Quantum Field Theory I

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March 8, 2024

Contents

Lecture 1

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Exam. The exam can be done whenever, just send an email at least ten days before. Half an hour to calculate something like in class, or generalize something, just technical stuff. It is possible to do QFT 1 and 2 together.

1 Introduction

The aim is to develop an alternative description of elementary particles and fundamental interactions using functional methods instead of canonical quantization. The path integral formulation of quantum mechanics is an example of functional method. Canonical quantization works by taking classical observable quantities and promoting them to operators obeying certain commutator relations. This was done in the relativistic formulation of quantum field theory in Theoretical Physics I.

The alternative, albeit equivalent, formulation of quantum mechanics is based on Feynman path integrals: the propagators are written in term of path integrals. Quantum Field Theory I and II reformulates quantum field theory in terms of a generalization of the quantum mechanical path integral to relativistic field theories. The content of Theoretical Physics I is studied using a functional approach.

One needs to formulate quantum field theories for particles of different spins: scalar bosons, spinor fermions and vector bosons. Gauge theories are quantized using functional methods. One does not look for spin $\frac{3}{2}$ and 2 fields, because quantum field theory is not suitable for their description: the theory is inconsistent because it is not renormalizable at every energy scale, in particular in the ultraviolet. For higher spins, there are problems in the propagation of particles in ordinary quantum field theory and one needs a more general approach.

The functional approach lets one study phenomena for which canonical quantization is not suitable.

*`https://github.com/M-a-s-o/notes`

1.1 Prerequisites

The prerequisites are the following.

Real Gaussian integral. Gaussian integrals are useful for many computations. In one dimension one has

$$\int_{\mathbb{R}} \mathrm{d}x\, \mathrm{e}^{-\frac{a}{2}x^2+bx} = \sqrt{\frac{2\pi}{a}}\mathrm{e}^{\frac{b^2}{2a}}$$

In n dimensions (considering only diagonal matrices) one has

$$\int_{\mathbb{R}^n} \mathrm{d}x_1 \cdots \mathrm{d}x_n\, \mathrm{e}^{-\frac{a_1}{2}x_1^2-\cdots-\frac{a_n}{2}x_n^2+b_1x_1+\cdots+b_nx_n} = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{a_1\cdots a_n}}\mathrm{e}^{\frac{b_1^2}{2a_1}+\cdots+\frac{b_n^2}{2a_n}}$$

Introducing the matrix and vectors

$$A = \mathrm{diag}(a_1, \dots, a_n)\,, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ a_n \end{bmatrix}\,, \quad b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

one obtains

$$\int_{\mathbb{R}^n} \mathrm{d}x_1 \cdots \mathrm{d}x_n\, \mathrm{e}^{-\frac{1}{2}x^\top Ax+b^\top x} = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det A}}\mathrm{e}^{\frac{1}{2}b^\top A^{-1}b}$$

which more generally holds for positive-definite symmetric matrices[1] A. This result is analytically continued to the cases where the exponent in the integrand has arbitrary signs or imaginary numbers while assuming the right-hand side keeps its validity.

Complex Gaussian integral. The complex Gaussian integral is the following

$$\int \prod_{j=1}^n \mathrm{d}z_j\, \mathrm{d}\bar{z}_j\, \mathrm{e}^{-\bar{z}^\top Az+\bar{b}^\top z+b^\top \bar{z}} = \frac{(2\pi)^n}{\det A}\mathrm{e}^{\bar{b}^\top A^{-1}b}$$

where A is a positive-definite hermitian matrix, b is a complex column vector and the bar is complex conjugation. Since $\mathbb{C} \simeq \mathbb{R}^2$, and the dimension is still n, one expects double the integrals.

There is also the generalization of Gaussian integrals for Grassmann odd variables suitable for spinors.

Average of a polynomial with Gaussian distribution. Consider the mean value of Gaussian-distributed variables (see Weinberg, eq. 9.A.10)

$$\begin{aligned}
\langle x_{k_1} \cdots x_{k_l} \rangle &\equiv \int \prod_{j=1}^n \mathrm{d}x_j\, x_{k_1} \cdots x_{k_l} \mathrm{e}^{-\frac{1}{2}x^\top Ax+b^\top x}\bigg|_{b=0} \\
&= \int \prod_{j=1}^n \mathrm{d}x_j\, \frac{\partial^l}{\partial b_{k_1} \cdots \partial b_{k_l}} \mathrm{e}^{-\frac{1}{2}x^\top Ax+b^\top x}\bigg|_{b=0} \\
&= \frac{\partial^l}{\partial b_{k_1} \cdots \partial b_{k_l}} \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det A}}\mathrm{e}^{\frac{1}{2}b^\top A^{-1}b}\bigg|_{b=0} \\
&= \begin{cases} 0\,, & l \text{ odd} \\ \dfrac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det A}} \displaystyle\sum_{\substack{\text{pairings} \\ \text{of } \{k_i\}}} \prod_{\{k_ik_j\}} A^{-1}_{k_ik_j}\,, & l \text{ even} \end{cases}
\end{aligned}$$

The last sum is over the pairings of $(k_1 \cdots k_l)$ — two pairings are the same if they differ only by the order of the pairs, or by the order of indices within a pair — and the product is over all such pairs.

One can compute averages through the derivatives of Gaussian integrals. From the first line (or the third), one may notice that if l is odd then the integral is null.

[1] See `https://en.wikipedia.org/wiki/Gaussian_integral`.

Functional calculus. Informally, functional calculus is need for infinite (non-countable) dimensional vectors (for example functions). From a discrete set of quantities q_i for which one knows how to take the derivative, one moves to the case of continuous variables where one works with functions $q(x)$.

Inner product. The inner product of two finite dimensional vector fields is

$$u \cdot v \equiv \sum_{i=1}^{n} u_i v_i$$

while for infinite dimensional vector fields one has

$$u \cdot v \equiv \int \mathrm{d}x \, u(x) v(x)$$

The inner product with respect to a matrix is

$$u^\top M v = \sum_{ij=1}^{n} u_i M_{ij} v_j \rightsquigarrow u^\top M v = \int \mathrm{d}x \, \mathrm{d}y \, u(x) M(x,y) v(y)$$

Identity operator. The identity operator is

$$q = Iq \iff q_i = \sum_j \delta_{ij} q_j \rightsquigarrow q(x) = \int \mathrm{d}y \, \delta(x-y) q(y)$$

The identity operator is the Dirac delta function.

Functional derivatives. The notation for functional derivatives is $\frac{\delta}{\delta q(x)}$. The concept of functional derivative can be defined by imposing a set of ansätze (pl. of ansatz):

- Linearity
$$\delta_q[F_1(q) + F_2(q)] = \delta_q F_1 + \delta_q F_2$$
- Leibniz rule
$$\delta_q[F_1(q) F_2(q)] = (\delta_q F_1) F_2 + F_1 \delta_q F_2$$
- It must hold
$$\delta_{q(x)} q(y) = \delta(y - x)$$

With these ansätze one can prove that the functional derivative enjoys the same properties as the regular derivative. For example

$$\delta_{q(x)} \int \mathrm{d}y \, q^P(y) = \int \mathrm{d}y \, P q^{P-1}(y) \, \delta_{q(x)} q(y) = P q^{P-1}(x)$$

Likewise

$$\delta_{q(x)} \int \mathrm{d}y \, f(y) \, \partial_y q(y) = \int \mathrm{d}y \, f(y) \, \partial_y \delta(x-y) = -\partial_x f(x)$$

where the result is obtained remembering that the Dirac delta is a distribution.

Generalization of Gaussian integrals to functional integrals. The Gaussian integral becomes

$$\int \prod_{j=1}^{n} \mathrm{d}q_j \, \mathrm{e}^{-\frac{1}{2} q^\top A q} = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det A}} \rightsquigarrow \int [\mathcal{D}q] \, \mathrm{e}^{-\frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, q(x) A(x,y) q(y)} = \frac{\text{const.}}{\sqrt{\text{“}\det A\text{”}}}$$

where $\mathcal{D}q$ is the functional measure that, along with the determinant, needs to be properly defined.

