\rangle &= \prod_{j\neq i} \left(1 - \psi_{\alpha_j} a^\dagger_{\alpha_j}\right) a_{\alpha_i} \left(1 - \psi_{\alpha_i} a^\dagger_{\alpha_i}\right) |0\rangle \\ &= \prod_{j\neq i} \left(1 - \psi_{\alpha_j} a^\dagger_{\alpha_j}\right) \psi_{\alpha_i} |0\rangle \\ &= \prod_{j\neq i} \left(1 - \psi_{\alpha_j} a^\dagger_{\alpha_j}\right) \psi_{\alpha_i} \left(1 - \psi_{\alpha_i} a^\dagger_{\alpha_i}\right) |0\rangle = \psi_{\alpha_i} |\psi\rangle \end{aligned}$$

As a last step we need **completeness relations**.
For **Bosons**:

$$\int \prod_\alpha \frac{d\bar{\phi}_\alpha \, d\phi_\alpha}{2\pi i} \, e^{-\sum_\alpha \bar{\phi}_\alpha \phi_\alpha} \, |\phi\rangle\langle\phi| \;=\; \mathbb{1}$$

For **Fermions**:

$$\int \prod_\alpha d\bar{\psi}_\alpha \, d\psi_\alpha \, e^{-\sum_\alpha \bar{\psi}_\alpha \psi_\alpha} \, |\psi\rangle\langle\psi| \;=\; \mathbb{1}$$

Convention: In the following we will use

$$\zeta \;=\; \begin{cases} 1 & \text{bosons} \\ -1 & \text{fermions} \end{cases} \qquad c \;=\; \begin{cases} 2\pi i & \text{bosons} \\ 1 & \text{fermions} \end{cases}$$

$$\phi \;\in\; \begin{cases} \mathbb{C} & \text{bosons} \\ \mathcal{G} & \text{fermions} \end{cases}$$

Now we can use the coherent states to express the many-body **partition function**:

$$
\begin{aligned}
Z &= \operatorname{tr}\left(e^{-\beta H}\right) = \sum_n \langle n|e^{-\beta H}|n\rangle \\
&= \sum_n \int \prod_\alpha \frac{d\bar{\phi}_\alpha \, d\phi_\alpha}{c} \, e^{-\sum_\alpha \bar{\phi}_\alpha \phi_\alpha} \langle n|\phi\rangle\langle\phi|e^{-\beta H}|n\rangle \\
&= \sum_n \int \prod_\alpha \frac{d\bar{\phi}_\alpha \, d\phi_\alpha}{c} \, e^{-\sum_\alpha \bar{\phi}_\alpha \phi_\alpha} \langle \zeta\phi|e^{-\beta H}|n\rangle\langle n|\phi\rangle \\
\rightarrow \quad Z &= \int \prod_\alpha \frac{d\bar{\phi}_\alpha \, d\phi_\alpha}{c} \, e^{-\sum_\alpha \bar{\phi}_\alpha \phi_\alpha} \langle \zeta\phi|e^{-\beta H}|\phi\rangle
\end{aligned}
$$

With the Hamiltonian

$$H = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + V(a_\alpha^\dagger, a_\alpha)$$

and repeating the procedure from the talk before (with $\tau = \beta/N$), we get:

$$Z = \int \prod_{i=0}^{N-1} \prod_\alpha \frac{d\bar{\phi}_{i,\alpha}\, d\phi_{i,\alpha}}{c}\, e^{-\tau \sum_{i=0}^{N-1} \sum_\alpha \bar{\phi}_{i,\alpha}\left[\frac{\phi_{i+1,\alpha}-\phi_{i,\alpha}}{\tau} + \varepsilon_\alpha \phi_{i+1,\alpha}\right] + V}$$

$$= \int_{\phi(\beta)=\zeta\phi(0)} D[\phi(\tau), \bar{\phi}(\tau)]\, e^{-\int_0^\beta d\tau \sum_\alpha \bar{\phi}_\alpha(\tau)(\partial_\tau + \varepsilon_\alpha)\phi_\alpha(\tau) + V(\bar{\phi}(\tau), \phi(\tau))}$$

Partition Function:

$$Z = \int D[\phi(\tau), \bar{\phi}(\tau)]\, e^{-\int_0^\beta d\tau \sum_\alpha \bar{\phi}_\alpha(\tau)(\partial_\tau + \varepsilon_\alpha)\phi_\alpha(\tau) + V(\bar{\phi}(\tau), \phi(\tau))}$$

Let us continue with **imaginary time-ordered** Green's functions (**Matsubara functions**): $(0 \leq \tau_i \leq \beta)$

$$G = \frac{1}{Z}\mathrm{tr}\left[e^{-\beta H}\mathrm{T}_\tau\left(A_1(\tau_1)...A_n(\tau_n)\right)\right] \quad , \qquad A(\tau) = e^{\tau H} A e^{-\tau H}$$

