Faculté de physique et ingénierie
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Quantum mechanics, path integrals and stochastic quantisation

UE3 Physique en laboratoire 2019 - 2020
M1 Magistère de physique fondamentale

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Summary

State of art on path integrals and stochastic quantisation

Work done on the subject

Secondary work done on the subject

‘’Thirty-one years ago, Dick Feynman told me about his 'sum over histories' version of quantum mechanics. The electron does anything it likes, he said. 'It goes in any direction at any speed, forward or backward in time, however it likes, and then you add up the amplitudes and it gives you the wave-function.' I said to him, 'You're crazy'. But he wasn't.’’

F.J. Dyson

Path-Integral formulation of quantum mechanics

Directly based on the notion of a propagator:

$$K(q,t|q_0,t_0) \;=\; \langle q|e^{-i\hat{H}(t-t_0)/\hbar}|q_0\rangle$$

Which is related to the evolution of the wave function by the Huygens principle:

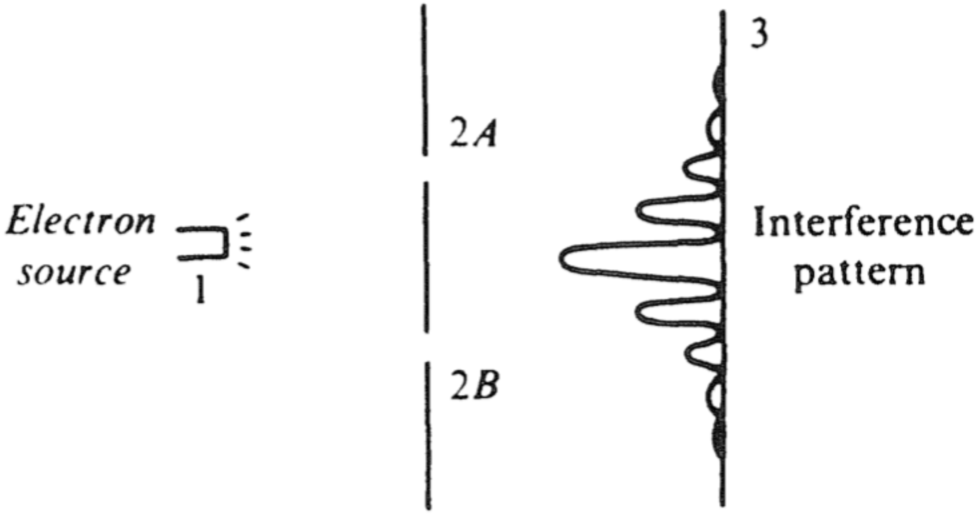
$$\psi(q,t) \;=\; \int \mathrm{d}q_0 \; K(q,t|q_0,t_0)\,\psi(q_0,t_0)$$

Path-Integral formulation of quantum mechanics

In the same way, it is also possible to introduce an intermediate point between ti and tf:

$$K(q_f t_f;\, q_i t_i) = \int K(q_f t_f;\, qt) K(qt;\, q_i t_i)\, dq$$

Example: with the Young slits:



$$P(3;\, 1) = |K(3;\, 1)|^2$$

$$K(3;\, 1) = K(3;\, 2A) K(2A;\, 1) + K(3;\, 2B) K(2B;\, 1)$$

Path-Integral formulation of quantum mechanics

By considering a free-particle with an Lagrangian as: $L = T - V$ we can generelize the propagator as:

$$\langle q_{\mathrm{f}} t_{\mathrm{f}} | q_{\mathrm{i}} t_{\mathrm{i}} \rangle = \lim_{n \to \infty} \left(\frac{m}{\mathrm{i} h \tau} \right)^{(n+1)/2} \int \prod_{1}^{n} \mathrm{d} q_j \exp \left\{ \frac{\mathrm{i}\tau}{\hbar} \sum_{0}^{n} \left[\frac{m}{2} \left(\frac{q_{j+1} - q_j}{\tau} \right)^2 - V \right] \right\}$$