Useful property. Starting from

$$e^{iq\cdot J} \equiv e^{i\int dy\, q(y)J(y)}$$

one may find its derivative

$$\begin{aligned}\delta_{J(x)} e^{iq\cdot J}|_{J=0} &= \delta_{J(x)} e^{i\int dy\, q(y)J(y)}|_{J=0} = \delta_{J(x)}\left[i\int dy\, q(y)J(y)\right] e^{iq\cdot J}|_{J=0} \\ &= iq(x)e^{iq\cdot J}|_{J=0} = iq(x)\end{aligned}$$

A function can be expressed as the derivative of an exponential with respect to a parameter. This parameter J is called the source of q. Since

$$q(x) = -i\,\delta_{J(x)} e^{iq\cdot J}|_{J=0}$$

then one may write any function of $q(x)$ as

$$G(q(x)) = G(-i\,\delta_{J(x)}) e^{iq\cdot J}|_{J=0}$$

To make sense of the right-hand expression, one may expand the function $G(x)$ in a Taylor series.

2 Feynman path integral in quantum mechanics

See Feynman–Hibbs, Srednicki, Anselmi, Cheng–Li. Quantum mechanics is a non-relativistic theory developed through the canonical quantization of observables (also called first quantization) $[\hat{x},\hat{p}] = i\hbar$, but it can also be equivalently formulated through Feynman's path integrals. In quantum field theory one can use the canonical quantization of fields (also called second quantization): expanding the free field in terms of plane waves, one promotes the Fourier coefficients to operators obeying (anti-)commutation relations

$$[a(\mathbf{k}), a^\dagger(\mathbf{k})] = (2\pi)^3\delta^{(3)}(\mathbf{k}-\mathbf{k}')$$

Though one may also use functional quantization which is developed in the following.

A massive particle. See Anselmi, Cheng–Li and Srednicki (for philosophy, application etc see Feynman–Hibbs). A simple case is the one of one massive particle in one dimension subject to a potential V. The Hamiltonian of the system is

$$H = \frac{p^2}{2m} + V(q)$$

where q is the position of the particle. The observables are promoted to operators

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})\,, \quad [\hat{q},\hat{p}] = i\hbar$$

The propagation of the particle is described by Schrödinger's equation

$$\hat{H}\,|\psi(t)\rangle = i\hbar\,\partial_t\,|\psi(t)\rangle$$

where $|\psi(t)\rangle$ is the state of the particle. Starting from the Hamiltonian, the corresponding Lagrangian is obtained by the Legendre transform

$$L(q,\dot{q}) = [p\dot{q} - H(p,q)]_{p=p(q,\dot{q})}$$

The expression of the momentum p in terms of q and $\dot{q}$ is obtain by solving Hamilton's equations

$$\dot{q} = \partial_p H\,, \quad \dot{p} = -\partial_q H$$

To describe the propagation of a particle one needs to know the probability of measuring such particle after some time. One would like an alternative mathematical formulation to ordinary quantum mechanics. Consider a particle at some initial point q_i and at some initial time t_i. Letting it propagate up to a final time t_f, one would like to compute the probability that the particle is at a final position q_f. Between the two measurements $t_i < t < t_f$, the particle is not being observed and it propagates. One can at most compute a probability amplitude given by

$$ {}_{\mathrm{S}}\langle q_f | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_f - t_i)} | q_i \rangle_{\mathrm{S}} \equiv {}_{\mathrm{H}}\langle q_f, t_f | q_i, t_i \rangle_{\mathrm{H}} $$

where $|q, t\rangle_{\mathrm{H}} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Ht} |q\rangle_{\mathrm{S}}$ is an instantaneous (and time independent) eigenvector of the time dependent position operator $Q(t)$ (see Srednicki, p. 43). Feynman observes that one does not know the precise path of the particle during its propagation, so the particle could take any path between the start and the end points. The only condition is that when $\hbar \to 0$, the classical limit, among the infinite number of possible paths between the start and the end, the only path available is the classical one, which is taken from the variational principle (called action principle in quantum field theory)

$$ \delta S = 0 \,, \quad \forall q \mid \delta q(t_i) = \delta q(t_f) = 0 $$

Feynman proposes that the probability amplitude should be the sum over all possible paths, each weighed by the probability of the particle to travel along such path: when taking the classical limit, the most probable path is the classical one. They weight of each path is

$$ \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(q_f, t_f, q_i, t_i)} $$

where the action is the classical one. The reason the weight is the above can be seen as follows. Interpreting the sum as an average, in the classical limit the weight oscillates rapidly and its average is zero. The classical path is the only one that can survive because the action is at a minimum, so minimal oscillation. Therefore, the path integral formulation is

$$ {}_{\mathrm{S}}\langle q_f | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_f - t_i)} | q_i \rangle_{\mathrm{S}} = \int [\mathcal{D}q] \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(q_f, t_f, q_i, t_i)} $$

The right-hand side is just a formal definition of the idea of path integral.

Lecture 2

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One would like to give an explicit prescription for the sum of all possible paths between two points

$$ \int [\mathcal{D}q] $$

Since one does not know how to deal with a continuum of paths, one can discretize the theory and then take the continuum limit. Time and space are discretized in equal-length steps

$$ \delta t = \frac{t_f - t_f}{N+1} $$

The position of the particle is no longer $q(t)$ but $q(t_j)$. The smaller is the step $\delta t \ll 1$, the better the discrete path approximates the Feynman path. Consecutive discrete points can be joined by straight segments giving the discrete path as

$$ q(t) = \frac{q_j - q_{j-1}}{\delta t}(t - t_{j-1}) + q_{j-1} \,, \quad j = 1, \dots, N+1 $$

where $q_0 \equiv q_i$ and $q_{N+1} \equiv q_f$. From the equation above, the time interval is

$$ t_f - t_i = (N+1)\delta t $$

so the probability amplitude becomes

$$ \begin{aligned} A &= {}_{\mathrm{S}}\langle q_f | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_f - t_i)} | q_i \rangle_{\mathrm{S}} = {}_{\mathrm{S}}\langle q_f | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\delta t\,(N+1)} | q_i \rangle_{\mathrm{S}} = {}_{\mathrm{S}}\langle q_f | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\delta t} \cdots \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\delta t} | q_i \rangle_{\mathrm{S}} \\ &= \int \prod_{j=1}^{N} \mathrm{d}q_j \, \langle q_f | \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,\delta t} \, | q_N \rangle \langle q_N | \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,\delta t} \, | q_{N-1} \rangle \cdots \langle q_1 | \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,\delta t} \, | q_i \rangle \end{aligned} $$

at the second line one has inserted N identities as the completeness relation in the position eigenstates

$$\int \mathrm{d}q \; |q\rangle\langle q| = I$$

Considering a generic factor, one notices

$$\langle q_{j+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H \,\delta t} \, |q_j\rangle = \langle q_{j+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[\frac{p^2}{2m} + V(q)]\,\delta t} \, |q_j\rangle$$

Since q and p do not compute, one cannot split the exponential the same way one does with numbers, but one has to apply the Zassenhaus formula (related to the Baker–Campbell–Hausdorff formula):

$$\mathrm{e}^{t(x+y)} = \mathrm{e}^{tx}\mathrm{e}^{ty}\mathrm{e}^{-\frac{1}{2}t^2[x,y]+o(t^2)}$$

The first order in t is just $\mathrm{e}^{t(x+y)} \approx \mathrm{e}^{tx}\mathrm{e}^{ty}$. Therefore, one has

$$\langle q_{j+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H \,\delta t} \, |q_j\rangle = \langle q_{j+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\,\delta t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q)\,\delta t} \, |q_j\rangle$$

The position states are eigenstates of the potential, but not of the momentum. One can insert a completeness relation in the momentum eigenstates between the two exponentials

$$\begin{aligned}\langle q_{j+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} H \,\delta t} \, |q_j\rangle &= \int \mathrm{d}p_j \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p_j^2}{2m}\,\delta t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_j)\,\delta t} \, \langle q_{j+1}|p_j\rangle \, \langle p_j|q_j\rangle \\ &= \int \frac{\mathrm{d}p_j}{2\pi\hbar} \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p_j^2}{2m}\,\delta t - \frac{\mathrm{i}}{\hbar}V(q_j)\,\delta t}\mathrm{e}^{\mathrm{i}p_j(q_{j+1}-q_j)}\end{aligned}$$

the operators can then act on their eigenstates producing the associated eigenvalue. At the second line one remembers

$$\langle q|p\rangle = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pq}}{\sqrt{2\pi\hbar}}$$

