Path integrals, propagators and density matrices

$$K(x,t;x',0) = \langle x|e^{-i\mathcal{H}t/\hbar}|x'\rangle \qquad \mathcal{H} = p^2/2M + V(q)$$

$$K(x,t;x',0) = \langle x|e^{-i\mathcal{H}(t-t_{N-1})/\hbar} \ldots e^{-i\mathcal{H}(t_k-t_{k-1})/\hbar} \ldots e^{-i\mathcal{H}t_1/\hbar}|x'\rangle$$

$$\int_{-\infty}^{+\infty} dx_k\, |x_k\rangle\langle x_k| = \mathbf{1} \quad (1 \leq k \leq N-1)$$

$$K(x,t;x',0) = \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dx_1 \ldots dx_k \ldots dx_{N-1} \langle x|e^{-i\mathcal{H}(t-t_{N-1})/\hbar}|x_{N-1}\rangle \times$$

$$\times \langle x_{N-1}| \ldots . |x_k\rangle\langle x_k|e^{-i\mathcal{H}(t_k-t_{k-1})/\hbar}|x_{k-1}\rangle\langle x_{k-1}|\ldots |x_1\rangle\langle x_1|e^{-i\mathcal{H}t_1/\hbar}|x'\rangle$$

$$t_k - t_{k-1} \equiv \epsilon = t/N \to 0 \text{ and } (N \to \infty)$$

$$K(x_k,t_k;x_{k-1},t_{k-1}) \approx \langle x_k| 1 - \frac{i\epsilon}{\hbar}\mathcal{H}\,|x_{k-1}\rangle \qquad x_N = x \text{ and } x_0 = x'$$

$$K(x_k,t_k;x_{k-1},t_{k-1}) \approx \langle x_k|x_{k-1}\rangle - \frac{i\epsilon}{\hbar}\langle x_k|\,\frac{p^2}{2M}\,|x_{k-1}\rangle - \frac{i\epsilon}{\hbar}\langle x_k|\,V(q)\,|x_{k-1}\rangle$$

$$\int_{-\infty}^{+\infty} dp_k\,|p_k\rangle\langle p_k| = \mathbf{1}$$

$$K(x_k,t_k;x_{k-1},t_{k-1}) \approx \int_{-\infty}^{+\infty} dp_k\,\langle x_k|p_k\rangle\langle p_k|x_{k-1}\rangle -$$

$$-\frac{i\epsilon}{\hbar}\int_{-\infty}^{+\infty} dp_k\;\frac{p_k^2}{2M}\,\langle x_k|p_k\rangle\langle p_k|x_{k-1}\rangle - \frac{i\epsilon}{\hbar}\int_{-\infty}^{+\infty} dp_k\;V(x_k)\,\langle x_k|p_k\rangle\langle p_k|x_{k-1}\rangle$$

$$\langle x_k | p_k \rangle = \frac{1}{\sqrt{2\pi\hbar}} \; e^{ip_k x_k/\hbar}$$

$$K(x_k, t_k; x_{k-1}, t_{k-1}) \approx \frac{1}{\sqrt{2\pi\hbar}} \int\limits_{-\infty}^{+\infty} dp_k \; \exp \frac{ip_k}{\hbar}(x_k - x_{k-1}) \times$$

$$\times \left(1 - \frac{i\epsilon}{\hbar} \left(\frac{p_k^2}{2M} + \; V(x_k) \right) \right)$$

$$K(x_k, t_k; x_{k-1}, t_{k-1}) = \frac{1}{\sqrt{2\pi\hbar}} \int\limits_{-\infty}^{+\infty} dp_k \; \exp \frac{ip_k}{\hbar}(x_k - x_{k-1}) \times$$

$$\times \exp \frac{i\epsilon}{\hbar} \left(\frac{p_k^2}{2M} + \; V(x_k) \right)$$

$$K(x_k, t_k; x_{k-1}, t_{k-1}) = \sqrt{\frac{M}{2\pi i\hbar\epsilon}} \; \exp \frac{i\epsilon}{\hbar} \left(\frac{M}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - \; V(x_k) \right)$$

$$K(x,t;x',0) = \int\limits_{-\infty}^{+\infty} ... \int\limits_{-\infty}^{+\infty} dx_1 \, ... dx_k \, ... dx_{N-1} \left[\prod_{k=1}^{N} \sqrt{\frac{M}{2\pi i \hbar \epsilon}} \; \right] \times$$

$$\times \; \exp \sum_{k=1}^{N} \frac{i\epsilon}{\hbar} \left(\frac{M}{2} \frac{(x_k - x_{k-1})^2}{\epsilon^2} - V(x_k) \right)$$