By identification:

$$\langle q_{\mathrm{f}} t_{\mathrm{f}} | q_{\mathrm{i}} t_{\mathrm{i}} \rangle = N \int \mathfrak{D} q \exp \left[\frac{\mathrm{i}}{\hbar} \int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} L(q, \dot{q}) \, \mathrm{d} t \right]$$

Some words about stochastic quantisation

''The basic idea of stochastic quantization is to consider the Euclidean path integral measure as the stationary distribution of a stochastic process'':

$$\langle \phi(x_1) \cdots \phi(x_n) \rangle = \frac{\int D\phi \exp\{-(1/\hbar) S_E\} \, \phi(x_1) \cdots \phi(x_n)}{\int D\phi \exp\{-(1/\hbar) S_E\}}$$

If we identify $h = kbT$ we may, as a statistical expectation value with respect to a system in equilibrium at a temperature T

S_E: Eudidean action

Some words about stochastic quantisation

To realize Euclidian action simulations with this idea, a ''fictious'' time need to be introduce: $\phi(x) \to \phi(x, t)$

Our field evolve with that fictious time by a stochastic differential equation as the Langevin equation:

$$\partial\phi(x, t)/\partial t = -\delta S_{\mathrm{E}}/\delta\phi(x, t) + \eta(x, t)$$

Finally, we get: $\lim_{t\to\infty} \langle \phi(x_1, t) \cdots \phi(x_k, t) \rangle_\eta = \langle \phi(x_1) \cdots \phi(x_k) \rangle$

Research strategy

- Realize a simulation of an Euclidian anharmonic oscillator and calculate correlation functions

- Find a way to extract the energy gap between the first excitate and fundamental state

- Return in the real time

The aim of this project

In quantum field theories, problems of some path integrals not well defined and not well simulated

To solve this problem with simple system of quantum mechanics and return after in quantum field theories

The energy gap symbolizes the smallest excitation of our systeme by adding a particule

How simulate a quantum anharmonic oscillator in an Euclidian time with stochastic quantisation ?

We have the action:

$$S_E = \int \frac{1}{2}\dot{\phi}^2 + \frac{1}{2}mw^2\phi^2 + \frac{\lambda}{4!}\phi^4 \mathrm{d}t$$

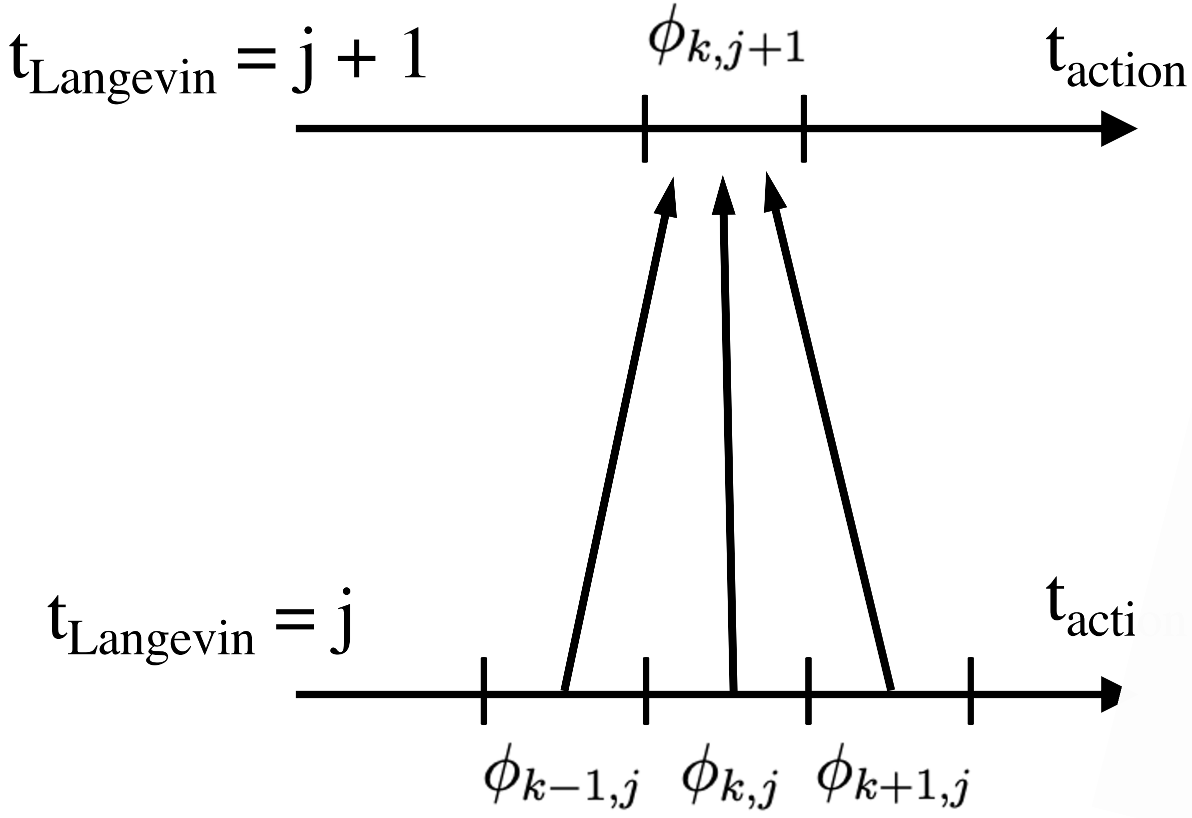
We need to introduce two discrete times: time of Langevin equation (j) and time of action (k):

