Path integral in quantum mechanics: an introduction

Rodrigo de León Ardón

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1 Classical Newtonian dynamics

Assume that the dynamics of a particle, with mass m, moving a long a line and subject to a force $F(x)$, is govern by the equation

$$m\ddot{x}(t) = F(x(t)). \tag{1}$$

The physical dimensions are $[m] = M$, $[x] = L$, $[t] = T$ and thus the force must have dimensions of $[F] = ML/T^2$. This immediately imply that are characteristics physical scales. For example consider $F = \alpha x$. Then the constant α must have dimensions $[\alpha] = M/T^2$.

Now, let us multiply the equation by $\dot{x}$ to obtain $\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}^2/2) = \dot{x}F(x)$. We see that for $\dot{x} = \text{const}.$ we must have $F = 0$. Moreover, if the force can be defined as

$$F(x) = -\frac{\mathrm{d}V(x)}{\mathrm{d}x}, \tag{2}$$

where $V(x)$ is the potential, we will obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m}{2}\dot{x}^2 + V(x)\right) = 0. \tag{3}$$

Hence, the quantity

$$E \equiv \frac{m}{2}\dot{x}^2 + V(x), \tag{4}$$

is a constant of motion. It has dimensions of $[E] = ML^2/T^2$ as well as the potential. Hence, the equation $m\ddot{x} = -V'$ has a constant of motion $E = \frac{m}{2}\dot{x}^2 + V(x)$. On the other hand, the equation is usually interpreted as a initial value problem and thus for an initial time t_1 we specify $x_1 = x(t_1)$ and $\dot{x}_1 = \dot{x}(t_1)$. This in turn sets the value of E to $E_1 = \frac{m}{2}\dot{x}_1^2 + V(x_1)$.

We can interpret these results in a different perspective by considering equation (4) as the starting point. We specify $x_1 = x(t_1)$ and $\dot{x}_1 = \dot{x}(t_1)$ and therefore we obtain

$$\frac{m}{2}\dot{x}_1^2 + V(x_1) = \frac{m}{2}\dot{x}^2 + V(x), \tag{5}$$

where for the right hand side $t \neq t_1$. Taking a temporal derivative we get

$$0 = \dot{x}(m\ddot{x} + V'). \tag{6}$$

Thus, either $\dot{x} = 0$ or $m\ddot{x} + V'$ for all $t \neq t_0$. If we consider $\dot{x} = 0$ we will have $0 = \frac{\mathrm{d}V}{\mathrm{d}t}$ and thus the potential is a constant and thus there is no force. Then, for a no trivial dynamics we consider $m\ddot{x} + V' = 0$ for all $t \neq t_0$. Notice that in some sense we have "derived" the equation.

This interpretation is exciting. To make more sense to it, first we consider an auxiliary variable p defined as

$$p = m\dot{x}. \tag{7}$$

Then, we will have

$$E = \frac{1}{2m}p^2 + V(x), \tag{8}$$

and now the initial data is x_1 and p_1. Following the previously discussed logic, we will obtain the expression $0 = \frac{p\dot{p}}{m} + V'\dot{x}$ and naively re-write it as $0 = \frac{p}{m}(\dot{p} + V')$ and obtain $\dot{p} = -V'$. This is the equation for p but we do not derive the equation for x, i.e. $p = m\dot{x}$. This is only a problem if we want to interpret p and x as independent variables. Notice that

$$0 = \frac{p\dot{p}}{m} + V'\dot{x} = \frac{p\dot{p}}{m} + V'\left(\dot{x} - \frac{p}{m}\right) + V'\frac{p}{m} = \frac{p}{m}(\dot{p} + V') + V'\left(\dot{x} - \frac{p}{m}\right). \tag{9}$$

By demanding that $\frac{p}{m} \neq 0$ and $V' \neq 0$ we obtain

$$\dot{p} = -V', \quad \dot{x} = \frac{p}{m}. \tag{10}$$

Hence, we can interpret p and x as independent variables. In order translate this demand in a manifest way let us define the function $H(x,p)$ subject to $H(x,p) = E$. This function has the form

$$H = \frac{1}{2m}p^2 + V(x), \tag{11}$$

and therefore

$$\frac{\partial H}{\partial p} = \frac{p}{m}, \quad \frac{\partial H}{\partial x} = V', \quad \frac{\partial^2 H}{\partial x \partial p} = \frac{\partial^2 H}{\partial p \partial x} = 0. \tag{12}$$