Since δt is infinitesimal, then one may substitute the potential with its value at the midpoint between two coordinates

$$V(q_j) \to V(\bar{q}_j)\,, \quad \bar{q}_j = \frac{q_{j+1}+q_j}{2}$$

Replacing every factor inside the probability amplitude, one gets

$$A = \int \prod_{j=1}^{N} \mathrm{d}q_j \, \prod_{k=0}^{N} \frac{\mathrm{d}p_k}{2\pi\hbar} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_k(q_{k+1}-q_k) - \frac{\mathrm{i}}{\hbar}H(p_k,\bar{q}_k)\,\delta t}$$

In the limit $N \to \infty$, equivalent to $\delta t \to 0$, one has

$$\begin{aligned}A &= \lim_{N\to\infty} \int \prod_{j=1}^{N} \mathrm{d}q_j \, \prod_{k=0}^{N} \frac{\mathrm{d}p_k}{2\pi\hbar} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_k \frac{q_{k+1}-q_k}{\delta t}\,\delta t - \frac{\mathrm{i}}{\hbar}H(p_k,\bar{q}_k)\,\delta t} \\ &= \lim_{N\to\infty} \int \prod_{j=1}^{N} \mathrm{d}q_j \, \prod_{k=0}^{N} \frac{\mathrm{d}p_k}{2\pi\hbar} \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_k \dot{q}_k\,\delta t - \frac{\mathrm{i}}{\hbar}H(p_k,\bar{q}_k)\,\delta t} \\ &\equiv \int [\mathcal{D}q\,\mathcal{D}p] \exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t \, \big[p(t)\dot{q}(t) - H(p(t),q(t))\big]\right]\end{aligned}$$

The last line is the definition of the path integral.

Since the explicit formula of the Hamiltonian is known

$$H = \frac{p^2}{2m} + V(q)$$

one can integrate over a momenta p_k to obtain

$$\begin{aligned}\int \mathrm{d}p_k \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p_k\dot{q}_k - \frac{p_k^2}{2m})\,\delta t} &= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi\hbar m}{\mathrm{i}\,\delta t}} \exp\left[-\frac{\dot{q}_k^2\,(\delta t)^2}{\hbar^2}\left(\frac{2\mathrm{i}}{\hbar}\frac{\delta t}{m}\right)^{-1}\right] \\ &= \left[\frac{m}{2\pi\hbar\mathrm{i}\,\delta t}\right]^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar}(\frac{q_{k+1}-q_k}{\delta t})^2\,\delta t}\end{aligned}$$

where one applies the analytic continuation of the Gaussian integral

$$\int \mathrm{d}x\, \mathrm{e}^{-\frac{a}{2}x^2+bx} = \sqrt{\frac{2\pi}{a}}\mathrm{e}^{\frac{b^2}{2a}}\,, \quad a = \frac{\mathrm{i}}{\hbar}\frac{\delta t}{m}\,, \quad b = \frac{\mathrm{i}}{\hbar}\dot{q}_k\,\delta t$$

At the second line, one replaces

$$\dot{q}_k \equiv \frac{q_{k+1}-q_k}{\delta t}$$

Performing the integration for every $k = 0, \dots, N$, the probability amplitude is then

$$A = \lim_{N\to\infty}\left[\frac{m}{2\pi\hbar\mathrm{i}\,\delta t}\right]^{\frac{N+1}{2}} \int \prod_{j=1}^{N} \mathrm{d}q_j \,\exp\left[\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{N}\delta t\left(\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2 - V\right)\right]$$

in the limit, the exponent is the classical Lagrangian (i.e. there are no operators)

$$\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{N}\delta t\left[\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2 - V\right] = \frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}\mathrm{d}t\, L(q,\dot{q})$$

The coefficient in square bracket of the amplitude is divergent but it compensates the infinitesimal nature of the integration measure. The path integral is then defined as

$$\int [\mathcal{D}q] \equiv \lim_{N\to\infty}\left[\frac{m}{2\pi\hbar\mathrm{i}\,\delta t}\right]^{\frac{N}{2}} \int \prod_{j=1}^{N-1}\mathrm{d}q_j$$

mind the rescaling $N+1 \to N$. To give a meaningful definition, time has to be discretized: continuous functions become discrete (like functions on a lattice).

Remark. See Feynman–Hibbs. If the path integral formulation is a consistent alternative prescription, then it concerns the computation of probability amplitudes, called kernels or Feynman propagators

$$K(q_f,t_f;q_i,t_i) \equiv \langle q_f|\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_f-t_i)}\,|q_i\rangle$$

The definition is independent of ordinary quantum mechanics and their operators. Probability amplitudes are weighed with the exponential of the classical action, the only sign of quantum mechanics is the appearance of Planck's constant $\hbar$.

One may notice that

- The weight $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S}$ is given in terms of the classical action

  $$S = \int_{t_i}^{t_f}\mathrm{d}t\, L(q(t),\dot{q}(t))$$

  The path integral is then referred to as the quantum integral.

- One may find a first equivalence with ordinary quantum mechanics. Consider the quantum mechanical wave function

  $$\begin{aligned}\psi(q,t) &= {}_{\mathrm{H}}\langle q,t|\psi\rangle = {}_{\mathrm{S}}\langle q|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\,|\psi\rangle = \int \mathrm{d}q'\;{}_{\mathrm{S}}\langle q|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t-t')}\,|q'\rangle\,\langle q',t'|\psi\rangle \\ &= \int \mathrm{d}q'\, K(q,t;q',t')\psi(q',t')\end{aligned}$$

  The kernel has the meaning of evolution operator. One may check that the wave function $\psi(q,t)$ satisfies Schrödinger's equation (see Anselmi, Feynman–Hibbs) thanks to the properties of the kernel.

Kernel of a free particle. The potential of a free particle is identically zero $V(q) = 0$. The kernel is

$$K_0(q_f, t_f; q_i, t_i) = \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar \mathrm{i}\,\delta t}\right]^{\frac{N}{2}} \int \prod_{j=1}^{N-1} \mathrm{d}q_j \,\exp\left[\frac{\mathrm{i}m}{2\hbar\delta t}\sum_{j=1}^{N}(q_j - q_{j-1})^2\right]$$

Its form is that of many Gaussian integrals, but they are not factorized, so a change of variables is necessary

$$\widetilde{q}_j = q_j - q_f\,, \quad \widetilde{q}_0 = q_i - q_f\,, \quad \widetilde{q}_N = 0\,, \quad \mathrm{d}q_j = \mathrm{d}\widetilde{q}_j$$

remembering that after rescaling? [r] one has

$$q_0 = q_i\,, \quad q_N = q_f$$

The sum in the exponent is then

$$\begin{aligned}
\sum_{j=1}^{N}(q_j - q_{j-1})^2 &= (q_1 - q_i)^2 + (q_2 - q_1)^2 + \cdots + (q_N - q_{N-1})^2 \\
&= [\widetilde{q}_1 - (q_i - q_f)]^2 + (\widetilde{q}_2 - \widetilde{q}_1)^2 + \cdots + (\cancel{\widetilde{q}_N} - \widetilde{q}_{N-1})^2 \\
&= (q_i - q_f)^2 - 2\widetilde{q}_1(q_i - q_f) + 2\widetilde{q}_1^2 + 2\widetilde{q}_2^2 + \cdots + 2\widetilde{q}_{N-1}^2 \\
&\quad -2\widetilde{q}_1\widetilde{q}_2 - 2\widetilde{q}_3\widetilde{q}_2 - \cdots - 2\widetilde{q}_{N-2}\widetilde{q}_{N-1} \\
&= (q_i - q_f)^2 + 2\widetilde{q}_1(q_f - q_i) + \widetilde{q}^\top \widetilde{M}\widetilde{q}
\end{aligned}$$

where one has a $N-1$ dimensional vector and square matrix

$$q = \begin{bmatrix} q \\ \vdots \\ q_{N-1}\end{bmatrix}\,, \quad \widetilde{M} = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ 0 & 0 & -1 & 2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