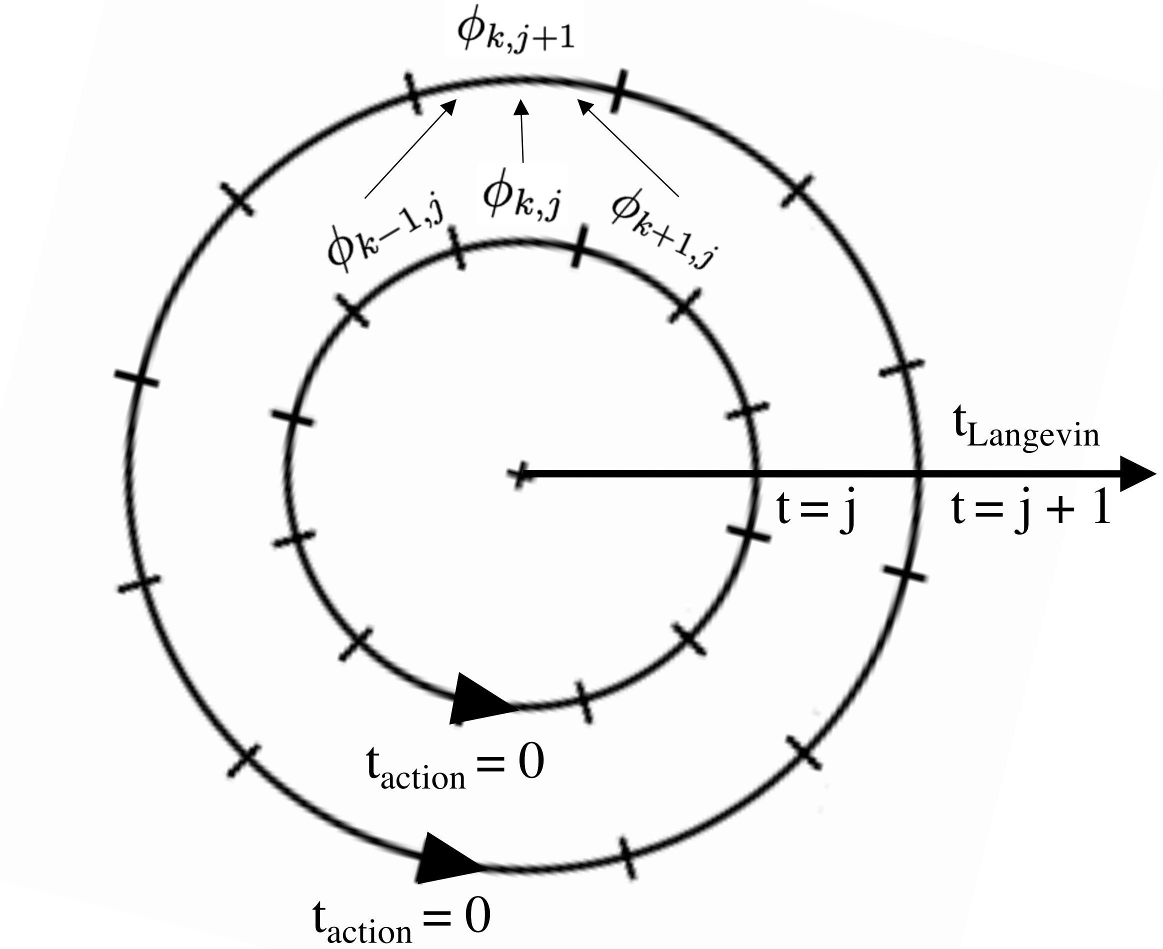
$$\phi \Longrightarrow \phi_{k,j}$$

We get the Langevin equation for this action:

$$\frac{\phi_{k,j+1} - \phi_{k,j}}{\Delta t_{Lan}} = \frac{\phi_{k+1,j} - 2\phi_{k,j} + \phi_{k-1,j}}{\Delta