Path integral

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Time evolution operator

- The time evolution operator is defined by

$$\left|\phi;t\right\rangle = U\left(t-t'\right)\left|\phi;t'\right\rangle$$

- and satisfy the following composition law:

$$U\left(t_1\right)U\left(t_2\right) = U\left(t_1+t_2\right)$$

$$U\left(t\right) = \left[U\left(t/N\right)\right]^N$$

Time evolution operator

- the time derivative of U is

$$U(\delta t + t) - U(t) = \left[U(\delta t) - 1\right] U(t) = \left(1 - \frac{i}{\hbar}\delta t H\right) U(t)$$

$$\frac{\partial U}{\partial t} = \frac{U(\delta t + t) - U(t)}{\delta t} = -\frac{i}{\hbar} H U(t)$$

- The solution for initial condition that $U(0) = 1$

$$U(t) = \exp\left(-\frac{i}{\hbar} H t\right)$$

Propagators

- To introduce the propagator K , defined as the function

$$K(rt,r't') = \langle r|U(t,t')|r'\rangle \theta(t-t')$$

- θ is the unit step (or Heaviside) function

$$\theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases} \qquad \frac{d\theta(t)}{dt} = \delta(t)$$

Propagators

- when $t \to t'$ $U(t,t') \to 1$

$$K(rt,r't') \to \langle r|r'\rangle = \delta(r-r')$$

- the propagator is a probability amplitude the amplitude for finding the system at some point *r* in configuration space at time *t* given that it was originally at *r*' at time *t*'.

$$K(rt,r't') = \langle r,t|r',t'\rangle \quad \text{for} \quad t > t'$$

Schrodinger equation

- the Schrodinger equation for U

$$\left[i\hbar \frac{\partial}{\partial t} - H(t) \right] |\psi, t\rangle = 0$$

$$|\psi, t\rangle = U(t, t') |\psi, t'\rangle$$

$$\left[i\hbar \frac{\partial}{\partial t} - H(t) \right] U(t, t') = 0$$

Schrodinger equation

- Schrodinger equation for K

$$\left[i\hbar\frac{\partial}{\partial t}-H(t)\right]K(rt,r't')$$

$$=\theta(t-t')\langle r|\left[i\hbar\frac{\partial}{\partial t}-H(t)\right]U(t,t')|r'\rangle+i\hbar\langle r|U(t,t')|r'\rangle\frac{\partial}{\partial t}\theta(t-t')$$

$$=i\hbar\delta(r-r')\delta(t-t')$$

- It is frequently called Green's function for the time-dependent Schrodinger equation.

Composition law

- The group property for U

$$U(t_3,t_2)U(t_2,t_1)=U(t_3,t_1)$$

- The composition of K

$$K(r_3t_3,r_1t_1)=\int K(r_3t_3,r_2t_2)K(r_2t_2,r_1t_1)dr_2$$

$$t_3>t_2>t_1$$

dimension of K

- A one-dimensional delta function $\delta(x)$ has dimension [l/L],

- (energy)[K]=$L^{-d}T^{-1}$ *h*

- [K]=L^{-d}

- When Hamiltonian is time-independent,

$$U(t,t') \to U(t-t') = \exp\left(-i\frac{Ht}{\hbar}\right)$$

$$K(rt,r't') \to K(r,r';t-t')$$

$$K(r,r';t) = \langle r| e^{-iHt/\hbar} |r'\rangle \theta(t)$$

- Let $\{\psi_{n\nu}(r)\}$ be a complete set of eigenfunctions of H, with energy eigenvalues E_n and ν the additional quantum numbers beyond energy in the case of degeneracy:

$$K(r,r';t) = \sum_{n\nu} e^{-iE_n t/\hbar} \varphi_{n\nu}(r) \varphi^*_{n\nu}(r') \theta(t)$$

recall that $$\sum_{n\nu} \varphi_{n\nu}(r) \varphi^*_{n\nu}(r') = \delta(r - r')$$

