Lecture 1

Path integral for second-quantized systems

Wavefunction obeys the Schrödinger's equation:

$$\psi(r, t+\delta t) = \left(1 - \frac{i\delta t}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V(r)\right)\right)\psi(r,t).$$

Employ the equality

$$\frac{1}{\sqrt{2\pi\xi}}\int_{-\infty}^{\infty}\exp\left(-\frac{(x-x')^2}{2\xi} + a\xi\right)f(x')dx' \approx f(x) + \xi\left(a + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right)f(x) + O(\xi^2),$$

Use $\xi = i\delta t\hbar/m$ and rewrite the Schrödinger's equation:

$$\psi(r, t+\delta t) = \frac{1}{(2\pi\xi)^{N/2}}\int \exp\left(-\frac{i\delta t}{\hbar}\left(-\frac{m}{2}\frac{(r-r')^2}{\delta t^2} + V(r)\right)\right)\psi(r',t)d^N r'.$$

Repeat N_t times

$$\psi(r_{N_t}, t + N_t\delta t) = \frac{1}{(2\pi\xi)^{N_t N/2}} \times$$
$$\times \int ... \int \exp\left(-\frac{i\delta t}{\hbar}\sum_{j=0}^{N_t-1}\left(-\frac{m}{2}\frac{(r_{j+1}-r_j)^2}{\delta t^2} + V(r_j, t)\right)\right)\psi(r_0, t)d^N r_0 ... d^N r_{N_t-1}.$$

Take the limit $\delta t \to 0$, at constant $N_t\delta t = t_2 - t_1$.

$$\psi(r_2, t_2) = \int \exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}\left(\frac{m\dot{x}^2(t')}{2} - V(x(t'))\right)dt'\right)\psi(r_1, t_1)Dx(t').$$

The factor $\frac{1}{(2\pi\xi)^{N_t N/2}}$ is included in $Dx(t')$.

Real-time evolution operator

$$U(t_1,t_2) \equiv e^{-i\hat{H}(t_2-t_1)} = \int \exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2}\left(\frac{m\dot{x}^2(t')}{2} - V(x(t'))\right)dt'\right)Dx(t')$$

has the imaginary-time counterpart $\Upsilon(\tau_1,\tau_2) \equiv e^{-\hat{H}(\tau_2-\tau_1)}$, determining the partition function $Z = \mathrm{Tr}\Upsilon(\beta,0)$.
Imaginary-time path integral reads

$$\Upsilon(\tau_1,\tau_2) = \int \exp\left(\frac{1}{\hbar}\int_{\tau_1}^{\tau_2}\left(-\frac{m\dot{x}^2(\tau')}{2} - V(x(\tau'))\right)d\tau'\right)Dx(\tau').$$

An arbitrary state of bosonic system

$$|X\rangle = \sum \alpha_{n_1,\dots,n_n} (\hat{a}_1^\dagger)^{n_1} \cdot \dots \cdot (\hat{a}_N^\dagger)^{n_N} \, |0\rangle$$

can be presented as

$$\Phi_X(\hat{a}_1^\dagger, \dots, \hat{a}_N^\dagger) \, |0\rangle \, .$$

Let's replace the operators $\hat{a}^\dagger$ with complex numbers a, so that many-body states are mapped to the multi-argument functions $\Phi_X(a_1, \dots, a_N)$.

Any quantum mechanical operator has its counter-part acting in the space of $\Phi(a)$. In particular, the creation-annihilation operators read:

$$\Phi_{\hat{a}_i^\dagger X} = a_i \Phi_X,$$

$$\Phi_{\hat{a}_i X} = \partial_{a_i} \Phi_X.$$

Scalar product with the vacuum:

$$\langle 0|X\rangle = \Phi_X(0).$$

Obtaining a scalar product of the two arbitrary states would require solving the partial-differential equation

$$\langle Y|X\rangle = \frac{1}{1-\partial_{\bar{b}}\partial_a} \bar{\Phi}_Y(b)\Phi_X(a)|_{a,b=0}$$

(expand the r.h.s. to check the expression!).

In the path-integral formalism, all the operators are expressed in the integral form. Let's derive the integral representation for the partial derivative. Start from the identity

$$a_1^n = e^{\frac{1}{2}\bar{a}_1 a_1} \partial^n_{-\frac{\bar{a}_1}{2}} e^{-\frac{1}{2}\bar{a}_1 a_1} = e^{\frac{1}{2}\bar{a}_1 a_1} \partial^n_{-\frac{\bar{a}_1}{2}} \int e^{-\frac{1}{2}(\bar{a}_0 a_0 + \bar{a}_1 a_0 - \bar{a}_0 a_1)} \frac{d^2 a_0}{2\pi}$$

($a_0, \bar{a}_0$ are complex conjugate, $a_1, \bar{a}_1$ are so far independent, and will be chosen conjugate afterwards). Apply $\partial^m_{a_1}$ to the both sides and calculate r.h.s.:

$$\partial^m_{a_1} a_1^n = \int e^{-\frac{1}{2}(\bar{a}_0 + \bar{a}_1)(a_0 - a_1)} \left(\frac{\bar{a}_0 + \bar{a}_1}{2} \right)^m a_0^n \frac{d^2 a_0}{2\pi}$$

Taylor-series expansion proves

$$R(\partial_{a_1}) F(a_1) = \int e^{-\frac{1}{2}(\bar{a}_0 + \bar{a}_1)(a_0 - a_1)} R\left(\frac{\bar{a}_0 + \bar{a}_1}{2} \right) F(a_0) \frac{d^{2N} a_0}{(2\pi)^N}$$

for arbitrary functions R, F dependent on N-component arguments.
In particular, $R = 1$ corresponds to the unitary operator.

