Path integration in Quantum Mechanics

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Contents

I. TRAJECTORIES IN CLASSICAL AND AND QUANTUM MECHANICS

The formal structure of quantum mechanics prevents us to use our intuition in interpreting the basic equations. The path integral formalism offers an alternative where some ingredients of classical mechanics can be salvaged.

The starting point of the mechanics is the concept of the state of motion, the set of information which specifies the history of a point particle as the function of the time. The Newton equation is second order in the time derivative hence we need two data per degree of freedom to identify the time evolution, described by the trajectory, $x(t)$. The Schrödinger equation is first order in the time derivative thus it is sufficient to specify the wave function at the initial time and the quantum mechanical state can be specified by the help of the coordinate alone. This is a well known problem, the Heisenberg uncertainty principle, $\Delta x\Delta p\geq\hbar/2$, forces us to use the coordinate or the momentum or a combination of the two to define the state of motion. The main victim of the restriction is the trajectory, $x(t)$. In fact, had we known the trajectory of a particle by a continuous monitoring of its location then we would have access to the coordinate and velocity, ie. the momentum simultaneously. The path integral formalism, guessed by Dirac and worked out in detail by Feynman, offers an alternative way to describe the transition amplitudes of a particle in quantum mechanics in terms of trajectories. Naturally the trajectory of this formalism is not unique, we have actually an integration over trajectories.

Imagine the propagation of a particle from the point S to D where a particle detector is placed in such a manner that a number of screens, each of them containing several small holes, are placed in between the source and the detector, c.f. Fig. 1. The particle propagates through the holes and the amplitude of detecting the particle, $\mathcal{A}$, is the sum over the possible ways of reaching the detector. This is a sum over rectangles from the source to the detector. In the limit when the screens are placed closed to each others thus the particle traverses the next screen after a short time of flight and the size of a hole become small and close to each others a rectangle approaches

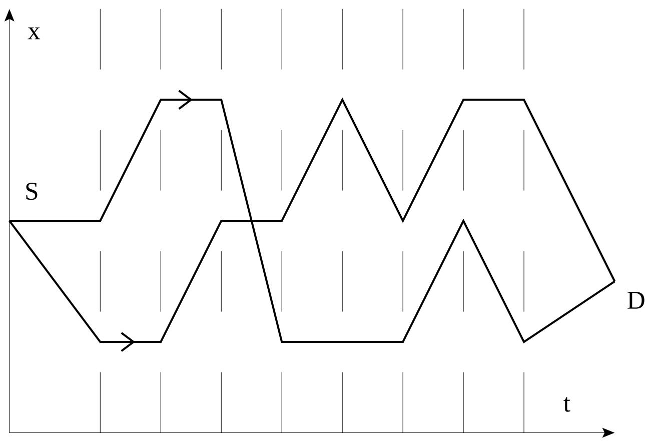

FIG. 1: The particle propagates from the source S to the location of the detector D through the holes of a system of screens. The amplitude of propagation is the sum of all possible ways of reaching the detector.

a trajectory and the amplitude can be written as

$$\mathcal{A} = \sum_{\text{path}} \mathcal{A}(\text{path}). \tag{1}$$

This result reintroduces a part of classical physics in quantum mechanics and offers a help to our intuition towards the understanding of quantum physics.

II. BROWNIAN MOTION

It is instructive to consider the problem of random walk where the path integral formalism arises in an intuitively clear and obvious manner.

The probabilistic description of a classical particle is based on the probability density $p(\boldsymbol{x}, t)$ and the probability current $\boldsymbol{j}(\boldsymbol{x}, t)$, satisfying the continuity equation

$$\partial_t p = -\boldsymbol{\nabla} \boldsymbol{j}. \tag{2}$$

Fick's equation relates the current to the inhomogeneity of the probability density

$$\boldsymbol{j} = -D \boldsymbol{\nabla} p, \tag{3}$$

in the absence of external forces, where D denotes the diffusion constant. The continuity equation allows us to write

$$\partial_t p = D \Delta p. \tag{4}$$

This equation, called the diffusion or heat equation can formally be related to the Schrödinger equation,

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi \tag{5}$$

by the Wick rotation, ie. the analytic continuation to complex time, $t_{Sch} \leftrightarrow -i\hbar t_{diff}$ and the replacement $\frac{\hbar^2}{2m} \leftrightarrow D$.

The Green function of the diffusion equation, (4), which corresponds to the initial condition $p(\boldsymbol{x}, t_i) = \delta(\boldsymbol{x} - \boldsymbol{x}_i)$ is called the Green function of eq. (4) and will be denoted by $G(\boldsymbol{x}, t_f; \boldsymbol{x}_i, t_i)$ for $t_f > t_i$. It is the conditional probability density that the particle is found at $\boldsymbol{x}$ at the time t_f assuming that its location was $\boldsymbol{x}_i$ at time t_i: $p(to \leftarrow from) = G(to; from)$. The solution of the diffusion equation which corresponds to the generic initial condition $p(\boldsymbol{x}, t_i) = p_i(\boldsymbol{x})$ can be written as

$$p(\boldsymbol{x}, t) = \int d^3y G(\boldsymbol{x}, t; \boldsymbol{y}, t_i) p_i(\boldsymbol{y}). \tag{6}$$

Te verify this claim we have to check two points:

1. Solution: The diffusion equation is linear hence this expression, a linear superposition of solutions is a solution, too.

2. Initial condition: It satisfies the desired initial condition,

$$\begin{aligned} p(\boldsymbol{x}, t_i) &= \int d^3y G(\boldsymbol{x}, t_i; \boldsymbol{y}, t_i) p_i(\boldsymbol{y}) \\ &= \int d^3y \delta(\boldsymbol{x} - \boldsymbol{y}) p_i(\boldsymbol{y}) \\ &= p_i(\boldsymbol{x}). \end{aligned} \tag{7}$$

The conditional probability,

$$p(A|B) = \frac{p(A \cap B)}{p(B)}, \tag{8}$$

gives $p(A \cap B) = p(A|B)p(B)$, and

$$p(A \cap B) = \sum_j p(A|B_j) p(B_j) \tag{9}$$

$B = \cup_j B_j$, $B_j \cap B_j = \emptyset$. The comparison of eqs. (6) and (9) where $p(B) = 1$ yields the interpretation of the Green function $G(\boldsymbol{x}, t_i; \boldsymbol{x}_i, t_i)$ as the conditional probability that the particle moves from $\boldsymbol{x}_i$ at t_i to $\boldsymbol{x}$ at t.

The expression (6) solves the diffusion equation for an arbitrary initial condition hence the equation

$$\partial_t G(\boldsymbol{x}, t, \boldsymbol{y}; t_i) = D\Delta_x G(\boldsymbol{x}, t; \boldsymbol{y}, t_i) \tag{10}$$

follows for the Green function. It is easy to verify that

$$G(\boldsymbol{x}, t_f, \boldsymbol{y}; t_i) = \frac{1}{[4\pi D(t_f - t_i)]^{d/2}} e^{-\frac{(\boldsymbol{x}-\boldsymbol{y})^2}{4D(t_f - t_i)}} \tag{11}$$

satisfies eq. (10) in dimension d and the initial condition $G(\boldsymbol{x}, t, \boldsymbol{y}; t) = \delta(\boldsymbol{x} - \boldsymbol{y})$ as $t \to t_i$.

The particle must be somewhere at a given, fixed intermediate time $t_i < t' < t$ during its motion from $\boldsymbol{x}_i$ to $\boldsymbol{x}$. Therefore the probability of moving from $\boldsymbol{x}_i$ to $\boldsymbol{x}$ can be written as

$$p(\boldsymbol{x}, t) = \int d^3z d^3y G(\boldsymbol{x}, t, ; \boldsymbol{z}, t') G(\boldsymbol{z}, t'; \boldsymbol{y}, t_0) p_i(\boldsymbol{y}). \tag{12}$$

The expression (6) of the left hand side, valid for arbitrary $p_i(\boldsymbol{y})$ yields the Chapman-Kolmogorov equation,

$$G(\boldsymbol{x}, t, \boldsymbol{x}_i; t_i) = \int d^3z G(\boldsymbol{x}, t, ; \boldsymbol{z}, t') G(\boldsymbol{z}, t'; \boldsymbol{x}_i, t_0). \tag{13}$$

By breaking the finite time of the propagation, $t - t_i$ into $N+1$ parts and applying the Chapman-Kolmogorov equation N-times one finds

$$\begin{aligned} G(\boldsymbol{x}, t; \boldsymbol{x}_i, t_i) &= \int d^3z_1 \cdots d^3z_N G(\boldsymbol{x}, t; \boldsymbol{z}_n, t_n) G(\boldsymbol{z}_n, t_n; \boldsymbol{z}_{n-1}, t_{n-1}) \cdots \\ &\quad \cdots G(\boldsymbol{z}_2, t_2; \boldsymbol{x}_1, t_1) G(\boldsymbol{z}_1, t_1; \boldsymbol{x}_i, t_i) \\ &= \frac{1}{(4\pi D\Delta t)^{3(N+1)/2}} \int d^3z_1 \cdots d^3z_N e^{-\frac{\Delta t}{4D} \sum_{n=0}^{N} (\frac{\boldsymbol{z}_{n+1} - \boldsymbol{z}_n}{\Delta t})^2}, \end{aligned} \tag{14}$$

where $t_n = t_i + n\Delta t$, $\Delta t = 1/(N+1)$, $\boldsymbol{z}_0 = \boldsymbol{x}_i$ and $\boldsymbol{z}_{N+1} = \boldsymbol{x}$. The right hand side can be considered as a summation over paths, made by piece wise linear functions which becomes an integral over paths in the continuum limit, $N \to \infty$, and can formally be written as

$$G(\boldsymbol{x}, t; \boldsymbol{x}_i, t_i) = \int D[\boldsymbol{x}] e^{-\frac{1}{4D} \int_{t_i}^{t} dt' \dot{\boldsymbol{x}}^2}, \tag{15}$$

where the integration is over trajectories with initial and end points $\boldsymbol{x}(t_i) = \boldsymbol{x}_i$ and $\boldsymbol{x}(t) = \boldsymbol{x}$, respectively and divergent normalization factor of the second line of eqs. (14) is included in the integral measure. Such an integration over trajectories is called Wiener process.

A word of caution about the continuous notation: Almost all trajectory of the Wiener process is non-differentiable. In other word, the differentiable trajectories have vanishing weight in the Wiener integral in the limit $N \to \infty$. The heuristic argument goes by inspecting the finite difference of trajectories with Δt-independent weight, they must have $\Delta x_n = x_{n+1} - x_n = \sqrt{\Delta t}$ according to eq. (14), therefore $v = \Delta x/\Delta t = \mathcal{O}\left(\Delta t^{-1/2}\right)$. The Wiener process is concentrated on fractals and the velocity, $\dot{x}$, appearing in the continuous notation of (15) must be handled symbolically, e.g. should be replaced by the discrete version, (14), as soon as it is used in a calculation.

