PATH INTEGRALS IN QM

2.1 PRELIMINARIES

In this lecture we introduce Path Integrals in the context of QM. Despite the simpler setting (QM compared to QFT), all the important features of Path Integrals will be discussed. We consider a point particle in one-dimension, and denote by $\hat{Q}$ the position operator, and by $\left|q\right\rangle$ the eigenstate corresponding to the eigenvalue q:

$$\hat{Q}\left|q\right\rangle = q\left|q\right\rangle \, . \tag{2.1}$$

The completeness condition for the states $\left|q\right\rangle$ is

$$\int \mathrm{d}q \left|q\right\rangle\!\left\langle q\right| = 1 \, . \tag{2.2}$$

The aim of this section is to find an expression for the quantum amplitude $\left\langle q't' \middle| qt \right\rangle$ for a system in state $\left|q\right\rangle$ at time t to evolve in state $\left|q'\right\rangle$ at time t',

$$\left\langle q't' \middle| qt \right\rangle = \left\langle q' \right| e^{-i\hat{H}(t'-t)} \left| q \right\rangle \, , \tag{2.3}$$

where $\hat{H}$ is the Hamiltonian of the system.

2.2 SETTING UP THE PATH INTEGRAL

In order to proceed with the calculation, let us define $T = t' - t$ to be the size of the time interval, and $\epsilon = T/n$, where n is an integer. Then

$$t_0 = t \tag{2.4}$$
$$t_k = t_0 = k\epsilon, \quad \text{for } k = 1, \ldots, n-1 \tag{2.5}$$
$$t_n = t + n\epsilon = t' \, . \tag{2.6}$$

$$\left\langle q' \right| e^{-i\hat{H}(t'-t)} \left| q \right\rangle = \left\langle q' \right| e^{-i\hat{H}T} \left| q \right\rangle \tag{2.7}$$
$$= \left\langle q' \right| \left(e^{-i\hat{H}\epsilon}\right) \ldots \left(e^{-i\hat{H}\epsilon}\right) \left| q \right\rangle , \tag{2.8}$$

where the expression in the second line contains n factors.

Inserting the completeness relation $n-1$ times,

$$\left\langle q't' \middle| qt \right\rangle = \int \prod_{k=1}^{n-1} dq_k \, \left\langle q' \right| \left(e^{-i\hat{H}\epsilon}\right) \left| q_{n-1} \right\rangle \left\langle q_{n-1} \right| \left(e^{-i\hat{H}\epsilon}\right) \left| q_{n-2} \right\rangle \ldots \left\langle q_1 \right| \left(e^{-i\hat{H}\epsilon}\right) \left| q \right\rangle \, . \tag{2.9}$$

For small ϵ we can expand the exponential to first order and evaluate the matrix elements:

$$e^{-i\hat{H}\epsilon} = 1 - i\hat{H}\epsilon + O(\epsilon^2) \tag{2.10}$$

$$\hat{H} = \frac{1}{2}\hat{P}^2 + V(\hat{Q})\,, \tag{2.11}$$

From the potential energy we get

$$\left\langle q_k\right| V(\hat{Q})|q_{k-1}\rangle = V(q_{k-1})\left\langle q_k\right| q_{k-1}\rangle \tag{2.12}$$

$$= V\left(\frac{q_k + q_{k-1}}{2}\right)\delta(q_k - q_{k-1}) \tag{2.13}$$

$$= \int \frac{dp}{2\pi} V\left(\frac{q_k + q_{k-1}}{2}\right) e^{ip(q_k - q_{k-1})} \tag{2.14}$$

In order to evaluate the contribution of the kinetic term, we introduce eigenstates of the momentum operator $\left|p\right\rangle$

$$\hat{P}\left|p\right\rangle = p\left|p\right\rangle \tag{2.15}$$

$$\left\langle q\middle|p\right\rangle = e^{ipq}\,, \tag{2.16}$$

and use the completeness of the states $\left|p\right\rangle$:

$$\left\langle q_k\right| \hat{P}^2|q_{k-1}\rangle = \int \frac{dp}{2\pi}\, p^2 e^{ip(q_k - q_{k-1})}\,. \tag{2.17}$$

