Path integration in open quantum systems

YUSUF KASIM & IVAN SAYCHENKO
SUPERVISOR: JANOS POLONYI

Outline

- Introduction
  - Malkovian evolution
  - Path integral for free particle
  - Path integral for a quadratic Lagrangian
- Electron in a magnetic field (Ivan)
  - Analytical computation
  - Parametrization with coupling running constants
- Numerical results for the harmonic oscillator (Yusuf)
  - Using path integral formalism
  - Using closed time path formalism

Introduction
Markovian evolution

Be the evolution operator : $U(t,t_0) \quad \text{with} \quad t \geqslant t_0$

Such that : $U(t,t_k)U(t_k,t_0) = U(t,t_0)$

$$U(t,t_0) = \mathbb{1}$$

$$\left(\frac{\partial U(t,t_0)}{\partial t}\right)_{t=t_0} = -\frac{H}{\hbar}$$

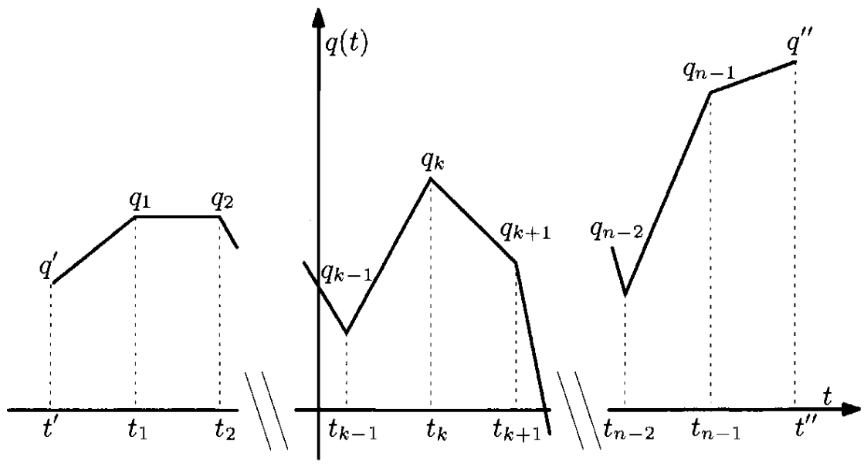
U describes the evolution of a state from t_0 to t. Be $G(y,t;x,t_0) = \langle y| U(t,t_0) |x\rangle$

Introduction
Markovian evolution

Let’s divide [x,y] in N+1 subintervals.

$$U(t,t_0) = U(t,t_N)U(t,t_{N-1})\cdots U(t_1,t_0)$$

$$\mathbb{1} = \int dx\, |x\rangle \langle x|$$



$$G(y,t;x,t_0) = \int_{x,t_0}^{y,t} dx_1 \cdots dx_N \langle y| U(t,t_N) |x_N\rangle \langle x_N| U(t,t_{N-1}) |x_{N-1}\rangle \cdots \langle x_1| U(t_1,t_0) |x\rangle$$

$$= \int_{x,t_0}^{y,t} [dx] \exp\left(i \frac{S[x]}{\hbar} \right)$$

J. Zinn-Justin Path Integrals in Quantum Mechanics, Oxford University Press, 2005

Path integral for a free particle

- Be a free particle, evolving from x (at t_0) to y (at t) : $\mathcal{L} = \frac{m}{2}\dot{x}$

$$G(y,t;x,t_0) = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{(N+1)/2}\int dx_1\ldots dx_N \exp\left(\frac{im}{\hbar 2\epsilon}\sum_{j=0}^{N}(x_{j+1}-x_j)^2\right) \qquad \epsilon = \frac{t}{N+1}$$

- decimation (renormalization theory) :

$$\frac{m}{2\pi i\hbar\epsilon}\int dx_1 \exp\left(\frac{im}{2\hbar\epsilon}(x_0-x_1)^2 + \frac{im}{2\hbar\epsilon}(x_1-x_2)^2\right) = \sqrt{\frac{m}{2\pi i\hbar(2\epsilon)}}\exp\left(\frac{im}{2\hbar(2\epsilon)}(x_2-x_0)^2\right)$$

$$G(y,t;x,t_0) = \sqrt{\frac{m}{2\pi i\hbar t}}\exp\left(\frac{im}{2\hbar t}(y-x)^2\right)$$

Path integral for a quadratic Lagrangian

- Be a harmonic oscillator into a magnetic field : $\mathcal{L} = \frac{m}{2}\dot{x} + b(t)x\dot{x} - \frac{1}{2}c(t)x^2 - e(t)x$

