2.2. The Path Integral Derived

The propagator from (q_a, t_a) to (q_b, t_b) is defined as

$$Z(q_a, t_a, q_b, t_b) = \langle q_b \mid U(t_b, t_a) \mid q_a \rangle \qquad t_b > t_a$$

For a t-independent H

$$Z(q_a, t_a, q_b, t_b) = \left\langle q_b \,\middle|\, e^{-iH(t_b - t_a)/\hbar} \,\middle|\, q_a \right\rangle$$
$$= \left\langle q_b \,\middle|\, e^{-iHt_b/\hbar} e^{iHt_a/\hbar} \,\middle|\, q_a \right\rangle$$

Following Swanson, we start by considering a 1-D system with a time-independent $H = H(P, Q)$.

Define

$$Q(t) = e^{iHt/\hbar} Q e^{-iHt/\hbar} \qquad P(t) = e^{iHt/\hbar} P e^{-iHt/\hbar} \qquad (2.26a)$$
$$\mid q, t \rangle = e^{iHt/\hbar} \mid q \rangle \qquad \mid p, t \rangle = e^{iHt/\hbar} \mid p \rangle \qquad (2.26)$$

Note that the corresponding Schrodinger states are

$$\mid q(t) \rangle_S = e^{-iHt/\hbar} \mid q \rangle \qquad \mid p(t) \rangle_S = e^{-iHt/\hbar} \mid p \rangle$$

For a t-independent H,

$$Z(q_a, t_a, q_b, t_b) = \langle q_b, t_b \mid q_a, t_a \rangle \qquad (2.30)$$

The set $\{ \mid q, t \rangle \}$ is complete since

$$\int_{-\infty}^{\infty} dq \mid q, t \rangle \langle q, t \mid = \int_{-\infty}^{\infty} dq\, e^{iHt/\hbar} \mid q \rangle \langle q \mid e^{-iHt/\hbar}$$
$$= \sum_{E, E'} \int_{-\infty}^{\infty} dq\, e^{iHt/\hbar} \mid E \rangle \langle E \mid q \rangle \langle q \mid E' \rangle \langle E' \mid e^{-iHt/\hbar}$$
$$= \sum_{E, E'} \int_{-\infty}^{\infty} dq\, e^{iEt/\hbar} \mid E \rangle \langle E \mid q \rangle \langle q \mid E' \rangle \langle E' \mid e^{-iE't/\hbar}$$
$$= \sum_{E, E'} e^{iEt/\hbar} \mid E \rangle \delta_{EE'} \langle E' \mid e^{-iE't/\hbar}$$
$$= \sum_{E} \mid E \rangle \langle E \mid$$
$$= I \qquad (2.27)$$

$$Q(t) \mid q, t \rangle = e^{iHt/\hbar} Q e^{-iHt/\hbar} e^{iHt/\hbar} \mid q \rangle$$
$$= e^{iHt/\hbar} Q \mid q \rangle$$
$$= e^{iHt/\hbar} q \mid q \rangle$$
$$= q \mid q, t \rangle \qquad (2.28)$$

→ $\mid q, t \rangle$ is an eigenstate of $Q(t)$ with eigenvalue q.

Similarly, $\mid p, t \rangle$ is an eigenstate of $P(t)$ with eigenvalue p.

Eq(2.26) gives

$$\langle q, t \mid = \langle q \mid e^{-iHt/\hbar}$$

so that

$$\langle q, -t \mid \psi(t) \rangle_S = \langle q \mid e^{iHt/\hbar} e^{-iHt/\hbar} \mid \psi \rangle = \langle q \mid \psi \rangle = \psi(q) \qquad (2.29)$$

Using eq(2.27), we have

$${}_S\langle \psi(-t_b) \mid \phi(-t_a) \rangle_S = \int_{-\infty}^{\infty} dq_a\, dq_b \langle \psi(-t_b) \mid q_b, t_b \rangle \langle q_b, t_b \mid q_a, t_a \rangle \langle q_a, t_a \mid \phi(-t_a) \rangle$$
$$= \int_{-\infty}^{\infty} dq_a\, dq_b\, \psi^*(q_b) Z(q_a, t_a, q_b, t_b) \phi(q_a) \qquad (2.31)$$

Let

$$\epsilon = \frac{t_b - t_a}{N} \qquad t_n = t_a + n\epsilon \qquad q_n = q(t_n) \qquad n = 0, \ldots N-1$$

with

$$t_0 = t_a \qquad t_N = t_b \qquad q_0 = q_a \; q_N = q_b$$

Using eq(2.27), we have

$$Z(q_a, t_a, q_b, t_b) = \int_{-\infty}^{\infty} d\,q_1 \ldots d\,q_{N-1} \langle q_b, t_b \mid q_{N-1}, t_{N-1} \rangle \tag{2.32}$$

$$\times \langle q_{N-1}, t_{N-1} \mid \ldots \mid q_1, t_1 \rangle \langle q_1, t_1 \mid q_a, t_a \rangle$$

Note that there're $N-1$ integrals while the integrand is a product of N propagators.

