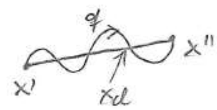
Lecture 2

9 Path integration via fluctuations around classical path

We still consider the free particle (only one classical path between x' and x'')

$$K_0(x'', x'; t) = \int_{x'=x(0)}^{x''=x(t)} \mathcal{D}[x(\tau)] \exp\left\{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}\tau\, \frac{m}{2}\,\dot{x}^2\right\}$$

Let $x(\tau) = x_{\mathrm{cl}}(\tau) + q(\tau)$; $\quad q$ is fluctuation around classical path with $q(0) = 0 = q(t)$.



$x_{\mathrm{cl}}(\tau) = \dfrac{x'' - x'}{t}\tau + x' \qquad$ linear motion

Consider free particle action

$$\begin{aligned}
S[x(\tau)] &= \frac{m}{2}\int_0^t \mathrm{d}\tau\, \dot{x}^2(\tau) = \frac{m}{2}\int_0^t \mathrm{d}\tau\, \left[\dot{x}_{\mathrm{cl}}(\tau) + \dot{q}(\tau)\right]^2(\tau) \\
&= \frac{m}{2}\int_0^t \mathrm{d}\tau\, \left[\dot{x}^2_{\mathrm{cl}}(\tau) + 2\dot{x}_{\mathrm{cl}}(\tau)\dot{q} + \dot{q}^2(\tau)\right](\tau) \\
&= S_{\mathrm{cl}} + m\dot{x}_{\mathrm{cl}} \underbrace{\int_0^t \mathrm{d}\tau\, \dot{q}}_{=q(t)-q(0)=0} + \frac{m}{2} \underbrace{\int_0^t \mathrm{d}\tau\, \dot{q}^2(\tau)}_{=q\dot{q}|_0^t - \int_0^t \mathrm{d}\tau\, q\ddot{q}} \\
&= S_{\mathrm{cl}} - \frac{m}{2}\int_0^t \mathrm{d}\tau\, q\ddot{q}
\end{aligned}$$

Path integral now reads

$$K_0(x'', x'; t) = \mathrm{e}^{(\mathrm{i}/\hbar)S_{\mathrm{cl}}} \int_{q(0)=0}^{q(t)=0} \mathcal{D}[q(\tau)] \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_0^t \mathrm{d}\tau\, q(\tau)\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\right) q(\tau)\right\}$$

Fluctuation operator: $\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\right)$ with Gauß integral

Consider the eigenvalue problem

$$-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\varphi_n(\tau) = \lambda_n \varphi_n(\tau) \qquad \text{with} \qquad \varphi(0) = 0 = \varphi(t)$$

Solution: $\quad \varphi_n(\tau) = \sqrt{\frac{2}{t}}\sin\left(\frac{n\pi}{t}\tau\right) \qquad$ with $\qquad \lambda_n = \left(\frac{n\pi}{t}\right)^2 > 0 \qquad n = 1, 2, 3, \ldots$

classical path is minimum of the action fucntional

Solutions are orthonormal: $\displaystyle\int_0^t \mathrm{d}\tau\, \varphi_n(\tau)\varphi_m(\tau) = \delta_{mn}$

Decompose $q(\tau)$ into these modes

$$q(\tau) = \sum_{n=1}^{\infty} c_n \varphi_n(\tau)$$

This is a linear transformation $q(\tau) \to c_n$.

The Jacobi determinate is a (unknown) constant.

$$\Longrightarrow \qquad \mathcal{D}[q(\tau)] = \mathcal{N}\prod_{n=1}^{\infty}\frac{\mathrm{d}c_n}{\sqrt{2\pi\mathrm{i}\hbar t/m}}$$

We also have

$$\int_0^t \mathrm{d}\tau\, q(\tau)\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\right) q(\tau) = \sum_{n=1}^{\infty}\lambda_n c_n^2$$

Hence the path integral reads

$$\begin{aligned} K_0(x'', x'; t) &= e^{(i/\hbar)S_{cl}} \mathcal{N} \prod_{n=1}^{\infty} \int \frac{dc_n}{\sqrt{2\pi i\hbar t/m}} \exp\left\{ i \frac{m\lambda_n}{2\hbar} c_n^2 \right\} \\ &= e^{(i/\hbar)S_{cl}} \mathcal{N} \prod_{n=1}^{\infty} \frac{1}{\sqrt{\lambda_n}} \stackrel{!}{=} \sqrt{\frac{m}{2\pi i\hbar t}}\, e^{(i/\hbar)S_{cl}} \end{aligned}$$