Assume $\tau_{i_1} \geq \tau_{i_2} \geq ... \geq \tau_{i_n}$. Then:

$$\begin{aligned} G &= \frac{\zeta^{\mathrm{P}}}{Z}\mathrm{tr}\left[e^{-\beta H} A_{i_1}(\tau_{i_1})...A_{i_n}(\tau_{i_n})\right] \\ &= \frac{\zeta^{\mathrm{P}}}{Z}\mathrm{tr}\left[e^{-(\beta-\tau_{i_1})H} A_{i_1} e^{-(\tau_{i_1}-\tau_{i_2})H} A_{i_2} ... e^{-(\tau_{i_{n-1}}-\tau_{i_n})H} A_{i_n} e^{-\tau_{i_n} H}\right] \end{aligned}$$

$$G = \frac{\zeta^{\mathrm{P}}}{Z}\mathrm{tr}\left[e^{-(\beta-\tau_{i_1})H}A_{i_1}e^{-(\tau_{i_1}-\tau_{i_2})H}A_{i_2}\ldots e^{-(\tau_{i_{n-1}}-\tau_{i_n})H}A_{i_n}e^{-\tau_{i_n}H}\right]$$

$$= \frac{\zeta^{\mathrm{P}}}{Z}\mathrm{tr}\left[e^{-\int_{\tau_{i_1}}^{\beta}d\tau H}A_{i_1}e^{-\int_{\tau_{i_2}}^{\tau_{i_1}}d\tau H}A_{i_2}\ldots A_{i_n}e^{-\int_{0}^{\tau_{i_n}}d\tau H}\right]$$

Now with the same insertions as before:

$$G = \frac{\zeta^{\mathrm{P}}}{Z}\int D[\phi,\bar{\phi}]\, e^{-\int_0^\beta d\tau\, \sum_\alpha \bar{\phi}_\alpha(\tau)\partial_\tau\phi_\alpha(\tau)+H(\phi,\bar{\phi})}A(\tau_{i_1})\ldots A(\tau_{i_n})$$

$$= \frac{1}{Z}\int D[\phi,\bar{\phi}]\, e^{-\int_0^\beta d\tau\, \sum_\alpha \bar{\phi}_\alpha(\tau)\partial_\tau\phi_\alpha(\tau)+H(\phi,\bar{\phi})}A(\tau_1)\ldots A(\tau_n)$$

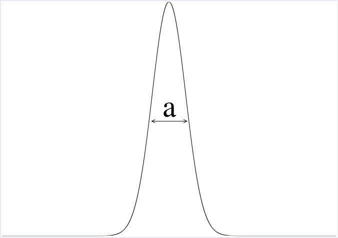
$\rightarrow$ **The functional integral is automatically time-ordered!**

Definition of the **one-particle Green's function**:

$$(\partial_\tau + \varepsilon_\alpha)\, G^0_{\alpha'}(\tau - \tau') = -\delta(\tau - \tau') \cdot \delta_{\alpha,\alpha'}$$

(real) **Gaussian integral**

$$a = \frac{1}{\sqrt{2\pi a}} \int_{-\infty}^{\infty} dx\, x^2 \cdot e^{-\frac{x^2}{2a}}$$



It can be shown that the functional integral converges to a **Grassmann-Gaussian** (fermions) or **complex Gaussian** (bosons) integral with **covariance** G^0.

As in the lecture we can Fourier transform to discrete **Matsubara frequencies**:

$$\phi(\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\phi(\tau) \qquad \bar{\phi}(\omega_n) = \int_0^\beta d\tau\, e^{-i\omega_n\tau}\bar{\phi}(\tau)$$

$$G_\alpha(\tau) \rightarrow G_\alpha(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_\alpha}$$

$$Z = \int D[\phi,\bar{\phi}]\, e^{\sum_{\omega_n,\alpha} \bar{\phi}_\alpha(\omega_n)(i\omega_n - \varepsilon_\alpha)\phi_\alpha(\omega_n) - V(\bar{\phi}(\omega_n),\phi(\omega_n))}$$

Expanding the potential term $e^{V(\bar{\phi},\phi)}$ in a power series leads to the usual **perturbation theory**

Wick's Theorem: (bosons)

$$(\bar{\phi}, A\phi) \equiv \sum_{x,y} \bar{\phi}(x) A(x,y) \phi(y) \simeq \sum_{\omega_n,\alpha} \bar{\phi}_\alpha(\omega_n)(i\omega_n - \varepsilon_\alpha)\phi_\alpha(\omega_n)$$

$$A = \left(G^0\right)^{-1} \rightarrow \sum_z G^0(x,z) A(z,y) = \delta(x-y)$$

$$\begin{aligned}
\rightarrow \phi(x)\, e^{(\bar{\phi},A\phi)} &= \sum_y \delta(x-y)\, \phi(y)\, e^{(\bar{\phi},A\phi)} \\
&= \sum_{y,z} G^0(x,z)\, A(z,y)\, \phi(y)\, e^{(\bar{\phi},A\phi)} \\
&= \sum_z G^0(x,z)\, \frac{\partial}{\partial \bar{\phi}(z)}\, e^{(\bar{\phi},A\phi)}
\end{aligned}$$

