Path integral formulation of NEQ Dynamics

We are interested in

$$\langle O(t) \rangle = \mathrm{tr}\left(O(\hat{x},\hat{p})\ \hat{\rho}(t) \right)$$

with

$$\hat{\rho}(t) = U(t,t_0)\ \hat{\rho}_0\ U^\dagger(t,t_0)$$

~~where for $\hat{H} = T(\hat{p}) + V(\hat{x})$ we have~~

$$U(t,t_0) = \exp\left(\frac{-i}{\hbar} \hat{H}(t-t_0) \right)$$

By inserting a complete set of states $\mathbb{1} = \int d^d x\ |x\rangle\langle x|$

$$\langle O(t) \rangle = \int_{\substack{x_0^+ x_0^- \\ x_f^+ x_f^-}} \underbrace{\langle x_f^- | \hat{O} | x_f^+ \rangle}_{\text{Operator matrix element}} \langle x_f^+ | U | x_0^+ \rangle \underbrace{\langle x_0^+ | \hat{\rho} | x_0^- \rangle}_{\text{Density matrix elements}} \langle x_0^- | U^\dagger | x_f^- \rangle$$

non-eq evolution

classically we had a simple picture between transitions between different states

$$P_{(x_0,p_0,t_0) \to (x_f,p_f,t_f)} = \delta\left(x_f - x_{cl}(x_0,p_0,t_f-t_0)\right) \delta\left(p_f - p_{cl}(x_0,p_0,t_f-t_0)\right)$$

can we have something concrete for QM as well

Expectation values take the structure

$$|x_0^+\rangle \xrightarrow{\langle x_f^+|U|x_0^+\rangle} |x_f^+\rangle$$

$$\langle x_0^+|\hat{\rho}_0|x_0^-\rangle \qquad\qquad \langle x_f^+|\hat{O}|x_f^-\rangle$$

$$\langle x_0^-| \xleftarrow{\langle x_0^-|U^\dagger|x_f^-\rangle} \langle x_f^-|$$

$$\xrightarrow{\text{time}}$$

Schwinger-Keldysh contour

$$\langle x_f^t | U | x_0^t \rangle = \langle x_f^t | e^{\frac{-i}{\hbar}\hat{H}(t-t_0)} | x_0^t \rangle$$

Idea: Split evolution in many small Δt-steps

$$e^{\frac{-i}{\hbar}\hat{H}\Delta t} = e^{\frac{-i}{\hbar}\left(T(\hat{p}) + V(\hat{x})\right)\Delta t}$$

$$= e^{\frac{-i}{\hbar}T(\hat{p})\Delta t} e^{\frac{-i}{\hbar}V(\hat{x})\Delta t} + O(\Delta t^2)$$

$$\langle x_f^t | e^{\frac{-i}{\hbar}\hat{H}(t-t_0)} | x_0^t \rangle = \langle x_f^t | \prod_{i=1}^{N} e^{\frac{-i}{\hbar}T(\hat{p})\Delta t} e^{\frac{-i}{\hbar}V(\hat{x})\Delta t} | x_0^t \rangle$$

$$= \langle x_f^t | \prod_{i=1}^{N} e^{\frac{-i}{\hbar}T(\hat{p})\Delta t} \int_{p_i} |p_i\rangle\langle p_i| \int_{x_i} |x_i\rangle\langle x_i| e^{\frac{-i}{\hbar}V(\hat{x})\Delta t} | x_0^t \rangle$$

$$= \int\left(\prod_{i=1}^{N} \frac{d^d p_i\, d^d x_i}{(2\pi\hbar)^d}\right) e^{-\frac{i}{\hbar}\sum_{i=1}^{N} H(x_i,p_i)\,\Delta t}$$

$$\langle x_f^t | \left(\prod_{i=1}^{N} |p_i\rangle \underbrace{\langle p_i | x_i\rangle}_{e^{-i\frac{p_i x_i}{\hbar}}} \langle x_i|\right) | x_0^t \rangle$$