Note: $\mathcal{N} \prod_{n=1}^{\infty} \frac{1}{\sqrt{\lambda_n}} = \underbrace{\mathcal{N}}_{\to\infty} \underbrace{\prod_{n=1}^{\infty} \left(\frac{t}{\pi n}\right)}_{\to 0} = \sqrt{\frac{m}{2\pi i\hbar t}}$

Compare with finite dimensional integral

$$\int_{\mathbb{R}^D} d^D\vec{x} \, \exp\left\{ \frac{i}{2} \vec{x}^T A \vec{x} \right\} = \sqrt{\frac{(2\pi i)^D}{\det A}}$$

This allow interpretation of path integral as determinant of fluctuation operator

$$\int_{q(0)=0}^{q(t)=0} \mathcal{D}[q(\tau)] \exp\left\{ \frac{i}{\hbar} \frac{m}{2} \int_0^t d\tau \; q(\tau) \left(-\frac{d^2}{d\tau^2} \right) q(\tau) \right\} = \frac{\mathcal{N}'}{\sqrt{\det\left(-\frac{d^2}{d\tau^2}\right)}} = \sqrt{\frac{m}{2\pi i\hbar t}}$$

Determinants of operators are not well defined but their quotients may be
$\Longrightarrow$ Theorem of Coleman later

10 The quasi-classical approximation

Recall path integral representation of propagator

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

with action functional

$$S[x(\tau)] = \int_0^t d\tau \, \left[\frac{m}{2} \dot{x}^2(\tau) - V(x(\tau)) \right] .$$

10.1 Basic idea

For $S[x] \gg \hbar$ only those paths significantly contribute, which are near a stationary path where $\delta S \approx 0$

$\Longrightarrow$ Hamilton's principle (constructive interference)

Consider only paths up to second order deviations around such a classical path.
Let x_{cl} be a classical path with $\delta S[x_{cl}(\tau)] = 0$ and $x_{cl}(0) = x'$, $x_{cl}(t) = x''$
Expand action functional to 2nd order in q, with $x(\tau) = x_{cl}(\tau) + q(\tau)$

$$\begin{aligned} S[x(\tau)] &= \int_0^t d\tau \, \left[\frac{m}{2} (\dot{x}_{cl} + \dot{q})^2 - V(x_{cl} + q) \right] \\ &\approx \int_0^t d\tau \, \left[\frac{m}{2} \dot{x}_{cl}^2 + m\dot{x}_{cl}\dot{q} + \frac{m}{2} \dot{q}^2 - V(x_{cl}) - V'(x_{cl})q - \frac{1}{2} V''(x_{cl})q^2 + O(q^3) \right] \\ &= S[x_{cl}] + \delta S + \delta^2 S + \cdots \end{aligned}$$

Here we have

- $O(q^0)$: $S[x_{\rm cl}] := \int_0^t \mathrm{d}\tau \, \left[\frac{m}{2}\,\dot{x}_{\rm cl}^2 - V(x_{\rm cl})\right]$ the classical action along $x_{\rm cl}$
- $O(q^1)$: $\delta S := \int_0^t \mathrm{d}\tau \, \left[m\dot{x}_{\rm cl}\dot{q} - V'(x_{\rm cl})q\right] = \underbrace{m\dot{x}_{\rm cl}q|_0^t}_{=0} - \int_0^t \mathrm{d}\tau\, q\, \underbrace{\left[m\ddot{x}_{\rm cl} - V'(x_{\rm cl})\right]}_{=0} q = 0$
- $O(q^2)$: $\delta^2 S := \int_0^t \mathrm{d}\tau \, \left[\frac{m}{2}\,\dot{q}^2 - \frac{1}{2}V''(x_{\rm cl})q^2\right] = \frac{m}{2}\int_0^t \mathrm{d}\tau\, q(\tau)\left[-\partial_\tau^2 - \frac{1}{m}V''(x_{\rm cl})\right] q(\tau)$

This expansion must be done for each classical path x_α obeying $x_\alpha(0) = x'$ and $x_\alpha(t) = x''$. Note, in general there exist several solutions to this boundary value problem! $\alpha = 1, 2, 3, \ldots$

$$\Longrightarrow \qquad K(x'', x'; t) = \sum_{x_\alpha} \mathcal{F}_\alpha(t)\, \exp\left\{\frac{\mathrm{i}}{\hbar} S_\alpha\right\} \qquad \text{with} \qquad S_\alpha := S[x_\alpha]$$

and

$$\mathcal{F}_\alpha(t) := \int_{q(0)=0}^{q(t)=0} \mathcal{D}[q(\tau)]\, \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_0^t \mathrm{d}\tau\, q(\tau)\left[-\partial_\tau^2 - \frac{1}{m}V''(x_\alpha)\right] q(\tau)\right\}$$