t_{action}} - mw^2\phi_{k,j} - \frac{\lambda}{3!}\phi_{k,j}^3 + \eta$$

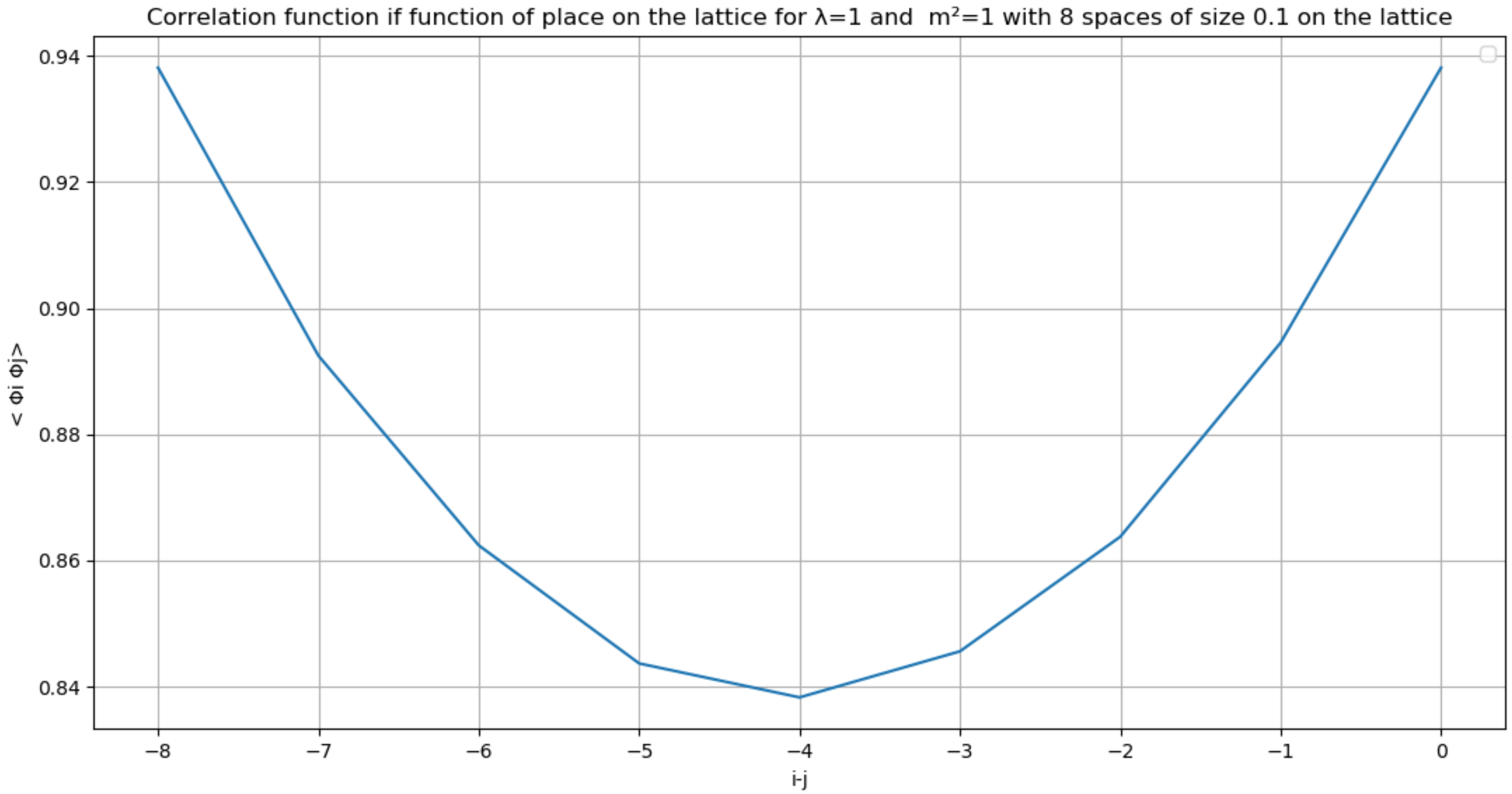
How simulate a quantum anharmonic oscillator in an Euclidian time with stochastic quantisation ?