- the propagator for a time-independent Hamiltonian is a Fourier series in time with the frequency spectrum

contour integration

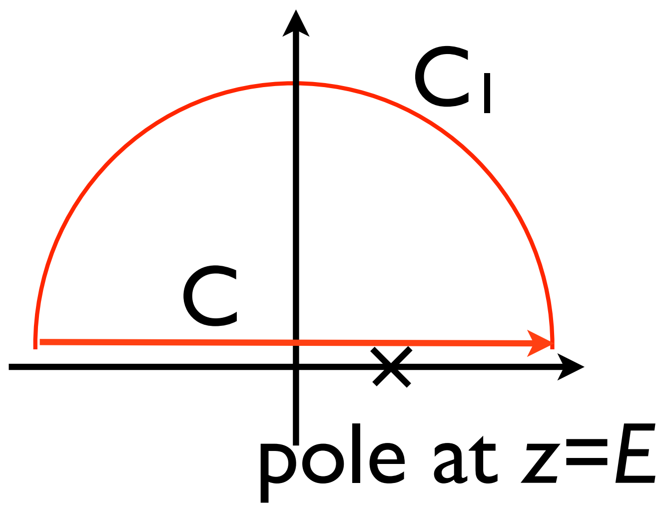
- consider the function defined by

$$f(E) = \int_C \frac{e^{-izt/\hbar}}{z-E} dz$$ pole at $z=E$

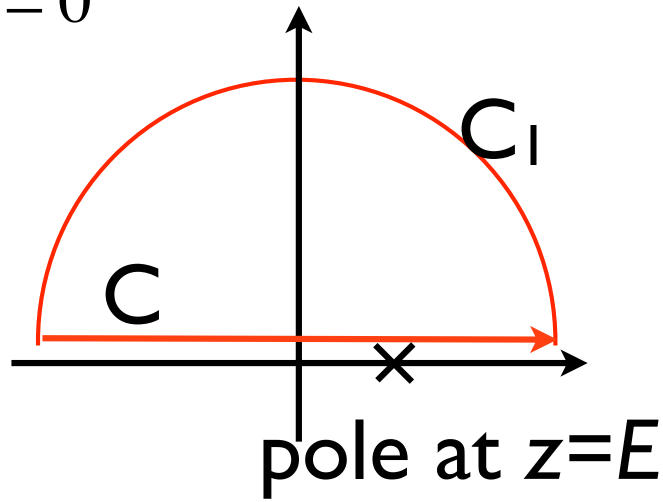
- where E is real, $z = \xi + i\eta$, and the contour C traverses $-\infty < \xi < \infty$ just above the real axis. $\eta \to 0^+$

- Analytical function

$$\int_{C+C_1} \frac{e^{-izt/\hbar}}{z-E} dz = 0$$



- At t<0 no pole, $f(E)+\int_{C_1}\frac{e^{-izt/\hbar}}{z-E}dz=0$



- $e^{\eta t/\hbar}\to 0$ at C1

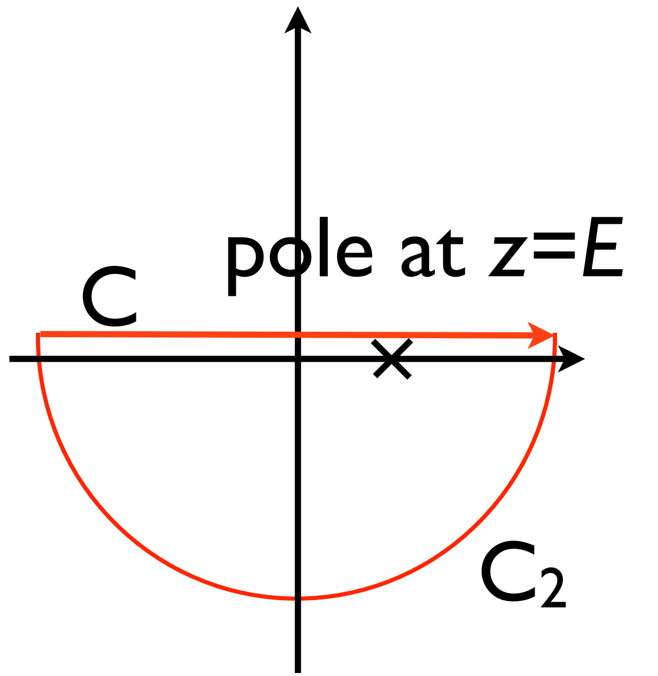
$$f(E)=\int_C\frac{e^{-i\varepsilon t/\hbar}}{\varepsilon-E}d\varepsilon=0$$