Recall previous section

$$\mathcal{F}_\alpha(t) = \mathcal{F}_0(t)\sqrt{\frac{\det(-\partial_\tau^2)}{\det\left(-\partial_\tau^2 - \frac{1}{m}V''(x_\alpha)\right)}} \qquad \text{where} \qquad \mathcal{F}_0(t) := \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}}$$

10.2 Theorem of Coleman

Let f_W be the unique solution of the initial value problem

$$\left[-\partial_\tau^2 - W(\tau)\right] f_W(\tau) = 0\,, \qquad f_W(0) = 0 \qquad \text{and} \qquad \dot{f}_W(\tau) = 1\,.$$

Then

$$\boxed{\frac{\det\left[-\partial_\tau^2 - U(\tau)\right]}{\det\left[-\partial_\tau^2 - V(\tau)\right]} = \frac{f_U(t)}{f_V(t)}}$$

where the determinant $\det A$ is the product of the eigenvalues of operator A on the function space $\mathcal{H} := \left\{\varphi \in L^2([0,t]) | \varphi(0) = 0 = \varphi(t)\right\}$.
That is, Coleman's theorem relates the initial value problem with the boundary value problem.

Proof: see Tutorial Exercise 4

10.3 Lemma related to the fluctuation operator

$$\boxed{f_{\frac{1}{m}V''(x_\alpha)}(t) = -m\left[\frac{\partial^2 S_\alpha}{\partial x''\partial x'}\right]^{-1}}$$

Proof:
Let $x_\alpha(\tau) \equiv x_\alpha(x'', x', \tau)$ i.e. $x_\alpha(x'', x', 0) = x'$, $x_\alpha(x'', x', t) = x''$.
Let $p'_\alpha := m\dot{x}_\alpha$ be the initial momentum at $\tau = 0$ $\Longrightarrow$ $p'_\alpha = p'_\alpha(x'')$.
Let $J(x', p'_\alpha, \tau) := \frac{\partial x_\alpha(\tau)}{\partial p'_\alpha}$ variation of classical path when changing initial momentum.

- Newton: $m\ddot{x}_\alpha = -V'(x_\alpha)$ $\Longrightarrow$ $m\ddot{J} = -\frac{\partial V'(x_\alpha)}{\partial p'_\alpha} = -V''(x_\alpha)\frac{\partial x_\alpha}{\partial p'_\alpha} = -V''(x_\alpha)\, J$

$$\Longrightarrow \qquad \left[-\partial_\tau^2 - \frac{1}{m}V''\left(x_\alpha(\tau)\right)\right] J(x', p'_\alpha, \tau) = 0$$

$J(x', p'_\alpha, 0) = \frac{\partial x'}{\partial p'_\alpha} = 0$ as x' and x'' are independent and p'_α only depends on x''.

$\dot{J}(x', p'_\alpha, 0) = \frac{\partial \dot{x}_\alpha(0)}{\partial p'_\alpha} = \frac{1}{m}\frac{\partial p'_\alpha}{\partial p'_\alpha} = \frac{1}{m}$

$mJ(x', p'_\alpha, t) = f_{\frac{1}{m}V''(x_\alpha)}(t)$ obeys conditions needed for Coleman's theorem

- Consider action

$$\begin{aligned}
\frac{\partial S_\alpha}{\partial x'} &= \int_0^t \mathrm{d}\tau \, \frac{\partial}{\partial x'} \left[\frac{m}{2}\dot{x}_\alpha^2 - V(x_\alpha)\right] = \int_0^t \mathrm{d}\tau \left[m\dot{x}_\alpha \frac{\partial \dot{x}_\alpha}{\partial x'} - V'(x_\alpha)\frac{\partial x_\alpha}{\partial x'}\right] = \\
&= \int_0^t \mathrm{d}\tau \left[m\dot{x}_\alpha \partial_\tau \frac{\partial x_\alpha}{\partial x'} - V'(x_\alpha)\frac{\partial x_\alpha}{\partial x'}\right] = \\
&= m\dot{x}_\alpha \frac{\partial x_\alpha}{\partial x'}\bigg|_0^t - \int_0^t \mathrm{d}\tau \, \underbrace{\left[m\ddot{x}_\alpha + V'(x_\alpha)\right]}_{=0} \frac{\partial x_\alpha}{\partial x'} \\
&= m\dot{x}_\alpha(x'', x', t) \underbrace{\frac{\partial}{\partial x'} \underbrace{x_\alpha(x'', x', t)}_{=x''}}_{=0} - \underbrace{m\dot{x}_\alpha(x'', x', 0)}_{=p'_\alpha} \frac{\partial x'}{\partial x'} = -p'_\alpha
\end{aligned}$$

$\Longrightarrow$

$$-\frac{\partial^2 S_\alpha}{\partial x'' \partial x'} = \frac{\partial p'_\alpha}{\partial x''} = \left(\frac{\partial x''}{\partial p'_\alpha}\right)^{-1} = \left[J(x', p'_\alpha, t)\right]^{-1}$$