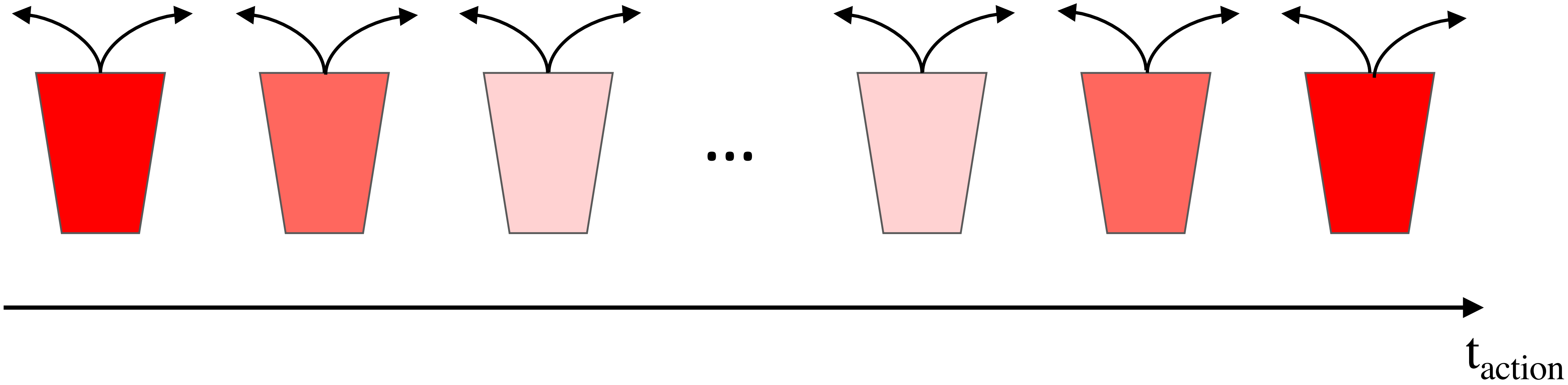
We need to introduce periodic boundary conditions