$$= \int\left(\prod_{i=1}^{N} \frac{d^d p_i\, d^d x_i}{(2\pi\hbar)^d}\right) e^{-\frac{i}{\hbar}\sum_{i=1}^{N} p_i x_i + H(x_i,p_i)\,\Delta t}$$

$$\langle x_f^t | \left(\prod_{i=1}^{N} |p_i\rangle\langle x_i|\right) | x_0^t \rangle$$

$$\left(\prod_{i=1}^{N} |p_i\rangle\langle x_i|\right) = |p_N\rangle\langle x_N|p_{N-1}\rangle \cdots\cdots \underbrace{\langle x_2|p_1\rangle}_{e^{i\frac{p_1 x_2}{\hbar}}}\langle x_1|$$

$$= |p_N\rangle\langle x_1|\; e^{\frac{i}{\hbar}\sum_{i=1}^{N-1} p_i x_{i+1}}$$

$$= \int d^d x_{N+1}\, |x_{N+1}\rangle\langle x_1|\; e^{\frac{i}{\hbar}\sum_{i=1}^{N} p_i x_{i+1}}$$

$\Rightarrow$

$$\langle x_f^t|\, e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\,|x_0^t\rangle$$

$$= \int d^d x_{N+1} \int\left(\prod_{i=1}^{N}\frac{d^d p_i\, d^d x_i}{(2\pi\hbar)^d}\right)\delta^d(x_{N+1}-x_f^t)\;\delta^d(x_1-x_0^t)$$

$$e^{\frac{i}{\hbar}\sum_{i=1}^{N}\left(p_i\frac{(x_{i+1}-x_i)}{\Delta t}-H(x_i,p_i)\right)\Delta t}$$

Now re-write $H(x_i,p_i) = T(p_i) + V(x_i)$

$$= \frac{p_i^2}{2m} + V(x_i)$$

and perform Gaussian integral

$$\int d^d p_i\;\; e^{\frac{i}{\hbar}\left[p_i\frac{(x_{i+1}-x_i)}{\Delta t}-\frac{p_i^2}{2m}\right]\Delta t}$$

$$= \left(\frac{2\pi m\hbar}{i\Delta t}\right)^{d/2} e^{\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{x_{i+1}-x_i}{\Delta t}\right)^2\right)\Delta t}$$

Define $\frac{x_{i+1}-x_i}{\Delta t} = \dot{x}_i$ we then have for the argument

$$\frac{1}{2} m \left(\frac{x_{i+1}-x_i}{\Delta t}\right)^2 - V(x_i) = L(x_i, \dot{x}_i)$$

such that

$$\langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} | x_0 \rangle$$

$$= \left(\frac{m}{2\pi\hbar i \Delta t}\right)^{\frac{dN}{2}} \int \left(\prod_{i=1}^{N+1} dx_i\right) \delta^d(x_{N+1}-x_f)\, \delta(x_1-x_0)$$

$$e^{\frac{i}{\hbar}\sum_{i=1}^{N} L(x_i, \dot{x}_i)\Delta t}$$

Now combine + and − branch
to go back and forth

$$\langle O(t)\rangle = \int d^d x_0^+ \int d^d x_0^- \int d^d x_f^+ \int d^d x_f^- \quad \langle x_f^- | \hat{O} | x_f^+ \rangle \langle x_0^+ | \hat{\rho} | x_0^- \rangle$$

$$\left(\frac{m}{2\pi\hbar\Delta t}\right)^{Nd} \int \left(\prod_{i=1}^{N+1} d^d x_i^+\right)\left(\prod_{i=1}^{N+1} d^d x_i^-\right)$$

$$\delta\left(x_{N+1}^+ - x_f^+\right) \quad \delta\left(x_{N+1}^- - x_f^-\right)$$
$$\delta\left(x_1^+ - x_0^+\right) \quad \delta\left(x_1^- - x_0^-\right)$$
$$e^{\frac{i}{\hbar}\sum_{i=1}^{N}\left(L(x_i^+, \dot{x}_i^+) - L(x_i^-, \dot{x}_i^-)\right)\Delta t}$$