III. PROPAGATOR

Let us consider a one dimensional non-relativistic particle described by the Hamiltonian

$$H = \frac{p^2}{2m} + U(x) \tag{16}$$

with $[x,p] = i\hbar$ and introduce the propagator or transition amplitude

$$\langle x_f | e^{-\frac{i}{\hbar}Ht} | x_i \rangle \tag{17}$$

between coordinate eigenstates.

The amplitude (17) is a complicated function of the variables t, x_i and x_f. We simplify the problem of finding it by computing it first for short time when it takes a simpler form and by constructing the finite time transition amplitude from the short time one. This latter step is accomplished by writing

$$\langle x_f | e^{-\frac{i}{\hbar}Ht} | x_i \rangle = \langle x_f | \left(e^{-\frac{i}{\hbar}H\Delta t}\right)^N | x_i \rangle \tag{18}$$

with $\Delta t = t/N$ and inserting a resolution of the identity,

$$\mathbb{1} = \int dx |x\rangle\langle x|, \tag{19}$$

between each operator,

$$\langle x_f | e^{-\frac{i}{\hbar}Ht} | x_i \rangle = \prod_{j=1}^{N-1} \int dx_j \langle x_N | e^{-\frac{i}{\hbar}H\Delta t} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{i}{\hbar}H\Delta t} | x_{N-2} \rangle \cdots \langle x_1 | e^{-\frac{i}{\hbar}H\Delta t} | x_0 \rangle, \tag{20}$$

where $x_0 = x_i$ and $x_N = x_f$. This relation which holds for any N becomes a path integral as $N \to \infty$. In fact, any trajectory between the given initial and final point can be approximated by a piece wise constant function when the length of the time interval Δt when the function is constant tends to zero.

In order to turn the simple path integral expression (20) into something useful we need a simple approximation for the short time transition amplitudes. There are $\mathcal{O}(N)$ of them multiplied together therefore it is enough to have $\mathcal{O}\left(N^{-1}\right) = \mathcal{O}\left(\Delta t\right)$ accuracy in obtaining them. The first guess would be

$$\begin{aligned}
\langle x|e^{-\frac{i}{\hbar}H\Delta t}|x'\rangle &\approx \langle x|1-\frac{i}{\hbar}H\Delta t|x'\rangle \\
&= \langle x|x'\rangle\left(1-\frac{i\Delta t}{\hbar}\frac{\langle x|H|x'\rangle}{\langle x|x'\rangle}\right) \\
&\approx \langle x|x'\rangle e^{\frac{i}{\hbar}\Delta t\frac{\langle x|H|x'\rangle}{\langle x|x'\rangle}}
\end{aligned} \tag{21}$$

but the problem is the orthogonality of the basis vectors $\langle x|x'\rangle = \delta(x-x')$. In fact, the small parameter in the expansion is $\Delta t/\langle x|x'\rangle$ which is diverging for $x \neq x'$. To avoid this problem we use two overlapping basis in an alternating manner. In case of continuous space the choice of the other, overlapping basis is rather natural. It will be a momentum basis, $|p\rangle$ with $p|q\rangle = q|q\rangle$. The corresponding resolution of the identity,

$$\mathbb{1} = \int \frac{dp}{2\pi\hbar}|p\rangle\langle p|, \tag{22}$$

inserted in Eqs. (21) yields

$$\begin{aligned}
\langle x|e^{-\frac{i}{\hbar}H\Delta t}|x'\rangle &= \int \frac{dp}{2\pi\hbar}\langle x|e^{-\frac{i}{\hbar}H\Delta t}|p\rangle\langle p|x'\rangle \\
&\approx \int \frac{dp}{2\pi\hbar}\langle x|1-\frac{i}{\hbar}H\Delta t|p\rangle\langle p|x'\rangle \\
&= \int \frac{dp}{2\pi\hbar}\langle x|p\rangle\langle p|x'\rangle\left(1-\frac{i\Delta t}{\hbar}\frac{\langle x|H|p\rangle}{\langle x|p\rangle}\right) \\
&\approx \int \frac{dp}{2\pi\hbar}e^{\frac{i}{\hbar}p(x-x')-\frac{i}{\hbar}\Delta t H(p,x)}
\end{aligned} \tag{23}$$

with

$$H(p,x) = \frac{\langle x|H|p\rangle}{\langle x|p\rangle} = \frac{p^2}{2m} + U(x). \tag{24}$$

By replacing this expression into Eq. (20) we arrive at a path integral in phase space,

$$\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle = \lim_{N\to\infty}\prod_{j=1}^{N-1}\int dx_j \prod_{k=1}^{N}\int \frac{dp_k}{2\pi\hbar}e^{\frac{i}{\hbar}\Delta t\sum_{\ell=1}^{N}[p_\ell\frac{x_\ell-x_{\ell-1}}{\Delta t}-H(p_\ell,x_\ell)]}, \tag{25}$$

with $x_0 = x_i$ and $x_N = x_f$ which can be written in a condensed, formal notation as

$$\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle = \int_{x(0)=x_i}^{x(t)=x_f} D[x]\int D[p]e^{\frac{i}{\hbar}\int d\tau[p(\tau)\dot{x}(\tau)-H(p(\tau),x(\tau))]} \tag{26}$$

by suppressing the regulator, Δt. The integration over coordinate or momentum trajectories of fixed or free initial and final points, respectively. We shall see that the continuous notation is as symbolic as for the Wiener measure, but notice here already that there is one more momentum integral than coordinate integration in eq. (25), preventing the quantum mechanical formalism to display canonical invariance which would follow only for canonical invariant integral measure, $\prod_j \int dx_j dp_j$.

The integrand in the exponent seems to be the Lagrangian of the analytical mechanics. However rather than relying on this classical analogy the momentum integral has to be performed in the quantum case. We start with Gauss' formula,

$$\int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}, \tag{27}$$

valid if for $a > 0$, yielding

$$\int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2+bx} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}} \tag{28}$$

after writing the exponent of the integrand in the form $-\frac{a}{2}(x-\frac{b}{a})^2+\frac{b^2}{2a}$ and carrying out the change of integration variable, $x \to x + \frac{b}{a}$. The integral

$$\int_{-\infty}^{\infty} dx e^{i\frac{a}{2}x^2+ibx} \tag{29}$$

with real a can be calculated by analytic continuation by assuming Im $a > 0$. The correct Riemann-sheet of the square root is chosen by requiring $\mathrm{Re}\frac{a}{i} > 0$, giving rise to the Fresnel integral,

$$\int_{-\infty}^{\infty} dx e^{i\frac{a}{2}x^2+ibx} = \sqrt{\frac{2\pi}{|a|}} e^{-i\frac{b^2}{2a}+i\mathrm{sign}(\mathrm{Re}\ a)\frac{\pi}{4}} \tag{30}$$

This result allows us to write the integral (25) as

$$\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \lim_{N\to\infty} \prod_{j=1}^{N-1} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int dx_j e^{\frac{i}{\hbar}\Delta t \sum_{\ell=1}^{N}[\frac{m}{2}(\frac{x_\ell-x_{\ell-1}}{\Delta t})^2-U(x_\ell)]} \tag{31}$$

in coordinate space which reads in condensed notation

$$\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle = \int_{x(0)=x_i}^{x(t)=x_f} D[x] e^{\frac{i}{\hbar}S[x]} \tag{32}$$

with

$$S[x] = \int d\tau L(x(\tau),\dot{x}(\tau)), \quad L = \frac{m}{2}\dot{x}^2 - U(x). \tag{33}$$

The expressions (26) and (32) are easy to memorize but are formal because the functional integration measure is defined by a limiting procedure, spelled out in the more involved expressions (25) and (31). The integration over the momentum recovers the Lagrangian (33) from the Hamiltonian

(16). Such an agreement with the Legendre transformation of Classical Mechanics is restricted to the Gaussian integration, i.e. Hamiltonians of the form (16), which are quadratic in the momentum and contain the dependence in the coordinate as an additive term.

We consider now few trivial but important generalizations of eq. (32). First seek the solution $\psi(t,x)$ of the Schrödinger equation, corresponding to the initial condition, $\psi(t_i,x) = \psi_i(x)$ by inserting a closing relation into

$$\psi(t,x) = \langle x|e^{-\frac{i}{\hbar}Ht}|\psi_i\rangle = \int dx_i \langle x|e^{-\frac{i}{\hbar}Ht}|x_i\rangle\langle x_i|\psi_i\rangle, \tag{34}$$

which we write as

$$\psi(t,x) = \int_{x(t)=x_f} D[x]e^{\frac{i}{\hbar}S[x]}\psi_i(x(t_i)) \tag{35}$$

where the integration of the initial point is carried out with the weight, given by the wave function of the initial state. Another generalization consists of the calculation of the matrix element

$$\begin{aligned}\langle\psi_f|e^{-\frac{i}{\hbar}Ht}|\psi_i\rangle &= \int dx_i dx_f \psi_f^*(x_f)\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle\psi_i(x_i)\\ &= \int D[x]e^{\frac{i}{\hbar}S[x]}\psi_f^*(x(t_f))\psi_i(x(t_i)).\end{aligned} \tag{36}$$

Finally, we generalize the results for a particle moving in a d-dimensional space. The steps leading to Eq. (25) can easily be repeated in this case leading to

$$\langle \boldsymbol{x}_f|e^{-\frac{i}{\hbar}Ht}|\boldsymbol{x}_i\rangle = \lim_{N\to\infty}\prod_{j=1}^{N-1}\int d^d x_j \prod_{k=1}^{N}\int \frac{d^d p_k}{(2\pi)^d} e^{\frac{i}{\hbar}\Delta t\sum_{\ell=1}^{N}[\boldsymbol{p}_\ell\cdot\frac{\boldsymbol{x}_\ell-\boldsymbol{x}_{\ell-1}}{\Delta t}-H(\boldsymbol{p}_\ell,\boldsymbol{x}_\ell)]} \tag{37}$$

with

$$H = \frac{\boldsymbol{p}^2}{2m} + U(\boldsymbol{x}) \tag{38}$$

which takes the form

$$\langle \boldsymbol{x}_f|e^{-\frac{i}{\hbar}Ht}|\boldsymbol{x}_i\rangle = \int_{\boldsymbol{x}(0)=\boldsymbol{x}_i}^{\boldsymbol{x}(t)=\boldsymbol{x}_f} D[\boldsymbol{x}]\int D[\boldsymbol{p}]e^{\frac{i}{\hbar}\int d\tau[\boldsymbol{p}(\tau)\dot{\boldsymbol{x}}(\tau)-H(\boldsymbol{p}(\tau),\boldsymbol{x}(\tau))]} \tag{39}$$

in condensed notation. The Lagrangian path integral reads in d-dimensions as

$$\begin{aligned}\langle \boldsymbol{x}_f|e^{-\frac{i}{\hbar}Ht}|\boldsymbol{x}_i\rangle &= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{d}{2}}\lim_{N\to\infty}\prod_{j=1}^{N-1}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{d}{2}}\int d^d x_j e^{\frac{i}{\hbar}\Delta t\sum_{\ell=1}^{N}[\frac{m}{2}(\frac{\boldsymbol{x}_\ell-\boldsymbol{x}_{\ell-1}}{\Delta t})^2-U(\boldsymbol{x}_\ell)]}\\ &= \int_{\boldsymbol{x}(0)=\boldsymbol{x}_i}^{\boldsymbol{x}(t)=\boldsymbol{x}_f} D[\boldsymbol{x}]e^{\frac{i}{\hbar}S[\boldsymbol{x}]}\end{aligned} \tag{40}$$

with

$$S[\boldsymbol{x}] = \int dt L(\dot{\boldsymbol{x}},\boldsymbol{x}), \quad L = \frac{m}{2}\dot{\boldsymbol{x}}^2 - U(\boldsymbol{x}). \tag{41}$$