Using eq(2.26), we have

$$\left\langle q_{j+1}, t_{j+1} \mid q_j, t_j \right\rangle = \left\langle q_{j+1} \mid e^{-i H t_{j+1}/\hbar} e^{i H t_j/\hbar} \mid q_j \right\rangle$$

$$= \left\langle q_{j+1} \mid e^{-i \epsilon H/\hbar} \mid q_j \right\rangle \tag{2.33}$$

Comment : eqs (2.32 – 3) can also be derived directly from

$$Z(q_a, t_a, q_b, t_b) = \left\langle q_b \,\middle|\, T\left[\exp\left(-\frac{i}{\hbar} \int_{t_a}^{t_b} d\,t\, H(t)\right)\right] \,\middle|\, q_a \right\rangle$$

by approximating the integral with a time – ordered sum & then inserting the identities

$$\int d\,q_j \left| q_j \right\rangle \left\langle q_j \right| = 1$$

behind each $e^{-i(t_{j+1}-t_j) H/\hbar}$ factor. Note that the result is valid for a t – dependent H.

Define the coordinate ordering operator C to move all momentum operators in a product to the left of all coordinate operators, e.g.,

$$C\left\{P\, Q\, P^2\right\} = P^3\, Q \tag{2.34}$$

Expanding $f(q, p)$ as a Taylor series in q & p, we have

$$f(q, p) = \sum_{m n} \alpha_{m n}\, q^n\, p^m$$

$$\rightarrow \qquad C\{f(Q, P)\} = \sum_{m n} \alpha_{m n}\, P^m\, Q^n$$

$$\therefore \qquad \langle p \mid C\{f(Q, P)\} \mid q \rangle = \sum_{m n} \alpha_{m n} \left\langle p \left| p^m q^n \right| q \right\rangle = f(q, p) \langle p \mid q \rangle \tag{2.35}$$

i.e., a coordinate ordered operator acts like a c-number function when one takes its matrix element between $\langle p \mid$ & $\mid q \rangle$.

Consider

$$H = a\,P + b\,Q$$

Using

$$\left[-\frac{i}{\hbar}\,\epsilon\, a\, P,\, -\frac{i}{\hbar}\,\epsilon\, b\, Q\right] = -\frac{\epsilon^2}{\hbar^2}\, a\, b\, [P, Q] = i\,\frac{\epsilon^2}{\hbar}\, a\, b$$

the BCH theorem eq(1.66) of §1.4 becomes

$$e^{-i\epsilon H/\hbar} = e^{-i\epsilon a P/\hbar}\, e^{-i\epsilon b Q/\hbar}\, e^{i\epsilon^2 a b/2\hbar} \tag{2.36}$$

$$= e^{-i\epsilon a P/\hbar}\, e^{-i\epsilon b Q/\hbar} + O(\epsilon^2)$$

$$= e^{-i\epsilon b Q/\hbar}\, e^{-i\epsilon a P/\hbar} + e^{-i\epsilon^2 a b/2\hbar}$$

$$= e^{-i\epsilon b Q/\hbar}\, e^{-i\epsilon a P/\hbar} + O(\epsilon^2)$$

Since the factor associated with the commutator is $O(\epsilon^2)$, we see that

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

$$\rightarrow \qquad e^{-i\epsilon H/\hbar} = e^{-i\epsilon P^2/2 m \hbar}\, e^{-i\epsilon V(Q)/\hbar} + O(\epsilon^2)$$

$$= e^{-i\epsilon V(Q)/\hbar}\, e^{-i\epsilon P^2/2m\hbar} + O(\epsilon^2) \tag{2.36a}$$

Thus, for propagators of infinitesimal time, quantum effects are negligible.

This statement can be extrapolated to finite times using the Trotter product formula

$$e^{t(A+B)} = \lim_{n\to\infty} \left(e^{tA/n}\, e^{tB/n} \right)^n \tag{2.38}$$

if A & B are bounded.

Using eqs(2.5 & 2.36a), eq(2.33) becomes

$$\langle q_{j+1}, t_{j+1} \mid q_j, t_j \rangle = \int_{-\infty}^{\infty} d p_j \, \langle q_{j+1} \mid p_j \rangle \langle p_j \mid e^{-i\epsilon H(P,Q)/\hbar} \mid q_j \rangle$$

$$= \int_{-\infty}^{\infty} d p_j \, \langle q_{j+1} \mid p_j \rangle \langle p_j \mid e^{-i\epsilon P^2/2m\hbar}\, e^{-i\epsilon V(Q)/\hbar} \mid q_j \rangle + O(\epsilon^2)$$

$$\approx \int_{-\infty}^{\infty} d p_j \exp\left\{ -\frac{i}{\hbar}\epsilon \left[\frac{p_j^2}{2m} + V(q_j) \right] \right\} \langle q_{j+1} \mid p_j \rangle \langle p_j \mid q_j \rangle \tag{2.39}$$

Reminder: eq(2.39) is the result of coordinate ordering.