- At t>0 pole residue

$$f(E)+\int_{C_2}\frac{e^{-izt/\hbar}}{z-E}dz=2\pi i e^{-iEt/\hbar}$$

- $e^{\eta t/\hbar}\to 0$ at C2

$$f(E)=\int_C\frac{e^{-i\varepsilon t/\hbar}}{\varepsilon-E}d\varepsilon=-2\pi i e^{-iEt/\hbar}$$



- one can express $$e^{-iEt/\hbar}\theta(t) = \frac{i}{2\pi}\int_C \frac{e^{-izt/\hbar}}{z-E}dz$$

$$K(r,r';t) = \frac{i}{2\pi}\int_C dz e^{-izt/\hbar}\sum_{n\nu}\frac{\varphi_{n\nu}(r)\varphi^*_{n\nu}(r')}{z-E_n}$$

$$= \frac{i}{2\pi}\int_C dE e^{-iEt/\hbar}\sum_{n\nu}\frac{\varphi_{n\nu}(r)\varphi^*_{n\nu}(r')}{E-E_n+i\varepsilon}$$

ε is positive infinitesimal

Green's Functions

- Green's function for the time-independent Schrodinger equation

$$G(r,r';E)=\sum_{n\nu}\frac{\varphi_{n\nu}(r)\varphi^{*}_{n\nu}(r')}{E-E_n+i\varepsilon}$$

$$K(r,r';t)=\frac{i}{2\pi}\int_C dE e^{-iEt/\hbar}G(r,r';E)$$

- G satisfies

$$(E-H)G(r,r';E)=\delta(r-r')$$

- Green's function has simple poles at the eigenvalues of the Hamiltonian, with residues R_n whose spatial dependence give the corresponding eigenfunctions:

$$R_n = \sum_{v} \varphi_{nv}(r) \varphi_{nv}^{*}(r')$$

- If the Hamiltonian has a spectrum that is partially or wholly continuous, then the poles coalesce into branch cuts.

- The inverse FT gives Green's function in terms of the propagator:

$$G(r,r';E) = \frac{1}{i\hbar}\int_0^{\infty} dt e^{izt/\hbar} K(r,r';t) \qquad z = E + i\varepsilon$$

- The integral runs only over positive times because, by definition, this propagator K vanishes for t < 0, and for that reason is called "causal" or "retarded." Propagators with other boundary conditions in time can also be defined.

Free particle propagator

- Free particle hamiltonian

$$H = \frac{p^2}{2m} \qquad U = \exp\left(\frac{-ip^2 t}{2m\hbar}\right)$$

- propagator $K(x, x'; t)$ only depends on $(x - x')$

$$K(x, x'; t) = \langle x | \exp\left(\frac{-ip^2 t}{2m\hbar}\right) | x' \rangle \theta(t)$$

$$= \int \frac{dp}{2\pi\hbar} \langle x | \exp\left(\frac{-ip^2 t}{2m\hbar}\right) | p \rangle \langle p | x' \rangle \theta(t)$$

$$= \int \frac{dp}{2\pi\hbar} e^{ip(x-x')/\hbar} e^{\frac{-ip^2 t}{2m\hbar}} \theta(t)$$

- One can define $K(x,x';t) \to K(x-x',t)$

$$K(x,t) = \int \frac{dp}{2\pi\hbar} \exp\left(\frac{ipx}{\hbar} - \frac{ip^2 t}{2m\hbar} \right) \theta(t)$$

$$= \int \frac{dp}{2\pi\hbar} \exp\left[\left(\frac{ip}{\hbar} \right) \left(x - \frac{pt}{2m} \right) \right] \theta(t)$$