$\epsilon \to 0$ $\epsilon = \Delta t_k \equiv t_k - t_{k-1}$

$$K(x,t;x',0) = \prod_{t'=0}^{t} \int\limits_{-\infty}^{\infty} \frac{dx(t')}{\mathcal{N}} \exp \frac{i}{\hbar} S[x(t')]$$

$$S[x(t')] = \int\limits_{0}^{t} dt' \left(\frac{1}{2} M \dot{x}^2 - V(x) \right)$$

$$K(x,t;x',0) = \int\limits_{x'}^{x} \mathcal{D}x(t') \exp \frac{i}{\hbar} S[x(t')]$$

Example 1; free particle

$$K(x,t;x',0) = \int_{-\infty}^{+\infty} ... \int_{-\infty}^{+\infty} dx_1 ... dx_{N-1} \times \prod_{k=1}^{N} \sqrt{\frac{M}{2\pi i\hbar\epsilon}}\ \exp \frac{i\epsilon}{\hbar}\left(\frac{M}{2}\frac{(x_k - x_{k-1})^2}{\epsilon^2}\right)$$

$$\int_{-\infty}^{\infty} du\ \sqrt{\frac{a}{\pi}}\ \exp -a(x-u)^2 \sqrt{\frac{b}{\pi}}\ \exp -b(u-y)^2 = \sqrt{\frac{ab}{\pi(a+b)}}\ \exp -\frac{ab}{a+b}(x-y)^2$$

$$\frac{M}{2\pi i\hbar\epsilon}\int_{-\infty}^{\infty} dx_1\ \exp \frac{iM}{2\hbar\epsilon}(x_2 - x_1)^2\ \ \exp \frac{iM}{2\hbar\epsilon}(x_1 - x')^2 = \sqrt{\frac{M}{2\pi i\hbar(2\epsilon)}}\ \exp \frac{iM}{2\hbar(2\epsilon)}(x_2 - x')^2$$

$$K(x,t;x',0) = \sqrt{\frac{M}{2\pi i\hbar t}}\ \exp \frac{iM}{2\hbar}\frac{(x-x')^2}{t}$$

Example 2; quadratic Lagrangean

$$L = \frac{1}{2}M\dot{x}^2 \; + \; b(t)x\,\dot{x} \; - \; \frac{1}{2}c(t)x^2 \; - e(t)\,x$$

$$y(t') = x(t') - x_c(t') \qquad\qquad M\ddot{x}_c \; + \; (c(t) \; + \; \dot{b}(t))x_c \; + e \; = 0$$

$$K(x, t; x', 0) = G(t)\exp\frac{i}{\hbar}S_c(x, x', t)$$

$$G(t) = \int_0^0 \mathcal{D}y(t')\exp\frac{i}{\hbar}\int_0^t dt'\left(\frac{1}{2}M\dot{y}^2 - \frac{1}{2}\,\tilde{c}(t)y^2\right) \qquad \tilde{c} = \; c \; + \; \dot{b}$$

$$G(t) = \lim_{N\to\infty,\,\epsilon\to 0}\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} dy_1 \ldots dy_k \ldots dy_{N-1}\left[\frac{M}{2\pi i\hbar\epsilon}\;\right]^{N/2} \times$$

$$\times \;\exp\frac{i}{\hbar}\sum_{k=1}^{N}\left[\frac{M}{2}\;\frac{(y_k - y_{k-1})^2}{\epsilon} \; - \; \frac{1}{2}\,\epsilon\,\tilde{c}_{k-1}\,y_{k-1}^2\right]$$

$$G(t) = \lim_{N\to\infty,\,\epsilon\to 0} \int\limits_{-\infty}^{\infty} \ldots \int\limits_{-\infty}^{\infty} dy_1 \ldots dy_k \ldots dy_{N-1} \left[\frac{M}{2\pi i\hbar\epsilon} \right]^{N/2} \times$$