Then, equation (9) gives

$$0 = \frac{\partial H}{\partial p}\left(\dot{p} + \frac{\partial H}{\partial x}\right) + \frac{\partial H}{\partial x}\left(\dot{x} - \frac{\partial H}{\partial p}\right) = \frac{\mathrm{d}H}{\mathrm{d}t}. \tag{13}$$

Recall that due to the form of H, it is an implicit function of time. If $\frac{\partial H}{\partial p} \neq 0$ and $\frac{\partial H}{\partial x}$ for all $t \neq t_1$, we obtain

$$\dot{p} = -\frac{\partial H}{\partial x}, \quad \dot{x} = \frac{\partial H}{\partial p}, \tag{14}$$

with x_1 and p_1 given. This is a completely different way of thinking because we can define H without considering the equation for x and p. The equations are obtained by demanding $H(x,p) = E$. In order to specify E, x_1 and p_1 must be given. If we define the condition $H(x,p) = E$ as an on-shell condition, then H is defined off-shell. For example, we can have the off-shell quantity

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial x}\dot{x} + \frac{\partial H}{\partial p}\dot{p}, \tag{15}$$

which on shell gives

$$\left.\frac{\mathrm{d}H}{\mathrm{d}t}\right|_{\text{on-shell}} = 0. \tag{16}$$

The obvious question is how to give, off-shell, the actual form of H? We know at least that it must contain a term proportional to p^2.

Let us use the knowledge of the Newton equation for the harmonic oscillator. Then, we know that

$$H(x,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2. \tag{17}$$

We then can interpret the system in a geometrical way. Consider $\mathbb{R}^3$ and the coordinates X, Y, Z. By setting

$$X = x, \quad Y = p, \quad Z = H(x,p), \tag{18}$$

We obtain an elliptic paraboloid $\mathbb{R}^3$ for $Z > 0$. When we go on-shell, i.e. $Z = E$, we obtain a curve perpendicular to this axis. This curve can be projected to the x-p plane and notice that the curve is parametrized by t. Now, in order to get a specific projected curve we must select E_1 which correspond to set x_1 and p_1.

So we learn that in general, the solutions to the equations corresponds to a curve in the x-p plane. This space is the domain of the function $H(x,p)$. Now, consider another function $A(x,p)$. Then,

$$\frac{\mathrm{d}}{\mathrm{d}t}A(x,p) = \frac{\partial A}{\partial x}\dot{x} + \frac{\partial A}{\partial p}\dot{p}. \tag{19}$$

On-shell we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}A(x,p) = \frac{\partial A}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial H}{\partial x}. \tag{20}$$

This motivates the definition of the following quantity

$$\frac{1}{\lambda}\{A(x,p), B(x,p)\} \equiv \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}. \tag{21}$$

The bracket $\{\cdot,\cdot\}$ is defined off-shell and we have introduced λ for dimensional reasons. Notice that $[\lambda] = [xp]$. Consider

$$\frac{1}{\lambda}\{p, H(x,p)\} = -\frac{\partial H}{\partial x}, \quad \frac{1}{\lambda}\{x, H(x,p)\} = \frac{\partial H}{\partial p}. \tag{22}$$

On-shell we find

$$\dot{p} = \frac{1}{\lambda}\{p, H(x,p)\}, \quad \dot{x} = \frac{1}{\lambda}\{x, H(x,p)\}. \tag{23}$$

We stress the difference between on-shell and off-shell. Suppose that we have a function $\mathcal{O}(x, p, t)$. Then, off-shell we have

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \frac{\partial \mathcal{O}}{\partial t} + \frac{\partial \mathcal{O}}{\partial x}\dot{x} + \frac{\partial \mathcal{O}}{\partial p}\dot{p}, \tag{24}$$

and on-shell

$$\frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} = \frac{\partial \mathcal{O}}{\partial t} + \frac{1}{\lambda}\{\mathcal{O}, H\}. \tag{25}$$

Equivalently, we can start off-shell with

$$\frac{1}{\lambda}\{\mathcal{O}, H\} = \frac{\partial \mathcal{O}}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial \mathcal{O}}{\partial p}\frac{\partial H}{\partial x}. \tag{26}$$

On-shell we find

$$\frac{1}{\lambda}\{\mathcal{O}, H\} = \frac{\partial \mathcal{O}}{\partial x}\dot{x} + \frac{\partial \mathcal{O}}{\partial p}\dot{p} = \frac{\mathrm{d}\mathcal{O}}{\mathrm{d}t} - \frac{\partial \mathcal{O}}{\partial t}. \tag{27}$$