Using eq(2.7), we have

$$\langle q_{j+1} \mid p_j \rangle \langle p_j \mid q_j \rangle = \frac{1}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar} \left[p_j (q_{j+1} - q_j) \right] \right\} \tag{2.40}$$

$$\rightarrow \qquad \langle q_{j+1}, t_{j+1} \mid q_j, t_j \rangle \approx \int_{-\infty}^{\infty} \frac{d p_j}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar}\epsilon \left[p_j \left(\frac{q_{j+1} - q_j}{\epsilon} \right) - H(p_j, q_j) \right] \right\}$$

Using

$$\lim_{\epsilon\to 0} \frac{q_{j+1} - q_j}{\epsilon} = \frac{d q_j}{d t} = \dot{q}_j \tag{2.41}$$

we have

$$\langle q_{j+1}, t_{j+1} \mid q_j, t_j \rangle \approx \int_{-\infty}^{\infty} \frac{d p_j}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar}\epsilon \left[p_j \dot{q}_j - H(p_j, q_j) \right] \right\}$$

$$= \int_{-\infty}^{\infty} \frac{d p_j}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar}\epsilon \mathcal{L}(p_j, q_j) \right\} \tag{2.42}$$

where

$$\mathcal{L}(p, q) = p\dot{q} - H(p, q) \tag{2.43}$$

is the Lagrangian density written in terms of the variables p & q.

Eq(2.32) thus becomes

$$\langle q_b, t_b \mid q_a, t_a \rangle = \int_{-\infty}^{\infty} d q_1 \ldots d q_{N-1} \int_{-\infty}^{\infty} \frac{d p_1}{2\pi\hbar} \ldots \frac{d p_{N-1}}{2\pi\hbar} \tag{2.44}$$

$$\times \exp\left\{ \frac{i}{\hbar}\epsilon \sum_{j=0}^{N-1} \mathcal{L}(p_j, q_j) \right\}$$

Note that there're $2(N-1)$ integrals and N terms in the exponent.

Now,

$$\lim_{\epsilon\to 0} \epsilon \sum_{j=0}^{N-1} \mathcal{L}(p_j, q_j) = \int_{t_a}^{t_b} d t\, \mathcal{L}(p, q)$$

$$= S(p, q, t_a, t_b) \tag{2.45}$$

is just the classical action.

Defining the path integral measure as

$$\mathcal{D} p \mathcal{D} q = \lim_{N\to\infty} \frac{d p_1}{2\pi\hbar} \ldots \frac{d p_{N-1}}{2\pi\hbar} d q_1 \ldots d q_{N-1} \tag{2.46}$$

eq(2.44) simplifies to

$$\langle q_b, t_b \mid q_a, t_a \rangle = \int_{q_a}^{q_b} \mathcal{D}\, p\, \mathcal{D}\, q\, e^{i S/\hbar}$$

$$= \int_{q_a}^{q_b} \mathcal{D}\, p\, \mathcal{D}\, q \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\, t\, \mathcal{L}(p, q) \right\} \quad (2.47)$$

It is easy to see that eq(2.47) remains valid for a time-dependent H of the form

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

where $b(t)$ is any function of t.

Extension to systems with n degrees of freedom is accomplished by replacing (q, p) with n-D vectors $(\boldsymbol{q}, \boldsymbol{p})$.

Eq(2.42) can be written as

$$\langle q_{j+1}, t_{j+1} \mid q_j, t_j \rangle \approx \int_{-\infty}^{\infty} \frac{d\, p_j}{2\, \pi\, \hbar} \exp\left\{ \frac{i}{\hbar} \epsilon \left[p_j\, \dot{q}_j - \frac{p_j^2}{2\, m} - V(q_j) \right] \right\}$$

Using eq(1.107) to evaluate the Gaussian integral, we have

$$\langle q_{j+1}, t_{j+1} \mid q_j, t_j \rangle \approx \sqrt{\frac{m}{2\, \pi\, i\, \hbar\, \epsilon}} \exp\left\{ \frac{i}{\hbar} \epsilon \left[\frac{1}{2}\, m\, \dot{q}_j^2 - V(q_j) \right] \right\}$$

$$= \sqrt{\frac{m}{2\, \pi\, i\, \hbar\, \epsilon}} \exp\left\{ \frac{i}{\hbar} \epsilon\, \mathcal{L}(\dot{q}, q) \right\} \quad (2.49)$$

where

$$\mathcal{L}(\dot{q}, q) = \frac{1}{2}\, m\, \dot{q}^2 - V(q) \quad (2.51)$$

Defining the path integral measure as

$$\overline{\mathcal{D}}\, q = \lim_{N \to \infty} \left(\frac{m}{2\, \pi\, i\, \hbar\, \epsilon} \right)^{N/2} d\, q_1 \ldots d\, q_{N-1} \quad (2.52)$$

we have

$$\langle q_b, t_b \mid q_a, t_a \rangle = \int_{q_a}^{q_b} \overline{\mathcal{D}}\, q\, e^{i S/\hbar}$$

$$= \int_{q_a}^{q_b} \overline{\mathcal{D}}\, q \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} d\, t\, \mathcal{L}(\dot{q}, q) \right\} \quad (2.50)$$

Finally, a velocity dependent potential leads to ambiguities in the path integral formulation (see Ex.2.6).