Hence

$$\left\langle q_k\right| e^{-i\hat{H}\epsilon}|q_{k-1}\rangle = \int \frac{dp}{2\pi}\,\exp\left\{i\epsilon\left[p\frac{q_k - q_{k-1}}{\epsilon} - H\left(p, \tilde{q}\right)\right]\right\} + O(\epsilon^2)\,, \tag{2.18}$$

where $\tilde{q} = \frac{q_k - q_{k-1}}{2}$. Therefore

$$\left\langle q' t'\middle|q t\right\rangle = \lim_{n\to\infty}\int \prod_{k=1}^{n-1} dq_k \prod_{j=1}^{n} \frac{dp_j}{2\pi} \times \tag{2.19}$$

$$\times \exp\left\{i\epsilon\sum_{m=1}^{n}\left[p_m\frac{q_m - q_{m-1}}{\epsilon} - H\left(p_m, \frac{q_m + q_{m-1}}{2}\right)\right]\right\}\,, \tag{2.20}$$

where $q_0 = q$, and $q_n = q'$. The limit above defines the *path integral* evaluation of the quantum amplitude, which we denote

$$\left\langle q' t'\middle|q t\right\rangle = \int \mathcal{D}q\mathcal{D}p\,\exp\left\{i\int_t^{t'} \mathrm{d}\tau\,\left[p\dot{q} - H(p, q)\right]\right\}\,. \tag{2.21}$$

2.3 Quadratic P dependence

For hamiltonians like the one above, *i.e.* hamiltonians that are only quadratic in the momentum $\hat{P}$, the expression above can be simplified by performing the integral over the momenta p_j:

$$\int \frac{dp}{2\pi}\,\exp\left\{i\epsilon\left[p\left(\frac{q_k - q_{k-1}}{\epsilon}\right) - \frac{1}{2}p^2\right]\right\} = (2\pi i\epsilon)^{-1/2}\,\exp\left\{i\epsilon\frac{1}{2}\left(\frac{q_k - q_{k-1}}{\epsilon}\right)^2\right\}\,. \tag{2.22}$$

Using this result, we can rewrite the path integral in Eq. (2.21) as

$$\langle q't'|qt\rangle = \lim_{n\to\infty} (2\pi i\epsilon)^{-n/2} \int \prod_{k=1}^{n-1} dq_k \, \exp\left\{ i\epsilon \sum_{m=1}^{n} \left[\frac{1}{2}\left(\frac{q_m - q_{m-1}}{\epsilon}\right)^2 - V\left(\frac{q_m + q_{m-1}}{2}\right)\right]\right\} . \tag{2.23}$$

Assuming that the limit exists, we have obtained the definition of the path integral as an integral over the position of the system only:

$$\langle q't'|qt\rangle = \int_{q,q'} \mathcal{D}q \exp\left\{ i\int_t^{t'} \mathrm{d}\tau \, \mathcal{L}(q,\dot{q})\right\} , \tag{2.24}$$

where $\mathcal{L}$ is the lagrangian of the system. Note that the suffix of the integral keeps track of the initial- and final-state configurations q and q'.

2.4 Correlators

We are now going to work out expressions for the matrix element of the position operator inbetween the initial and final state considered above.

2.4.1 One-point Function

The first example that we are going to consider is the matrix element

$$\langle q't'|\, \hat{Q}(\bar{t})|qt\rangle = \langle q'|\, e^{-i\hat{H}(t'-t)}\hat{Q}e^{-i\hat{H}(\bar{t}-t)}\, |q\rangle , \tag{2.25}$$

where we assume $t < \bar{t} < t'$, and we have used

$$\hat{Q}(t) = e^{i\hat{H}t}\hat{Q}e^{-i\hat{H}t} . \tag{2.26}$$

Proceeding as we did in the previous section, we can write

$$\langle q't'|\, \hat{Q}(\bar{t})|qt\rangle = \langle q'|\left(e^{-i\hat{H}\epsilon}\right)\ldots\left(e^{-i\hat{H}\epsilon}\right)\hat{Q}\left(e^{-i\hat{H}\epsilon}\right)\ldots\left(e^{-i\hat{H}\epsilon}\right)|q\rangle , \tag{2.27}$$

where we assumed that $\bar{t} = t_k$, and the first and second ellipses denote respectively $(n-k)$, and k factors of $\left(e^{-i\hat{H}\epsilon}\right)$. Performing the same manipulations as before we obtain

$$\langle q't'|\, \hat{Q}(\bar{t})|qt\rangle = \lim_{n\to\infty} \int \prod_{k=1}^{n-1} dq_k \prod_{j=1}^{n} \frac{dp_j}{2\pi}\, q_k \times \tag{2.28}$$

$$\times \exp\left\{ i\epsilon \sum_{m=1}^{n} \left[p_m \frac{q_m - q_{m-1}}{\epsilon} - H\left(p_m, \frac{q_m + q_{m-1}}{2}\right)\right]\right\} . \tag{2.29}$$