- Split x to "classical" path (Euler-Lagrange solution) + fluctuations : $x = \bar{x} + y$ with $y(t_i) = y(t_f) = 0$

- Taylor expansion of the action : $S[x] = S[\bar{x}] + \left(\frac{\delta S}{\delta x}\right)_{\bar{x}} y + \frac{1}{2}\left(\frac{\delta^2 S}{\delta x^2}\right)_{\bar{x}} y^2$

$$G(y,t;x,t_0) = \int_{x,t_0}^{y,t} [dx] \exp\left(i\frac{S[\bar{x}]}{\hbar}\right) \exp\left(i\frac{1}{2\hbar}\delta^2 S[x] y^2\right)$$

$$= \exp\left(i\frac{S_{cl}(y,t;x,t_0)}{\hbar}\right) \int_{0,t_0}^{0,t} [dy] \exp\left(i\frac{1}{2\hbar}\delta^2 S[x] y^2\right)$$

$$= \sqrt{\frac{m}{2\pi i\hbar f(t)}} \exp\left(i\frac{S_{cl}(y,t;x,t_0)}{\hbar}\right)$$

Electron in a magnetic field
Analytical computation

Be an electron in a magnetic field B defined by : $\mathbf{B} = B\mathbf{e_z}$

with potential vector $\mathbf{A} = By\mathbf{e_x} + Bx\mathbf{e_y}$

$$S[\mathbf{x}] = \int_{t_i}^{t_f} dt \frac{m}{2}\dot{\mathbf{x}}^2(t) + \frac{e}{c}\dot{\mathbf{x}}(t) \cdot \mathbf{A}(\mathbf{x}(t))$$

$$= \sum_{j=1}^{N+1} p_{x\ j}(x_j - x_{j-1}) - \frac{p_{x\ j}^2}{2m} - \frac{1}{2m}\left(p_y - \frac{e}{c}Bx_j\right)^2$$

« 2D harmonic oscillator like », corresponding to a quadratic Lagrangian

Electron in a magnetic field
Analytical computation

$$G(\mathbf{y}, t_f; \mathbf{x}; t_i) = \left(\frac{M}{2\pi i\hbar t}\right)^{3/2} \frac{\omega_L t/2}{sin(\omega_L t/2)} exp\left(\frac{i}{\hbar} S_{cl}\right)$$

$$S_{cl} = \frac{m}{2}\left(\frac{z_f - z_i}{t} + \frac{\omega_L}{2} cot\left(\frac{\omega_L t}{2}\right)((x_f - x_i)^2 + (y_f - y_i)^2) + \omega_L(x_i y_f - x_f y_i) + \omega_L(x_f y_f - x_i y_i)\right)$$

Notes :

-In classical mechanics, the electron describes circles in the xy-plane.

-the electron is free along z-axis

Parametrization with coupling running constants

Let's parametrize the action using running coupling constants :

$$S_{cl}^{\perp} = \frac{m(t)}{2t}(\mathbf{y}-\mathbf{x})^2 + \frac{m(t)\omega_L}{2}|\mathbf{x}\times\mathbf{y}| + \frac{m(0)\omega_L}{2}[\mathbf{x}\cdot\mathbf{y}]_{t_i}^{t_f}$$

With the running mass : $m(t) = \frac{1}{2}\omega_L t \; cot\left(\frac{\omega_L t}{2}\right)$

And Landau (cyclotron) frequency : $\omega_L = \frac{e}{m(0)c}B$

Numerical simulations

- We tried doing simulations for a harmonic oscillator using Monte Carlo simulations and the metropolis algorithm.
- The basis of the metropolis algorithm is to take a random change in one variable and check the change in action and following the principle of least action decide the probability of taking or rejecting a move
- The propagator for the harmonic oscillator is given by:

$$G(x,t;x^{'}) = \sqrt{\frac{m}{2\pi\hbar i\Delta t}}\exp\left\{-\frac{i}{\hbar}xD^{-1}x\right\}$$