- characteristic length $l = \frac{pt}{m}$

$$p = \frac{\hbar}{l} \qquad l = \sqrt{\frac{\hbar t}{m}}$$

- Dimensionless variable

$$\xi = \frac{x}{l} = \sqrt{\frac{m}{\hbar t}}x \qquad \eta = \frac{p}{\hbar}l = \sqrt{\frac{t}{m\hbar}}p$$

$$\begin{aligned}
K(x,t) &= \frac{\theta(t)}{2\pi l}\int_{-\infty}^{\infty} d\eta \exp\left[i\eta\left(\xi - \frac{\eta}{2}\right)\right] \\
&= \frac{\theta(t)}{2\pi l}\int_{-\infty}^{\infty} d\eta \exp\left[-\frac{i\eta^2}{2} + i\xi\eta\right] \\
&= \frac{\theta(t)}{2\pi l}\int_{-\infty}^{\infty} d\eta \exp\left[-\frac{i(\eta-\xi)^2}{2} + \frac{i\xi^2}{2}\right] \\
&= \frac{\theta(t)}{2\pi l} e^{i\xi^2/2}\int_{-\infty}^{\infty} d\eta' e^{-i\eta'^2/2}
\end{aligned}$$

Gaussian integral

- if *a* is real

$$I(a)=\int_{-\infty}^{\infty} dx e^{-ax^2/2}=\frac{1}{\sqrt{a}}\int_{-\infty}^{\infty} du e^{-u^2/2}=\sqrt{\frac{2\pi}{a}}$$

- For complex $a=|a|e^{i\theta}$, the integral is defined by analytic continuation provided $-\frac{\pi}{2}\le\theta\le\frac{\pi}{2}$

$$I(a)=\sqrt{\frac{2\pi}{|a|}}e^{-i\theta/2}$$

- When *a* is pure imaginary $a=\pm i\lambda$

$$I(a)=\sqrt{\frac{2\pi}{i|\lambda|}}$$

$$
\begin{aligned}
K(x,t) &= \frac{\theta(t)}{2\pi l} e^{i\xi^2/2} \int_{-\infty}^{\infty} d\eta' e^{-i\eta'^2/2} \\
&= \frac{\theta(t)}{2\pi l} \sqrt{\frac{2\pi}{i}} e^{ix^2/2l^2} \\
&= \theta(t) \sqrt{\frac{m}{2\pi i\hbar t}} e^{imx^2/2\hbar t}
\end{aligned}
$$

Feynman Path Integral

- Consider the simplest situation, a single particle in one dimension, with the Hamiltonian

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

- The object of interest is the propagator,

$$K(b,a) = \langle x_b | U(t_b, t_a) | x_a \rangle \theta(t_b - t_a)$$

- Breaking the evolution from a to b into a large sequence of κ, small forward steps in time of duration τ by means of the composition law for U;
- Evaluating each small step explicitly;
- Showing that these steps sum to the form, $\sum_{P} \exp(iS/\hbar)$ where S is the classical action for some path P composed of linear segments from a to b;
- taking the limit defined by $t_b - t_a = \kappa\tau$

$$\tau \to 0$$

$$\kappa \to \infty$$

- The sequence of steps is a product of K, unitary transformations:

$$K(b,a)=\langle x_b|U(t_b,t_b-\tau)\cdots U(t_a+2\tau,t_a+\tau)U(t_a+\tau,t_a)|x_a\rangle\theta(t_b-t_a)$$

- Define $t_a=t_0$, $t_b=t_\kappa$, $t_k=t_0+k\tau$

$$\begin{aligned}K(b,a)&=\int dx_{\kappa-1}\cdots dx_2\,dx_1\langle x_\kappa|U(t_{\kappa-1}+\tau,t_{\kappa-1})|x_{\kappa-1}\rangle\cdots\\&\quad\cdots\langle x_2|U(t_1+\tau,t_1)|x_1\rangle\langle x_1|U(t_0+\tau,t_0)|x_0\rangle\\&=\int dx_{\kappa-1}\cdots dx_2\,dx_1\langle x_\kappa|e^{-iH(t_{\kappa-1})\tau/\hbar}|x_{\kappa-1}\rangle\cdots\\&\quad\cdots\langle x_2|e^{-iH(t_1)\tau/\hbar}|x_1\rangle\langle x_1|e^{-iH(t_0)\tau/\hbar}|x_0\rangle\end{aligned}$$

- Approximation 1

$$e^{-iH(t_j)\tau/\hbar} \simeq 1 - \frac{i}{\hbar} H\left(t_j\right)\tau$$

- however it spoil the unitary property as expressed in the composition law, and thereby abandon the superposition principle.

