

Ch 6: Path integrals in quantum mechanics

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

$$[Q, P] = i \quad (\hbar = 1)$$

Probability amplitude for the particle to start at q' at t' , and end at position q'' at t'' :

$$\langle q'' | e^{-iH(t'' - t')} | q' \rangle$$

$|q'\rangle, |q''\rangle$: eigenstates of Q

Heisenberg pic: $Q(t) = e^{iHt} Q e^{-iHt}$.

$Q(t)|q, t\rangle = q|q, t\rangle$: instantaneous eigenstate

$$|q, t\rangle = e^{iHt} |q\rangle$$

$$Q|q\rangle = q|q\rangle$$

Transition amplitude: $\langle q'', t'' | q', t' \rangle$.

Divide time interval $T = t'' - t'$ into $N+1$ equal pieces, introduce N complete sets of position eigenkets:

$$\langle q''t'' | q', t' \rangle = \int_{j=1}^N \prod_j dq_j \langle q'' | e^{-iH\delta t} | q_N \rangle \langle q_N | e^{-iH\delta t} | q_{N-1} \rangle \\ \times \dots \langle q_1 | e^{-iH\delta t} | q' \rangle$$

The integrals over the q s all run from $-\infty$ to $+\infty$.

Campbell-Baker-Hausdorff formula:

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]} + \dots$$

$$\therefore e^{-iH\delta t} = e^{-i\frac{1}{2m}P^2\delta t} e^{-iV(Q)\delta t} e^{\underbrace{O(\delta t^2)}_{\text{can be ignored}}}$$

can be ignored
in the small δt limit

$$\langle q_2 | e^{-iH\delta t} | q_1 \rangle = \langle q_2 | e^{-i\frac{1}{2m}P^2\delta t} e^{-iV(Q)\delta t} | q_1 \rangle$$

$$= \int_{-\infty}^{\infty} dp_1 \langle q_2 | e^{-i\frac{1}{2m}P^2\delta t} | p_1 \rangle \langle p_1 | e^{-iV(Q)\delta t} | q_1 \rangle$$

$$= \int_{-\infty}^{\infty} dp_1 \underbrace{\langle q_2 | p_1 \rangle}_{\frac{e^{ip_1 q_2}}{\sqrt{2\pi}}} \underbrace{\langle p_1 | q_1 \rangle}_{\frac{e^{-ip_1 q_1}}{\sqrt{2\pi}}} e^{-i\frac{1}{2m}p_1^2\delta t} e^{-iV(q_1)\delta t}$$

$$= \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} e^{ip_1(q_2-q_1)} e^{-i\frac{p_1^2\delta t}{2m}} e^{-iV(q_1)\delta t}$$

3

$$= \int_{-\infty}^{\infty} \frac{dp_1}{2\pi} e^{-iH(p_1, q_1)\delta t} e^{ip_1(q_2 - q_1)}$$

More general hamiltonian: worry about ordering of P and Q in any term that contains both.

Weyl-ordering:

$$H(P, Q) := \int \frac{dx}{2\pi} \frac{dk}{2\pi} e^{inxP + ikQ} \int dp dq e^{-ixp - ikg} H(p, q)$$

Then*,

$$H(p_1, q_1) \rightarrow H(p_1, \bar{q}_1), \quad \bar{q}_1 := \frac{q_1 + q_2}{2}$$

Our hamiltonian is Weyl-ordered, so this replacement makes no difference in the limit $\delta t \rightarrow 0$.

Adopting Weyl-ordering for the general case:

$$\begin{aligned} \langle q'', t'' | q', t' \rangle &= \int \prod_{k=1}^N dq_k \prod_{j=0}^N \frac{dp_j}{2\pi} e^{ip_j(q_{j+1} - q_j)} \\ &\times e^{-iH(p_j, \bar{q}_j)\delta t}, \quad \bar{q}_j := \frac{1}{2}(q_j + q_{j+1}) \\ &q_0 = q', \quad q_{N+1} = q'' \end{aligned}$$

* This is not clear to me.

