PATH INTEGRAL FORMULATION OF NON-EQUILILBRIUM DYNAMICS

Below we provide a brief description of the construction of the non-equilibrium path integral for quantum mechanical systems. Details of the derivation can also be found e.g. in J. Berges lecture notes `https://arxiv.org/abs/1503.02907` or in any graduate level textbook on Quantum mechanics or Quantum Field Theory.

1. Construction of the Path Integral

We are interested in computing the real-time evolution of a generic local observable $O(\hat{x},\hat{p})$, which in the Schroedinger picture can be expressed as

$$O(t) = \mathrm{tr}\Big(O(\hat{x},\hat{p})\hat{\rho}(t)\Big) \tag{1}$$

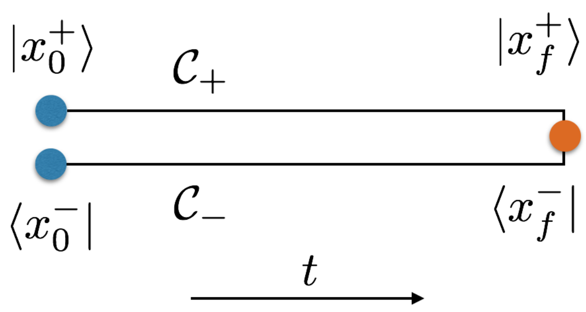
where $\hat{\rho}(t) = e^{-i\hat{H}t/\hbar}\ \hat{\rho}_0\ E^{+i\hat{H}t/\hbar}$ is the time dependent density operator for an arbitrary initial state $\hat{\rho}_0$. We will assume that the Hamiltonian of the system be of the form

$$H(\hat{x},\hat{p}) = T(\hat{p}) + V(\hat{x}), \qquad \text{with} \qquad T(\hat{p}) = \frac{\hat{p}^2}{2m}. \tag{2}$$

Inserting complete sets of states we can perform the usual construction to express the expectation value as

$$O(t) = \int_{x_f^+\, x_f^-\, x_0^+\, x_0^-} \langle x_f^-|O(\hat{x},\hat{p})|x_f^+\rangle\, \langle x_f^+|e^{-i\hat{H}t/\hbar}|x_0^+\rangle\, \langle x_0^-|e^{+i\hat{H}t/\hbar}|x_f^-\rangle\, \langle x_0^+|\hat{\rho}_0|x_0^-\rangle. \tag{3}$$

One finds that the general expression features three distinct pieces, related to the initial conditions, the non-equilibrium evolution and the operator matrix elements. Specifically, the non-equilibrium evolution is described by the product of a forward amplitude $\langle x_f^+|e^{-i\hat{H}t/\hbar}|x_0^+\rangle$ and (the complex conjugate of) a backward amplitude $\langle x_0^-|e^{+i\hat{H}t/\hbar}|x_f^-\rangle$.



Graphically, the expression in Eq. (3) can be represented as in Fig. 1 by a closed time path $\mathcal{C} = \mathcal{C}_+ + \mathcal{C}_-$, which is usually referred to as the Schwinger-Keldysh contour. In the following, the variables and states representing the dynamics on the upper branch $\mathcal{C}_+$ of the will be labeled with superscript $+$, while the variables and states representing representing the dynamics on the lower branch $\mathcal{C}_-$ of the contour will be labeled with $-$ superscripts.

1.1. **Construction of the path integral for the transition amplitude.** By discretizing the time direction into N discrete time steps of size Δt the transition matrix element on the + branch of the Schwinger-Keldysh contour can be rewritten as