On the other hand, consider the fundamental expression

$$\{x, p\} = \lambda. \tag{28}$$

What is the physical meaning of λ? The constant is only relevant if we consider the bracket. Otherwise is not fundamental since it does not appear directly in the equations of motion. But if we consider it to be meaningful, we will have

$$[\lambda] = (ML)\frac{L}{T}, \tag{29}$$

and therefore

$$[x] = \sqrt{\frac{T}{M}[\lambda]}, \quad [p] = \sqrt{\frac{M}{T}[\lambda]}, \quad [H] = \frac{[\lambda]}{T}. \tag{30}$$

Now if we work in a system in which the velocity is dimensionless, i.e. $L = T$, and the mass is measured in terms of inverse length, i.e. $M = 1/L$, we obtain

$$[x] = L, \quad [p] = \frac{1}{L}, \quad [H] = \frac{1}{L}, \tag{31}$$

and λ is dimensionless so we can set $\lambda = 1$. At this stage this seems completely nonsense, later we will see that it is completely reasonable and that the bracket due indeed has a fundamental role.

Now we are in position to generalize the system and called the objects by their names. Suppose that we now have N particles over the line. Then, instead of consider a x-p plane, we have $\mathbb{R}^{2N}$ space, this is called phase-space. The p's are the momenta for each particle. A point in phase-space is given by $(\mathbf{x}, \mathbf{p}) = (x^1, \ldots, x^N, p_1, \ldots, p_N)$. Therefore, the Hamiltonian function is written as $H = H(\mathbf{x}, \mathbf{p})$, the Poisson bracket as

$$\begin{aligned} \frac{1}{\lambda}\{A(\mathbf{x},\mathbf{p}), B(\mathbf{x},\mathbf{p})\} &\equiv \sum_i^N \left(\frac{\partial A}{\partial x^i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x^i} \right), \\ &= \nabla_{\mathbf{x}} A \cdot \nabla_{\mathbf{p}} B - \nabla_{\mathbf{p}} A \cdot \nabla_{\mathbf{x}} B. \end{aligned} \tag{32}$$

and

$$\{x^i, x^j\} = 0, \quad \{p_i, p_j\} = 0, \quad \{x^i, p_i\} = \lambda \delta^i_j. \tag{33}$$

Again, the equations of motion are obtained from the on-shell condition $H(\mathbf{x}, \mathbf{p}) = E$ where E is the energy of the system. Recall that H can be seen as a $2N$-dimensional surface in an extended phase space $\mathbb{R}^{2N+1}$, as discussed for the harmonic oscillator. On shell we obtain a $(2N-1)$-dimensional surface and its projection to to phase space is denoted as Ω. Per each E there is a hypersurface Ω_E. Initial conditions will select one among all of them and the solution $(\mathbf{x}(t), \mathbf{p}(t))$ corresponds to a curve defined on Ω_E. Notice that only for $N = 1$, Ω_E correspond to curve and if the particles move in $\mathbb{R}^n$ we consider $2nN$ instead of $2N$. The equations of motion are

$$\dot{p}_i = -\frac{\partial H}{\partial x^i}, \quad \dot{x}^i = \frac{\partial H}{\partial p_i}. \tag{34}$$

which can be written as

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{x}} H, \quad \dot{\mathbf{x}} = \nabla_{\mathbf{p}} H. \tag{35}$$

With this notation, the off-shell quantity $\mathrm{d}H/\mathrm{d}t$ can be written as

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \nabla_{\mathbf{x}} H \cdot \dot{\mathbf{x}} + \nabla_{\mathbf{p}} H \cdot \dot{\mathbf{p}}. \tag{36}$$

Now let us consider how the hamiltonian H changes under perturbations. Let H' be the hamiltonian of the perturbed system and H the hamiltonian of the unperturbed system. For the later, we assume that we have a solution of $\dot{\mathbf{p}} = -\nabla_{\mathbf{x}} H$, $\dot{\mathbf{x}} = \nabla_{\mathbf{p}} H$ with $(\mathbf{x}(t = t_1), \mathbf{p}(t = t_1))$ given. The $(2N-1)$-dimensional surface Ω_{E_1} is defined and we know the curve on Ω_{E_1}. For the moment, let us think H' as a completely independent system with repspect to H and the position and momenta are label by $\mathbf{x}'$ and $\mathbf{p}'$. The on-shell condition $H' = E'$ will give $\dot{\mathbf{p}}' = -\nabla_{\mathbf{x}'} H'$, $\dot{\mathbf{x}}' = \nabla_{\mathbf{p}'} H'$ and $\Omega_{E'}$. In order to relate both systems, we see that E' must be of the form $E' \approx E + \varepsilon$ where the energy ε is considered to be small. Then, the $\Omega_{E'}$ hypersurface corresponds to the Ω_E hypersurface with small perturbations. Then, we can consider $\mathbf{x}' = \mathbf{x} + \delta\mathbf{x}$ and $\mathbf{p}' = \mathbf{p} + \delta\mathbf{p}$ where the functions $\delta\mathbf{x}$ and $\delta\mathbf{p}$ are small and parametrize these perturbations. To clarify we can denote them as $\delta\mathbf{x} = \epsilon_1\vec{\eta}(\mathbf{x})$ and $\delta\mathbf{p} = \epsilon_2\vec{\zeta}(\mathbf{p})$ where ϵ_1 and ϵ_2 are small parameters that control the perturbation.