Wick's Theorem: (bosons)

$$\phi(x)\, e^{(\bar{\phi},A\phi)} \;=\; \sum_z G^0(x,z)\,\frac{\partial}{\partial\bar{\phi}(z)}\, e^{(\bar{\phi},A\phi)}$$

yields

$$\begin{aligned}
& \int D[\phi,\bar{\phi}] e^{(\bar{\phi},A\phi)} \phi(\tau_1)...\phi(\tau_n)\bar{\phi}(\tau_{n+1})...\bar{\phi}(\tau_{2n}) \\
= & \int D[\phi,\bar{\phi}] \sum_z G^0(\tau_1,z)\,\phi(\tau_2)...\bar{\phi}(\tau_{2n})\,\frac{\partial e^{(\bar{\phi},A\phi)}}{\partial\bar{\phi}(z)} \\
= & -\int D[\phi,\bar{\phi}] e^{(\bar{\phi},A\phi)} \sum_z G^0(\tau_1,z)\cdot\delta(z-\tau_i) \\
& \qquad \cdot\phi(\tau_2)...\phi(\tau_n)\bar{\phi}(\tau_{n+1})...\bar{\phi}(\tau_{i-1})\bar{\phi}(\tau_{i+1})...\bar{\phi}(\tau_{2n})
\end{aligned}$$

Wick: $\langle\phi(\tau_1)...\bar{\phi}(\tau_{2n})\rangle_0 \;=\;$ sum over all contractions

n-particle Green's Function:

$$
\begin{aligned}
G(\tau_1,\alpha_1;\dots;\tau_n,\alpha_n|\tau_1',\alpha_1';\dots;\tau_n',\alpha_n') \\
&= \zeta^n \langle \mathrm{T}_\tau \left(a_{\alpha_1}(\tau_1)\dots a_{\alpha_n}(\tau_n) a^\dagger_{\alpha_n'}(\tau_n')\dots a^\dagger_{\alpha_1'}(\tau_1') \right)\rangle \\
&= \zeta^n \langle \phi_{\alpha_1}(\tau_1)\dots\phi_{\alpha_n}(\tau_n)\bar{\phi}_{\alpha_n'}(\tau_n')\dots\bar{\phi}_{\alpha_1'}(\tau_1')\rangle
\end{aligned}
$$

Generating Functionals:

$$
\begin{aligned}
W(\rho,\bar{\rho}) &= \frac{1}{Z}\int D[\phi,\bar{\phi}] e^{(\bar{\phi},A\phi)+V(\phi,\bar{\phi})}\, e^{-(\bar{\phi},\rho)-(\bar{\rho},\phi)} \\
W_c(\rho,\bar{\rho}) &= \log\frac{1}{Z}\int D[\phi,\bar{\phi}] e^{(\bar{\phi},A\phi)+V(\phi,\bar{\phi})}\, e^{-(\bar{\phi},\rho)-(\bar{\rho},\phi)}
\end{aligned}
$$

Why are these functionals called **generating**?

$$\left.\frac{\partial W(\rho,\bar\rho)}{\partial \rho_{\alpha_1}(\tau_1)}\right|_{\rho=\bar\rho=0} = \frac{-\zeta}{Z}\int D[\phi,\bar\phi]e^{(\bar\phi,A\phi)+V(\phi,\bar\phi)}\bar\phi_{\alpha_1}(\tau_1)$$

$\rightarrow$ Derivatives of W generate expectation values of the fields, i.e. **Green's functions**.

$\rightarrow$ The derivatives of W_c generate **connected Green's functions**, for example

$$\left.\frac{\partial^2 W_c(\rho,\bar\rho)}{\partial\bar\rho_{\alpha_1}(\tau_1)\partial\rho_{\alpha_2}(\tau_2)}\right|_{\rho=\bar\rho=0}$$

$$= \left.\frac{\partial}{\partial\bar\rho_{\alpha_1}(\tau_1)}\right|_{..}\frac{-\zeta}{W}\int D[\phi,\bar\phi]e^{(\bar\phi,A\phi)+V(\phi,\bar\phi)}\,e^{-(\bar\phi,\rho)-(\bar\rho,\phi)}\bar\phi_{\alpha_2}(\tau_2)$$

$$= \zeta\langle\phi_{\alpha_1}(\tau_1)\bar\phi_{\alpha_2}(\tau_2)\rangle - \zeta\langle\phi_{\alpha_1}(\tau_1)\rangle\cdot\langle\bar\phi_{\alpha_2}(\tau_2)\rangle$$

Summary and Overview

- Coherent states are the eigenstates of the annihilation operators of a many-body system
- The functional integral formalism is the counterpart of the single-particle path integral
- The functional integral formalism produces automatically imaginary time-ordered products
- Once established it is a very powerful, elegant and general tool kit
- Most of the current (analytical) publications in condensed matter theory use this formalism