$$\begin{aligned} \langle x_f^+|e^{-i\hat{H}t/\hbar}|x_0^+\rangle &= \lim_{N\to\infty} \langle x_f^+|\prod_{i=0}^{N} e^{-i\hat{H}\Delta t/\hbar}|x_0^+\rangle \\ &= \lim_{N\to\infty} \langle x_f^+|\left(\prod_{i=0}^{N}\int_{x_i\, p_i} |p_i\rangle\langle p_i|e^{-iT(\hat{p})\Delta t/\hbar}e^{-iV(\hat{x})\Delta t/\hbar}|x_i\rangle\langle x_i|\right)|x_0^+\rangle \\ &= \lim_{N\to\infty} \langle x_f^+|\left(\prod_{i=0}^{N}\int_{x_i\, p_i} |p_i\rangle\langle p_i|e^{-iH(x_i,p_i)\Delta t/\hbar}|x_i\rangle\langle x_i|\right)|x_0^+\rangle\,, \\ &= \lim_{N\to\infty} \langle x_f^+|\left(\prod_{i=0}^{N}\int_{x_i\, p_i} |p_i\rangle e^{-ip_ix_i/\hbar}e^{-iH(x_i,p_i)\Delta t/\hbar}\langle x_i|\right)|x_0^+\rangle \\ &= \lim_{N\to\infty} \langle x_f^+|\left(\prod_{i=0}^{N}\int_{x_i\, p_i} |p_i\rangle\langle x_i|\right) e^{\frac{i}{\hbar}\sum\limits_{i=0}^{N}\left(-p_ix_i-H(x_i,p_i)\Delta t\right)}|x_0^+\rangle, \end{aligned} \tag{4}$$

where we neglected higher order contributions in Δt, which would enter through the non-commutativity of T and V but which vanish in the limit $N\to\infty$. By evaluating the product according to

$$\prod_{i=0}^{N}|p_i\rangle\langle x_i| \;=\; |p_N\rangle\Big(\prod_{i=0}^{N-1}\langle x_{i+1}|p_i\rangle\Big)\langle x_0| \;=\; |p_N\rangle e^{i\sum\limits_{i=1}^{N-1}p_ix_{i+1}}\langle x_0| \;=\; \int_{x_{N+1}}|x_{N+1}\rangle\langle x_0|\, e^{i\sum\limits_{i=1}^{N}p_ix_{i+1}} \tag{5}$$

we obtain the following expression for the transition amplitude:

$$\begin{aligned} \langle x_f^+|e^{-i\hat{H}t/\hbar}|x_0^+\rangle \;=\; \lim_{N\to\infty}\left(\prod_{i=1}^{N+1}\int_{x_i}\right)\left(\prod_{i=1}^{N}\int_{p_i}\right)e^{\frac{i}{\hbar}\sum_{i=0}^{N}\left(p_i\frac{x_{i+1}-x_i}{\Delta t}-H(x_i,p_i)\right)\Delta t} \\ \delta^{(d)}(x_f^+-x_{N+1})\;\;\delta^{(d)}(x_0^+-x_1). \end{aligned} \tag{6}$$

Now inserting the assumed form of the Hamiltonian (2), we perform the Gauian integrals according to

$$\int_{p_i} e^{\frac{i}{\hbar}\left(p_i\frac{(x_{i+1}-x_i)}{\Delta t}-\frac{p_i^2}{2m}\right)} = \left(\frac{2\pi m\hbar}{i\Delta t}\right)^{\frac{d}{2}} e^{\frac{im}{2\hbar}\left(\frac{(x_{i+1}-x_i)}{\Delta t}\right)^2\Delta t}. \tag{7}$$

We now rewrite $\dot{x}_i \equiv (x_{i+1}-x_i)/\Delta t$ to recover the Lagrange function in the exponent,

$$\frac{1}{2}m\dot{x}_i^2 - V(x_i) = L(x_i,\dot{x}_i). \tag{8}$$

Then the transition amplitude takes the form

$$\langle x_f^+|e^{-i\hat{H}t/\hbar}|x_0^+\rangle = \lim_{N\to\infty}\left(\prod_{i=1}^{N+1}\int_{x_i}\right)\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{\frac{Nd}{2}} e^{\frac{i}{\hbar}\sum\limits_{i=1}^{N}L(x_i,\dot{x}_i)\Delta t}\delta^{(d)}(x_f^+-x_{N+1})\delta^{(d)}(x_0^+-x_1). \tag{9}$$