The kernel is then

$$\begin{aligned}
K_0(q_f, t_f; q_i, t_i) &= \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar \mathrm{i}\,\delta t}\right]^{\frac{N}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar\,\delta t}(q_f - q_i)^2} \int \prod_{j=1}^{N-1} \mathrm{d}\widetilde{q}_j \,\exp\left[\frac{\mathrm{i}m}{2\hbar\,\delta t}\left[\widetilde{q}^\top \widetilde{M}\widetilde{q} + 2\widetilde{q}_1(q_f - q_i)\right]\right] \\
&= \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar \mathrm{i}\,\delta t\,N}\right]^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar\,\delta t}(q_f - q_i)^2}\mathrm{e}^{-\frac{\mathrm{i}m}{2\hbar\,\delta t}(q_f - q_i)^2\frac{N-1}{N}} \\
&= \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar \mathrm{i}\,\delta t\,N}\right]^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar\,\delta t\,N}(q_f - q_i)^2} = \left[\frac{m}{2\pi\hbar \mathrm{i}\,\Delta t}\right]^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar\,\Delta t}(q_f - q_i)^2}
\end{aligned}$$

at the second line one remembers that

$$\int \prod_{i=1}^{N-1} \mathrm{d}x_i \,\mathrm{e}^{-\frac{1}{2}x^\top M x + b^\top x} = \frac{(2\pi)^{\frac{N-1}{2}}}{\sqrt{\det M}}\mathrm{e}^{\frac{1}{2}b^\top M^{-1} b}$$

where

$$M = -\frac{\mathrm{i}m}{\hbar\,\delta t}\widetilde{M}\,, \quad \det\widetilde{M} = N\,, \quad (\widetilde{M}^{-1})_{11} = \frac{N-1}{N}\,, \quad b_1 = \frac{\mathrm{i}m}{\delta t}(q_f - q_i)$$

At the last line, one notices that

$$\delta t = \frac{t_f - t_i}{N} = \frac{\Delta t}{N}$$

With this specific example, one may notice that the divergence of δt is compensated to give a finite result.

Properties of the kernel. A few properties:

- The equal-time limit is
$$\lim_{t_f\to t_i} K_0(q_f,t_f;q_i,t_i)=\delta(q_f-q_i)$$
equivalent to $q_f\to q_i$. This is consistent with an expression of the Dirac delta given by
$$\lim_{\varepsilon\to 0}\frac{1}{\sqrt{2\pi\varepsilon}}\mathrm{e}^{-\frac{q^2}{2\varepsilon}}=\delta(\varepsilon)$$
[r]
- The kernel satisfies Schrödinger's equation
$$\mathrm{i}\hbar\,\partial_t K_0=-\frac{\hbar^2}{2m}\,\partial_q^2 K_0$$
This can be checked for
$$K_0(q,t;0,0)=\sqrt{\frac{m}{2\pi\hbar\mathrm{i}t}}\mathrm{e}^{\frac{\mathrm{i}m}{2\hbar t}q^2}$$
It follows that the wave function
$$\psi(q,t)=\int \mathrm{d}q'\,K_0(q,t;q',t')\psi(q',t')$$
satisfies Schrödinger's equation because its dependence on time comes from the kernel.
- Composition law
$$K_0(q,t;q_0,t_0)=\int \mathrm{d}q'\,K_0(q,t;q',t')K_0(q',t';q_0,t_0)$$
This can be seen from
$$K_0(q,t,;q_0,t_0)=\left[\frac{m}{2\pi\hbar\mathrm{i}(t-t_0)}\right]^{\frac{1}{2}}\mathrm{e}^{\frac{\mathrm{i}m}{2\hbar}\frac{(q-q_0)^2}{t-t_0}}$$
but working backwards: integrating to obtain such expression. The integral is not trivial since in the exponents one has
$$\begin{aligned}\frac{\mathrm{i}m}{2}\left[\frac{(q-q')^2}{t-t'}+\frac{(q'-q_0)^2}{t'-t_0}\right]&=\frac{\mathrm{i}m}{2}\left[\frac{[(t'-t_0)q+(t-t')q_0+(t_0-t)q']^2}{(t-t_0)(t-t')(t'-t_0)}+\frac{(q-q_0)^2}{t-t_0}\right]\\&=\frac{\mathrm{i}m}{2}\frac{(q-q_0)^2}{t-t_0}+\frac{\mathrm{i}m}{2}\left[-\frac{q'}{(t-t')(t'-t_0)}+\delta q\right]\end{aligned}$$
[r] idk if true
where δq is some shift and one can substitute the bracket with another variable.

Exercise. Finish the calculation.

Lecture 3

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2.1 Quadratic potential

See Srednicki, Schulman cap 6. From now on one sets $\hbar=1$. Consider a one dimensional massive particle in a quadratic potential
$$V(q)=\frac{1}{2}c(t)q^2$$
The Lagrangian is
$$L(q,\dot q)=\frac{1}{2}m\dot q^2-\frac{1}{2}c(t)q^2$$

One would like to compute the kernel, the Feynman propagator

$$K(q_b, t_b; q_a, t_a) = \int_{q_a,t_a}^{q_b,t_b} [\mathcal{D}q] \, \mathrm{e}^{\mathrm{i}S}$$

The following procedure works well for quadratic potentials. One can expand a generic trajectory $q(t)$ around a classical trajectory $\bar{q}(t)$ (that is, solution of the classical equations of motion obtained from the variational principle)

$$q(t) = \bar{q}(t) + \delta q(t)$$

This fluctuation does not apply to the end points $\delta q(t_a) = \delta q(t_b) = 0$. The variation of the action is

$$\delta S = \int \mathrm{d}t \, \frac{\delta S}{\delta q(t)} \, \delta q(t) = 0 \,, \quad \forall \delta q(t) \implies \frac{\delta S}{\delta q(t)} = 0$$

For the quadratic potential, the equations of motion are

$$m\ddot{\bar{q}} + c(t)\bar{q} = 0$$

The path integral sums all the fluctuations δq from the classical path. To find the kernel, one needs to compute the action

$$S[\bar{q} + \delta q, \dot{\bar{q}} + \delta\dot{q}]$$

First method. There are two methods to compute the kernel. The first one is

$$S = \int \mathrm{d}t \, \left[\frac{1}{2}m\dot{q}^2 - \frac{1}{2}c(t)q^2\right] = \int \mathrm{d}t \, \left[\frac{1}{2}m(\dot{\bar{q}} + \delta\dot{q})^2 - \frac{1}{2}c(t)(\bar{q} + \delta q)^2\right] = \cdots = S[\bar{q}] + S[\delta q]$$

[r] This result is particular to quadratic potentials.

Second method. The second method utilizes functional derivatives and the equivalent of the Taylor series

$$S[\bar{q} + \delta q] = S[\bar{q}] + \delta_q S|_{\bar{q}} \, \delta q + \frac{1}{2} \, \delta_q^2 S|_{\bar{q}} \, (\delta q)^2$$

The expansion ends at second order because the potential is quadratic. [r] The linear term is zero because $\bar{q}$ is the solution to the classical equations of motion, thus extremizing the action. Only the last term has to be computed

$$\delta_q^2 S \, (\delta q)^2 = \delta_q(\delta_q S \, \delta q) \, \delta q = \int \mathrm{d}t'' \, \frac{\delta}{\delta q(t'')} \left[\int \mathrm{d}t' \, \frac{\delta S}{\delta q(t')} \delta q(t')\right] \delta q(t'')$$

The inner integral is

$$\begin{aligned}\int \mathrm{d}t' \, \frac{\delta S}{\delta q(t')} \, \delta q(t') &= \int \mathrm{d}t' \int \mathrm{d}t \, \frac{\delta L(q(t))}{\delta q(t')} \, \delta q(t') \\ &= \int \mathrm{d}t' \, \mathrm{d}t \, [m\dot{q}(t) \, \partial_t \delta(t - t') - c(t)q(t)\delta(t - t')] \, \delta q(t') \\ &= \int \mathrm{d}t \, [-m\dot{q}(t)\delta\dot{q}(t) - c(t)q(t)\delta q(t)]\end{aligned}$$

where one remembers

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}c(t)q^2 \,, \quad \frac{\delta q(t)}{\delta q(t')} = \delta(t - t')$$

in particular

$$\frac{\delta\dot{q}^2(t)}{\delta q(t')} = \frac{\delta\dot{q}^2(t)}{\delta\dot{q}(t)} \frac{\delta\dot{q}(t)}{\delta q(t')} = 2\dot{q}(t) \, \partial_t \frac{\delta q(t)}{\delta q(t')} = 2\dot{q}(t) \, \partial_t \delta(t - t')$$