Now in the limit $N \to \infty$, $\Delta t \to 0$
and we have

$$\sum_{i=1}^{N} \Delta t \, L(x_i^+, \dot{x}_i^+) \longrightarrow \int_{t_0}^{t_f} dt \, L(x^+, \dot{x}^+) = S_{cl}(x^+; t_0, t_f)$$

the integral measure becomes a <u>functional integral</u>

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

Hence we have the following compact form

$$\langle O(t)\rangle = \int d^dx_0^+ \int d^dx_0^- \int d^dx_f^+ \int d^dx_f^- \underbrace{\langle x_0^+|\hat{\rho}|x_0^-\rangle}_{\text{initial condition}} \underbrace{\langle x_f^-|\hat{O}|x_f^+\rangle}_{\text{observable}}$$

$$\underbrace{\int_{x_0^+}^{x_f^+}\mathcal{D}x^+ \int_{x_0^-}^{x_f^-}\mathcal{D}x^- \; e^{\frac{i}{\hbar}\left(S(x^+|t_0,t_f) - S(x^-|t_0,t_f)\right)}}_{\text{non-equilibrium evolution / transition amplitude}}$$

Now how does this dolale / differ from classical dynamics:

Classically we have sum over different trajectories, each satisfying

$$\left.\frac{\delta S_{cl}}{\delta x_{cl}}\right|_{x_{cl}} = 0$$

Now in Quantum theory we have x^+ and x^- under path-integral

<u>change variables:</u>

$$x_{cl} = \frac{x^+ + x^-}{2}$$

$$\tilde{x} = \frac{1}{\hbar}(x^+ - x^-)$$

$$J = \frac{\partial(x^+, x^-)}{\partial(x_{cl}, \tilde{x})} = \begin{pmatrix} +1 & +\frac{\hbar}{2} \\ +1 & -\frac{\hbar}{2} \end{pmatrix} \qquad |\det J| = \hbar$$

→ can absorb into definition of functional integral of $Dx_{cl}\, D\tilde{x}$ =

$$x^+ = x_{cl} + \frac{\hbar}{2}\tilde{x}$$

$$x^- = x_{cl} - \frac{\hbar}{2}\tilde{x}$$

Now what is action

$$S_{cl}(x^+) - S_{cl}(x^-) = S_{cl}\left(x_{cl}+\frac{\hbar}{2}\tilde{x}\right) - S_{cl}\left(x_{cl}-\frac{\hbar}{2}\tilde{x}\right)$$

Expand in Taylor Series

$$= \frac{\delta S_{cl}}{\delta x_{cl}}\Big|_{x_{cl}} \hbar\tilde{x} + 2\left(\frac{\hbar}{2}\right)^3 \frac{\tilde{x}^3}{3!}\frac{\delta^3 S_{cl}}{\delta x_{cl}^3} + \dots$$

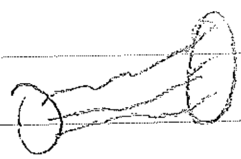
In field theory terms in $V(x)$ with powers larger than x^4 are usually not considered, so the series terminates

We then have

$$\int_{x_0^+}^{x_f^+} Dx^+ \int_{x_0^-}^{x_f^-} Dx^- \, e^{i/\hbar\left(S(x^+|t_0,t_f) - S(x^-|t_0,t_f)\right)}$$

$$= \int_{x_0^{cl}}^{x_f^{cl}} Dx_{cl}\int_{\tilde{x}_0}^{\tilde{x}_f} D\tilde{x}\; e^{i\left(\frac{\delta S_{cl}}{\delta x_{cl}}\tilde{x} + \frac{\hbar^2}{24}\frac{\delta^3 S_{cl}}{\delta x_{cl}^3}\tilde{x}^3\right)}$$

If we drop $\hbar^2$ terms we can perform the integrals over $\tilde{x}$ yielding $\delta\left(\frac{\delta S}{\delta x_{cl}}\right)$



$\Rightarrow$ Classical trajectories are recovered in the limit $\hbar \to 0$

Beware that quantum corrections ($\hbar$ terms) are also "hiding" in initial conditions and observables as seen in our discussion of Wigner-Weyl quantization