Note that now there is an extra factor of q_k in the integrand, corresponding to the insertion of the operator $\hat{Q}(\bar{t})$. The limit above is denoted

$$\langle q't' | \hat{Q}(\bar{t}) | qt \rangle = \int \mathcal{D}q\mathcal{D}p \, q(\bar{t}) \exp\left\{ i \int_t^{t'} d\tau \, \left[p\dot{q} - H(p,q) \right] \right\} \tag{2.30}$$

$$= \int_{qq'} \mathcal{D}q \, q(\bar{t}) \exp\left\{ i \int_t^{t'} d\tau \, \mathcal{L}(q,\dot{q}) \right\} . \tag{2.31}$$

2.4.2 Two-point function

Let us now consider the slightly more complicated case of the matrix element of the product of two position operators

$$\left\langle q't' \right| \hat{Q}(\bar{t}_1)\hat{Q}(\bar{t}_2) \left| qt \right\rangle , \tag{2.32}$$

where now we assume $\bar{t}_1 = t_k$, $\bar{t}_2 = t_\ell$, $t < \bar{t}_2 < \bar{t}_1 < t'$. We can write this correlator as:

$$\left\langle q't' \right| \hat{Q}(\bar{t}_1)\hat{Q}(\bar{t}_2) \left| qt \right\rangle = \left\langle q' \right| \left(e^{-i\hat{H}\epsilon} \right) \ldots \hat{Q} \ldots \hat{Q} \ldots \left(e^{-i\hat{H}\epsilon} \right) \left| q \right\rangle , \tag{2.33}$$

where the three ellipses here denote respectively $(n-k)$, $(k-\ell)$, and ℓ factors of $\left(e^{-i\hat{H}\epsilon}\right)$. Proceeding exactly as above yields:

$$\left\langle q't' \right| \hat{Q}(\bar{t}_1)\hat{Q}(\bar{t}_2) \left| qt \right\rangle = \int_{qq'} \mathcal{D}q \, q(\bar{t}_1)q(\bar{t}_2) \exp\left\{ i \int_t^{t'} d\tau \, \mathcal{L}(q,\dot{q}) \right\} . \tag{2.34}$$

There is a subtlety here that it is worth noting. The ordering of times in Eq. (2.32) matters, while it clearly does not in the RHS of Eq. (2.34) where $q(\bar{t}_1)$ and $q(\bar{t}_1)$ are just integration variables. If $\bar{t}_2 > \bar{t}_1$, then the RHS of Eq. (2.34) corresponds to

$$\left\langle q't' \right| \hat{Q}(\bar{t}_2)\hat{Q}(\bar{t}_1) \left| qt \right\rangle . \tag{2.35}$$

Both results can be summarised as

$$\left\langle q't' \right| T\left(\hat{Q}(\bar{t}_1)\hat{Q}(\bar{t}_2) \right) \left| qt \right\rangle = \int_{qq'} \mathcal{D}q \, q(\bar{t}_1)q(\bar{t}_2) \exp\left\{ i \int_t^{t'} d\tau \, \mathcal{L}(q,\dot{q}) \right\} , \tag{2.36}$$

where we have introduced the T-ordered product of operators:

$$T\left(\hat{Q}(t)\hat{Q}(t') \right) = \theta(t-t')\hat{Q}(t)\hat{Q}(t') + \theta(t'-t)\hat{Q}(t')\hat{Q}(t) . \tag{2.37}$$

You can easily verify that the derivation can be extended to an arbitrary number of insertions of the operator $\hat{Q}$:

$$\left\langle q't' \right| T\left(\hat{Q}(\bar{t}_1) \ldots \hat{Q}(\bar{t}_n) \right) \left| qt \right\rangle = \int_{qq'} \mathcal{D}q \, q(\bar{t}_1) \ldots q(\bar{t}_n) \exp\left\{ i \int_t^{t'} d\tau \, \mathcal{L}(q,\dot{q}) \right\} . \tag{2.38}$$