$$\times \, \exp \frac{i}{\hbar} \sum_{k=1}^{N} \left[\frac{M}{2} \frac{(y_k - y_{k-1})^2}{\epsilon} - \frac{1}{2}\, \epsilon \, \tilde{c}_{k-1} \, y_{k-1}^2 \right]$$

$$\zeta = \begin{pmatrix} y_1 \\ . \\ . \\ y_{N-1} \end{pmatrix}$$

$$\sigma = \frac{M}{2i\hbar} \begin{pmatrix} 2 & -1 & . & 0 & 0 \\ -1 & 2 & . & 0 & 0 \\ . & . & . & . & . \\ 0 & 0 & . & 2 & -1 \\ 0 & 0 & . & -1 & 2 \end{pmatrix} + \frac{i\epsilon}{2\hbar} \begin{pmatrix} \tilde{c}_1 & 0 & . & 0 & 0 \\ 0 & \tilde{c}_2 & . & 0 & 0 \\ . & . & . & . & . \\ 0 & 0 & . & \tilde{c}_{N-2} & 0 \\ 0 & 0 & . & 0 & \tilde{c}_{N-1} \end{pmatrix}$$

$$G(t) = \lim_{N\to\infty,\,\epsilon\to 0} \left[\frac{M}{2\pi i\hbar\epsilon} \right]^{N/2} \int d^{N-1}\zeta \exp -\zeta^T \, \sigma \, \zeta$$

$$\sigma = U^\dagger \ \sigma_D \ U$$

$$\int d^{N-1}\zeta \exp -\zeta^T \ \sigma \ \zeta = \int d^{N-1}\xi \exp -\xi^T \ \sigma_D \ \xi = \prod_{\alpha=1}^{N-1} \sqrt{\frac{\pi}{\sigma_\alpha}} = \frac{\pi^{(N-1)/2}}{\sqrt{\det \sigma}}$$

$$G(t) = \lim_{N\to\infty,\, \epsilon\to 0} \left(\left(\frac{M}{2\pi i\hbar} \right) \frac{1}{\epsilon} \frac{1}{\left(\frac{2i\hbar\epsilon}{M}\right)^{N-1} \det \sigma} \right)^{1/2}$$

$$f(t) = \lim_{N\to\infty,\, \epsilon\to 0} \left(\epsilon \left(\frac{2i\hbar\epsilon}{M} \right)^{N-1} \det \sigma \right) \qquad \left(\frac{2i\epsilon\hbar}{M} \right)^{N-1} \det \sigma =$$

$$\det \left[\begin{pmatrix} 2 & -1 & . & 0 & 0 \\ -1 & 2 & . & 0 & 0 \\ . & . & . & . & . \\ 0 & 0 & . & 2 & -1 \\ 0 & 0 & . & -1 & 2 \end{pmatrix} - \frac{\epsilon^2}{M} \begin{pmatrix} \tilde{c}_1 & 0 & . & 0 & 0 \\ 0 & \tilde{c}_2 & . & 0 & 0 \\ . & . & . & . & . \\ 0 & 0 & . & \tilde{c}_{N-2} & 0 \\ 0 & 0 & . & 0 & \tilde{c}_{N-1} \end{pmatrix} \right]$$

$$\equiv \det \tilde{\sigma}_{N-1} \equiv p_{N-1}$$

$$p_{j+1} = \left(2 - \frac{\epsilon^2}{M}\ \tilde{c}_{j+1}\right) p_j - p_{j-1}, \qquad j = 1, ..., N-2$$

$$p_1 = 2 - (\epsilon^2 c_1/M) \qquad\qquad p_0 = 1$$

$$\frac{p_{j+1} - 2p_j + p_{j-1}}{\epsilon^2} = \frac{\tilde{c}_{j+1} p_j}{M}$$

$$\varphi(t) \equiv \epsilon p_j \qquad\qquad \frac{d^2\varphi(t)}{dt^2} = -\frac{\tilde{c}(t)\varphi(t)}{M}$$

$$\varphi(0) = \epsilon p_0 \to 0 \qquad\qquad \frac{d\varphi(t)}{dt} = \epsilon\left(\frac{p_1 - p_0}{\epsilon}\right) = 2 - \frac{\epsilon^2 c_1}{M} - 1 \to 1$$

$$\frac{d^2 f(t)}{dt^2} + \frac{\tilde{c}(t) f(t)}{M} = 0 \quad f(0) = 0 \qquad df(t)/dt|_{t=0} = 1$$

$$K(x,t;x',0) = \sqrt{\frac{M}{2\pi i\hbar f(t)}}\exp\frac{i}{\hbar}S_c(x,x',t)$$