IV. DIRECT CALCULATION OF THE PATH INTEGRAL

A. Free particle

Let us start with the path integral for a one dimensional free particle with finite N,

$$\begin{aligned} G_0(x_f, x_i, t) &= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \left(\prod_{j=1}^{N-1} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int dx_j \right) e^{\frac{im}{2\hbar\Delta t}\sum_{\ell=1}^{N}(x_\ell - x_{\ell-1})^2} \\ &= \left(\prod_{j=1}^{N-1} \int dx_j \right) \prod_{\ell=1}^{N} f(x_\ell - x_{\ell-1}, \Delta t), \end{aligned} \tag{42}$$

where $x_0 = x_i$ and $x_N = x_f$, $\Delta t = T/N$ and

$$f(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} e^{\frac{im}{2\hbar t}x^2}. \tag{43}$$

We shall calculate this expression by a successive integration. For this end let us consider the single integral

$$\int dz f(x-z, t_1) f(z-y, t_2) = N \int dz e^{i\frac{a}{2}z^2 + ibz + ic}, \tag{44}$$

with $a = \frac{m}{\hbar}\frac{t_1+t_2}{t_1 t_2}$, $b = -\frac{m}{\hbar}\frac{yt_1+xt_2}{t_1 t_2}$, $c = \frac{m}{2\hbar}(\frac{x^2}{t_1} + \frac{y^2}{t_2})$, and $N = \frac{m}{2\pi i\hbar\sqrt{t_1 t_2}}$. The straightforward application of the Fresnel integral yields

$$\begin{aligned} \int dz f(x-z, t_1) f(z-y, t_2) &= N\sqrt{\frac{2\pi i}{a}} e^{-i\frac{b^2}{2a} + ic} \\ &= \sqrt{\frac{m}{2\pi i\hbar(t_1+t_2)}} e^{i\frac{m}{2\hbar}\left[-\frac{(yt_1+xt_2)^2}{t_1 t_2(t_1+t_2)} + \frac{x^2}{t_1} + \frac{y^2}{t_2}\right]} \\ &= f(x-y, t_1+t_2), \end{aligned} \tag{45}$$

in other words, the integrand $f(x,t)$ is self reproducing during the integration. This property can be used to successively integrate in (42) with the result

$$G_0(x_f, x_i, t) = f(x_f - x_i, t) = \sqrt{\frac{m}{2\pi i\hbar t}} e^{\frac{im}{2\hbar t}(x_f - x_i)^2}. \tag{46}$$

To check the result we calculate the free propagator in the operator formalism, too. The time evolution operator is diagonal in momentum space,

$$e^{-\frac{i}{\hbar}Ht} = \int \frac{dp}{2\pi\hbar} |p\rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} \langle p|, \tag{47}$$

and the propagator, its matrix element in the coordinate basis, is

$$\begin{aligned}\langle x_f|e^{-\frac{i}{\hbar}Ht}|x_i\rangle &= \int \frac{dp}{2\pi\hbar}\langle x_f|p\rangle e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}\langle p|x_i\rangle \\ &= \int \frac{dp}{2\pi\hbar}e^{-\frac{i}{\hbar}\frac{p^2}{2m}t+\frac{i}{\hbar}p(x_f-x_i)} \\ &= \sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{im}{2t\hbar}(x_f-x_i)^2}.\end{aligned} \tag{48}$$

As a useful exercise let us calculate the spread of the wave packet

$$\psi_i(x) = \frac{e^{-\frac{x^2}{2\Delta x^2}}}{\sqrt{\Delta x\sqrt{2}}}, \tag{49}$$

without using the momentum representation,

$$\psi(t,x) = \frac{1}{\sqrt{\Delta x\sqrt{2}}}\sqrt{\frac{m}{2\pi i\hbar t}}\int dy e^{\frac{im}{2t\hbar}(x-y)^2-\frac{y^2}{2\Delta x^2}} \tag{50}$$

what we write in the form

$$\psi(t,x) = N\int dy e^{-\frac{a}{2}y^2+by+c} \tag{51}$$

with $N = \sqrt{\frac{m}{2\sqrt{2}\pi i\hbar t\Delta x}}$, $a = \frac{1}{\Delta x^2} - i\frac{m}{t\hbar}$, $b = -i\frac{m}{t\hbar}x$ and $c = i\frac{m}{2t\hbar}x^2$. The Gaussian integral gives

$$\begin{aligned}\psi(t,x) &= N\sqrt{\frac{2\pi}{a}}e^{\frac{b^2}{2a}+c} \\ &= N\sqrt{\frac{2\pi}{a}}e^{-\frac{\frac{m^2}{t^2\hbar^2}}{2}\frac{\frac{1}{\Delta x^2}+i\frac{m}{t\hbar}}{\frac{1}{\Delta x^4}+\frac{m^2}{t^2\hbar^2}}x^2+c} \\ &= N\sqrt{\frac{2\pi}{a}}e^{-\frac{m^2\Delta x^2}{2(t^2\hbar^2+m^2\Delta x^4)}x^2}e^{-i\frac{m^3\Delta x^4}{2t\hbar(t^2\hbar^2+m^2\Delta x^4)}x^2+c},\end{aligned} \tag{52}$$

a wave packet of width

$$\Delta x(t) = \sqrt{t^2v^2+\Delta x^2}, \tag{53}$$

with $v = \frac{\hbar}{m\Delta x}$.

B. Stationary phase (semiclassical) approximation

The semiclassical approximation of the path integral consists of the approximation by assuming that the action changes fast in units of $\hbar$. A simple integral

$$I = \int dx e^{\frac{i}{\hbar}S(x)} \tag{54}$$

can be approximated in the limit $\hbar \to 0$ by restraining the domain of integration to the regions where the exponent of the integrand changes slowly, $x \sim x_0$, $S'(x_0) = 0$. Let us suppose that there is a single point x_0 where this equation is satisfied and write

$$\begin{aligned} I &= \int dx e^{\frac{i}{\hbar}S(x_0)+\frac{i}{\hbar}(x-x_0)S'(x_0)+\frac{i}{2\hbar}(x-x_0)^2S''(x_0)+\mathcal{O}\left((x-x_0)^3\right)} \\ &= e^{\frac{i}{\hbar}S(x_0)} \int dy e^{\frac{i}{2\hbar}y^2S''(x_0)+\frac{i}{\hbar}\mathcal{O}\left(y^3\right)} \\ &= e^{\frac{i}{\hbar}S(x_0)} \sqrt{\frac{2\pi\hbar}{|S''(x_0)|}} e^{i\mathrm{sign}(ReS''(x_0))\frac{\pi}{4}} \left(1 + \mathcal{O}\left(\hbar^3\right)\right). \end{aligned} \tag{55}$$

In case of several locally constant regions, $S'(x_j) = 0$, $j = 1 \ldots N$ we sum over thes regions,

$$I = \sum_{j=1}^{N} e^{\frac{i}{\hbar}S(x_j)} \sqrt{\frac{2\pi\hbar}{|S''(x_j)|}} e^{i\mathrm{sign}(ReS''(x_j))\frac{\pi}{4}} \left(1 + \mathcal{O}\left(\hbar^3\right)\right). \tag{56}$$

This approximation can easily be extended to the path integral,

$$\mathcal{A} = \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x] e^{\frac{i}{\hbar}S[x]} \tag{57}$$

where the dominant contribution comes from the domain of integration where the phase of the integrand changes the slowest manner with the trajectories, around the classical trajectory,

$$\frac{\delta S[x]}{\delta x(t)}_{|x=x_{cl}} = 0. \tag{58}$$

By expanding the exponent around the classical trajectory we find

$$\begin{aligned} \mathcal{A} &= \int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x] e^{\frac{i}{\hbar}S[x_{cl}]+\frac{i}{\hbar}\int dt[x(t)-x_{cl}(t)]\frac{\delta S[x]}{\delta x(t)}+\frac{i}{2\hbar}\int dtdt'[x(t)-x_{cl}(t)]\frac{\delta^2 S[x]}{\delta x(t)\delta x(t')}[x(t')-x_{cl}(t')]+\mathcal{O}\left((x-x_{cl})^3\right)} \\ &= e^{\frac{i}{\hbar}S[x_{cl}]} \int_{y(t_i)=0}^{y(t_f)=0} D[y] e^{\frac{i}{2\hbar}\int dtdt' y(t)\frac{\delta^2 S[x]}{\delta x(t)\delta x(t')}y(t')+\frac{i}{\hbar}\mathcal{O}\left(y^3\right)}. \end{aligned} \tag{59}$$

Since $y \sim \sqrt{\hbar}$ the $\mathcal{O}\left(y^3\right)$ term can be neglected in the formal limit $\hbar \to 0$ whee the path integral is reduced to the product of a phase factor, containing the classical action and a path integral of a quadratic action with vanishing initial and and points. This limit corresponds to the semiclassical limit when the initial and the final point of the propagation, x_i and x_f, respectively, are held fixed.