- Proof completed

10.4 Van Vleck-Pauli-Morette formula

Above result together with $f_0(t) = t$ for the free particle (see below) we arrive at

$$\frac{\det\left[-\partial_\tau^2\right]}{\det\left[-\partial_\tau^2 - \frac{1}{m}V''(x_\alpha(\tau))\right]} = \frac{f_0(t)}{f_{\frac{1}{m}V''(x_\alpha)}(t)} = -\frac{t}{m}\frac{\partial^2 S_\alpha}{\partial x'' \partial x'}$$

Hence

$$\mathcal{F}_\alpha(t) = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \left(-\frac{t}{m}\frac{\partial^2 S_\alpha}{\partial x'' \partial x'}\right)^{1/2} = \sqrt{\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 S_\alpha}{\partial x'' \partial x'}}$$

Van Vleck-Pauli-Morette formula:

$$\boxed{K(x'', x'; t) = \sum_{x_\alpha} \sqrt{\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 S_\alpha}{\partial x'' \partial x'}} \exp\left\{\frac{\mathrm{i}}{\hbar}S_\alpha\right\}}$$

In d dimension

$$K(x'', x'; t) = \sum_{x_\alpha} \sqrt{\left(\frac{\mathrm{i}}{2\pi\hbar}\right)^d \det\left(\frac{\partial^2 S_\alpha}{\partial x''_a \partial x'_b}\right)} \exp\left\{\frac{\mathrm{i}}{\hbar}S_\alpha\right\}$$

10.5 Examples

- Free particle: $V(x) = 0$

$$\begin{aligned}
&-\partial_\tau^2 f_0(\tau) = 0 \quad \Longrightarrow \quad f_0(\tau) = a\tau + b \\
&f_0(0) = 0 \quad \Longrightarrow \quad b = 0\,, \quad \dot{f}_0(0) = 1\,, \quad \Longrightarrow \quad a = 1 \quad \Longrightarrow \quad f_0(t) = t
\end{aligned}$$

Single classical path

$$S_{\mathrm{cl}}(x'', x'; t) = \frac{m}{2t}\left(x'' - x'\right)^2 \qquad \Longrightarrow \qquad \frac{\partial^2 S_{\mathrm{cl}}}{\partial x'' \partial x'} = -\frac{m}{t}$$

Check Lemma:

$$f_0(t) = -m\left[\frac{\partial^2 S_{\mathrm{cl}}}{\partial x'' \partial x'}\right]^{-1} = -m\left(-\frac{t}{m}\right) = t \qquad \text{Q.E.D.}$$

- Harmonic oscillator: $V(x) = \frac{m}{2}\omega^2 x^2 \qquad \Longrightarrow \qquad \frac{1}{m}V''(x) = \omega^2$

  $\left(-\partial_\tau^2 - \omega^2\right) f_{\omega^2}(\tau) = 0 \qquad \Longrightarrow \qquad f_{\omega^2}(\tau) = a\sin(\omega\tau) + b\cos(\omega\tau)$
  $f_{\omega^2}(0) = 0 \quad \Longrightarrow \quad b = 0\,, \qquad \dot{f}_{\omega^2}(0) = 1\,, \quad \Longrightarrow \quad a = \frac{1}{\omega} \qquad \Longrightarrow \qquad f_{\omega^2}(t) = \frac{1}{\omega}\sin(\omega t)$

  Classical action: Homework problem 6

  $$S_{\rm cl}(x'', x'; t) = \frac{m\omega}{2\sin(\omega t)}\left[(x''^2 + x'^2)\cos(\omega t) - 2x''x'\right] \qquad \Longrightarrow \qquad \frac{\partial^2 S_{\rm cl}}{\partial x''\partial x'} = -\frac{m\omega}{\sin(\omega t)}$$

  Check Lemma:

  $$f_{\omega^2}(t) = -m\left[-\frac{m\omega}{\sin(\omega t)}\right]^{-1} = \frac{\sin(\omega t)}{\omega} \qquad \text{Q.E.D.}$$

For application to Green's function see Exercise 5.
Eigenvalues: $\quad \lambda_n = \left(\frac{\pi n}{t}\right)^2 - \omega^2\,, \qquad$ assume $\quad \pi n < \omega t < \pi(n+1)$
$\Longrightarrow$ first n eigenvalues are negative; each contributes a phase factor $\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}}$ (Morse index!)
See also Tutorial Exercise 3 and Homework Problem 7.

Tutorial Exercise 4.