1.2. **Non-equilibrium path integral.** By repeating the same steps for the backward amplitude $\langle x_0^-|e^{+i\hat{H}t/\hbar}|x_f^-\rangle$ on the $-$ branch of the contour, we are now able to express operator expectation values $\langle O(t)\rangle$ as a path integral. Collecting all the terms in Eq. (3) we obtain for the expectation value

$$\begin{aligned} O(t) = \lim_{N\to\infty}\int_{x_f^+\,x_f^-\,x_0^+\,x_0^-}\langle x_f^-|\hat{O}|x_f^+\rangle\,\langle x_0^+|\hat{\rho}|x_0^-\rangle\left(\frac{m}{2\pi\hbar\Delta t}\right)^{\frac{Nd}{2}}\left(\prod_{i=1}^{N+1}\int_{x_i^+\,x_i^-}\right)e^{\frac{i}{\hbar}\sum\limits_{i=1}^{N}\left\{L(x_i^+,\dot{x}_i^+)-L(x_i^-,\dot{x}_i^-)\right\}} \\ \delta^{(d)}(x_f^+-x_{N+1}^+)\;\;\delta^{(d)}(x_0^+-x_1^+)\;\;\delta^{(d)}(x_f^--x_{N+1}^-)\;\;\delta^{(d)}(x_0^--x_1^-). \end{aligned} \tag{10}$$

Note that in the limit $N\to\infty$ we have

$$\sum_{i=1}^{N}L(x_i^+,\dot{x}_i^+)\longrightarrow\int_{t_0}^{t}\mathrm{d}\tilde{t}\,L(x^+,\dot{x}^+) = S_{\mathrm{cl}}(x^+,t,t_0) \tag{11}$$

and the integral measure becomes a *functional integral*

$$\int_{x_0^+}^{x_f^+} \mathscr{D}x^+ \equiv \lim_{N\to\infty} \left(\prod_{i=1}^{N} \int \frac{\mathrm{d}^d x_i^+}{\left(\frac{2\pi\hbar\Delta t}{m}\right)^{\frac{d}{2}}} \right) \int \mathrm{d}^d x_{N+1}\, \delta^{(d)}(x_f^+ - x_{N+1}^+)\ \delta^{(d)}(x_0^+ - x_1^+), \tag{12}$$

such that finally we can express the expectation value as

$$O(t) = \underbrace{\int_{x_0^+ x_0^-} \langle x_0^+|\hat{\rho}|x_0^-\rangle}_{\text{Initial conditions}} \underbrace{\int_{x_f^+ x_f^-} \langle x_f^-|\hat{O}|x_f^+\rangle}_{\text{Operator matrix element}} \underbrace{\int_{x_0^+}^{x_f^+} \mathscr{D}x^+ \int_{x_0^-}^{x_f^-} \mathscr{D}x^-\ e^{\frac{i}{\hbar}\left\{S_{\rm cl}(x^+,t,t_0) - S_{\rm cl}(x^-,t,t_0)\right\}}}_{\text{Non-equilibrium evolution}}. \tag{13}$$

Note that in contrast to the classical dynamics, where a classical trajectory contributes with a single path, the quantum mechanical path integral describes an average over all possible paths from $x_0^+ \to x_f^+$ in the amplitude and $x_0^- \to x_f^-$ in the complex conjugate amplitude. Each path is "weighted" with a complex exponential factor $e^{\frac{i}{\hbar}\delta S_{\rm cl}}$, where $\delta S_{\rm cl}$ denotes difference of the action on the $+,-$ branches of the Schwinger-Keldysh contour.