- Where D^{-1} is the inverse of the Feynman green function that we get from functional derivative of the generator functional

$$D^{-1} = \frac{m}{2}(\partial_t)^2 - m\omega^2 + i\epsilon$$

Numerical simulations

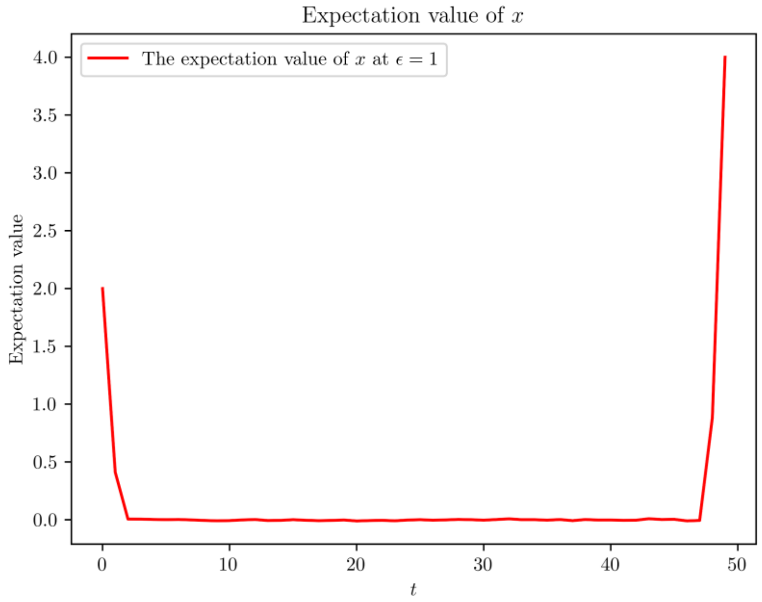
- The extra imaginary term $i\epsilon$ comes from the generator function which is the Feynman Green function
- The expectation value for an observable x is given by
- $< x > = \frac{\int dx P(x) x}{\int dx\, P(x)}$
- But if the probability is given by a complex number it becomes more difficult. We can then use a small trick

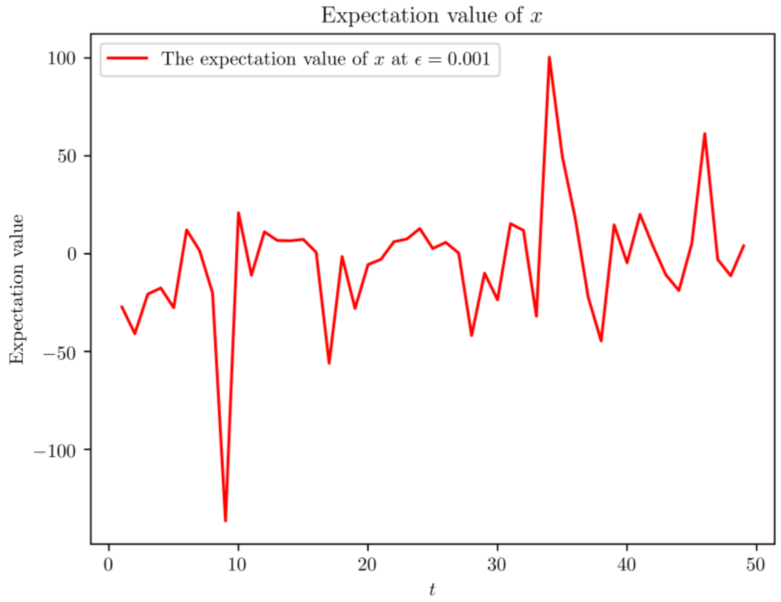
$$< x >= \frac{\frac{\int dx P'(x) e^{i\phi} x}{\int dx P'(x)}}{\frac{\int dx P'(x) e^{i\phi}}{\int dx P'(x)}} = \frac{< e^{i\phi} x >}{< e^{i\phi} >}$$

- Where P' is the absolute magnitude of the probability and ϕ is the polar angle

Numerical simulations

- In our case the ϵ will be the guidance for the metropolis and will stabilize of ϕ.
- We found that at low values of ϵ the integral diverges and for us $\epsilon \to 0$ so we run into a problem where we need to keep ϵ around $\epsilon = 1$ even if it's not very physical

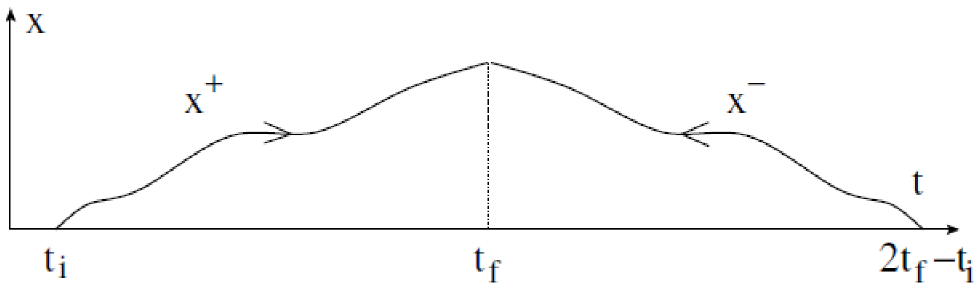




Numerical simulations
CTP formalism

- The Closed Time Path (CTP) formalism can be summed by the imagining the world line of a system and then reversing the time arrow at the end and thus creating two world lines one in the "positive" time direction and the other in the "negative" direction
- Introducing semi-holonomic forces (non conservative forces)
- We will thus have 2 "actions" for each subsystem
- And we can then define a new effective action