11 Path integrals in polar coordinates

Assume central potential $V(\vec{x}) = V(r)$ with $r = |\vec{x}|$
Lagrangian:

$$L(\dot{\vec{x}}, \vec{x}) = \frac{m}{2}\dot{\vec{x}}^2 - V(r) = \frac{m}{2}\left[\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\varphi}^2\right] - V(r)$$

Polar coordinates:

$$\begin{aligned} x &= r\sin\theta\cos\varphi & \quad & r \in [0\infty[\,, \quad \theta \in [0,\pi]\,, \quad \varphi \in [0, 2\pi[\\ y &= r\sin\theta\sin\varphi & & \mathrm{d}^3\vec{x} = r^2\mathrm{d}r\,\sin\theta\mathrm{d}\theta\,\mathrm{d}\varphi \\ z &= r\cos\theta & & \end{aligned}$$

Path Integral:

$$K(\vec{x}'', \vec{x}'; t) = \lim_{N\to\infty}\prod_{j=1}^{N-1}\int \mathrm{d}^3\vec{x}_j \prod_{j=1}^{N}\left(\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{3/2}\mathrm{e}^{(\mathrm{i}/\hbar)S_j}$$

Short-time action:

$$S_j := \frac{m}{2\varepsilon}|\Delta\vec{x}_j|^2 - V(r_j)\varepsilon$$

Note

$$|\Delta\vec{x}_j|^2 = |\vec{x}_j - \vec{x}_{j-1}|^2 = r_j^2 + r_{j-1}^2 - 2r_j r_{j-1}\cos\Theta_j$$

$$\cos\Theta_j := \frac{\vec{x}_j\cdot\vec{x}_{j-1}}{r_j r_{j-1}} = \cos\theta_j\cos\theta_{j-1} + \sin\theta_j\sin\theta_{j-1}\Delta\varphi_j$$

11.1 Performing the angular integration

$$\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2\varepsilon}\left[-2r_j r_{j-1}\cos\Theta_j\right]\right\} = \exp\left\{\frac{m r_j r_{j-1}}{\mathrm{i}\hbar\varepsilon}\cos\Theta_j\right\}$$

Gegenbauer expansion formula (recall QM scattering on sph. sym. potential or Rayleigh's expansion)

$$\mathrm{e}^{\mathrm{i}z\cos\Theta} = \left(\frac{2}{\mathrm{i}z}\right)^{\nu}\Gamma(\nu)\sum_{\ell=0}^{\infty}(\ell+\nu)C_\ell^\nu(\cos\Theta)\mathrm{I}_{\ell+\nu}(\mathrm{i}z)$$

C_ℓ^ν: Gegenbauer polynomial, ultra spherical polynomial

$\nu = \frac{1}{2}$ $\quad C_\ell^{1/2}(\cos\Theta) = P_\ell(\cos\Theta)$ Legendre polynomial

$\nu = \frac{d-2}{2}$ appears in d dimension, $\quad d = 3 \to \nu = \frac{1}{2}$

I_μ: modified Bessel function

Γ: Gamma function

Now we let $\nu = \frac{1}{2}$, $\quad z = -\frac{mr_jr_{j-1}}{\hbar\varepsilon}$, $\quad \Gamma(1/2) = \sqrt{\pi}$

$$\begin{aligned}\exp\left\{\frac{\mathrm{i}m}{2\varepsilon\hbar}|\Delta\vec{x}_j|^2\right\} &= \exp\left\{\frac{\mathrm{i}m}{2\varepsilon\hbar}(r_j^2+r_{j-1}^2)\right\}\sqrt{\frac{2\pi\mathrm{i}\hbar\varepsilon}{mr_jr_{j-1}}}\\ &\quad\times\sum_{\ell_j=0}^{\infty}\left(\ell_j+\frac{1}{2}\right)\mathrm{I}_{\ell_j+\frac{1}{2}}\left(\frac{mr_jr_{j-1}}{\mathrm{i}\hbar\varepsilon}\right)P_{\ell_j}(\cos\Theta_j)\end{aligned}$$

Short-time propagator:

$$\begin{aligned}K(\vec{x}_j,\vec{x}_{j-1};\varepsilon) &= \left(\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}\right)^{3/2}\sqrt{\frac{\pi\mathrm{i}\hbar\varepsilon}{2mr_jr_{j-1}}}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{m}{2\varepsilon}(r_j^2+r_{j-1}^2)-V(r_j)\varepsilon\right]\right\}\\ &\quad\times\sum_{\ell_j=0}^{\infty}(2\ell_j+1)\mathrm{I}_{\ell_j+\frac{1}{2}}\left(\frac{mr_jr_{j-1}}{\mathrm{i}\hbar\varepsilon}\right)P_{\ell_j}(\cos\Theta_j)\\ &= \frac{m}{\mathrm{i}\hbar\varepsilon\sqrt{r_jr_{j-1}}}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{m}{2\varepsilon}(r_j^2+r_{j-1}^2)-V(r_j)\varepsilon\right]\right\}\\ &\quad\times\sum_{\ell_j=0}^{\infty}\left(\frac{2\ell_j+1}{4\pi}\right)\mathrm{I}_{\ell_j+\frac{1}{2}}\left(\frac{mr_jr_{j-1}}{\mathrm{i}\hbar\varepsilon}\right)P_{\ell_j}(\cos\Theta_j)\end{aligned}$$