1.3. **Change of variables & classical trajectories.** We would like to investigate what the path integral formula (13) reveals when expanded around a classical trajectory, or around $\hbar = 0$. Classically, we have a single variables x describing the position of a particle along a classical trajectory where the action is stationary, i.e.

$$\frac{\delta S_{\rm cl}}{x} = 0. \tag{14}$$

Conversely, in the quantum mechanical path integral, we have two coordinates $x^\pm$ describing all possible paths of propagation on the forward $(+)$ and backward $(-)$ branches of the Schwinger-Keldysh contour. Nevertheless, remnants of classical behavior in the quantum mechanical path integral can be identified by performing a change of variables according to

$$x_{\rm cl} = \frac{x^+ + x^-}{2}, \qquad \tilde{x} = \frac{1}{\hbar}(x^+ - x^-), \tag{15}$$

We find that the action becomes[1]

$$S_{\rm cl}(x^+,t,t_0) - S_{\rm cl}(x^-,t,t_0)\ =\ \frac{\delta S_{\rm cl}}{\delta x_{\rm cl}}\Big|_{x_{\rm cl}} \hbar\tilde{x} + 2\left(\frac{\hbar}{2}\right)^3 \frac{\tilde{x}^3}{3!}\frac{\delta^3 S_{\rm cl}}{\delta x_{\rm cl}^3}\Big|_{x_{\rm cl}} + \cdots. \tag{16}$$

where in most instances, the theories under consideration only contain terms up to quartic power $O(\hat{x}^4)$ in the potential, and the series ends at the given order. Noting that the Jacobian $|\det J| = \hbar$ of the transformation can be absorbed into the definition measures $\mathscr{D}x_{cl}\mathscr{D}\tilde{x}$, the path integrals in (13) then takes the form

$$\int_{x_0^+}^{x_f^+} \mathscr{D}x^+ \int_{x_0^-}^{x_f^-} \mathscr{D}x^-\ e^{\frac{i}{\hbar}\left\{S_{\rm cl}(x^+,\dot{x}^+,t,t_0) - S_{\rm cl}(x^-,\dot{x}^-,t,t_0)\right\}} \tag{17}$$

$$= \int_{x_0^{\rm cl}}^{x_f^{\rm cl}} \mathscr{D}x_{\rm cl} \int_{\tilde{x}_0}^{\tilde{x}_f} \mathscr{D}\tilde{x}\ \ \exp\left\{ i\left[\frac{\delta S_{\rm cl}}{\delta x_{\rm cl}}\Big|_{x_{\rm cl}} \tilde{x}\ +\ \frac{\hbar^2}{24}\frac{\delta^3 S_{\rm cl}}{\delta x_{\rm cl}^3}\Big|_{x_{\rm cl}} \tilde{x}^3 \right]\right\}. \tag{18}$$

Now one finds that in the limit $\hbar \to 0$, the integrations over $\tilde{x}$ can be performed explicitly, yielding

$$\int_{\tilde{x}_0}^{\tilde{x}_f} \mathscr{D}\tilde{x}\ \ \exp\left\{ i \frac{\delta S_{\rm cl}}{\delta x_{\rm cl}}\Big|_{x_{\rm cl}} \tilde{x} \right\}\ =\ \delta\left(\frac{\delta S_{\rm cl}}{\delta x_{\rm cl}}\right), \tag{19}$$

and one recovers classical trajectories, each satisfying the principle of a stationary action

$$\frac{\delta S}{\delta x_{\rm cl}}\Big|_{x_{\rm cl}} = 0. \tag{20}$$

Note that in addition to the $O(\hbar^2)$ (and higher) quantum corrections to classical dynamics, the path integral in Eq. (13) also contains quantum corrections to the initial conditions and operator expectation values, encoded in the operator matrix elements.

[1]Note that strictly speaking, the functional Taylor expansion of the action around $x_{\rm cl}$ takes the form $S_{\rm cl}(x^+,t,t_0) - S_{\rm cl}(x^-,t,t_0) = \int_{t_0}^{t} dt'\ \frac{\delta S}{\delta x_{\rm cl}(t')}\Big|_{x_{\rm cl}(t')} \tilde{x}(t') + \cdots$, and we suppress the integrals in the following to lighten the notation.