The second derivative is then

$$\begin{aligned}\delta_q^2 S\,(\delta q)^2 &= \int \mathrm{d}t''\,\frac{\delta}{\delta q(t'')}\left[\int \mathrm{d}t\,\left[-m\dot{q}(t)\delta\dot{q}(t) - c(t)q(t)\delta q(t)\right]\right]\delta q(t'') \\ &= \int \mathrm{d}t''\,\mathrm{d}t\,[-m\,\partial_t\delta(t-t'')\,\delta\dot{q}(t)\,\delta q(t'') - c(t)\delta(t-t'')\,\delta q(t)\,\delta q(t'')] \\ &= \int \mathrm{d}t\,\left[m(\delta\dot{q})^2 - c(t)[\delta q(t)]^2\right]\end{aligned}$$

This is exactly the original action but with δq instead of q (and a missing factor of $1/2$). Therefore

$$S[\bar{q}+\delta q] = S[\bar{q}] + \frac{1}{2}\,\delta_q^2 S|_{\bar{q}}\,(\delta q)^2 = S[\bar{q}] + S[\delta q]$$

Remark. This method of the Taylor expansion is more general and can be applied to arbitrary potentials of the form $V(q,g)$ where $g \ll 1$ is a coupling constant. Starting from the cubic term of the Taylor series, one has contributions only from the potential since the kinetic term is quadratic.

Kernel. The kernel becomes

$$K(q_b,t_b;q_a,t_a) = \mathrm{e}^{\mathrm{i}S[\bar{q}]}\int_{0,t_a}^{0,t_b}[\mathcal{D}\delta q]\,\mathrm{e}^{\mathrm{i}S[\delta q]} \equiv \mathrm{e}^{\mathrm{i}S[\bar{q}]}K(0,t_b;0,t_a)$$

To compute the kernel, one has to discretize time

$$\frac{t_b - t_a}{N+1} = \delta t \implies K(0,t_b;0,t_a) = \lim_{N\to\infty}\left[\frac{m}{2\pi\mathrm{i}\,\delta t}\right]^{\frac{1}{2}}\int\prod_{j=1}^{N}\mathrm{d}(\delta q_j)\,\mathrm{e}^{\mathrm{i}S[\delta q]}$$

where the action is discretized also

$$\mathrm{i}S[\delta q] = \sum_{j=0}^{N}\mathrm{i}\left[\frac{m}{2\,\delta t}(\delta q_{j+1}-\delta q_j)^2 - \frac{1}{2}\delta t\,c_j(\delta q_j)^2\right],\quad c_j = c(t_a+\delta t\,j)\,,\quad \delta q_j = \delta q\,(t_a+\delta t\,j)$$

keeping in mind that the extremes have to be constant

$$\delta q_0 = \delta q(t_a) = 0\,,\quad \delta q_{N+1} = \delta q(t_b) = 0$$

[r] Considering a vector

$$\eta = \begin{bmatrix}\delta q_1\\ \vdots \\ \delta q_N\end{bmatrix}$$

by completing the square? [r], the action can be rewritten as

$$\mathrm{i}S[\delta q] = -\eta^\top A\eta\,,\quad A = \frac{m}{2\pi\mathrm{i}\,\delta t}\begin{bmatrix}2-\frac{(\delta t^2)}{m}c_1 & -1 & 0 & \cdots \\ -1 & 2-\frac{(\delta t^2)}{m}c_2 & -1 & \cdots \\ 0 & -1 & 2-\frac{(\delta t)^2}{m}c_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots\end{bmatrix}$$

The kernel is then

$$\begin{aligned}K(0,t_b;0,t_a) &= \lim_{N\to\infty}\left[\frac{m}{2\pi\mathrm{i}\,\delta t}\right]^{\frac{N+1}{2}}\int \mathrm{d}^N\eta\,\mathrm{e}^{-\eta^\top A\eta} = \lim_{N\to\infty}\left[\frac{m}{2\pi\mathrm{i}\,\delta t}\right]^{\frac{N+1}{2}}\frac{\pi^{\frac{N}{2}}}{\sqrt{\det A}} \\ &= \lim_{N\to\infty}\left[\frac{m}{2\pi\mathrm{i}\,\delta t}\frac{\pi^N}{(\frac{2\pi\mathrm{i}\,\delta t}{m})^N\det A}\right]^{\frac{1}{2}} = \lim_{N\to\infty}\left[\frac{m}{2\pi\mathrm{i}}\frac{1}{\delta t(\frac{2\pi\mathrm{i}\,\delta t}{m})^N\det A}\right]^{\frac{1}{2}}\end{aligned}$$

At the second equality of the first line one applies the Gaussian integral (notice there is no $1/2$). Let the denominator be

$$F_N(t_b, t_a) \equiv \delta t \left(\frac{2\pi \mathrm{i}\, \delta t}{m}\right)^N \det A = \delta t\, P_N$$

and

$$P_N \equiv \left(\frac{2\pi \mathrm{i}\, \delta t}{m}\right)^N \det A = \det \begin{bmatrix} 2 - \frac{(\delta t)^2}{m} c_1 & -1 & 0 & \cdots \\ -1 & 2 - \frac{(\delta t)^2}{m} c_2 & -1 & \cdots \\ 0 & -1 & 2 - \frac{(\delta t)^2}{m} c_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

One can find a recursion relation for a generic P_j given by

$$P_{j+1} = \left(2 - \frac{(\delta t)^2}{m} c_{j+1}\right) P_j - P_{j-1}\,, \quad j = 1, \dots, N\,, \quad P_0 = 1\,, \quad P_1 = 2 - \frac{(\delta t)^2}{m} c_1$$

This relation can be rewritten as

$$\delta t\, \frac{P_{j+1} - 2P_j + P_{j-1}}{\delta t^2} = -\frac{c_{j+1}}{m} P_j\, \delta t$$

Letting

$$F_j = \delta t\, P_j \equiv \varphi_j = \varphi(t_a + \varepsilon j)$$

the previous equation becomes

$$\frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{(\delta t)^2} = -\frac{c_{j+1}}{m} \varphi_j$$

For $\delta t \to 0$ the identity above becomes a second order differential equation

$$\mathrm{d}_t^2 \varphi(t) = -\frac{c(t)}{m} \varphi(t)$$

The initial value problem is

$$\varphi(t = t_a) = \delta t\, P_0 \to 0\,, \quad \mathrm{d}_t \varphi(t = t_a) = \delta t\, \frac{P_1 - P_0}{\delta t} = 2 - \frac{\delta t^2}{m} c_1 - 1 \to 1$$

The quantity needed to compute in the kernel $K(0, t_b; 0, t_a)$ is $F(t_b, t_a) = \varphi(t = t_b)$. The full kernel is thus

$$K(q_b, t_b; q_a, t_a) = \mathrm{e}^{\mathrm{i}S[\bar{q}]} K(0, t_b; 0, t_a) = \mathrm{e}^{\mathrm{i}S[\bar{q}]} \left[\frac{m}{2\pi \mathrm{i} F(t_b, t_a)}\right]^{\frac{1}{2}}$$

where one has

$$F(t, t_a) = \varphi(t)$$

which satisfies

$$m\, \mathrm{d}_t^2 F(t, t_a) + c(t) F(t, t_a) = 0\,, \quad F(t_a, t_a) = 0\,, \quad \mathrm{d}_t F(t_a, t_a) = 1$$