First result of a simulation



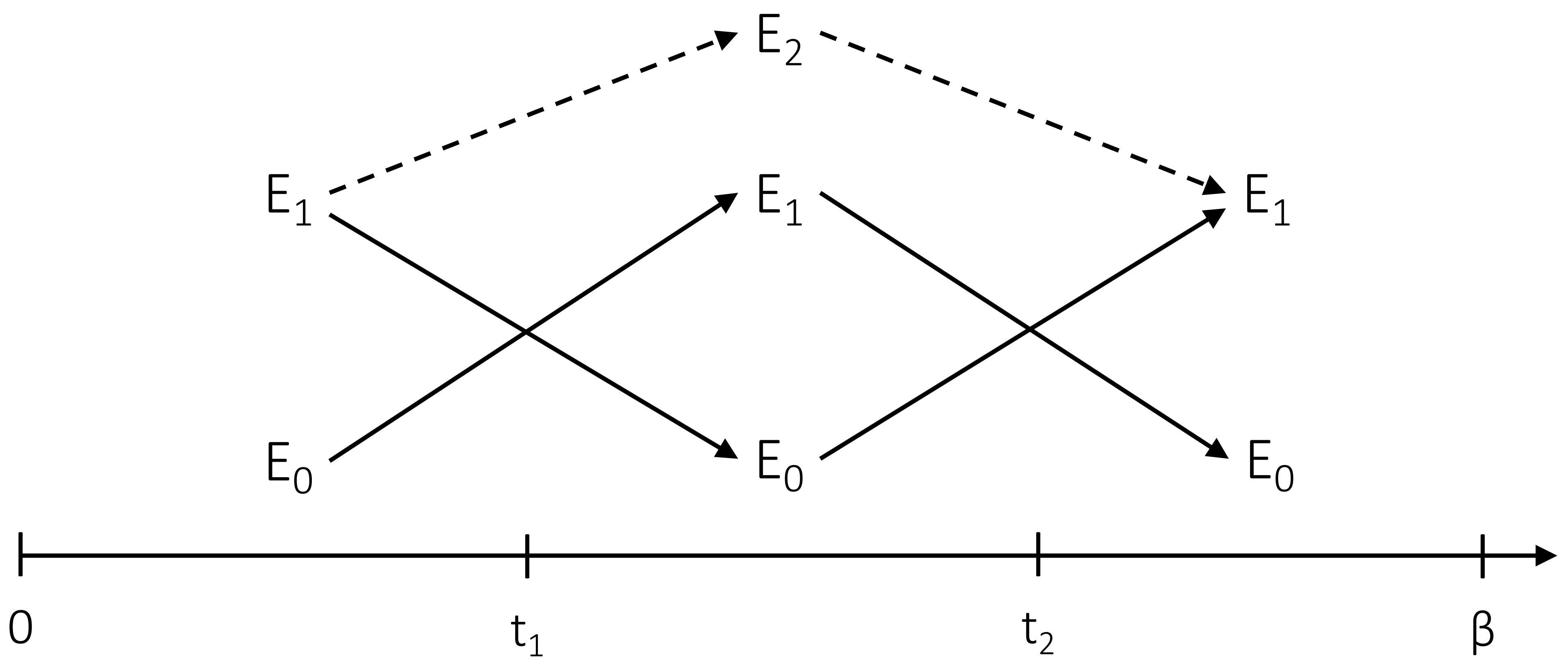
What is problematic with this kind of simulation ?

It is due to the periodic boundary conditions:



We cannot see a real relaxation of the initial excited states

How to extract this energy gap with its conditions with this periodic boundary condition ?



How to extract this energy gap with its conditions with this periodic boundary condition ?

Theoretically this leads us to the following formula:

$$< \phi(t)\phi(t') >= \sum_n < n|U(t_0,t_1)x(t_1)U(t_1,t_2)x(t_2)U(t_2,\beta)|n >$$

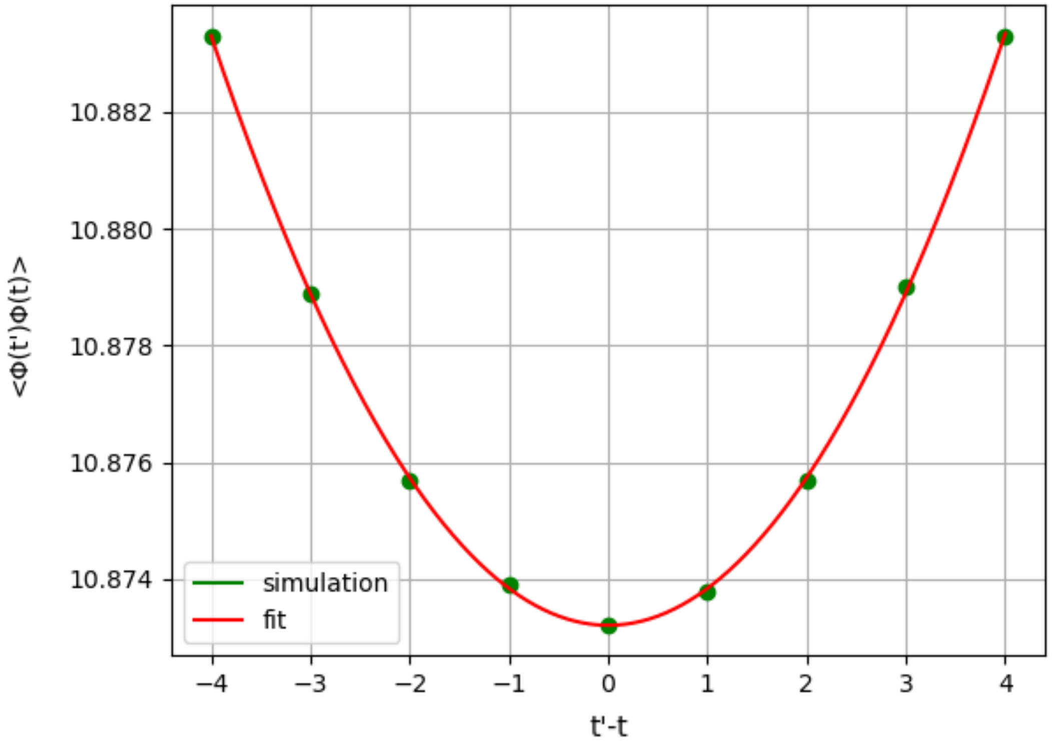
With: $\hat{x}(t) = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)$ and with $t' = t_2$ and $t = t_1$