Let $\dot{q}_j := \frac{q_{j+1} - q_j}{\delta t}$ and take formal limit
of $\delta t \rightarrow 0$:

$$\langle q'', t'' | q', t' \rangle = \int Dq Dp e^{i \int_{t'}^{t''} dt [p(t) \dot{q}(t) - H(p(t), q(t))]}$$

If $H(p, q)$ is no more than quadratic in p ,
then p integral is gaussian. If the term that
is quadratic in p is independent of q , then
the prefactors generated by the gaussian integrals
are all constants and can be absorbed into the
definition of Dq . The result of integrating
out p is then

$$\langle q'', t'' | q', t' \rangle = \int Dq e^{i \int_{t'}^{t''} dt L(q(t), \dot{q}(t))}$$

where $L(q, \dot{q})$ is computed by first finding
the stationary point of the p integral
by solving

$$0 = \frac{\partial}{\partial p} (p \dot{q} - H(p, q)) = \dot{q} - \frac{\partial H(p, q)}{\partial p}$$

for p in terms q, \dot{q} and then plugging this solution back into $p\dot{q} - H$ to get L .

Examine $\langle q'', t'' | Q(t_1) | q', t' \rangle$, $t' < t_1 < t''$:

$$\begin{aligned} \langle q'', t'' | Q(t_1) | q', t' \rangle &= \langle q'' | e^{-iH(t''-t_1)} Q e^{-iH(t_1-t')} | q' \rangle \\ &= \int Dp Dq q(t_1) e^{iS} \end{aligned}$$

$$S := \int_{t'}^{t''} dt (p\dot{q} - H)$$

Consider $\int Dp Dq q(t_1) q(t_2) e^{iS}$. This requires $Q(t_1)$ and $Q(t_2)$ but their order depends on the order of t_1 and t_2 :

$$\int Dp Dq q(t_1) q(t_2) e^{iS} = \langle q'', t'' | T\{Q(t_1) Q(t_2)\} | q', t' \rangle$$

Functional derivatives:

$$\frac{\delta}{\delta f(t_1)} f(t_2) = \delta(t_1 - t_2)$$

$$H(p, q) \rightarrow H(p, q) - f(t)q(t) - h(t)p(t)$$

$$\begin{aligned}
 & \langle q'', t'' | q', t' \rangle_{f,h} = \int Dp Dq e^{i \int_{t'}^{t''} dt (pq - H + fq + hp)} \\
 & \frac{1}{i} \frac{\delta}{\delta f(t_1)} \langle q'', t'' | q', t' \rangle_{f,h} = \int Dp Dq q(t_1) e^{i \int_{t'}^{t''} dt (pq - H + fq + hp)} \quad \uparrow \\
 & \frac{1}{i} \frac{\delta}{\delta f(t_1)} \frac{1}{i} \frac{\delta}{\delta f(t_2)} \langle q'', t'' | q', t' \rangle_{f,h} = \int Dp Dq q(t_1) q(t_2) e^{i \int_{t'}^{t''} dt (pq - H + fq + hp)} \\
 & \frac{1}{i} \frac{\delta}{\delta h(t_1)} \langle q'', t'' | q', t' \rangle_{f,h} = \int Dp Dq p(t_1) e^{i S_{f,h}}
 \end{aligned}$$

...

At the end, set $f=h=0$:

$$\langle q'', t'' | T\{Q(t_1) \dots P(t_n) \dots\} | q', t' \rangle$$

$$= \left[\frac{1}{i} \frac{\delta}{\delta f(t_1)} \right] \dots \left[\frac{1}{i} \frac{\delta}{\delta h(t_n)} \right] \dots \langle q'', t'' | q', t' \rangle \Big|_{f=h=0}$$

Suppose we are also interested in initial and final states other than position eigenstates. Then, we must multiply by the wave functions for these states and integrate. We will be interested, in particular, in the ground

state as both the initial and final states.
Also, we will take the limits $t' \rightarrow -\infty$ and
 $t'' \rightarrow +\infty$:

$$\langle 0 | 0 \rangle_{f,h} = \lim_{\substack{t' \rightarrow -\infty \\ t'' \rightarrow +\infty}} \int dq'' dq' \psi_0^*(q'') \langle q'', t'' | q', t' \rangle_{f,h} \psi_0(q')$$

↓
 ↓
 ground-state
 wavefunction

Too cumbersome. Need to simplify.