For the harmonic oscillator (forced or not)

$$\tilde{c}(t) = c(t) = M\omega^2$$

$$\frac{d^2 f(t)}{dt^2} + \omega^2 f(t) = 0$$

$$f(t) = \frac{\sin(\omega t)}{\omega}$$

The effects of $e(t)$ or $b(t) = b$ will show up only in $S_c(x,x',t)$.

Stationary phase (or semi-classical) approximation

$$K(x,t;x',0) = \int_{x'}^{x} \mathcal{D}q(t') \exp \frac{i}{\hbar} S[q(t')]$$

$$S[q(t')] = \int_{0}^{t} dt' \, L(q(t'), \dot{q}(t'), t')$$

When $\hbar \to 0$ we must expand the action about a stationary path

$$S[q(t')] = S[q_c(t')] + \int_{0}^{t} dt' \, \delta q(t') \left. \frac{\delta S[q(t')]}{\delta q(t')} \right|_{q=q_c} +$$

$$+ \frac{1}{2} \int_{0}^{t} \int_{0}^{t} dt' dt'' \, \delta q(t') \, \delta q(t'') \left. \frac{\delta^2 S[q(t')]}{\delta q(t') \, \delta q(t'')} \right|_{q=q_c} + \ldots$$

$$S[q(t')] = S[q_c(t')] + \int_0^t dt' \left\{ \left.\frac{\partial L}{\partial q}\right|_{q_c} \delta q(t') + \left.\frac{\partial L}{\partial \dot{q}}\right|_{q_c} \delta \dot{q}(t') \right\} +$$

$$+\frac{1}{2}\int_0^t dt' \left\{ \left.\frac{\partial^2 L}{\partial q^2}\right|_{q_c} \delta q(t')\,\delta q(t') + 2\left.\frac{\partial^2 L}{\partial \dot{q}\partial q}\right|_{q_c} \delta \dot{q}(t')\,\delta q(t') + \right.$$

$$\left. + \left.\frac{\partial^2 L}{\partial \dot{q}^2}\right|_{q_c} \delta \dot{q}(t')\,\delta \dot{q}(t') \right\} + \ldots$$

$$q_c(0) = x',\; q_c(t) = x,\; \text{and } \delta q(t') \equiv q(t') - q_c(t') \Rightarrow \delta q(t) = \delta q(0) = 0$$

$$S[q(t')] = S[q_c(t')] + \int_0^t dt'\,\delta q(t') \left\{ \left.\frac{\partial L}{\partial q}\right|_{q_c} - \frac{d}{dt'}\left.\frac{\partial L}{\partial \dot{q}}\right|_{q_c} \right\} +$$

$$+\frac{1}{2}\int_0^t dt'\,\delta q(t') \left\{ \left[\left.\frac{\partial^2 L}{\partial q^2}\right|_{q_c} - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial \dot{q}\partial q}\right|_{q_c} \right) \right] - \right.$$

$$\left. - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial \dot{q}^2}\right|_{q_c} \right) \frac{d}{dt'} - \frac{\partial^2 L}{\partial \dot{q}^2}\frac{d^2}{dt'^2} \right\} \delta q(t')$$

Equation for an extremum; the first functional derivative

$$\left.\frac{\partial L}{\partial q}\right|_{q_c} - \frac{d}{dt'}\left.\frac{\partial L}{\partial \dot{q}}\right|_{q_c} = 0$$