- Approximation 2 (Baker-Campbell-Hausdorff theorem)

$$e^{-iH(t_j)\tau/\hbar} \simeq e^{-iT\tau/\hbar} e^{-iV\tau/\hbar}$$

$$\langle x_{k+1} | e^{-iH(t_0)\tau/\hbar} | x_k \rangle \simeq \langle x_{k+1} | e^{-iT\tau/\hbar} e^{-iV\tau/\hbar} | x_k \rangle$$

$$= e^{-iV(x_k,t_k)\tau/\hbar} \langle x_{k+1} | e^{-iT\tau/\hbar} | x_k \rangle$$

$$= e^{-iV(x_k,t_k)\tau/\hbar} K(x_{k+1} - x_k, \tau)$$

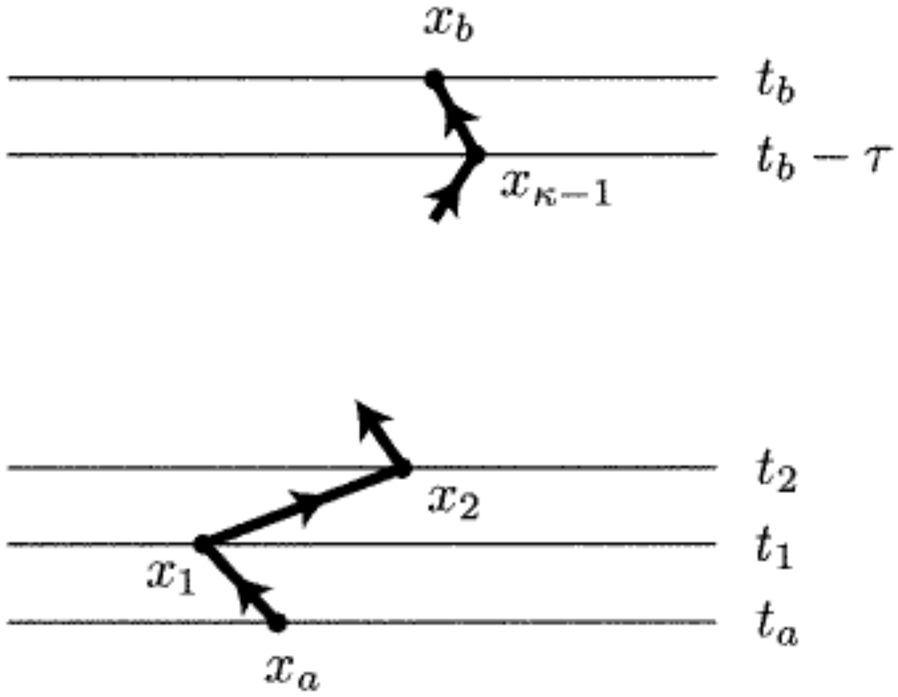
- K(x,t) is the free particle propagator

$$\langle x_{k+1} | e^{-iT\tau/\hbar} | x_k \rangle = \sqrt{\frac{m}{2\pi i\hbar\tau}} e^{-im(x_{k+1}-x_k)^2/2\hbar\tau}$$

$$\langle x_{k+1} | e^{-iH(t_0)\tau/\hbar} | x_k \rangle \simeq \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\frac{i}{\hbar}\left[\frac{m(x_{k+1} - x_k)^2}{2\tau} - V(x_k, t_k)\tau\right]$$

$$K(b,a)=\left(\frac{m}{2\pi i\hbar\tau}\right)^{\kappa/2}\int dx_{\kappa-1}\cdots dx_2\,dx_1$$

$$\times\exp\sum_k\frac{i\tau}{\hbar}\left[\frac{m\left(x_{k+1}-x_k\right)^2}{2\tau^2}-V\left(x_k,t_k\right)\right]$$



- The ratio $(x_{k+1}-x_k)/\tau$, as $\tau \rightarrow 0$, is the velocity in this step.

$$\frac{m\left(x_{k+1}-x_k\right)^2}{2\tau^2}-V\left(x_k,t_k\right)=\frac{1}{2}m\left[\dot{x}\left(t_k\right)\right]^2-V\left(x_k,t_k\right)=L\left(x_k,\dot{x}\left(t_k\right),t_k\right)$$