Simple harmonic oscillator. The parameter is

$$c(t) = m\omega^2$$

The differential equation above becomes

$$\ddot{F} + \omega^2 F = 0\,, \quad F(t_a) = 0\,, \quad \dot{F}(t_a) = 1$$

whose solution is

$$F(t, t_a) = \frac{1}{\omega} \sin[\omega(t - t_a)]$$

The desired quantity is then

$$F(t_b,t_a)=\frac{1}{\omega}\sin[\omega(t_b-t_a)]=\frac{1}{\omega}\sin\omega T\,,\quad T\equiv t_b-t_a$$

To compute the kernel one has to find the action and path for the classical equations of motion. The Lagrangian is

$$L=\frac{1}{2}m\dot{q}^2-\frac{1}{2}m\omega^2q^2$$

The equations of motion are

$$m\ddot{q}+m\omega^2q=0\,,\quad q(t_a)=q_a\,,\quad q(t_b)=q_b$$

The solution is therefore

$$q(t)=\frac{1}{\sin\omega T}[q_b\sin\omega(t-t_a)+q_a\sin\omega(t_b-t)]$$

Its derivative is

$$\dot{q}(t)=\frac{\omega}{\sin\omega T}[q_b\cos\omega(t-t_a)-q_a\cos\omega(t_b-t)]$$

The action is

$$\begin{aligned}S&=\int\mathrm{d}t\left[\frac{1}{2}m\dot{q}^2-\frac{1}{2}m\omega^2q^2\right]=\frac{1}{2}mq\dot{q}\bigg|_{t_a}^{t_b}-\int\mathrm{d}t\left[\frac{1}{2}mq\ddot{q}+\frac{1}{2}m\omega^2q^2\right]\\&=\frac{1}{2}m\bar{q}(t_b)\dot{\bar{q}}(t_b)-\frac{1}{2}m\bar{q}(t_a)\dot{\bar{q}}(t_a)=\cdots\\&=\frac{m\omega}{2\sin\omega T}[(q_a^2+q_b^2)\cos\omega T-2q_aq_b]\end{aligned}$$

At the first equality one integrates by parts. The last bracket is zero

$$\frac{1}{2}mq(\ddot{q}+\omega^2q)|_{\bar{q}}=0$$

on the classical path since the equations of motion are

$$\ddot{\bar{q}}+\omega^2\bar{q}=0$$

Finally, the kernel is

$$K(q_b,t_b;q_a,t_a)=\left[\frac{m\omega}{2\pi\mathrm{i}\sin\omega T}\right]^{\frac{1}{2}}\exp\left[\frac{\mathrm{i}m\omega}{2\sin\omega T}\big((q_a^2+q_b^2)\cos\omega T-2q_aq_b\big)\right]$$

For any quadratic potential, the kernel can be computed by solving the differential equation of $F(t,t_a)$. For other potentials, one has to use perturbative approaches.

2.2 Partition function

The kernel is defined as

$$K(q_f,t_f;q_i,0)={}_{\mathrm{S}}\langle q_f|\mathrm{e}^{-\mathrm{i}Ht_f}\,|q_i\rangle_{\mathrm{S}}=\int[\mathcal{D}q]\,\mathrm{e}^{\mathrm{i}S[q]}$$

The partition function is the integral of a periodic kernel (i.e. its initial and final points coincide)

$$Z(t)=\int\mathrm{d}q\,K(q,t;q,0)$$

Relation to statistical mechanics. This definition coincides with the statistical mechanical definition

$$Z(t) = \mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}\hat{H}t}$$

Setting the system in a box, one has a discrete energy spectrum E_n with corresponding energy states $|n\rangle$. The identity can be decomposed as

$$I = \sum_n |n\rangle\langle n|$$

The kernel is then

$$\begin{aligned} K(q_f, t_f; q_i, 0) &= \langle q_f|\,\mathrm{e}^{-\mathrm{i}Ht_f}\,|q_i\rangle = \sum_n \langle q_f|\,\mathrm{e}^{-\mathrm{i}Ht_f}\,|n\rangle\,\langle n|q_i\rangle = \sum_n \mathrm{e}^{-\mathrm{i}E_n t_f}\,\langle q_f|n\rangle\,\langle n|q_i\rangle \\ &= \sum_n \mathrm{e}^{-\mathrm{i}E_n t_f}\psi_n^\dagger(q_f)\psi_n(q_i) \end{aligned}$$

The partition function is then

$$\begin{aligned} Z(t) &= \int \mathrm{d}q\, K(q, t; q, 0) = \int \mathrm{d}q\, \sum_n \mathrm{e}^{-\mathrm{i}E_n t}\psi_n^\dagger(q)\psi_n(q) \\ &= \sum_n \mathrm{e}^{-\mathrm{i}E_n t}\int \mathrm{d}q\,|\psi_n(q)|^2 = \sum_n \mathrm{e}^{-\mathrm{i}E_n t} \end{aligned}$$

remembering that the wave function is normalized such that the above integral (i.e. the probability) is unity. Finally one notices that

$$Z(t) = \mathrm{Tr}\,\mathrm{e}^{-\mathrm{i}\hat{H}t} = \sum_n \mathrm{Tr}\Big[\mathrm{e}^{-\mathrm{i}\hat{H}t}\,|n\rangle\langle n|\Big] = \sum_n \langle n|\,\mathrm{e}^{-\mathrm{i}\hat{H}t}\,|n\rangle = \sum_n \mathrm{e}^{-\mathrm{i}E_n t}$$

at the second equality one inserts the identity inside the trace (remembering that $\mathrm{Tr}(A+B) = \mathrm{Tr}\,A + \mathrm{Tr}\,B$) and the cyclic property of the trace noting that the Hamiltonian is diagonal on the energy eigenstates $|n\rangle$.

Exercise. .[r] Compute the partition function of the harmonic oscillator. Use Taylor expansion. One may also prove that the harmonic oscillator energy spectrum is

$$E_n = \hbar\omega\left[n + \frac{1}{2}\right]$$

2.3 Correlation function

Two-point correlation function. A two-point correlation function for an operator O_{H} in the Heisenberg picture

$$O_{\mathrm{H}}(t) = \mathrm{e}^{\mathrm{i}Ht}O_{\mathrm{S}}\mathrm{e}^{-\mathrm{i}Ht}$$

is given by

$$C(t_1, t_2, t_f, t_i) = {}_{\mathrm{H}}\langle q_f, t_f|\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|q_i, t_i\rangle_{\mathrm{H}}$$

Considering $t_i < t_2 < t_1 < t_f$ one has

$$C(t_1, t_2, t_f, t_i) = \langle q_f, t_f|\,O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\,|q_i, t_i\rangle = \langle q_f|\,\mathrm{e}^{-\mathrm{i}H(t_f - t_1)}O_{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H(t_1 - t_2)}O_{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H(t_2 - t_i)}\,|q_i\rangle$$

Supposing that O_{S} is a function of $\hat{q}$ only, then one has

$$\begin{aligned} &C(t_1, t_2, t_f, t_i) = \\ &\quad = \int \mathrm{d}q_1\,\mathrm{d}q_2\;\langle q_f|\,\mathrm{e}^{-\mathrm{i}H(t_f - t_1)}O_{\mathrm{S}}(q_1)\,|q_1\rangle\langle q_1|\,\mathrm{e}^{-\mathrm{i}H(t_1 - t_2)}O_{\mathrm{S}}(q_2)\,|q_2\rangle\langle q_2|\,\mathrm{e}^{-\mathrm{i}H(t_2 - t_i)}\,|q_i\rangle \end{aligned}$$

where one has substituted the operators O with their eigenvalues, so the ones above are functions (as hinted by the presence of an explicit function argument). One obtains

$$C(t_1, t_2, t_f, t_i) = \int \mathrm{d}q_1\,\mathrm{d}q_2\,K(q_f, t_f; q_1, t_1)O(q_1)K(q_1, t_1; q_2, t_2)O(q_2)K(q_2, t_2; q_i, t_i)$$

This corresponds to a path integral where one integrates all paths between q_f and q_1, then measures with the operator, integrates the paths between q_1 and q_2, measures with other operator and finally integrates to the beginning (between q_2 and q_i).