2.5 Generating functional

2.5.1 Functional derivative

Consider a functional F that associates a number, which we denote $F[u]$, to a given function $u(x)$. The functional derivative describes the change of the functional to an infinitesimal variation of the function u:

$$u(x) \mapsto u(x) + \delta u(x)\,.$$

We define

$$\delta F = F[u+\delta u] - F[u] = \int dx\, \frac{\delta F}{\delta u(x)} \delta u(x)\,. \tag{2.39}$$

You can see the analogy to the case of a function of several variables, where the variation to a change δx_k in the variables is given by

$$\delta F = F(x+\delta x) - F(x) = \sum_k \frac{\partial F}{\partial x_k} \delta x_k\,. \tag{2.40}$$

In particular we have

$$\frac{\delta}{\delta f(x)} f(y) = \delta(x-y)\,, \tag{2.41}$$

again to be compared with its discrete analogue

$$\frac{\partial}{\partial x_j} x_i = \delta_{ij}\,. \tag{2.42}$$

2.5.2 Sources in the path integral

Let $f(t)$ and $h(t)$ be two functions, we can add so-called source terms to the path integral, and define

$$\left\langle q't' \middle| qt \right\rangle_{f,h} = \int \mathcal{D}p\mathcal{D}q\, \exp\left\{ i \int_t^{t'} d\tau\, \left[p(\tau)\dot{q}(\tau) - H(p(\tau), q(\tau)) + f(\tau)q(\tau) + h(\tau)p(\tau) \right] \right\}\,. \tag{2.43}$$

Taking functional derivatives with respect to the source fields yields e.g.

$$\begin{aligned} &\left(\frac{1}{i} \frac{\delta}{\delta f(\bar{\tau})} \right) \left\langle q't' \middle| qt \right\rangle_{f,h} = \\ &\qquad = \int \mathcal{D}p\mathcal{D}q\, q(\bar{\tau})\, \exp\left\{ i \int_t^{t'} d\tau\, \left[p(\tau)\dot{q}(\tau) - H(p(\tau), q(\tau)) + f(\tau)q(\tau) + h(\tau)p(\tau) \right] \right\}\,, \end{aligned} \tag{2.44}$$

$$\left(\frac{1}{i}\frac{\delta}{\delta f(\bar{\tau}_1)}\right)\left(\frac{1}{i}\frac{\delta}{\delta f(\bar{\tau}_2)}\right)\left\langle q't'\middle|qt\right\rangle_{f,h} =$$
$$= \int \mathcal{D}p\mathcal{D}q\; q(\bar{\tau}_1)q(\bar{\tau}_2)\,\exp\left\{i\int_t^{t'} d\tau\,\left[p(\tau)\dot{q}(\tau) - H(p(\tau),q(\tau)) + f(\tau)q(\tau) + h(\tau)p(\tau)\right]\right\}, \tag{2.45}$$

and similarly for the derivatives with respect to h pulling down factors of p in the integrand.

As we have seen in the previous section, we have

$$\left\langle q't'\right| T\left(\hat{Q}(t_1)\ldots\hat{Q}(t_n)\right)\left|qt\right\rangle =$$
$$= \left(\frac{1}{i}\frac{\delta}{\delta f(t_1)}\right)\ldots\left(\frac{1}{i}\frac{\delta}{\delta f(t_n)}\right)\left\langle q't'\middle|qt\right\rangle_{f,h}\Bigg|_{f=h=0}. \tag{2.46}$$

2.6 Projection onto the ground state

It is useful to be able to compute the amplitude for the system to evolve from the vacuum state at time t into the vacuum state at time t' under the action of the external sources f, h. Having computed $\left\langle q't'\middle|qt\right\rangle$, the above amplitude is given by

$$\langle 0,t'|0,t\rangle = \int dq dq'\; \phi_0(q')^*\,\left\langle q't'\middle|qt\right\rangle_{f,h}\,\phi_0(q)\,, \tag{2.47}$$

where $\phi_0(q) = \left\langle q\middle|0\right\rangle$ is the wave function of the ground state, and $|n\rangle$ denote the eigenstates of the Hamiltonian. Eq. (2.47) yields the right amplitude, but requires the convolution of $\left\langle q't'\middle|qt\right\rangle$ with the ground state wave function. We shall now describe a procedure that allows the compute the vacuum-to-vacuum amplitude directly as a path integral.