- Lagrangian $L=T-V$

$$\sum_k \tau L\left(x_k,\dot{x}\left(t_k\right),t_k\right)=\int_{t_a}^{t_b} dt' L\left(x\left(t'\right),\dot{x}\left(t'\right),t'\right)=S_{ba}\left[x\left(t\right)\right]$$

- The functional $S_{ba}[x(t)]$ is the classical action for motion along the arbitrary path $x(t)$.

$$K(b,a)=\left(\frac{m}{2\pi i\hbar\tau}\right)^{\kappa/2}\int dx_{\kappa-1}\cdots\int dx_2\int dx_1\exp\frac{i}{\hbar}S_{ba}\left[x(t)\right]$$

- In this expression the path x(t) is unrestricted except at the and points, and is not just one selected by the classical equation of motion, i.e., not just a path that minimizes the action. In the limit $\tau \to 0$, the integrals over the intermediate points (x_1 ... x_{K-1}) therefore include all paths from a to b.

- It is customary to write this last equation as

$$K(b,a)=\left(\frac{m}{2\pi i\hbar\tau}\right)^{\kappa/2}\int_a^b \mathcal{D}\left(x(t)\right)\exp\frac{i}{\hbar}S_{ba}\left[x(t)\right]$$

- Because the phase oscillates rapidly to not contribute in the integral. if the path is sufficiently erratic if

$$\left|x_{k+1} - x_k\right| \geq l = \sqrt{\frac{\hbar\tau}{m}}$$

- For a fixed time-slice parameter τ, a sufficiently large mass will suppress paths that are far from the differentiable classical path.

- For any mass, there is a τ sufficiently small to suppress paths that jump about in space by an amount that violates $\left|x_{k+1} - x_k\right| \leq l$

Free-Particle Path Integral

- Let $x(t)$ be an arbitrary path, $Q(t)$ the classical path from (x_a, t_a) to (x_b, t_b)

$$Q(t) = \frac{x_b - x_a}{t_b - t_a} t + x_a$$

- $y(t)$ be the deviation from the classical path.

$$y(t) = x(t) - Q(t)$$

$$y(t_a) = y(t_b) = 0$$

- First-order deviations from the classical path leave the action unchanged,

$$\dot{x}^2(t) = \left[\dot{Q}(t) + \dot{y}(t)\right]^2 \simeq \dot{Q}^2(t) + \dot{y}^2(t)$$

$$S_{ba}\left[Q(t) + y(t)\right] = \frac{1}{2}m\int_{t_a}^{t_b} dt\left[\dot{Q}^2(t) + \dot{y}^2(t)\right]$$

- The first term is the classical action,

$$S_{cl}(b,a) = \frac{1}{2}m\int_{t_a}^{t_b} dt\dot{Q}^2(t) = \frac{1}{2}m\frac{\left(x_b - x_a\right)^2}{t_b - t_a}$$

- The separation of arbitrary paths into the classical path and the departure there from thus results in

$$K(b,a) = F(t_b - t_a)\exp\left[\frac{i}{\hbar}S_{cl}(b,a)\right]$$

- F(b,a) is the integral over all paths from y=0 back to y=0 during the interval t_b - t_a :

$$F(t_b - t_a) = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}(y(t))\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\frac{1}{2}m\dot{y}^2(t)\right]$$

$$F(t) = \int dy K(0,t;y,t')K(y,t';0,0)$$

$$= F(t-t')F(t')\int dy \exp\frac{i}{\hbar}\left[S_{cl}(0,t;y,t') + S_{cl}(y,t';0,0)\right]$$

$$= F(t-t')F(t')\int dy \exp\frac{imy^2}{2\hbar}\left(\frac{1}{t-t'} + \frac{1}{t'}\right)$$

$$= F(t-t')F(t')\sqrt{\frac{2\pi i\hbar}{m}}\sqrt{\frac{(t-t')t'}{t}}$$

$$S_{cl}(0,t;y,t') + S_{cl}(y,t';0,0) = \frac{1}{2}m\left(\frac{y^2}{t-t'} + \frac{y^2}{t'}\right)$$

$$F(t) \propto \frac{1}{\sqrt{t}} \qquad F(t) = \sqrt{\frac{m}{2\pi i\hbar t}}$$

$$K(b,a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}} \exp\left[\frac{i}{\hbar} S_{cl}(b,a)\right]$$

$$= \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}} \exp\left[\frac{im}{2\hbar} \frac{(x_b - x_a)^2}{t_b - t_a}\right]$$