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Inserting the explicit expression of the kernels, one obtains

$$C = \int \mathrm{d}q_1 \, \mathrm{d}q_2 \, O(q_1)O(q_2) \int [\mathcal{D}q^{\gamma_1}] \, \mathrm{e}^{\mathrm{i}S_{\gamma_1}} \int [\mathcal{D}q^{\gamma_2}] \, \mathrm{e}^{\mathrm{i}S_{\gamma_2}} \int [\mathcal{D}q^{\gamma_3}] \, \mathrm{e}^{\mathrm{i}S_{\gamma_3}}$$

Discretizing the path integrals

$$\int [\mathcal{D}q] \, \mathrm{e}^{\mathrm{i}S[q]} \to \frac{1}{A} \int \prod_{j=1}^{N} \frac{\mathrm{d}q_j}{A} \mathrm{e}^{\mathrm{i}S} \,, \quad A = \frac{2\pi\mathrm{i}\,\delta t}{m}$$

gives

$$\begin{aligned} C &= \frac{1}{A^3} \int \prod_{j=1}^{N_1} \frac{\mathrm{d}q_j}{A} \, \mathrm{d}q_2 \prod_{k=1}^{N_2} \frac{\mathrm{d}q_k}{A} \, \mathrm{d}q_1 \prod_{l=1}^{N_3} \frac{\mathrm{d}q_l}{A} O(q_1)O(q_2)\mathrm{e}^{\mathrm{i}S_\Gamma} \\ &= \frac{1}{A} \int \prod_{j=1}^{N_1} \frac{\mathrm{d}q_j}{A} \frac{\mathrm{d}q_2}{A} \prod_{k=1}^{N_2} \frac{\mathrm{d}q_k}{A} \frac{\mathrm{d}q_1}{A} \prod_{l=1}^{N_3} \frac{\mathrm{d}q_l}{A} O(q_1)O(q_2)\mathrm{e}^{\mathrm{i}S_\Gamma} \end{aligned}$$

where $\Gamma = \gamma_1 \cup \gamma_2 \cup \gamma_3$. The first integral is for $\gamma_1 : q_i < q_j < q_2$, the second is for $gama_2 : q_2 < q_k < q_1$ and the third is for $\gamma_3 : q_1 < q_l < q_f$. In the limit $N_i \to \infty$, the measure is

$$[\mathcal{D}q]_\Gamma = \frac{1}{A} \int \prod_{j=1}^{N_1} \frac{\mathrm{d}q_j}{A} \frac{\mathrm{d}q_2}{A} \prod_{k=1}^{N_2} \frac{\mathrm{d}q_k}{A} \frac{\mathrm{d}q_1}{A} \prod_{l=1}^{N_3} \frac{\mathrm{d}q_l}{A}$$

Therefore, the two-point correlation function is

$$C(t_1, t_2) = \langle q_f, t_f | \, \mathcal{T}\{O_\mathrm{H}(t_1)O_\mathrm{H}(t_2)\} \, |q_i, t_i\rangle = \int [\mathcal{D}q] \, O(q(t_1))O(q(t_2))\mathrm{e}^{\mathrm{i}S}$$

This is an intermediate step. The actual quantity is the Green function.

2.4 Green function

See Cheng–Li. The Green function is a particular correlation function where the initial and final states are the ground state $|0\rangle$

$$G(t_1 \cdots t_n) = \langle 0| \, \mathcal{T}\{O_\mathrm{H}(t_1) \cdots O_\mathrm{H}(t_n)\} \, |0\rangle$$

The definition can be generalized to different operators within the same time-ordered product.

Two-point Green function. One would like to compute the Green function with the path integral. The two-point Green function is given by

$$G(t_1, t_2) = \langle 0| \, \mathcal{T}\{O_\mathrm{H}(t_1)O_\mathrm{H}(t_2)\} \, |0\rangle = \int \mathrm{d}q \, \mathrm{d}q' \, \langle 0|q't'\rangle \, \langle q't'| \, \mathcal{T}\{O_\mathrm{H}(t_1)O_\mathrm{H}(t_2)\} \, |qt\rangle \, \langle qt|0\rangle$$

The expectation value in the middle can be computed through the correlation function. The bra-kets are the wave function

$$\langle qt|0\rangle = \langle q| \, \mathrm{e}^{-\mathrm{i}Ht} \, |0\rangle = \langle q| \, \mathrm{e}^{-\mathrm{i}E_0 t} \, |0\rangle = \mathrm{e}^{-\mathrm{i}E_0 t}\varphi_0(q)$$

In quantum field theory, the energy levels can be shifted so one sets $E_0 = 0$. Therefore

$$\langle qt|0\rangle = \varphi_0(q) \,, \quad \langle 0|q't'\rangle = \varphi_0^*(q')$$

The Green function is then

$$\begin{aligned} G(t_1, t_2) &= \int \mathrm{d}q \, \mathrm{d}q' \, \varphi_0^*(q')\varphi'(q) \int [\mathcal{D}q] \, O(q(t_1))O(q(t_2))\mathrm{e}^{\mathrm{i}S} \\ &= \int [\mathcal{D}q] \, \varphi_0^*(q')\varphi_0(q)O(q(t_1))O(q(t_2))\mathrm{e}^{\mathrm{i}S} \end{aligned}$$

at the second line one incorporates the integrals $\mathrm{d}q\,\mathrm{d}q'$ into the path integral. One would like to elaborate the above prescription in order to eliminate $\varphi_0^*(q')\varphi_0(q)$.

[r] The correlation function is

$$C(t',t) = \langle q't'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|qt\rangle = \int \mathrm{d}Q\,\mathrm{d}Q'\ \langle q't'|Q'T'\rangle\,\langle Q'T'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|QT\rangle\,\langle QT|qt\rangle$$

[r] Letting E_n be the energy eigenvalue with corresponding eigenstate $|n\rangle$, the wave function is

$$\langle n|q\rangle = \varphi_n(q)$$

[r]

$$\begin{aligned}\langle q't'|Q'T'\rangle &= \langle q'|\,\mathrm{e}^{-\mathrm{i}H(t'-T')} = \sum_n \langle q'|\,\mathrm{e}^{-\mathrm{i}H(t'-T')}\,|n\rangle\,\langle n|Q'\rangle = \sum_n \mathrm{e}^{-\mathrm{i}E_n(t'-T')}\varphi_n^*(q')\varphi_n(Q') \\ &= \varphi_0^*(q')\varphi_0(Q') + \sum_{n>0} \mathrm{e}^{-\mathrm{i}E_n(t'-T')}\varphi_n^*(q')\varphi_n(Q')\end{aligned}$$

The times t and t' can be freely moved around the number line since they are not integrated. One observes that in the limit $t' \to -\mathrm{i}\infty$ (like Wick's rotation), the exponential tends to zero (remember that the energy is positive since $E_0 = 0$). Therefore

$$\lim_{t'\to-\mathrm{i}\infty} \langle q't'|Q'T'\rangle = \varphi_0^*(q')\varphi_0(Q')$$

Similarly

$$\lim_{t\to\mathrm{i}\infty} \langle QT|qt\rangle = \varphi_0^*(Q)\varphi_0(q)$$

Performing a similar calculation one has

$$\lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} \langle q't'|qt\rangle = \varphi_0^*(q')\varphi_0(q)$$

Taking the above limit for the correlator, one has

$$\begin{aligned}\lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} C(t,t') &= \lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} \langle q't'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|qt\rangle \\ &= \int \mathrm{d}Q\,\mathrm{d}Q'\ \varphi_0^*(q')\varphi_0(Q')\,\langle Q'T'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|QT\rangle\,\varphi_0^*(Q)\varphi_0(q) \\ &= \varphi_0^*(q')\varphi_0(q)\int \mathrm{d}Q\,\mathrm{d}Q'\ \varphi_0(Q')\varphi_0^*(Q)\,\langle Q'T'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|QT\rangle \\ &= \lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} \langle q't'|qt\rangle\,G(t_1,t_2)\end{aligned}$$

[r] Therefore, the Green function is

$$G(t_1,t_2) = \lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} \frac{\langle q't'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)O_{\mathrm{H}}(t_2)\}\,|qt\rangle}{\langle q't'|qt\rangle}$$

This operation is similar to a normalization: the Green function is a correlation function normalized to the product of the two states.