In the limit $(t_2-t_1)>>1$ and $(\beta-t_2)>>1$:

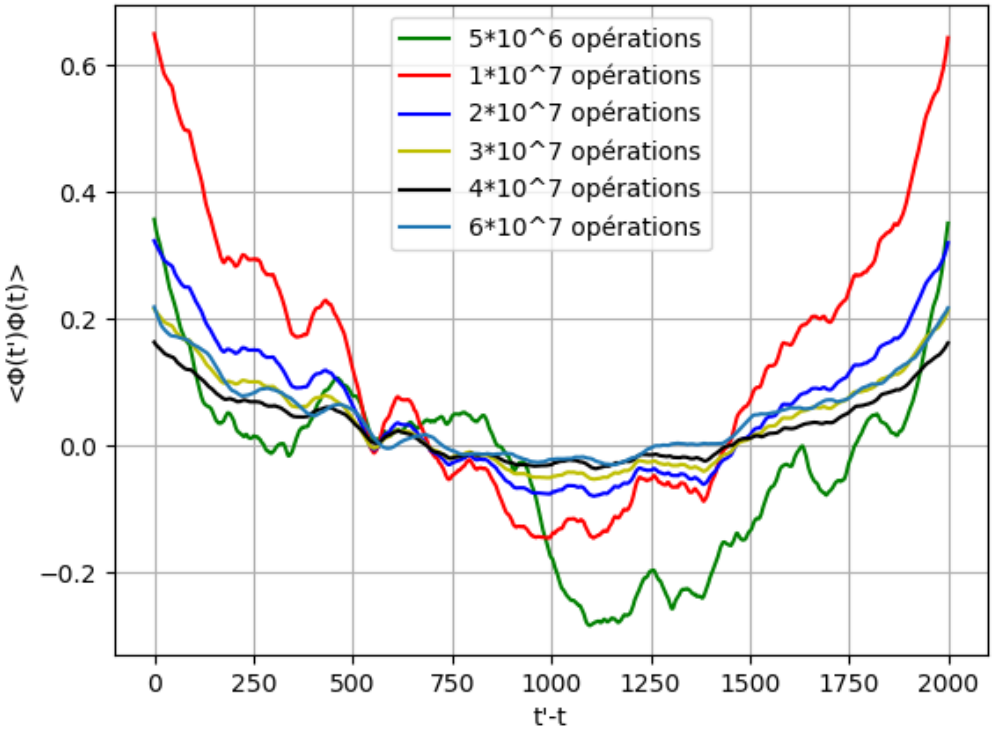
$$< \phi(t)\phi(t') >= \frac{1}{2}e^{-E_0 t_1}e^{-E_1(t_2-t_1)}e^{-E_0(\beta-t_2)} + \frac{1}{2}e^{-E_1 t_1}e^{-E_0(t_2-t_1)}e^{-E_1(\beta-t_2)}$$