Eigenvalue problem; the second functional derivative

$$\left[\left.\frac{\partial^2 L}{\partial q^2}\right|_{q_c} - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial \dot{q}\partial q}\right|_{q_c}\right) - \frac{d}{dt'}\left(\left.\frac{\partial^2 L}{\partial \dot{q}^2}\right|_{q_c}\frac{d}{dt'}\right)\right]\delta q(t') = \lambda \delta q(t')$$

$$-M\frac{d^2}{dt'^2}\delta q(t') - V''(q_c(t'))\delta q(t') = \lambda \delta q(t') \qquad \delta q(t) = \delta q(0) = 0$$

$$\delta q(t') = \sum_n c_n \varphi_n(t') \qquad \int_0^t dt' \varphi_n(t')\varphi_m(t') = \delta_{mn}$$

$$S[q(t')] = S[q_c(t')] + \sum_n \frac{1}{2}\lambda_n c_n^2$$

$$K(x,t;x',0) \approx \exp\frac{i}{\hbar}S[q_c]\int\ldots\int\frac{\mathcal{J}}{\mathcal{N}}\,dc_0\,dc_1\ldots dc_n\ldots\;\exp\frac{i}{2\hbar}\sum_{n=0}^{\infty}\lambda_n c_n^2$$

Jacobian of $\prod_{t'=0}^{t} dq(t')$ to $\prod_{n=0}^{N} dc_n$. Defining $\frac{1}{\mathcal{N}_R} \equiv \lim_{n\to\infty}\left[\frac{\mathcal{J}}{\mathcal{N}}(2\pi i\hbar)^{n/2}\right]$

⬇

$$K(x,t;x',0) \approx \frac{1}{\mathcal{N}_R}\frac{1}{\sqrt{\det[M\partial_{t'}^2 + V''(q_c)]}}\exp\frac{i}{\hbar}S[q_c]$$

Computing determinants; Coleman's theorem

$$\det\left[\frac{-\partial_{t'}^2 + W^{(1)}(t') - \lambda}{-\partial_{t'}^2 + W^{(2)}(t') - \lambda}\right] = \frac{\psi_\lambda^{(1)}(t')}{\psi_\lambda^{(2)}(t')}$$

$$[-\partial_{t'}^2 + W^{(i)}(t')]\psi_\lambda^{(i)}(t') = \lambda\psi_\lambda^{(i)}(t')$$

$$\psi_\lambda^{(i)}(0) = 0 \quad \text{and} \quad \partial_{t'}\psi_\lambda^{(i)}(t')|_{t'=0} = 1$$

$$\frac{\det[-\partial_{t'}^2 + W(t')]}{\psi_0(t)} \quad \Rightarrow \quad \mathcal{N}_R = \sqrt{2\pi i\hbar/M}$$

It can be shown that

$$G(t) \equiv \sqrt{\frac{M}{2\pi i\hbar f(t)}} = \sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_c(x,x',t)}{\partial x \partial x'}}$$

$$G(t) = \sqrt{\det\left(\frac{i}{2\pi\hbar}\frac{\partial^2 S_c(\mathbf{x},\mathbf{x}',t)}{\partial x_i \partial x'_j}\right)}$$

But, there is the easy way

$$\int_{-\infty}^{+\infty} dx\, K(x,t;x',0)K^*(x,t;x'',0) = \delta(x'-x'')$$

Imaginary time path integrals

$$\rho_N(x,x',\beta) = \langle x|e^{-\mathcal{H}\beta/\hbar}|x'\rangle \qquad \beta \equiv 1/k_BT \quad \text{and} \quad t = -i\hbar\beta$$

$$\rho_N(x,x',\beta) = \int_{x'}^{x} \mathcal{D}x(\tau)\exp -\frac{1}{\hbar}S_E[x(\tau)] \qquad \mathcal{Z} = \mathrm{tr}\rho_N = \int \rho_N(x,x,\beta)\,dx$$

$$S_E[x(\tau)] = \int_0^{\hbar\beta}\left(\frac{1}{2}M\dot{x}^2 + V(x(\tau))\right)d\tau$$

Integral of the functional $F[x(\tau)] = \exp -\frac{1}{\hbar}\int_0^{\hbar\beta} V(x(\tau))d\tau$ over the

Wiener measure

$$d_W(x,t) = dx_1 ... dx_{N-1}\prod_{k=1}^{N}\sqrt{\frac{M}{2\pi\hbar^2\epsilon}}\,\exp -\frac{M\epsilon}{2\hbar^2}\frac{(x_k - x_{k-1})^2}{\epsilon^2}$$