- Recall that

$$K(x,t) = \theta(t)\sqrt{\frac{m}{2\pi i\hbar t}} e^{imx^2/2\hbar t}$$

brute-force evaluation

$$F\left(t_b - t_a\right) = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}\left(y(t)\right) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{1}{2} m\dot{y}^2(t)\right]$$

$$F\left(t_b - t_a\right) = \left(\frac{m}{2\pi i\hbar\tau}\right)^{\kappa/2} \int dy_{\kappa-1}\cdots dy_2\, dy_1 \exp\frac{im}{2\hbar\tau}\sum_k \left(y_{k+1} - y_k\right)^2$$

- Introduce dimensionless variables, $\eta_k = \sqrt{\frac{m}{\hbar\tau}}\, y_k$

$$F\left(t_b - t_a\right) = \left(\frac{m}{2\pi i\hbar\tau}\right)^{\kappa/2} \left(\frac{\hbar\tau}{m}\right)^{(\kappa-1)/2} \int d\eta_{\kappa-1}\cdots d\eta_2\, d\eta_1 \exp\frac{i}{2}\sum_k \left(\eta_{k+1} - \eta_k\right)^2$$

$$= \left(\frac{m}{\hbar\tau}\right)^{1/2} \left(\frac{1}{2\pi i}\right)^{\kappa/2} \int d\eta_{\kappa-1}\cdots d\eta_2\, d\eta_1 \exp\frac{i}{2}\sum_k \left(\eta_{k+1} - \eta_k\right)^2$$

- The argument of the exponential is a quadratic form,

$$\sum_k \left(\eta_{k+1} - \eta_k\right)^2 = 2\left(\eta_1^2 + \eta_2^2 + \cdots + \eta_{\kappa-1}^2 - \eta_1\eta_2 - \eta_2\eta_3 - \cdots - \eta_{\kappa-2}\eta_{\kappa-1}\right)$$

$$= \mathbf{v}^T \Lambda \mathbf{v}$$

$$\mathbf{v} = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \vdots \\ \eta_{\kappa-2} \\ \eta_{\kappa-1} \end{pmatrix} \qquad \Lambda = \begin{pmatrix} 2 & -1 & 0 & \cdots & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ \vdots & & & \ddots & & \\ & & & & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix}$$

- diagonalizing Λ, one gets the eigenvalues $\{\lambda\}$ and eigenvectors $\{\zeta\}$

- reduces F to a product of Gaussian integrals.

$$\sum_k \left(\eta_{k+1} - \eta_k\right)^2 = \sum_k \lambda_k \zeta_k^2$$

$$d\eta_{\kappa-1} \cdots d\eta_2 d\eta_1 = d\zeta_{\kappa-1} \cdots d\zeta_2 d\zeta_1$$

- All λ are positive,

$$F\left(t_b - t_a\right) = \left(\frac{m}{2\pi i\hbar\tau}\right)^{1/2} \prod_k \int \frac{d\zeta_k}{\sqrt{2\pi i}} \exp\left(\frac{i}{2}\lambda_k \zeta_k^2\right)$$

$$F(t) = \left(\frac{m}{2\pi i\hbar\tau} \right)^{1/2} \prod_k \int \frac{d\zeta_k}{\sqrt{2\pi i}} \exp\left(\frac{i}{2} \lambda_k \zeta_k^2 \right)$$

$$= \left(\frac{m}{2\pi i\hbar\tau} \right)^{1/2} \prod_k \frac{1}{\sqrt{\lambda_k}}$$

$$= \left(\frac{m}{2\pi i\hbar\tau \det\Lambda} \right)^{1/2}$$

$$= \left(\frac{m}{2\pi i\hbar t} \right)^{1/2}$$

$$\det\Lambda = \prod_k \lambda_k = \kappa + 1$$