C. Quadratic potential

We consider a particle with the Lagrangian

$$L = \frac{m}{2}\dot{x}^2 - \frac{m\omega^2(t)}{2}x^2, \tag{60}$$

as the next example. The integral we seek in this case for finite N is

$$I_N = \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{\frac{N+1}{2}} \prod_{j=1}^{N} \int dy_j e^{\frac{i}{\hbar}\sum_{\ell=1}^{N+1}\left[\frac{m}{2\Delta t}(y_\ell - y_{\ell-1})^2 - \Delta t\frac{m\omega_{\ell-1}^2}{2}y_{\ell-1}^2\right]} \tag{61}$$

with $y_0 = y_N = 0$, $\Delta t = T/N$ and $\omega_\ell = \omega(\Delta t \ell)$. We shall use the vector notation, $\vec{y} = (y_0, y_1, \ldots, y_\ell)$ for the trajectory and write

$$I_N = \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{(N+1)/2} \int d^N y e^{\frac{i}{2}\vec{y}A_N\vec{y}^{\text{tr}}}, \tag{62}$$

where

$$A_N = \frac{m}{\hbar\Delta t}\begin{pmatrix} 1 & -1 & 0 & \ldots & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 \\ 0 & -1 & 2 & \ldots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \ldots & 2 & -1 \\ 0 & 0 & 0 & \ldots & -1 & 1 \end{pmatrix} - \frac{m\Delta t}{\hbar}\begin{pmatrix} \omega_0^2 & 0 & 0 & \ldots & 0 & 0 \\ 0 & \omega_1^2 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \omega_2^2 & \ldots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \ldots & \omega_{\ell-1}^2 & 0 \\ 0 & 0 & 0 & \ldots & 0 & \omega_\ell^2 \end{pmatrix}. \tag{63}$$

The matrix A_N can be brought into a diagonal form by a suitable basis transformation and the Fresnel integral yields in the basis where it is diagonal

$$\begin{aligned} I_N &= \Big(\frac{m}{2\pi i\hbar\Delta t}\Big)^{\frac{N+1}{2}} \prod_{j=1}^{N}\sqrt{\frac{2\pi i}{\lambda_j}} \\ &= \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\prod_{j=1}^{N}\sqrt{\frac{m}{\hbar\Delta t\lambda_j}}, \end{aligned} \tag{64}$$

where λ_j denotes the eigenvalues. We have $\lambda_j > 0$ for sufficient small Δt since the second derivative of the kinetic energy is a negative semi-definite operator. We write this expression as

$$I_N = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\frac{1}{\sqrt{\det\frac{\hbar\Delta t}{m}A_N}} \tag{65}$$

and introduce the notation

$$D_N = \det\frac{\hbar\Delta t}{m}A_N = \det\left[\begin{pmatrix} 1 & -1 & 0 & \ldots & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 \\ 0 & -1 & 2 & \ldots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \ldots & 2 & -1 \\ 0 & 0 & 0 & \ldots & -1 & 1 \end{pmatrix} - \Delta t^2\begin{pmatrix} \omega_0^2 & 0 & 0 & \ldots & 0 & 0 \\ 0 & \omega_1^2 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \omega_2^2 & \ldots & 0 & 0 \\ & & & \ddots & & \\ 0 & 0 & 0 & \ldots & \omega_{N-1}^2 & 0 \\ 0 & 0 & 0 & \ldots & 0 & \omega_N^2 \end{pmatrix}\right]. \tag{66}$$

It is easy to verify the recursive relation

$$D_{n+1} = (2 - \Delta t^2 \omega_{n+1}^2) D_n - D_{n-1}. \tag{67}$$

The corresponding initial conditions are $D_0 = 0$ and $D_1 = 1 - \Delta t^2 \omega_0^2$. We define in this manner a function $\phi(n\Delta t) = \Delta t D_n$ which satisfy the equation

$$\ddot{\phi}(t) = -\omega^2(t)\phi(t), \tag{68}$$

together with the initial conditions $\phi(t_i) = 0$, $\dot{\phi}(t_i) = 1$. The solution of this initial condition problem, $\phi(t, t_i)$ gives

$$\begin{aligned} \lim_{N\to\infty} I_N &= \int_{y(t_i)=0}^{y(t_f)=0} D[y] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(y(t),\dot{y}(t))} \\ &= \sqrt{\frac{m}{2\pi i\hbar\phi(t_f, t_i)}}. \end{aligned} \tag{69}$$

This result allows us to find the path integral with the quadratic Lagrangian, (60),

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(x(t),\dot{x}(t))} = \sqrt{\frac{m}{2\pi i\hbar\phi(t_f, t_i)}} e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(x_{cl}(t),\dot{x}_{cl}(t))}, \tag{70}$$

where the classical trajectory, $x_{cl}(t)$ solves the equation of motion

$$\ddot{x}_{cl}(t) = -\omega^2(t) x_{cl}(t), \tag{71}$$

together with the boundary conditions $x_{cl}(t_i) = x_i$ and $x_{cl}(t_f) = x_f$.

As a simple example we consider the case of the harmonic oscillator, $\omega(t) = \omega$, where

$$S[x_{cl}] = \int_{t_i}^{t_f} dt L(x_{cl}(t), \dot{x}_{cl}(t)) = \frac{m\omega}{2\sin\omega T}\left[(x_f^2 + x_i^2)\cos\omega T - 2x_i x_f\right], \tag{72}$$

with $T = t_f - t_i$ and $\phi(t, t_i) = \frac{\sin\omega T}{\omega}$, giving the exact result

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} D[x] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\frac{m}{2}\dot{x}^2 - \frac{m\omega^2}{2}x^2\right]} = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T}\left[(x_f^2+x_i^2)\cos\omega T - 2x_i x_f\right]}. \tag{73}$$

V. MATRIX ELEMENTS

So far we have considered the direct calculation of the transition amplitude within the path integral formalism. But there are cases when the calculation of the path integral with the given action is too difficult and we resort to a perturbation series instead. We need the matrix element of more general expressions, obtained by inserting different operators into the time evolution operator, for instance

$$\langle x_f | e^{-\frac{i}{\hbar}H(t-t')} F(x) e^{-\frac{i}{\hbar}Ht'} | x_i \rangle. \tag{74}$$

Such a matrix element can be obtained within the path integral formalism in a natural manner. In fact, we have

$$\begin{aligned}
\langle x_f|e^{-\frac{i}{\hbar}H(t-t')}F(x)e^{-\frac{i}{\hbar}Ht'}|x_i\rangle &= \int dx_1'dx_2'\langle x_f|e^{-\frac{i}{\hbar}H(t-t')}|x_1'\rangle \underbrace{\langle x_1'|F(x)|x_2'\rangle}_{\delta(x_1'-x_2')F(x_1')}\langle x_2'|e^{-\frac{i}{\hbar}Ht'}|x_i\rangle \\
&= \int dx'\langle x_f|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle F(x')\langle x'|e^{-\frac{i}{\hbar}Ht'}|x_i\rangle \\
&= \int dx' \int_{x(t')=x'}^{x(t)=x_f} D[x]e^{\frac{i}{\hbar}\int dtL(x(t),\dot{x}(t))}F(x')\int_{x(0)=x_i}^{x(t')=x'} D[x]e^{\frac{i}{\hbar}\int dtL(x(t),\dot{x}(t))} \\
&= \int_{x(0)=x_i}^{x(t)=x_f} D[x]e^{\frac{i}{\hbar}\int dtL(x(t),\dot{x}(t))}F(x(t') \qquad (75)
\end{aligned}$$

where it was used in the last equation that the integration over trajectories from $x(0) = x_i$ to $x(t') = x'$ and from $x(t') = x'$ to $x(t) = x_f$ together with the integration over x' is equivalent with the integration over trajectories from $x(0) = x_i$ to $x(t) = x_f$. The generalization of this procedure for n insertions is

$$\begin{aligned}
&\langle x_f|e^{-\frac{i}{\hbar}H(t-t_n)}F_n(x)e^{-\frac{i}{\hbar}H(t_n-t_{n-1})}F_{n-1}(x)e^{-\frac{i}{\hbar}H(t_{n-1}-t_{n-2})}\cdots e^{-\frac{i}{\hbar}H(t_2-t_1)}F_1(x)e^{-\frac{i}{\hbar}Ht_1}|x_i\rangle \\
&= \int_{x(0)=x_i}^{x(t)=x_f} D[x]e^{\frac{i}{\hbar}S[x]}\prod_{j=1}^{n}F_j(x(t_j)) \qquad (76)
\end{aligned}$$

with $t_i \leq t_j \leq t_f$. It is useful to rewrite these equations by introducing a dummy time variable for the time-independent Hamiltonian, $H = H(t)$ and for the observable $x(t)$ and by using the time ordered product of Appendix C in the Schrödinger representation,

$$\langle x_f|T[e^{-\frac{i}{\hbar}\int_0^{t_f}dt'H(t')}\prod_{j=1}^{n}F_j(x(t_j))]|x_i\rangle = \int_{x(0)=x_i}^{x(t)=x_f} D[x]e^{\frac{i}{\hbar}S[x]}\prod_{j=1}^{n}F_j(x(t_j)). \qquad (77)$$

A slight extension to arbitrary matrix elements, $\langle x_f| \to \langle\psi_f|$, $|x_i\rangle \to |\psi_i\rangle$, can easily be found by convolution,

$$\begin{aligned}
&\langle\psi_f|T[e^{-\frac{i}{\hbar}\int_0^{t_f}dt'H(t')}\prod_{j=1}^{n}F_j(x(t_j))]|\psi_i\rangle \\
&= \int dx_i dx_f \psi_f^*(x_f)\langle x_f|T[e^{-\frac{i}{\hbar}\int_0^{t_f}dt'H(t')}\prod_{j=1}^{n}F_j(x(t_j))]|x_i\rangle\psi_i(x_i) \\
&= \int dx_i dx_f \psi_f^*(x_f)\psi_i(x_i)\int_{x(0)=x_i}^{x(t)=x_f} D[x]e^{\frac{i}{\hbar}S[x]}\prod_{j=1}^{n}F_j(x(t_j)) \qquad (78)
\end{aligned}$$

The generalization of (78) for analytic functionals

$$F[x(t)] = \sum_{n=0}^{\infty}\frac{1}{n!}\prod_{j=1}^{n}\int dt_j f_n(t_1,\ldots,t_n)x(t_1)\cdots x(t_j), \qquad (79)$$

in terms of the generating functional

$$Z[j] = \int D[x] e^{\frac{i}{\hbar}S[x]+\frac{i}{\hbar}\int dt x(t) j(t)} \tag{80}$$

is

$$\begin{aligned}\langle\psi_f|T[e^{-\frac{i}{\hbar}\int_0^{t_f} dt' H(t')}\prod_{j=1}^{n} F[x(t)]]|\psi_i\rangle &= \int D[x] e^{\frac{i}{\hbar}S[x]} F[x(t)] \\ &= F\left[\frac{\delta}{\delta\frac{i}{\hbar}j(t)}\right] Z[j]_{|j=0}.\end{aligned} \tag{81}$$

The proof follows by noting that the factor $x^n(t)$ is generated by acting with the differential operator $(\frac{\hbar}{i})^n\delta^n/\delta x(t)^n$.