Partition function

$$Z = \mathrm{Tr} e^{-\beta \hat{\mathrm{H}}}$$

Elementary evolution operator $\hat{\Upsilon}_{\delta\tau} = 1 - \delta\tau \hat{H}(\hat{a}^\dagger, \hat{a})$ with the normal-ordered $\hat{H}(\hat{a}^\dagger, \hat{a})$ maps to $\Upsilon_{\delta\tau} = 1 - \delta\tau H(a, \partial_a)$, that equals

$$S_{\tau+\delta\tau,\tau} = \int \left(1 - \delta\tau H\left(a_{\tau+\delta\tau}, \frac{\bar{a}_{\tau+\delta\tau} + \bar{a}_\tau}{2}\right)\right) e^{-\frac{1}{2}(\bar{a}_\tau + \bar{a}_{\tau+\delta\tau})(a_\tau - a_{\tau+\delta\tau})} \frac{d^{2N} a_\tau}{(2\pi)^N}$$

We put $\delta\tau H$ back in the exponent, and introduce $N_\tau = \beta/\delta\tau$ time slices:

$$\Upsilon_{\beta,0} = \int .. \int e^{-\delta\tau \sum_j \left(\frac{\bar{a}_j + \bar{a}_{j+1}}{2} \frac{a_j - a_{j+1}}{\delta\tau} + H\left(a_{j+1}, \frac{\bar{a}_{j+1} + \bar{a}_j}{2}\right)\right)} \frac{d^{2N(N_\tau - 1)} a}{(2\pi)^{N(N_\tau - 1)}}.$$

Integration is over all but last-grid variables.
Z is the convolution of υ with the unitary operator $\int e^{-\delta\tau \frac{\bar{a}_{N_\tau} + \bar{a}_1}{2} \frac{a_{N_\tau} - a_1}{\delta\tau}} \frac{d^{2N} a_{N_\tau}}{(2\pi)^N}$.
In the path-integral notation

$$Z = \int e^{-\int (-\bar{a}_\tau \partial_\tau a_\tau + H(a_\tau, \bar{a}_\tau)) d\tau} D\bar{a}, a.$$

Comment 0. "Kinetic" part is purely imaginary:

$$\sum_j \frac{1}{2}(\bar{a}_j + \bar{a}_{j+1})(a_j - a_{j+1}) = -i \sum_j (a'_j a''_{j+1} - a''_j a'_{j+1})$$

Comment 1. The real-time evolution operator reads

$$U = \int e^{-i\int \sum_j (-\bar{a}_t(-i\partial_t)a_t + H(a_t, \bar{a}_t))dt} D\bar{a}, a.$$

Comment 2. For a typical path $|a_j - a_{j+1}| \approx 1$ (independent of $\delta\tau$), so what is $\partial_\tau a_\tau$ and even a_τ? "Discrete" expressions must be kept in mind.

Comment 3. The only approximations in the discrete scheme are about the series expansion of the exponent. For numerical implementations, one can develop a higher-order scheme with respect to $\delta\tau$.

Comment 4. There are many confusions about the notation ($a \leftrightarrow \bar{a}$ etc).

States of the fermionic system

$$|X\rangle = \sum_{k_x=0,1} \alpha_{k_1,\ldots,k_n} (\hat{c}_1^{\dagger})^{k_1} \cdot \ldots \cdot (\hat{c}_n^{\dagger})^{k_n} \, |0\rangle$$

Gunter Grassmann (1809-1877)

are mapped on the functions of Grassmann variables

$$\Phi_X(c_1, \ldots, c_N) \, |0\rangle \, .$$

Definitions:

$$c_i c_j + c_j c_i = 0.$$

$$\int dc = 0, \quad \int c dc = 1.$$

Felix Berezin (1931-1980)

Mapped creation-annihilation operators:

$$\Phi_{\hat{c}_i^\dagger X} = c_i \Phi_X \, ,$$

$$\Phi_{\hat{c}_i X} = \int \Phi_X dc_i .$$

Examples

$$e^{ac} = 1 + ac$$

$$e^{a_1 c_1 \bar{c}_1 + a_2 c_2 \bar{c}_2} = 1 + a_1 c_1 \bar{c}_1 + a_2 c_2 \bar{c}_2 + a_1 a_2 c_1 \bar{c}_1 c_2 \bar{c}_2$$

Rotating to the eigenspace of Hermitian A, prove that

$$\iint e^{(\bar{c}Ac) + a(\bar{\xi}c) + \bar{a}(\xi\bar{c})} d^n c d^n \bar{c} = \det A \; e^{-a\bar{a}(\bar{\xi}A^{-1}\xi)}$$

($\bar{c}, c, \bar{\xi}, \xi$ are vectors with Grassmann components). In particular:

$$\iint e^{(\bar{c}Ac)} d^n c d^n \bar{c} = \det A$$

(actually valid not only for Hermitian A – consider the Taylor series of $e^{(\bar{c}Ac)}$ for the proof).

The integral representation:

$$\left(\int dc_1\right)^m c_1^n = \int e^{-\frac{1}{2}(\bar{c}_0+\bar{c}_1)(c_0-c_1)} \left(\frac{\bar{c}_0+\bar{c}_1}{2}\right)^m c_0^n \; 2d\bar{c}_0 dc_0, \qquad n,m=0,1$$

allows to write the fermionic path-integral

$$Z = \int e^{-\int(-\bar{c}_\tau \partial_\tau c_\tau + H(c_\tau,\bar{c}_\tau))d\tau} D\bar{c}, c.$$

N.B. Grassmann variables always appear pairwise in the path integral.