Recall spherical harmonics $Y_{\ell m}(\theta,\varphi)$:

$$\left(\frac{2\ell_j+1}{4\pi}\right)P_{\ell_j}(\cos\Theta_j) = \sum_{m_j=-\ell_j}^{\ell_j}Y_{\ell_jm_j}(\theta_j,\varphi_j)Y^*_{\ell_jm_j}(\theta_{j-1},\varphi_{j-1})$$

and

$$\int_0^\pi \mathrm{d}\theta_j\sin\theta_j\int_0^{2\pi}\mathrm{d}\varphi_j\,Y_{\ell_jm_j}(\theta_j,\varphi_j)Y^*_{\ell_{j+1}m_{j+1}}(\theta_j,\varphi_j) = \delta_{\ell_j\ell_{j+1}}\delta_{m_jm_{j+1}}$$

Angular integration becomes trivial

$$K(\vec{x}'',\vec{x}';t) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{4\pi}P_\ell(\cos\Theta)K_\ell(r'',r';t)$$

with $\cos\Theta := \frac{\vec{x}''\cdot\vec{x}'}{r''r'}$ and radial path integral

$$K_\ell(r'',r';t) := \lim_{N\to\infty}\prod_{j=1}^{N-1}\int_0^\infty \mathrm{d}r_j\,r_j^2\prod_{j=1}^{N}k_\ell(r_j,r_{j-1};\varepsilon)$$

where the radial short-time propagator is given by

$$k_\ell(r_j,r_{j-1};\varepsilon) := \frac{m}{\mathrm{i}\hbar\varepsilon\sqrt{r_jr_{j-1}}}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\frac{m}{2\varepsilon}(r_j^2+r_{j-1}^2)-V(r_j)\varepsilon\right]\right\}\mathrm{I}_{\ell+\frac{1}{2}}\left(\frac{mr_jr_{j-1}}{\mathrm{i}\hbar\varepsilon}\right)$$

11.2 Discussion of radial path integral

Consider asymptotic expression of Bessel function

$$I_\nu(z) = \frac{\mathrm{e}^z}{\sqrt{2\pi z}}\left\{1-\frac{\nu^2-1/4}{2z}+O(z^{-2})\right\} \qquad \text{for} \qquad \mathrm{Re}\,z>0\,,$$

recall

$$z = \frac{m r_j r_{j-1}}{\mathrm{i}\hbar\varepsilon} \qquad \text{and} \qquad \operatorname{Im} m > 0 \Leftrightarrow \operatorname{Re} z > 0 \qquad \text{and} \qquad \frac{1}{z} = O(\varepsilon)$$

Within a path integral we may set

$$I_\nu(z) \approx \frac{1}{\sqrt{2\pi z}} \exp\left\{ z - \frac{\nu^2 - 1/4}{2z} \right\}$$

This allows us to express the short-time propagator as

$$k_\ell(r_j, r_{j-1}; \varepsilon) \approx \frac{m}{\mathrm{i}\hbar\varepsilon\sqrt{r_j r_{j-1}}} \sqrt{\frac{\mathrm{i}\hbar\varepsilon}{2\pi m r_j r_{j-1}}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S_j^{(\ell)}} = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar\varepsilon}} \frac{1}{r_j r_{j-1}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S_j^{(\ell)}}$$

with radial short-time action

$$\begin{aligned} S_j^{(\ell)} &:= \frac{m}{2\varepsilon}(r_j^2 + r_{j-1}^2) - V(r_j)\varepsilon - \frac{m r_j r_{j-1}}{\varepsilon} - \frac{(\ell + \frac{1}{2})^2 - \frac{1}{4}}{2 m r_j r_{j-1}} \hbar^2 \varepsilon \\ &= \frac{m}{2\varepsilon} \Delta r_j^2 - \left(V(r_j) + \frac{\ell(\ell+1)}{2 m r_j r_{j-1}} \right) \varepsilon \end{aligned}$$

and radial effective potential

$$V_{\text{eff}}(r_j) = V(r_j) + \frac{\ell(\ell+1)}{2m\hat{r}_j^2}$$

Comments:

- Centrifugal potential shows up as expected
- Becomes problematic for explicit integration due to singular term $\sim 1/r^2$ for $r \searrow 0$
- Always remember that this originally comes from a Bessel function. The radial part of Brownian motion in $\mathbb{R}^3$ is not a Wiener but a Bessel process (later)

11.3 The radial harmonic oscillator

Here we have $V(r) = \frac{m}{2}\omega^2 r^2$. For short-time action we choose arithmetic mean of squared distance

$$V(r_j) = \frac{m\omega^2}{4}(r_j^2 + r_{j-1}^2)$$

Short-time propagator

$$k_\ell(r_j, r_{j-1}; \varepsilon) = \frac{m}{\mathrm{i}\hbar\varepsilon\sqrt{r_j r_{j-1}}} \exp\left\{ \frac{\mathrm{i}}{\hbar} \left[\frac{m}{2\varepsilon}(r_j^2 + r_{j-1}^2) - \frac{m\omega^2}{4}(r_j^2 + r_{j-1}^2)\varepsilon \right] \right\} \mathrm{I}_{\ell+\frac{1}{2}} \left(\frac{m r_j r_{j-1}}{\mathrm{i}\hbar\varepsilon} \right)$$

Let $\sin\phi := \omega\varepsilon \quad \to \quad \cos\phi = \sqrt{1 - \sin^2\phi} = 1 - \frac{1}{2}\omega^2\varepsilon^2 + O(\varepsilon^4)$ approx. only in potential term

$$k_\ell(r_j, r_{j-1}; \varepsilon) = \frac{m\omega}{\mathrm{i}\hbar\sin\phi\sqrt{r_j r_{j-1}}} \exp\left\{ \frac{\mathrm{i}}{\hbar} \frac{m\omega}{2}(r_j^2 + r_{j-1}^2)\cot\phi \right\} \mathrm{I}_{\ell+\frac{1}{2}} \left(\frac{m\omega r_j r_{j-1}}{\mathrm{i}\hbar\sin\phi} \right)$$

Define

$$v_\lambda(\eta'', \eta'; \phi) := \frac{1}{\mathrm{i}\sin\phi} \exp\left\{ \mathrm{i}(\eta'' + \eta')\cot\phi \right\} \mathrm{I}_\lambda \left(\frac{2\sqrt{\eta''\eta'}}{\mathrm{i}\sin\phi} \right)$$

with $\operatorname{Re}\lambda > 0, \quad 0 < \eta'', \eta' < \infty, \quad 0 < \phi < \pi$.

Using Weber's formula in its modified form (see exercise 7) where $\operatorname{Re}\lambda > 0$ and $\operatorname{Re}\alpha > 0$

$$\int_0^\infty \mathrm{d}r\, r\, \mathrm{e}^{\alpha r^2} \mathrm{I}_\lambda\left(\frac{ar}{\mathrm{i}}\right) \mathrm{I}_\lambda\left(\frac{br}{\mathrm{i}}\right) = \frac{\mathrm{i}}{2\alpha} \exp\left\{ -\frac{\mathrm{i}}{4\alpha}(a^2 + b^2) \right\} \mathrm{I}_\lambda\left(-\frac{\mathrm{i}ab}{2\alpha} \right)$$

one can show

$$\boxed{\int_0^\infty \mathrm{d}\eta\, v_\lambda(\eta'',\eta;\phi'')v_\lambda(\eta,\eta';\phi') = v_\lambda(\eta'',\eta';\phi''+\phi')}$$

Now we let $\eta_j := \frac{m\omega}{2\hbar}r_j^2$ and write

$$k_\ell(r_j,r_{j-1};\varepsilon) = \frac{m\omega}{\hbar}\,(r_j r_{j-1})^{-1/2}\,v_{\ell+\frac{1}{2}}(\eta_j,\eta_{j-1};\phi)$$

Explicit path integration:

$$\begin{aligned}
K_\ell(r'',r';t) \;&:= \lim_{N\to\infty}\prod_{j=1}^{N-1}\int_0^\infty \mathrm{d}r_j\, r_j^2 \prod_{j=1}^{N} k_\ell(r_j,r_{j-1};\varepsilon)\\
&= \frac{m\omega}{\hbar}\frac{1}{\sqrt{r''r'}}\lim_{N\to\infty}\prod_{j=1}^{N-1}\int_0^\infty \underbrace{\mathrm{d}r_j\, r_j\frac{m\omega}{\hbar}}_{=\mathrm{d}\eta_j}\prod_{j=1}^{N} v_{\ell+\frac{1}{2}}(\eta_j,\eta_{j-1};\phi)\\
&= \frac{m\omega}{\hbar}\frac{1}{\sqrt{r''r'}}\lim_{N\to\infty} v_{\ell+\frac{1}{2}}(\eta'',\eta';N\phi)\\
&\qquad \lim_{N\to\infty} N\phi = \lim_{N\to\infty}\left(N\arcsin\frac{\omega t}{N}\right) = \omega t\\
&= \frac{m\omega}{\hbar}\frac{1}{\sqrt{r''r'}} v_{\ell+\frac{1}{2}}(\eta'',\eta';\omega t)\\
&= \frac{1}{\sqrt{r''r'}}\frac{m\omega}{\mathrm{i}\hbar\sin\omega t}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m\omega}{2}(r''^2+r'^2)\cot\omega t\right\}\mathrm{I}_{\ell+\frac{1}{2}}\left(\frac{m\omega r''r'}{\mathrm{i}\hbar\sin\omega t}\right)
\end{aligned}$$