$$\tilde{S}[\tilde{x}] = S[x_+] - S[x_-]$$



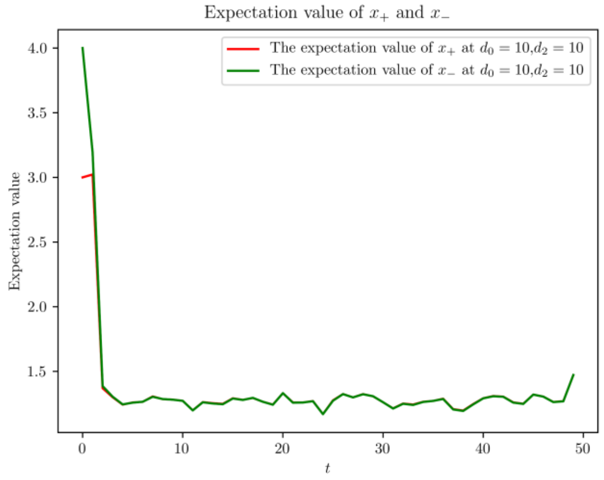
Positive and negative systems, J.Polonyi 2016

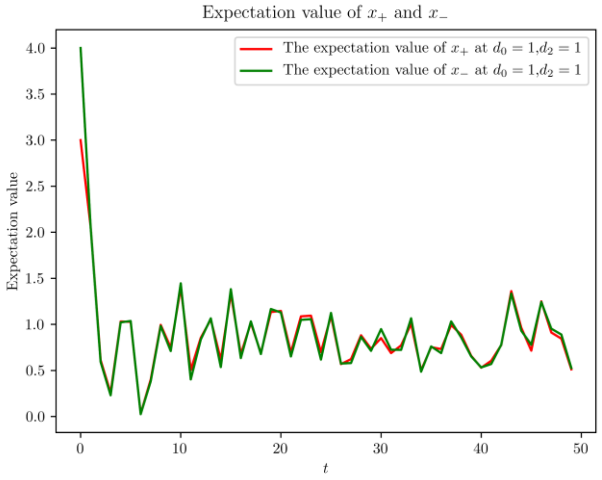
CTP formalism

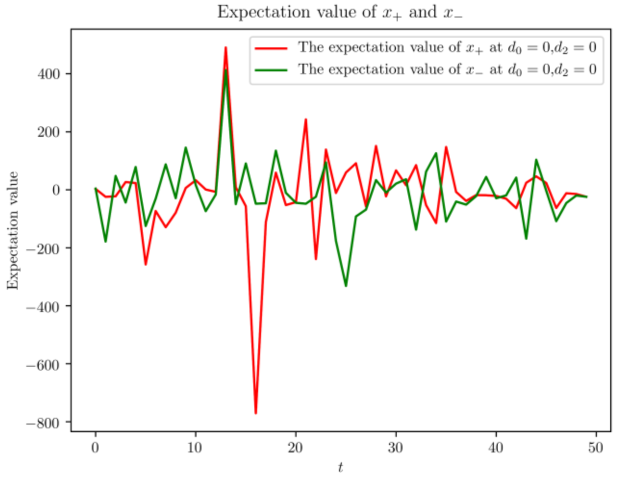
- If we take the harmonic oscillator Lagrangian and add a semi-holonomic friction term and after removing the non-unitary terms we can the final Lagrangian for the harmonic oscillator given by:

$$\mathcal{L} = m\dot{x}\dot{x}^d - m\nu x^d \dot{x} - m\omega x^d x + \frac{i}{2} d_2 \dot{x}^{d2} + \frac{i}{2} d_0 x^{d2}$$

- Where $x = (x_+ + x_-)/2$ and $x^d = x_+ - x_-$. ν is the friction term and d_0, d_2 will describe the decoherence between the positions and velocity, respectively.
- The d_0, d_2 will stabilize the metropolis algorithm here.
- Physically they represent the decoherence between the system and the environment and this show the importance of the openness of the system







CTP formalism

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