Results of simulations

Test of the shape of formula



Results of more realistic simulation

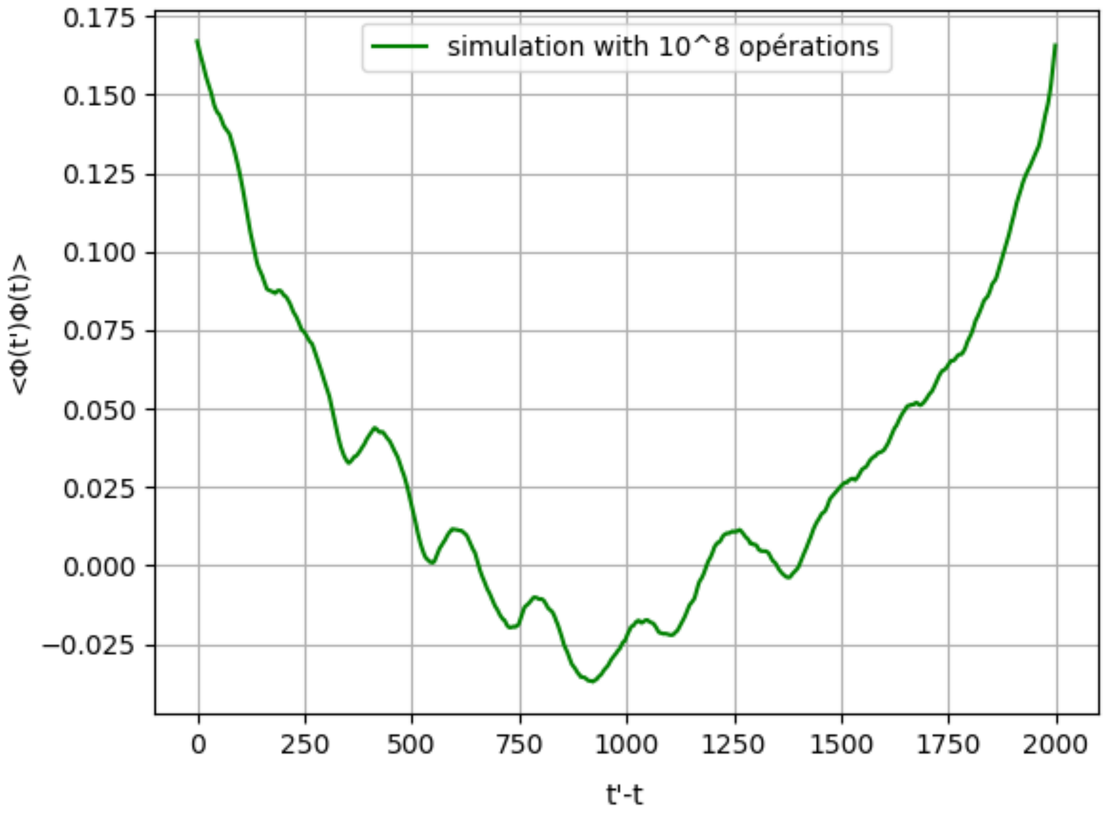


How to verify that the theory works?

With the harmonic oscillator, we know that the energy gap is equal to ω:

$$w_{simulation} = \frac{2}{\Delta t}\sin(\frac{w\Delta t}{2})$$

Problematic with this simulation



Increase the simulation time to improve the statistical equilibrium

Code a program allowing better extraction of the energy gap

Work done but not presented

Bibliography:

- Study of the formalism of the path integral
- Study of the instantons (tunnel effect of particules in double-well potential)
- Semi-classical approximations

Simulation:

- Brownian motion with Langevin equation
- Brownian motion with complex Langevin equation
- Simple action as quadratic and quartic
- Correction of the stability with transformation as rotation or polynomial

Bibliography

Damgaard, P. H., & Hüffel, H. (1987). Stochastic quantization. *Physics Reports*, *152*(5-6), 227-398.

Ryder, L. H. (1996). *Quantum field theory* (2nd ed.). Cambridge ; New York: Cambridge University Press.

Courses of Mr POLONYI