Recall

$$K(\vec{x}'',\vec{x}';t) = \sum_{\ell=0}^{\infty} K_\ell(r'',r';t)\sum_{m-\ell}^{\ell} Y_{\ell m}(\theta'',\varphi'')Y^*_{\ell m}(\theta',\varphi')$$

For $\omega t = n\pi$, i.e. $t = nT/2$, $n\in\mathbb{N}$, above expressions are to be understood in a distributional sense. See Homework problem 7.

Spectral properties:
Consider Hille-Hardy formula

$$\begin{aligned}
&\frac{1}{1-\rho^2}\exp\left\{-\frac{1}{2}(x^2+y^2)\frac{1+\rho^2}{1-\rho^2}\right\}\mathrm{I}_\nu\left(\frac{2xy\rho}{1-\rho^2}\right) =\\
&\qquad = (xy)^\nu\exp\left\{-\frac{1}{2}(x^2+y^2)\right\}\sum_{n=0}^{\infty}\frac{n!\rho^{2n+\nu}}{\Gamma(n+\nu+1)}\,\mathrm{L}_n^{(\nu)}(x^2)\mathrm{L}_n^{(\nu)}(y^2)
\end{aligned}$$

$\mathrm{L}_n^{(\nu)}$: Associated Laguerre polynomials and $\rho\in\mathbb{C}\backslash\{-1,+1\}$.

Let $x = r'/r_0$, $y = r''/r_0$, $r_0 := \sqrt{\hbar/m\omega}$, $\nu = \ell+1/2$ and $\rho = \mathrm{e}^{-\mathrm{i}\omega t}$, $\omega t\neq n\pi$.
Note that

$$\frac{2\rho}{1-\rho^2} = \frac{2\mathrm{e}^{-\mathrm{i}\omega t}}{1-\mathrm{e}^{-2\mathrm{i}\omega t}} = \frac{1}{\mathrm{i}\sin\omega t}\,,\qquad \frac{1+\rho^2}{1-\rho^2} = \frac{\cos\omega t}{\mathrm{i}\sin\omega t} = \frac{1}{\mathrm{i}}\,\cot\omega t$$

Radial propagator

$$\begin{aligned}
K_\ell(r'',r';t) \;&= \frac{1}{\sqrt{xy}}\frac{2\rho}{1-\rho^2}\exp\left\{-\frac{1}{2}(x^2+y^2)\frac{1+\rho^2}{1-\rho^2}\right\}\mathrm{I}_{\ell+\frac{1}{2}}\left(\frac{2xy\rho}{1-\rho^2}\right)\\
&= \frac{2\rho}{\sqrt{xy}}(xy)^{\ell+\frac{1}{2}}\exp\left\{-\frac{1}{2}(x^2+y^2)\right\}\sum_{n=0}^{\infty}\frac{n!\rho^{2n+\ell+\frac{1}{2}}}{\Gamma(n+\ell+\frac{3}{2})}\,\mathrm{L}_n^{(\ell+\frac{1}{2})}(x^2)\mathrm{L}_n^{(\ell+\frac{1}{2})}(y^2)\\
&\overset{!}{=} \sum_{n=0}^{\infty}\mathrm{e}^{-(\mathrm{i}/\hbar)E_n t}R_{n\ell}(r'')R_{n\ell}(r')
\end{aligned}$$

with $\rho^{2n+\ell+\frac{1}{2}} = \mathrm{e}^{-\mathrm{i}\omega t(2n+\ell+\frac{3}{2})}$ we arrive at

$$E_n = \hbar\omega(2n + \ell + \tfrac{3}{2})$$
$$R_{n\ell}(r) = \sqrt{\frac{2n!}{\Gamma(n + \ell + \frac{3}{2})}} \left(\frac{r}{r_0}\right)^{\ell} \mathrm{e}^{-r^2/2r_0^2}\, \mathrm{L}_n^{(\ell+\frac{1}{2})}\left(r^2/r_0^2\right)$$

A long way to a well-know result, but our first explicit non-trivial path integral!