This definition of two-point Green function can be generalized to n points

$$G(t_1\cdots t_n) = \lim_{\substack{t'\to-\mathrm{i}\infty\\ t\to\mathrm{i}\infty}} \frac{\langle q't'|\,\mathcal{T}\{O_{\mathrm{H}}(t_1)\cdots O_{\mathrm{H}}(t_n)\}\,|qt\rangle}{\langle q't'|qt\rangle}$$

In this way, the Green function does not explicitly depend on the ground state.

2.5 Generating functional

Suppose to compute the Green function of an operator O. One can always introduce the generating functional for Green functions

$$W[J] = \lim_{\substack{t' \to -\mathrm{i}\infty \\ t \to \mathrm{i}\infty}} \frac{1}{\langle q't'|qt\rangle} \int [\mathcal{D}q] \exp\left[\mathrm{i}\int_t^{t'} \mathrm{d}\tau \left[L(\tau) + J(\tau)O_{\mathrm{H}}(q(\tau))\right]\right]$$

Applying to W an arbitrary number of derivatives with respect to J one brings the operator in front of the exponential. In this way one obtains the desired Green function

$$G(t_1 \cdots t_n) = \left.\frac{\delta^n W[J]}{\delta J(t_1) \cdots J(t_n)}\right|_{J=0}$$

The function J is called the source of the operator O_{H}.

The generating functional is a modification of a path integral that one would get without any insertion of operators but with the source different from zero

$$W[J] = \langle 0|0\rangle_J$$

With no source, one has

$$W[0] = \langle 0|0\rangle = 1$$

This is in accordance with the prescription of the Green function without any insertion of operators: the ratio is unity.

2.6 Euclidean space

By performing a Wick rotation the time coordinate $\tau = -\mathrm{i}\tau_{\mathrm{E}}$. The limits become

$$t' \to -\mathrm{i}\infty \rightsquigarrow t'_{\mathrm{E}} \to \infty$$

likewise

$$t \to \mathrm{i}\infty \rightsquigarrow t_{\mathrm{E}} \to -\infty$$

The exponential of the Lagrangian becomes

$$\exp\left[\mathrm{i}\int \mathrm{d}\tau\, L(\tau)\right] \rightsquigarrow \exp\left[\int \mathrm{d}\tau_{\mathrm{E}}\, L(-\mathrm{i}\tau_{\mathrm{E}})\right]$$

Considering the Lagrangian of a one-dimensional particle in a potential

$$L = \frac{1}{2}m\dot{q}^2 - V(q) = \frac{1}{2}m(\mathrm{d}_\tau q)^2 - V(q) \rightsquigarrow L(-\mathrm{i}\tau_{\mathrm{E}}) = -\frac{1}{2}m\dot{q}_{\mathrm{E}}^2 - V(q) \equiv -L_{\mathrm{E}}$$

the exponential is then

$$\exp\left[\mathrm{i}\int \mathrm{d}\tau\, L(\tau)\right] \rightsquigarrow \exp\left[-\int \mathrm{d}\tau_{\mathrm{E}}\, L_{\mathrm{E}}\right]$$

The ground energy can always be set to zero, so the energies are always positive and the exponential is no longer a phase but decays.

Generating functional. The generating functional becomes

$$W_{\mathrm{E}}[J] = \lim_{\substack{t' \to \infty \\ t \to -\infty}} \frac{1}{\langle q't'|qt\rangle} \int [\mathcal{D}q] \exp\left[-\int \mathrm{d}\tau_{\mathrm{E}}[L_{\mathrm{E}} + JO_{\mathrm{H}}(\tau_{\mathrm{E}})]\right]$$

2.7 Arbitrary dimensions

The formalism developed can be generalized to D dimensions. If a particle propagates in D dimensions, the configuration point is

$$\mathbf{q} = (q^1, \dots q^D)$$

The kernel is

$$\begin{aligned} K(\mathbf{q}_f, t_f; \mathbf{q}_i, t_i) &= \int [\mathcal{D}\mathbf{q}]\, \mathrm{e}^{\mathrm{i}S[\mathbf{q}]} = \lim_{N\to\infty} \frac{1}{A} \int \prod_{j=1}^{N} \frac{\mathrm{d}\mathbf{q}_j}{A^D} \mathrm{e}^{\mathrm{i}S[\mathbf{q}_j]} \\ &= \lim_{N\to\infty} \left[\frac{m}{2\pi\mathrm{i}\,\delta t}\right]^{\frac{ND+1}{2}} \int \prod_{j=1}^{N} \mathrm{d}\mathbf{q}_j\, \mathrm{e}^{\mathrm{i}S[\mathbf{q}_j]} \end{aligned}$$

Conclusion. Some phenomena are easier described through the path integral formulation of quantum mechanics, like tunnelling and scattering.

3 Scalar boson fields

In quantum field theory, canonical quantization is limited and cumbersome. One uses the functional approach which generalizes the quantum mechanical path integral.

In order to go towards increasing complexity, one starts from real scalar boson fields, then fermions, then gauge fields and gauge theories. QFT I is about scalar boson, while QFT II starts from fermions. Between the two there is a bit of conformal field theory.

Spin zero particles are described by scalar fields. Neutral particles are real scalar fields $\varphi(x)$.

3.1 Canonical quantization

One may start from neutral particles. For free massive scalar fields, the Lagrangian density is given by

$$\mathcal{L} = \frac{1}{2}\eta^{\mu\nu}\,\partial_\mu\varphi\,\partial_\nu\varphi - \frac{1}{2}m^2\varphi^2$$

where the metric η convention is timelike, mostly minus. The corresponding action is

$$S = \int \mathrm{d}^4x\,\mathcal{L}$$

Applying the action principle $\delta S = 0$ one obtains the classical equations of motion that have to have boundary conditions: integrating over all space-time one imposes that the fields go to zero sufficiently fast. For a scalar field, the equations of motion are Klein–Gordon's

$$(\Box + m^2)\varphi(x) = 0\,, \quad \Box \equiv \partial_\mu\partial^\mu = \partial_0^2 - \nabla^2$$

The action is

$$S = \int \mathrm{d}^4x \left[\frac{1}{2}\dot{\varphi}^2 - \frac{1}{2}|\nabla\varphi|^2 - \frac{1}{2}m^2\varphi^2\right]$$

The canonical momentum is

$$\pi(x) = \frac{\delta\mathcal{L}}{\delta\dot{\varphi}(x)} = \dot{\varphi}(x)$$

The most general solution for Klein–Gordon equation is

$$\varphi(x) = \varphi_+(x) + \varphi_-(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^{\frac{3}{2}}\sqrt{2k^0}}[a_+(\mathbf{k})\mathrm{e}^{\mathrm{i}k^\mu x_\mu} + a_-(\mathbf{k})\mathrm{e}^{-\mathrm{i}k^\mu x_\mu}]\,, \quad k^0 = \sqrt{|\mathbf{k}|^2 + m^2}$$

The reality condition given by the neutral nature of the boson field implies

$$[a_-(\mathbf{k})]^\dagger = a_+(\mathbf{k})$$

The Fourier coefficients can be expressed in terms of the fields as

$$a_\pm(\mathbf{k}) = \mp\frac{\mathrm{i}}{(2\pi)^{\frac{3}{2}}\sqrt{2k^0}} \int \mathrm{d}^3k\,\mathrm{e}^{\mp\mathrm{i}kx}\overleftrightarrow{\partial_0}\varphi(x)\,, \quad f\overleftrightarrow{\partial_0}g \equiv f\,\partial_0 g - (\partial_0 f)g$$

Exercise. Check that the previous expressions give back φ.

Canonical quantization. Canonical quantization of the fields (called second quantization) is implemented by promoting the Fourier coefficients $a_\pm(\mathbf{k})$ to be operators obeying the commutation relation

$$[a_-(\mathbf{k}), a_+(\mathbf{k}')] = \delta^{(3)}(\mathbf{k} - \mathbf{k}') \leftrightarrow [a(\mathbf{k}), a^\dagger(\mathbf{k})] = \delta^{(3)}(\mathbf{k} - \mathbf{k}')$$

The number operator is

$$N(\mathbf{k}) \equiv a^\dagger(\mathbf{k}) a(\mathbf{k})$$

while the total number is

$$N = \int \mathrm{d}^3 k \, N(\mathbf{k})$$