Matrix elements of observables composed by the coordinate and the momentum can be calculated in a similar manner, by the use of the generating functional

$$\begin{aligned}Z[j,k] &= \lim_{N\to\infty}\prod_{j=1}^{N-1}\int dx_j \prod_{k=1}^{N}\int\frac{dp_k}{2\pi} e^{\frac{i\Delta t}{\hbar}\sum_{\ell=1}^{N}[p_\ell\frac{x_\ell-x_{\ell-1}}{\Delta t}-\frac{p_\ell^2}{2m}-U(x_\ell)+x_\ell j_\ell+p_\ell k_\ell]} \\ &= \int_{x(0)=x_i}^{x(t)=x_f} D[x]D[p] e^{\frac{i}{\hbar}\int dt[x(t)\dot{x}(t)-H(p(t),x(t))+x(t)j(t)+p(t)k(t)]},\end{aligned} \tag{82}$$

which can be written after integrating out the momentum as

$$\begin{aligned}Z[j,k] &= \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\lim_{N\to\infty}\prod_{j=1}^{N-1}\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int dx_j e^{\sum_{\ell=1}^{N}[\frac{im}{2\Delta t\hbar}(x_\ell-x_{\ell-1}+\Delta t k_\ell)^2-\frac{i\Delta t}{\hbar}U(x_\ell)+x_\ell j_\ell]} \\ &= \int D[x] e^{\frac{i}{\hbar}\int d\tau[\frac{m}{2}\dot{x}^2(\tau)+\frac{m}{2}k^2(\tau)+m\dot{x}(\tau)k(\tau)-U(x(\tau))+x(\tau)j(\tau)]}.\end{aligned} \tag{83}$$

The insertion of the mixed observable $F[p(t),x(t')]$ is found as

$$\begin{aligned}\int_{x(0)=x_i}^{x(t)=x_f} D[x] e^{\frac{i}{\hbar}\int dt L(x(t),\dot{x}(t))} F[x(t),p(t')] &= F\left[\frac{\hbar}{i}\frac{\delta}{\delta j(t)},\frac{\hbar}{i}\frac{\delta}{\delta k(t')}\right] Z[j,k]_{|j=k=0} \\ &= \langle x_f|e^{-\frac{i}{\hbar}Ht} T[F[\hat{x}_H(t),\hat{p}_H(t')]]|x_i\rangle.\end{aligned} \tag{84}$$

VI. EXPECTATION VALUES

Usually one needs an expectation value rather than transition an amplitude. It is not difficult to generalize the expressions for the expectation value $\langle\psi(t)|A|\psi(t)\rangle$ between the ground state, $|\psi(t) = |0\rangle$ with vanishing energy, $H|0\rangle = 0$. The time dependence of the operator $F[x(t)]$ in (78) can be retained by using the Heisenberg representation c.f. Appendix C to define the expectation value

$$
\begin{aligned}
& \langle 0|T[\prod_{j=1}^{n} F_j(x(t_j))]|0\rangle_H \\
= \ & \langle 0|e^{\frac{i}{\hbar}Ht_n}F_n(x)e^{-\frac{i}{\hbar}Ht_n}e^{\frac{i}{\hbar}Ht_{n-1}}F_{n-1}(x)e^{-\frac{i}{\hbar}Ht_{n-1}}\cdots e^{\frac{i}{\hbar}Ht_1}F_1(x)e^{-\frac{i}{\hbar}Ht_1}|0\rangle_S \\
= \ & \langle 0|e^{\frac{i}{\hbar}Ht_n}F_n(x)e^{-\frac{i}{\hbar}H(t_n-t_{n-1})}F_{n-1}(x)e^{-\frac{i}{\hbar}H(t_{n-1}-t_{n-2})}\cdots e^{-\frac{i}{\hbar}H(t_2-t_1)}F_1(x)e^{-\frac{i}{\hbar}Ht_1}|0\rangle_S. \quad (85)
\end{aligned}
$$

Next we use the stability of the ground state during the time evolution,

$$
e^{-\frac{i}{\hbar}Ht}|0\rangle = |0\rangle, \tag{86}
$$

to insert an "invisible" factor $e^{-\frac{i}{\hbar}Ht}$ beside the bra,

$$
\begin{aligned}
& \langle 0|T[\prod_{j=1}^{n} F_j(x(t_j))]|0\rangle_H \\
= \ & \langle 0|e^{-\frac{i}{\hbar}H(t-t_n)}F_n(x)e^{-\frac{i}{\hbar}H(t_n-t_{n-1})}F_{n-1}(x)e^{-\frac{i}{\hbar}H(t_{n-1}-t_{n-2})}\cdots e^{-\frac{i}{\hbar}H(t_2-t_1)}F_1(x)e^{-\frac{i}{\hbar}Ht_1}|0\rangle_S \quad (87)
\end{aligned}
$$

to find

$$
\begin{aligned}
\langle 0|T[\prod_{j=1}^{n} F_j(x(t_j))]|0\rangle_H &= \langle 0|T[e^{-\frac{i}{\hbar}\int_0^{t_f}dt'H(t')}\prod_{j=1}^{n} F_j(x(t_j))]|0\rangle_S \\
&= \int D[x]e^{\frac{i}{\hbar}S[x]}\prod_{j=1}^{n} F_j(x(t_j) \qquad (88)
\end{aligned}
$$

where the convolution with the ground state wave function is suppressed for better lisibility.

The argument above, introduced by Feynman, relates the ground expectation values transition amplitude between the ground state with operator insertions and provides the starting point for the perturbation expansion. In number of cases one is interested in expectation values between non-sationary state where eq. (86) does not apply. The expectation values of an observable A at time t can be written in the form

$$
\begin{aligned}
\langle A(t)\rangle &= \langle\psi_i|e^{\frac{i}{\hbar}Ht}Ae^{-\frac{i}{\hbar}Ht}|\psi_i\rangle \\
&= \mathrm{Tr}[e^{-\frac{i}{\hbar}Ht}\rho(t_i)e^{\frac{i}{\hbar}Ht}A] = \mathrm{Tr}[\rho_S(t)A_S] \\
&= \mathrm{Tr}[\rho(t_i)e^{\frac{i}{\hbar}Ht}Ae^{-\frac{i}{\hbar}Ht}] = \mathrm{Tr}[\rho_H A_H(t)] \qquad (89)
\end{aligned}
$$

for a general initial state, defined by the density matrix, e.g. $\rho_i = |\psi_i\rangle\langle\psi_i|$ fo the initial pure state $|\psi_i\rangle$.

The path integral expressions for (89) can easily be derived. First we give the path integral formulas for the density matrix for a given time t. There will be two path integrals, one for the bra and the other is for the ket of the initial density matrix,

$$\rho(x^+,x^-,t) = \int dx_i^+ dx_i^- \int_{x^+(0)=x_i}^{x^+(t)=x^+} D[x^+] \int_{x^-(0)=x_i}^{x^-(t)=x^-} D[x^-] e^{\frac{i}{\hbar}S[x^+]-\frac{i}{\hbar}S[^-]}\rho_i(x_i^+,x_i^-) \tag{90}$$

giving the density matrix at time t. The expectation values (89) for $A = F(x)$ can be obtained by means of the generating functional

$$Z[j^+,j^-] = \int D[x^+]D[x^-]e^{\frac{i}{\hbar}S[x^+]-\frac{i}{\hbar}S[x^-]+\frac{i}{\hbar}\int dt[x^+(t)j^+(t)+x^-(t)j^-(t)]} \tag{91}$$

where the convolution with the density matrix is suppressed. In fact, the insertion the operator in question into either time axis yields

$$\langle F(x(t))\rangle = \mathrm{Tr}[\rho_H F(x_H(t))] = F\left[\frac{\hbar}{i}\frac{\delta}{\delta j^\pm(t)}\right] Z[j^+,j^-]_{|j^\pm=0}. \tag{92}$$

The equation is valid for both signs for Hermitian operators $F(x)$. There is no difficulty in extending these formulas for observables containing the coordinate and the momentum at arbitrary time,

$$\langle F[x(t),p(t')]\rangle = \mathrm{Tr}[\rho_H T[x_H(t),p_H(t')]] = F\left[\frac{\hbar}{i}\frac{\delta}{\delta j^\pm(t)},\frac{\hbar}{i}\frac{\delta}{\delta k^\pm(t')}\right] Z[j^+,k^+,j^-,k^-]_{|j^\pm=k^\pm=0}. \tag{93}$$

VII. PERTURBATION EXPANSION

The importance of the path integral integral formalism should be clear by now, it can be use to obtain matrix elements and expectation values. But its usefulness is not clear because the path integral has only been calculated for noninteracting particles. When the interaction, the non-Gaussian part of the action is weak compared to the quadratic part then one expects perturbation expansion be applicable. It is actually much more simple than in the operator formalism because we face only c-numbers in the path integrals. We split the action into a free quadratic term and the rest which is assumed to contain only a weak anharmonic potential $U(x)$,

$$S = S_0 + \int dt U(x(t)), \tag{94}$$

we have

$$\begin{aligned}\langle\psi_f|e^{-\frac{i}{\hbar}Ht}|\psi_i\rangle &= \int D[x]e^{\frac{i}{\hbar}S_0[x]-\frac{i}{\hbar}\int dt' U(x(t'))} \\ &= \sum_{n=0}^\infty \frac{(-i)^n}{n!\hbar^n}\prod_{j=1}^n\int dt_j \int D[x]e^{\frac{i}{\hbar}S_0[x]}\prod_{j=1}^n U(x(t_j))\end{aligned} \tag{95}$$

which can be written as

$$\langle\psi_f|e^{-\frac{i}{\hbar}Ht}|\psi_i\rangle = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!\hbar^n}\prod_{j=1}^{n}\int dt_j\langle\psi_f|T[e^{-\frac{i}{\hbar}\int dt' H_0(t')}\prod_{j=1}^{n}U(x(t_j))]|\psi_i\rangle. \qquad (96)$$

The last equation shows that the propagation in the presence of a potential can be viewed as a sequence of interactions with the potential separated by free propagation.

Another, more compact expression of the perturbation series can be given by the help of the free generator functional

$$Z_0[j] = \int D[x]e^{\frac{i}{\hbar}S_0[x]+\frac{i}{\hbar}\int dt x(t)j(t)}, \qquad (97)$$

which allows us to write (95) as

$$\begin{aligned}\langle\psi_f|e^{-\frac{i}{\hbar}Ht}|\psi_i\rangle &= \sum_{n=0}^{\infty}\frac{(-i)^n}{n!\hbar^n}\prod_{j=1}^{n}\int dt_j\prod_{j=1}^{n}U\left(\frac{\delta}{\delta\frac{i}{\hbar}j(t_j)}\right)Z_0[j]_{|j=0}\\ &= e^{-\frac{i}{\hbar}U(\frac{\delta}{\delta\frac{i}{\hbar}j(t_j)})}Z_0[j]_{|j=0}. \qquad (98)\end{aligned}$$

This form of the perturbation expansion can easier be visualized by Feynman diagrams.

VIII. PROPAGATION ALONG FRACTAL TRAJECTORIES

A classical particle moves along a trajectory with analytic dependence on the time as long as the potential is analytic. This is different in Quantum Mechanics. The reason is that the spacial separation $|x-y|$ scales with the square root of the time of the propagation, $\sqrt{t}$ in the free propagator

$$\langle x|e^{t\frac{i\hbar}{2m}\partial_t^2}|y\rangle = \sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{im}{2\hbar t}(x-y)^2}, \qquad (99)$$

yielding diverging velocity, $|x-y|/t \approx 1/\sqrt{t}$ Another way to see this is to note that the typical trajectories satisfy $|x-y| \approx \sqrt{\Delta t\hbar/m}$ in the path integral (31). In fact, the contributions of the trajectories with $(x-y)^2 \gg \Delta t\hbar/m$ are suppressed by the rapidly oscillating phase of the integrand and the trajectories with $(x-y)^2 \ll \Delta t\hbar/m$ have small entropy. But the most detailed result comes from Eq. (31) in the limit $t \to \infty$ when the dependence of the numerical values of the path integral on the final point x_f is negligible. We can then shift the integration variables $x_\ell \to x_\ell + x_{\ell+1}$ which decouples them and give

$$\langle\Delta x^2\rangle \approx i\frac{\Delta t\hbar}{m}\langle 1\rangle. \qquad (100)$$

This result expresses the fact that fine the time resolution becomes longer the trajectory appears. The rescaling $\Delta t \to \lambda\Delta t$ induces the rescaling

$$L = \sum \sqrt{\Delta x^2} \to \frac{1}{\sqrt{\lambda}} \sum \sqrt{\Delta x^2} = \lambda^{-1/2} L \tag{101}$$

of the length of the trajectory, a scaling law characteristic of fractals.