The energy eigenstates are

$$\hat{H}\left|n\right\rangle = E_n\left|n\right\rangle\,, \tag{2.48}$$

and their wave functions are denoted as

$$\phi_n(q) = \left\langle q\middle|n\right\rangle\,. \tag{2.49}$$

We assume that the vacuum energy vanishes, $E_0 = 0$. We want to evaluate the amplitude

$$\langle Q'T'|QT\rangle_{f,h} \tag{2.50}$$

where the sources h and f have support in the interval $[t, t']$, with $T < t < t' < T'$. The sources behind switched off between T and t, we can readily compute

$$\left\langle qt\middle|QT\right\rangle = \int \mathcal{D}q\mathcal{D}p\,\exp\left\{i\int_T^t \mathrm{d}\tau\,\left[p\dot{q} - H(p,q)\right]\right\} \tag{2.51}$$
$$= \left\langle q\right|\exp\left[-i\hat{H}(t-T)\right]\left|Q\right\rangle \tag{2.52}$$
$$= \sum_n \phi_n(q)\phi_n(Q)^* e^{-iE_n(t-T)}\,. \tag{2.53}$$

We can now analytically continue the result to $T_I = (1 - i\epsilon)T$, and consider the limit $T \to -\infty$:

$$\lim_{T\to-\infty} \left\langle qt \middle| QT_I \right\rangle = \phi_0(q)\phi_0(Q)^* \,. \tag{2.54}$$

A similar result can be obtained for $\left\langle Q'T' \middle| q't' \right\rangle$. We can therefore write

$$\langle Q'T'|QT\rangle_{f,h} = \int \mathrm{d}q'\,\mathrm{d}q \left\langle Q'T' \middle| q't' \right\rangle \left\langle q't' \middle| qt \right\rangle_{f,h} \left\langle qt \middle| QT \right\rangle \,. \tag{2.55}$$

And therefore

$$\lim_{\substack{T'\to\infty \\ T\to-\infty}} \frac{\langle Q', (1-i\epsilon)T'|Q,(1-i\epsilon)T\rangle_{f,h}}{\phi_0(Q)^*\phi_0(Q')} = \int \mathrm{d}q'\,\mathrm{d}q\; \phi_0(q')^* \left\langle q't' \middle| qt \right\rangle_{f,h} \phi_0(q) \,. \tag{2.56}$$

The expresson on the RHS is the vacuum-to-vacuum amplitude, $\langle 0, t'|0, t\rangle_{f,h}$, that we want to compute. The expression on the LHS is the limit of the path integral for $T \to \infty$, $T' \to \infty$. The only dependence on the boundary values Q and Q' appears in the denominator on LHS: it is a normalization factor independent of f and h, which disappears when taking derivatives with respect to the sources. Instead of analytically continuing to complex values of T and T', we can simply add an imaginary part to the Hamiltonian,

$$\hat{H} \to (1 - i\epsilon)\hat{H} \,. \tag{2.57}$$

Taking the limit $T \to \infty$, $T' \to \infty$, we obtain the amplitude

$$\langle 0|0\rangle_{f,h} = \int \mathcal{D}p\mathcal{D}q\; \exp\left\{ i\int_{-\infty}^{\infty} \mathrm{d}\tau \left[p\dot{q} - (1-i\epsilon)H(p,q) + fq + hp \right] \right\} \tag{2.58}$$

2.7 Weyl ordering

If we are interested in more general Hamiltonians, with terms that involve products of $\hat{P}$ and $\hat{Q}$, then we need to give a prescription for the ordering of the operators in the Hamiltonian, so that the quantum mechanical amplitude is actually described by the path integral.

As discussed by Berezin in 1971, the mid-point prescription we adopted in Eq. (2.23) is equivalent to the Weyl-ordering of the Hamiltonian.

The Weyl product of two operators $\hat{A}$ and $\hat{B}$ is defined by considering the operator $\left(\alpha\hat{A} + \beta\hat{B}\right)^n$, and expanding it in powers of α and β:

$$\left(\alpha\hat{A} + \beta\hat{B}\right)^n = \sum_k \frac{n!}{k!l!}\,\alpha^k\beta^l \left[\hat{A}^k\hat{B}^l\right] \,. \tag{2.59}$$

The quantity in the square bracket is the Weyl ordered product of $\hat{A}^k$ and $\hat{B}^l$.