Let $H|n\rangle = E_n|n\rangle$, $E_0 = 0$.

$$\begin{aligned} |q', t'\rangle &= e^{iHt'} |q'\rangle \\ &= \sum_{n \geq 0} e^{iHt'} |n\rangle \langle n | q' \rangle \\ &= \sum_{n \geq 0} \psi_n^*(q') e^{iE_n t'} |n\rangle \end{aligned}$$

$$H \rightarrow (1 - i\varepsilon) H$$

$$\begin{aligned} |q', t'\rangle &= \sum_{n \geq 0} \psi_n^*(q') e^{i(1-i\varepsilon)E_n t'} |n\rangle \\ &= \sum_{n \geq 0} \psi_n^*(q') e^{iE_n t'} |n\rangle e^{\varepsilon E_n t'} \end{aligned}$$

As $t' \rightarrow -\infty$, only the ground state contributes:

$$\lim_{t' \rightarrow -\infty} |q', t'\rangle \Big|_{H \rightarrow (1-i\varepsilon)H} = \psi_0^*(q') |0\rangle$$

Next, multiply by an arbitrary function $\chi(q')$ and integrate over q' . The only requirement is that $\langle 0|\chi \rangle \neq 0$. We then have a constant times $|0\rangle$ and this constant can be absorbed into the normalization of the path integral.

Similarly, $H \rightarrow (1-i\varepsilon)H$ picks the ground state in $\langle q'', t'' | = \langle q'' | e^{-iHt''}$ in the limit $t'' \rightarrow +\infty$.

\therefore if we use $(1-i\varepsilon)H$ instead of H , we can be cavalier (=careless) about the boundary conditions on the endpoints of the path. Any reasonable boundary conditions will result in the ground state as both initial and final states.

$$\langle 0|0 \rangle_{f,h} = \int Dp Dq e^{i \int_{-\infty}^{\infty} dt [p\dot{q} - (1-i\varepsilon)H + fq + h p]}$$

Suppose now $H = H_0 + H_1$ and we know the solution of H_0 , treating H_1 as perturbation.

9

suppress iε.

$$\begin{aligned} & i \int_{-\infty}^{\infty} dt (pq - H_0(p, q) - H_1(p, q) + fq + hp) \\ \langle 0 | 0 \rangle_{f, h} &= \int Dp Dq e^{-i \int_{-\infty}^{\infty} dt H_1\left(\frac{1}{i} \frac{\delta}{\delta p(t)}, \frac{1}{i} \frac{\delta}{\delta q(t)}\right)} \\ &= e^{i \int_{-\infty}^{\infty} dt (pq - H_0(p, q) + fq + hp)} \\ &\quad \times \int Dp Dq e^{-i \int_{-\infty}^{\infty} dt H_1\left(\frac{1}{i} \frac{\delta}{\delta p(t)}, \frac{1}{i} \frac{\delta}{\delta q(t)}\right)} \end{aligned}$$

The trick was as follows: We can extract each power of q w/ an f -derivative. Why not expand H_1 in a power series about q , replace each q w/ an f -derivative, and resum to obtain the original form of H_1 . Simil for p .

If H_1 depends only on q , if we are interested only in time-ordered products of Q s, if H is no more than quadratic in P , and if the term quadratic in P doesn't involve Q ,

then

$$\langle 0 | 0 \rangle_f = e^{i \int_{-\infty}^{\infty} dt L_1\left(\frac{1}{i} \frac{\delta}{\delta p(t)}\right)} \int Dq e^{i \int_{-\infty}^{\infty} dt [L_0(q, q) + fq]}$$

where $L_1(q) = -H_1(q)$.