We can now see better the formal feature of the expressions (26) and (32): the velocity $\dot{x}$ appearing in them is diverging and ill defined! The quadratic terms p^2 or $\dot{x}^2$ alone in the exponents of Eqs. (32) or (26), respectively, would be enough to smoothen out the trajectories and to render $\dot{x}$ finite by the oscillating phase of the integrand. But these quadratic expressions are multiplied by Δt. This factor reduces the impact of the kinetic energy and we loose one power of Δt in the denominator of $\langle \dot{x}^2 \rangle$.

The propagation along fractals is not a mathematical artifact, rather it represents a central part of Quantum Mechanics. Its suppression cancels Heisenberg commutation relation. We shall check this by calculating the matrix elements of the operator $[x, p]$

$$\begin{aligned} \langle [x,p] \rangle &= \langle x_f | T[[p,x] e^{-\frac{i}{\hbar}\int_0^t d\tau H(\tau)}] | x_i \rangle \\ &= \langle x_f | T[(x_{\ell+1} p_{\ell+1} - p_{\ell+1} x_\ell) e^{-\frac{i}{\hbar}\int_0^t d\tau H(\tau)}] | x_i \rangle, \end{aligned} \tag{102}$$

where the index ℓ corresponds to the time the commutator is inserted in the matrix element and the time ordering is used to arrive at the desired order of the coordinate and momentum operators. The infinitesimal propagator (23) shows that the first term on the right hand side of Eq. (102) is indeed the matrix element of xp. We find

$$\langle [x,p] \rangle = \left(\frac{\hbar}{i}\right)^2 \left(\frac{\delta}{\delta j_{\ell+1}} \frac{\delta}{\delta k_{\ell+1}} - \frac{\delta}{\delta j_\ell} \frac{\delta}{\delta k_{\ell+1}} \right) Z[j,k]_{|j=k=0} \tag{103}$$

by means of the generating functional Eq. (83). One differentiation with respect to $ik_\ell/\hbar$ brings down the factor $m(x_\ell - x_{\ell-1})/\Delta t$ as expected from classical mechanics and we find the familiar looking result

$$\begin{aligned} \langle [x,p] \rangle &= \langle x_{\ell+1} m \frac{x_{\ell+1} - x_\ell}{\Delta t} - x_\ell m \frac{x_{\ell+1} - x_\ell}{\Delta t} \rangle \\ &= \frac{m}{\Delta t} \langle (x_{\ell+1} - x_\ell)^2 \rangle \\ &\approx i\hbar \langle 1 \rangle. \end{aligned} \tag{104}$$

Note that a smearing of the singularity of the fractals, the replacement of the scaling law (100) by

$$\langle \Delta x^2 \rangle \approx i \frac{\Delta t^{1+\epsilon} \hbar}{m} \langle 1 \rangle, \tag{105}$$

with $\epsilon > 0$ leads to

$$\langle [x,p]\rangle \approx i\hbar\langle 1\rangle \Delta t^{\epsilon} \to 0, \tag{106}$$

and the loss of the canonical commutation relation. In other words, the scaling law, (100), is an essential part of quantum mechanics, its slightest weakening reduces quantum mechanics to classical physics.

IX. EXTERNAL ELECTROMAGNETIC FIELD

In the presence of an external vector potential $\boldsymbol{A}$ the path integral (40) is changed into

$$\begin{aligned}\langle \boldsymbol{x}_f|e^{-\frac{i}{\hbar}Ht}|\boldsymbol{x}_i\rangle &= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{d}{2}} \lim_{N\to\infty}\prod_{j=1}^{N-1}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{d}{2}}\int d^d x_j \\ &\quad\times e^{\frac{i}{\hbar}\Delta t\sum_{\ell=1}^{N}[\frac{m}{2}(\frac{\boldsymbol{x}_\ell-\boldsymbol{x}_{\ell-1}}{\Delta t})^2-U(\boldsymbol{x}_\ell)+\frac{e}{c}\frac{\boldsymbol{x}_\ell-\boldsymbol{x}_{\ell-1}}{\Delta t}\cdot\boldsymbol{A}(\frac{\boldsymbol{x}_\ell+\boldsymbol{x}_{\ell-1}}{2})]} \\ &= \int_{\boldsymbol{x}(0)=\boldsymbol{x}_i}^{\boldsymbol{x}(t)=\boldsymbol{x}_f} D[x]e^{\frac{i}{\hbar}\int d\tau L(\boldsymbol{x}(\tau),\dot{\boldsymbol{x}}(\tau))}\end{aligned} \tag{107}$$

where

$$L = \frac{m}{2}\dot{\boldsymbol{x}}^2 - U(\boldsymbol{x}) + \frac{e}{c}\dot{\boldsymbol{x}}\cdot\boldsymbol{A}(\boldsymbol{x}). \tag{108}$$

The compact, cutoff independent notation is even more misleading than in the absence of external vector potential due to the need of the mid-point prescription, appearing explicitly in the first equation of (107). To see the origin of this unexpected complication we assume that the vector potential is actually evaluated at an intermediate point

$$\boldsymbol{x} = (1-\eta)\boldsymbol{x}_\ell + \eta\boldsymbol{x}_{\ell-1} \tag{109}$$

in the Eq. (107) and follow an inverse argument in proving the path integral formulas. Let us denote the value of the path integral (107) by $\psi(\boldsymbol{x}_f,t)$ and find its equation of motion. The propagator (17) reads for time dependent Hamiltonian as

$$\langle x_f|T[e^{-\frac{i}{\hbar}\int d\tau H(\tau)}]|x_i\rangle \tag{110}$$

and the equation of motion should be the Schrödinger equation. The strategy is similar than the direct construction of the path integral: an infinitesimal change of time. The increase $t \to t + \Delta t$

corresponds one more integration in the regulated path integral, therefore we have

$$
\begin{aligned}
\psi(\boldsymbol{x}, t+\Delta t) \;=\; & \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{3/2} \int d^d x' \\
& \exp\left[\frac{im}{2\hbar\Delta t}(\boldsymbol{x}-\boldsymbol{x}')^2 - \frac{i}{\hbar}\Delta t U(\boldsymbol{x}+\eta(\boldsymbol{x}'-\boldsymbol{x})) \right. \\
& \left. + \frac{ie}{c\hbar}(\boldsymbol{x}-\boldsymbol{x}')\cdot \boldsymbol{A}(\boldsymbol{x}+\eta(\boldsymbol{x}'-\boldsymbol{x}))\right]\psi(\boldsymbol{x}', t). \qquad (111)
\end{aligned}
$$

The integral is dominated by the contributions $\boldsymbol{x}' \approx \boldsymbol{x}$ for small Δt due to the rapidly oscillating phase of the integrand and we make an expansion for small $\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{x}'$,

$$
\begin{aligned}
\psi(\boldsymbol{x}, t+\Delta t) \;=\; & \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{3/2} \int d^d y \exp\left[\frac{im\boldsymbol{y}^2}{2\hbar\Delta t} - \frac{i}{\hbar}\Delta t U + \frac{ie}{c\hbar}\boldsymbol{y}\cdot\boldsymbol{A} \right. \\
& \left. + \frac{i}{\hbar}\Delta t \eta \boldsymbol{y}\cdot\boldsymbol{\partial}U - \frac{ie\eta}{c\hbar}y_j y_k \partial_k A_j + \cdots \right] \\
& \times \left[1 - \boldsymbol{y}\cdot\boldsymbol{\partial} + \frac{1}{2}(\boldsymbol{y}\cdot\boldsymbol{\partial})^2 + \cdots \right]\psi(\boldsymbol{x}, t) \qquad (112)
\end{aligned}
$$

where the $U = U(\boldsymbol{x})$ and $\boldsymbol{A} = \boldsymbol{A}(\boldsymbol{x})$. The nest step is the expansion of the integrand,

$$
\begin{aligned}
\psi(\boldsymbol{x}, t+\Delta t) \;=\; & \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{3/2} \int d^d y e^{\frac{im}{2\hbar\Delta t} y_j (\delta_{jk} - \frac{2\Delta t e\eta}{mc}\partial_k A_j) y_k} \\
& \left[1 - \frac{i\Delta t}{\hbar}U + \frac{ie}{c\hbar}\boldsymbol{y}\cdot\boldsymbol{A} - \frac{e^2}{2c^2\hbar^2}(\boldsymbol{y}\cdot\boldsymbol{A})^2 + \frac{i\Delta t\eta}{\hbar}\boldsymbol{y}\cdot\boldsymbol{\partial}U + \cdots \right] \\
& \times \left[1 - \boldsymbol{y}\cdot\boldsymbol{\partial} + \frac{1}{2}(\boldsymbol{y}\cdot\boldsymbol{\partial})^2 + \cdots \right]\psi(\boldsymbol{x}, t) \\
=\; & \left(\frac{m}{2\pi i \Delta t \hbar}\right)^{3/2} \int d^d y e^{\frac{im}{2\hbar\Delta t} y_j (\delta_{jk} - \frac{2\Delta t e\eta}{mc}\partial_k A_j) y_k} \\
& \left[1 - \boldsymbol{y}\cdot\boldsymbol{\partial} + \frac{1}{2}(\boldsymbol{y}\cdot\boldsymbol{\partial})^2 - \frac{i\Delta t}{\hbar}U + \frac{ie}{c\hbar}\boldsymbol{y}\cdot\boldsymbol{A} - \frac{ie}{c\hbar}(\boldsymbol{y}\cdot\boldsymbol{A})(\boldsymbol{y}\cdot\boldsymbol{\partial}) \right. \\
& \left. - \frac{e^2}{2c^2\hbar^2}(\boldsymbol{y}\cdot\boldsymbol{A})^2 + \frac{i\Delta t\eta}{\hbar}\boldsymbol{y}\cdot\boldsymbol{\partial}U + \cdots \right]\psi(\boldsymbol{x}, t). \qquad (113)
\end{aligned}
$$

Finally, the Gaussian integration can easily be carried out,

$$
\begin{aligned}
\psi(\boldsymbol{x}, t+\Delta t) \;=\; & \frac{1}{\sqrt{\det B}}\left[1 + \frac{i\hbar\Delta t}{2m}\boldsymbol{\partial}\cdot B^{-1}\cdot\boldsymbol{\partial} - \frac{i\Delta t}{\hbar}U + \frac{\Delta t e}{mc}\boldsymbol{A}\cdot B^{-1}\cdot\boldsymbol{\partial} \right. \\
& \left. - \frac{i\Delta t e^2}{2mc^2\hbar}\boldsymbol{A}\cdot B^{-1}\cdot\boldsymbol{A} + \cdots \right]\psi(\boldsymbol{x}, t), \qquad (114)
\end{aligned}
$$

where

$$
B_{jk} = \delta_{jk} - \frac{2\Delta t e\eta}{mc}\partial_k A_j. \qquad (115)
$$

The expansion of B in Δt further simplifies the result,

$$\begin{aligned}\psi(\boldsymbol{x}, t+\Delta t) &= \left(1+\frac{\Delta te\eta}{mc}\boldsymbol{\partial}\cdot\boldsymbol{A}\right)\left[1+\frac{i\hbar\Delta t}{2m}\boldsymbol{\partial}\cdot B^{-1}\cdot\boldsymbol{\partial}-\frac{i\Delta t}{\hbar}U\right.\\ &\quad\left.+\frac{\Delta te}{mc}\boldsymbol{A}\cdot B^{-1}\cdot\boldsymbol{\partial}-\frac{i\Delta te^2}{2mc^2\hbar}\boldsymbol{A}\cdot B^{-1}\cdot\boldsymbol{A}+\cdots\right]\psi(\boldsymbol{x}, t)\\ &= \left[1+\frac{\Delta te\eta}{mc}\boldsymbol{\partial}\cdot\boldsymbol{A}+\frac{i\hbar\Delta t}{2m}\Delta-\frac{i\Delta t}{\hbar}U+\frac{\Delta te}{mc}\boldsymbol{A}\cdot\boldsymbol{\partial}\right.\\ &\quad\left.-\frac{i\Delta te^2}{2mc^2\hbar}\boldsymbol{A}\cdot\boldsymbol{A}+\cdots\right]\psi(\boldsymbol{x}, t).\end{aligned} \tag{116}$$

The equation of motion is

$$\begin{aligned}i\hbar\partial_t\psi(\boldsymbol{x}, t) &= \left[\frac{i\hbar e\eta}{mc}\boldsymbol{\partial}\cdot\boldsymbol{A}-\frac{\hbar^2}{2m}\Delta+U+\frac{i\hbar e}{mc}\boldsymbol{A}\cdot\boldsymbol{\partial}+\frac{e^2}{2mc^2}\boldsymbol{A}^2\right]\psi(\boldsymbol{x}, t) \qquad (117)\\ &= \left[\frac{1}{2m}\left(\frac{\hbar}{i}\boldsymbol{\partial}-\frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right)^2+U(\boldsymbol{x})+\frac{i\hbar e(\eta-\frac{1}{2})}{mc}\boldsymbol{\partial}\cdot\boldsymbol{A}(\boldsymbol{x})\right]\psi(\boldsymbol{x}, t)\end{aligned}$$

where the cutoff is removed, $\Delta t \to 0$. The lesson of this calculation is that contrary to the naive expectation the η-dependence survives the removal of the cutoff and we must use the mid-point prescription, $\eta = 1/2$ in order to recover the standard Schrödinger equation. This unexpected effect, namely that the details at time scale Δt remain visible at finite time after the limit $\Delta t \to 0$ has been taken is called quantum anomaly.

X. ÎTO INTEGRAL

The surprising persistence of the η-dependence found in the previous section is the result of the fractal nature of the typical trajectories in the path integral. We shall show this by identifying a characteristic feature of ordinary time integrals occurring within the path integral.

The usual properties, such as the rule of change of variable, of a Riemann integral is usually derived by replacing the integral with a sum and by performing appropriate limit. These rules may change if the functions in question are not regular. Let us consider the following change of variable:

$$\int_{t_i}^{t_f} dt\dot{x}(t)\frac{df(x)}{dx} = \int_{x_i}^{x_f} dx\frac{df(x)}{dx} = f(x_f) - f(x_i), \tag{118}$$

valid for continuously differentiable functions $x(t)$ and $f(x)$.

What happens if $x(t)$ is a fractal, in particular, a typical trajectory in the path integral? To find the answer we perform the calculation at small but finite Δt. We start with the safe identity

$$f(x_f) - f(x_i) = \sum_{j=1}^{N}[f(x_j) - f(x_{j-1})], \tag{119}$$

where $x_0 = x_i$ and $x_N = x_f$. In the next step we check the sensitivity of the right hand side on the choice of the point where the integrand is evaluated. For this end we introduce the η parameter by defining the point of evaluation

$$x_{j-1}^{(\eta)} = (1-\eta)x_j + \eta x_{j-1}, \tag{120}$$

the notation $f_j = f(x_j^{(\eta)})$, $\Delta_j = x_j - x_{j-1}$ and write for Eq. (119)

$$\begin{aligned} f(x_f) - f(x_i) &\approx \sum_{j=1}^{N} \Bigg[\left(f(x_{j-1}^{(\eta)}) + \eta\Delta_j \frac{df(x_{j-1}^{(\eta)})}{dx} + \frac{\eta^2}{2}\Delta_j^2 \frac{d^2 f(x_{j-1}^{(\eta)})}{dx^2} \right) \\ &\quad - \left(f(x_{j-1}^{(\eta)}) + (\eta-1)\Delta_j \frac{df(x_{j-1}^{(\eta)})}{dx} + \frac{(\eta-1)^2}{2}\Delta_j^2 \frac{d^2 f(x_{j-1}^{(\eta)})}{dx^2} \right) \Bigg] \\ &= \sum_{j=1}^{N} \left[\Delta_j f'(x_{j-1}^{(\eta)}) + \left(\eta - \frac{1}{2}\right) \Delta_j^2 f''(x_{j-1}^{(\eta)}) \right]. \end{aligned} \tag{121}$$

The scaling law, (100), yields

$$f(x_f) - f(x_i) = \int_{x_i}^{x_f} dx \frac{df(x)}{dx} + \left(\eta - \frac{1}{2}\right) \frac{i\hbar}{m} \int_{x_i}^{x_f} dt \frac{d^2 f(x)}{dx^2}, \tag{122}$$

a modification of partial integration rule. The functions are assumed to be sufficiently regular and differentiable in standard integral and differential calculus. But the transformation of integrals for fractals (100) requires to keep one order of magnitude more in the finite difference, Δt or Δx and the result is a modification of the usual rules, like (122).

XI. QUANTIZATION RULES IN POLAR COORDINATES

The fact that the path integral is dominated by nowhere differentiable, fractal trajectories requires the modification of certain rules of standard analysis. This explains the circumstance that the quantum mechanics does not display canonical invariance as its classical counterpart, in particular, its rules depend on the choice of coordinate system. We demonstrate this feature by working out the naive rules of quantization in polar coordinates.

These rules for a free particle in the usual coordinate systems are the following: One starts with the Lagrangian

$$L_0 = \frac{m}{2}\dot{\boldsymbol{x}}^2, \tag{123}$$

defines the momentum

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{x}}}, \tag{124}$$

and construct the Hamiltonian,

$$H_0 = \dot{\boldsymbol{x}}\boldsymbol{p} - L_0, \tag{125}$$

expressed in terms of the momentum

$$H_0 = \frac{\boldsymbol{p}^2}{2m}. \tag{126}$$

The canonical commutation relations,

$$[x_j, p_k] = i\hbar\delta_{j,k}, \tag{127}$$

give rise to the representation $p_j = \frac{\hbar}{i}\partial_{x_j}$ and the Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2, \tag{128}$$

which possesses translational and rotational symmetry,

$$[H_0, \boldsymbol{p}] = [H_0, \boldsymbol{L}] = 0, \tag{129}$$

where the momentum $\boldsymbol{p}$ and angular momentum $\boldsymbol{L}$ generates translations and rotations, respectively.

One uses the parametrization

$$\boldsymbol{x} = \begin{cases} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{cases} \tag{130}$$

in polar coordinates where the free Lagrangian

$$\tilde{L}_0 = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) \tag{131}$$

yields the momenta

$$\begin{aligned} p_r &= \frac{\delta L_0}{\delta\dot{r}} = m\dot{r}, \\ p_\theta &= \frac{\delta L_0}{\delta\dot{\theta}} = mr^2\dot{\theta}, \\ p_\phi &= \frac{\delta L_0}{\delta\dot{\phi}} = mr^2\sin^2\theta\dot{\phi}. \end{aligned} \tag{132}$$

The Hamiltonian is therefore of the form

$$\begin{aligned} \tilde{H}_0 &= p_r\dot{r} + p_\theta\dot{\theta} + p_\phi\dot{\phi} - L \\ &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2\sin^2\theta}. \end{aligned} \tag{133}$$

The corresponding operators are determined by the canonical commutation relations,

$$[r, p_r] = [\theta, p_\theta] = [\phi, p_\phi] = i\hbar \tag{134}$$

with the solution

$$p_r = \frac{\hbar}{i}\frac{\partial}{\partial r}, \quad p_\theta = \frac{\hbar}{i}\frac{\partial}{\partial \theta}, \quad p_\phi = \frac{\hbar}{i}\frac{\partial}{\partial \phi}. \tag{135}$$

These operators lead to the Hamilton operator

$$\tilde{H}_0 = -\frac{\hbar^2}{2m}\left[\partial_r^2 + \frac{1}{r^2}\left(\partial_\theta^2 + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\right]. \tag{136}$$

It is not difficult to see that this operator does not possess the usual symmetries, namely $[\tilde{H}_0, \boldsymbol{p}] \neq 0$, $[\tilde{H}_0, \boldsymbol{L}] \neq 0$.

The correct Hamiltonian is obtained by means of the Laplace-Beltrami operator,

$$H_0 = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\phi^2\right)\right], \tag{137}$$

which differs from $\tilde{H}_0$,

$$H_0 = \tilde{H}_0 + i\frac{\hbar}{2m}\left(\frac{2}{r}p_r + \cot\theta p_\theta\right) \tag{138}$$

The difference, an $\mathcal{O}(\hbar)$ term, is called Îto potential because the derivation of the Hamilton function, defined by the exponent of the phase space path integral, produces the result (138) and shows that the Îto potential arises from the scaling law (100).

Appendix A: Bracket formalism

The bracket formalismis of Dirac is very well suited to the need of linear algebra and quantum mechanics in particular. It consists of thefollowing two steps:

1. The scalar products, (ϕ, ψ) and $(\phi, A\psi)$ where A is an operator are written as $\langle\phi|\psi\rangle$ and $\langle\phi|A|\psi\rangle$, respectively.

2. The symbols bra, $\langle\phi|$, and ket, $|\psi\rangle$ are used independently. (This is the main point, the previous one faciliates this use only.) The ket denotes a vector, an element of a linear space, $|\psi\rangle \in \mathcal{H}$ and the bra stands for a linear functional over the vector field, $\langle\phi| : \mathcal{H} \to C$. The bras and kets form two equivalent linear spaces, namely there is an invertible linear map, connecting them if $\mathcal{H}$ is a Hilbert space.

The advantages of the bracket formalism can be seen in the following rules:

1. Projector onto the vector $|\psi\rangle$:

$$P_{|\psi\rangle} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{A1}$$

2. Closing relation of a basis $\{|n\rangle\}$:

$$\mathbb{1} = \sum_n |n\rangle\langle n|. \tag{A2}$$

In the case of a continuous spectrum the sum is replaced by an integral.

3. Projection of a vector $|\psi\rangle$ onto a basis $\{|n\rangle\}$:

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle. \tag{A3}$$

4. One formally defines the eigenstates of the coordinate and the momentum operators, $\hat{x}$ and $\hat{p}$, respectively, as $\hat{x}|x\rangle = x|x\rangle$, $\hat{p}|p\rangle = p|p\rangle$ and impose the closing relations,

$$\mathbb{1} = \int dx|x\rangle\langle x| = \int \frac{dp}{2\pi\hbar}|p\rangle\langle p|. \tag{A4}$$

The convention of the normalization of the state $|p\rangle$, leading to the denominator in the second integral is motivated below by the Fourier theorem.

5. The wave function of the state $|\psi\rangle$ is defined as $\psi(x) = \langle x|\psi\rangle$. The closing relation gives

$$\psi(x) = \langle x|\psi\rangle = \langle x|\mathbb{1}|\psi\rangle = \int dy\langle x|y\rangle\langle y|\psi\rangle = \int dy\langle x|y\rangle\psi(y) \tag{A5}$$

implies $\langle x|y\rangle = \delta(x-y)$.

6. The wave function of the image of the state $|\psi\rangle$ after the action of the operator A is

$$[A\psi](x) = \langle x|A|\psi\rangle. \tag{A6}$$

eg. $\langle x|\hat{p}|p\rangle = \frac{\hbar}{i}\nabla\langle x|p\rangle = p\langle x|p\rangle \to \psi_p(x) = \langle x|p\rangle = ce^{\frac{i}{\hbar}xp}$.

7. Wave function in momentum space is given by $\tilde{\psi}(p) = \langle p|\psi\rangle$. The closing relation gives in this case

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \langle p|\mathbb{1}|\psi\rangle = \int \frac{dq}{2\pi\hbar}\langle p|q\rangle\langle q|\psi\rangle, \tag{A7}$$

leading to $\langle p|q\rangle = 2\pi\hbar\delta(p-q)$.

8. Fourier theorem for the wave function,

$$\tilde{\psi}(p) = \int dx e^{-\frac{i}{\hbar}px}\psi(x), \qquad \psi(x) = \int \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}px}\tilde{\psi}(p) \tag{A8}$$

can be written by means of the closing relations and $c = 1$ as

$$\begin{aligned}\tilde{\psi}(p) &= \langle p|\psi\rangle = \langle p|\mathbb{1}|\psi\rangle = \int dx \langle p|x\rangle\langle x|\psi\rangle = \int dx e^{-\frac{i}{\hbar}px}\psi(x),\\ \psi(x) &= \langle x|\psi\rangle = \langle x|\mathbb{1}|\psi\rangle = \int dp \langle x|p\rangle\langle p|\psi\rangle = \int \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}px}\tilde{\psi}(p)\end{aligned} \tag{A9}$$

The linear space, obtained by extending the original Hilbert space with the basis vectors $|x\rangle$ and $|p\rangle$ is called a rigged Hilbert space.

Appendix B: Functional derivative

The functionals are defined by mens of lattice discretization. A continuous function $f(t)$ defined in the interval $t_i < t < t_f$ is approximated by the values $\{f_j = f(t_j)\}$, $t_j = t_i + j\Delta t$, $\Delta t = (t_f - t_i)/N$, $j = 1, \ldots, N$ of a piecewise constant function for large but finite N. The functional derivatives of the functional

$$F[f] = \int_{t_i}^{t_f} dt f(t) g(t) = \Delta t \sum_{j=1}^{N} f_j g_j \tag{B1}$$

are defined by

$$\frac{\delta^n F[f]}{\delta f(\tau_1) \cdots \delta f(\tau_n)} = \frac{1}{\Delta t^n} \frac{\partial^n F[f]}{\partial f_1 \cdots \partial f_n}, \tag{B2}$$

where $t_{j-1} \le \tau_j < t_j$. The singular prefactor $1/\Delta t^n$ is needed to assure the identity

$$\frac{\delta F[f]}{\delta f(t)} = g(t). \tag{B3}$$

The generalization of the Taylor expansion for multi-variable functions,

$$f(\boldsymbol{x} + \boldsymbol{\epsilon}) = \sum_{n=0}^{\infty} \frac{(\boldsymbol{\epsilon} \cdot \boldsymbol{\partial})^n}{n!} f(\boldsymbol{x}) \tag{B4}$$

is the functional Taylor expansion reads as

$$F[x + \epsilon] = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int_{t_i}^{t_f} dt \epsilon(t) \frac{\delta}{\delta x(t)} \right)^n F[x]. \tag{B5}$$

Appendix C: Representations of time dependence

Sometime it is useful to make time-dependent basis transformation in representing the time dependence. One usually encounter the following three cases:

1. Schrödinger representation

The traditional way to represent the time dependence, generated by a time-independen Hamiltonian H, is letting the states to follow the time-dependence prescribed by Schrödinger's equation

$$i\hbar\partial_t|\psi(t)\rangle_S = H|\psi(t)\rangle_S, \tag{C1}$$

leading to

$$|\psi(t)\rangle_S = e^{-\frac{i}{\hbar}(t-t_i)H}|\psi(t_i)\rangle_S. \tag{C2}$$

The time is treated as a number, without replacing it with an operator. Hence the time-dependence is trivial for the observables and we can restrict our attention the time-independent operators, $i\hbar\partial_t A_S = 0$. The different representations will agree at the initial time, t_i.

2. Heisenberg representation

The classical fields acquire non-trivial time-dependence in field theory. the quantum generalization, quantum field theory, contains field operators with non-trivial time-dependence. This makes is necessary to reformulate the time dependence in terms of opeartors. The simplest possibility is to perform a time-dependent basisi transformation in te Schrödingr picture which stops the states,

$$|\Psi(t)\rangle_H = e^{\frac{i}{\hbar}(t-t_i)H}|\Psi(t)\rangle_S. \tag{C3}$$

The transformaiotn of the opeerators is inferred by requiring that the matrix elements are identical in the two representations,

$$\langle\psi(t)|_S A_S|\psi(t)\rangle_S = \underbrace{\langle\psi(t_i)|e^{\frac{i}{\hbar}(t-t_i)H}}_{\langle\psi(t)|_S} A_S \underbrace{e^{-\frac{i}{\hbar}(t-t_i)H}|\psi(t_i)\rangle}_{|\psi(t)\rangle_S} = \langle\psi(t_i)|\underbrace{e^{\frac{i}{\hbar}(t-t_i)H}A_S e^{-\frac{i}{\hbar}(t-t_i)H}}_{A(t)_H}|\psi(t_i)\rangle, \tag{C4}$$

which induces the transformation

$$A_H(t) = e^{\frac{i}{\hbar}(t-t_i)H}A_S e^{-\frac{i}{\hbar}(t-t_i)H}. \tag{C5}$$

Therefore, the operators satisfy the Heisenberg equation of motion,

$$i\hbar\partial_t A_H(t) = [A_H, H], \tag{C6}$$

with the initial conditions $A_H(t_i) = A_S$.

3. Interaction representation

The perturbation expansion can be applied for the Hamiltonian $H = H_0 + H_1$ where H_0 and H_1 represent the free, easily diagonalizable dominant part and the small, complicated interaction part, respectively. The perturbation expansion for the Heisenberg equation is rather cumbersome a reasonable compromise between the two preceding representations to place the time dependence, generated by the simple part of the Hamiltonian into the operators and leave the complicated but supposedly small part of the time dependence for the states where the usual Rayleigh-Schrödinger perturbation expansion is relatively simple.

For this end we define

$$|\Psi(t)\rangle_i = e^{\frac{i}{\hbar}(t-t_i)H_0}|\Psi(t)\rangle_S \tag{C7}$$

which induces the transformation

$$A_i(t) = e^{\frac{i}{\hbar}(t-t_i)H_0}A_S e^{-\frac{i}{\hbar}(t-t_i)H_0} \tag{C8}$$

for the operators. The state vector satisfies the equation of motion

$$\begin{aligned} i\hbar\partial_t|\Psi(t)\rangle_i &= -H_0|\Psi(t)\rangle_i + e^{\frac{i}{\hbar}(t-t_i)H_0}(H_0+H_1)|\Psi(t)\rangle_S \\ &= -H_0|\Psi(t)\rangle_i + e^{\frac{i}{\hbar}(t-t_i)H_0}(H_0+H_1)e^{-\frac{i}{\hbar}(t-t_i)H_0}e^{\frac{i}{\hbar}(t-t_i)H_0}|\Psi(t)\rangle_S \\ &= H_{1i}(t)|\Psi(t)\rangle_i \end{aligned} \tag{C9}$$

is indeed a Schrödinger equation involving the interaction only. The operators follow the free Heisenberg equation,

$$i\hbar\partial_t A_i(t) = [A_i, H_0]. \tag{C10}$$

4. Schrödinger equation with time dependent Hamiltonian

The interaction representation requires the solution of Schrödinger's equation with time dependent Hamiltonian,

$$i\hbar\partial_t|\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \tag{C11}$$

To obtain it in a closed form one introduces the time-ordered product, a modified multiplication rule for operators depending on the time. For a chain of operators $A_1(t_1), \cdots, A_n(t_n)$ the time ordered product is defined by acting with the operators in the order of ascending time values. For two operators we have

$$T[A(t_A)B(t_B)] = \Theta(t_A - t_B)A(t_A)B(t_B) + \Theta(t_B - t_A)B(t_B)A(t_A), \tag{C12}$$

where

$$\Theta(t) = \begin{cases} 1 & t > 1, \\ \frac{1}{2} & t = 0, \\ 0 & t < 0. \end{cases} \tag{C13}$$

The solution of Schrödinger's equation is

$$|\Psi(t)\rangle = U(t, t_i)|\Psi(t_i)\rangle \tag{C14}$$

where

$$U(t, t_i) = T[e^{-\frac{i}{\hbar}\int_{t_i}^{t} dt' H(t')}]. \tag{C15}$$

To prove this result it is sufficient to show that the time evolution operator $U(t_2, t_1)$ satisfies the equation of motion

$$i\hbar\partial_t U(t, t_i) = H(t)U(t, t_i). \tag{C16}$$

This can easily be done by writing

$$\begin{aligned} i\hbar\partial_t U(t, t_i) &= i\partial_t T[e^{-\frac{i}{\hbar}\int_{t_i}^{t} dt' H(t')}] \\ &= i\hbar\partial_t \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar})^n}{n!} \int_{t_i}^{t} dt_1 \cdots \int_{t_i}^{t} dt_n T[H(t_1) \cdots H(t_n)], \end{aligned} \tag{C17}$$

and noting that the derivative ∂_t generates n-times the same integrand,

$$\begin{aligned} i\hbar\partial_t U(t, t_i) &= \hbar \sum_{n=0}^{\infty} \frac{n(-\frac{i}{\hbar})^n}{n!} \int_{t_i}^{t} dt_2 \cdots \int_{t_i}^{t} dt_n T[H(t)H(t_1) \cdots H(t_{n-1})] \\ &= H(t) \sum_{n=1}^{\infty} \frac{(-\frac{i}{\hbar})^{n-1}}{(n-1)!} \int_{t_i}^{t} dt_1 \cdots \int_{t_i}^{t} dt_{n-1} T[H(t_1) \cdots H(t_{n-1})] \\ &= H(t)U(t, t_i). \end{aligned} \tag{C18}$$