We can use these linear splittings ff-shell to obtain

$$H'(\mathbf{x}',\mathbf{p}') \approx H'(\mathbf{x}',\mathbf{p}')\big|_{\mathbf{x}'=\mathbf{x},\mathbf{p}'=\mathbf{p}} + \nabla_{\mathbf{x}'}H'\big|_{\mathbf{x}'=\mathbf{x},\mathbf{p}'=\mathbf{p}}\cdot\delta\mathbf{x} + \nabla_{\mathbf{p}'}H'\big|_{\mathbf{x}'=\mathbf{x},\mathbf{p}'=\mathbf{p}}\cdot\delta\mathbf{p}. \tag{37}$$

In order to recover the on-shell condition $E' \approx E + \varepsilon$, then we must have that

$$H'(\mathbf{x}',\mathbf{p}')\big|_{\mathbf{x}'=\mathbf{x},\mathbf{p}'=\mathbf{p}} = H(\mathbf{x},\mathbf{p}), \tag{38}$$

and thus

$$H'(\mathbf{x}',\mathbf{p}') \approx H(\mathbf{x},\mathbf{p}) + \nabla_{\mathbf{x}}H\cdot\delta\mathbf{x} + \nabla_{\mathbf{p}}H\cdot\delta\mathbf{p}. \tag{39}$$

To justify the above expression notice, for example, that $\frac{\partial H'}{\partial x'^i} = \frac{\partial x^j}{\partial x'^i}\frac{\partial H'}{\partial x^j}$ and $\frac{\partial x'^i}{\partial x^j} = \delta^i_j + \epsilon_1\frac{\partial \eta^i}{\partial x^j}$. Then, $\frac{\partial H'}{\partial x'^i} = \left(\delta^j_i + O(\epsilon_1)\right)\frac{\partial}{\partial x^j}(H + O(\epsilon_1)) = \frac{\partial H}{\partial x^i} + O(\epsilon_1)$.

Therefore, on-shell we obtain

$$E' \approx E - \dot{\mathbf{p}}\cdot\delta\mathbf{x} + \dot{\mathbf{x}}\cdot\delta\mathbf{p}. \tag{40}$$

It remains to contemplate the initial conditions. Since we know them for the unperturbed system we need to specify them for $t = t_1$. Notice that the case in which the perturbation are zero, basically we have that the perturbations modify the curve but not the hypersurface. Therefore, the displacements $\delta\mathbf{x}$ and $\delta\mathbf{p}$ play no physical roll and thus they can be interpreted as virtual. They generate virtual curves. In order to justify this interpretation and provide an example of their usefulness, consider the off-shell quantity $\mathbf{p}'\dot{\mathbf{x}'} - H'(\mathbf{x}',\mathbf{p}')$. We find that

$$\mathbf{p}'\cdot\dot{\mathbf{x}}' - H'(\mathbf{x}',\mathbf{p}') \approx \mathbf{p}\cdot\dot{\mathbf{x}} - H(\mathbf{x},\mathbf{p}) + \mathbf{p}\cdot\frac{\mathrm{d}}{\mathrm{d}t}\delta\mathbf{x} + \delta\mathbf{p}\cdot\dot{\mathbf{x}} - \nabla_{\mathbf{x}}H\cdot\delta\mathbf{x} - \nabla_{\mathbf{p}}H\cdot\delta\mathbf{p}. \tag{41}$$

Notice that the above can be written as

$$\mathbf{p}'\cdot\dot{\mathbf{x}}' - H'(\mathbf{x}',\mathbf{p}') \approx \mathbf{p}\cdot\dot{\mathbf{x}} - H(\mathbf{x},\mathbf{p}) + \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{p}\cdot\delta\mathbf{x}) + (\dot{\mathbf{p}} + \nabla_{\mathbf{x}}H)\cdot\delta\mathbf{x} - (\dot{\mathbf{x}} - \nabla_{\mathbf{p}}H)\cdot\delta\mathbf{p}. \tag{42}$$

Due to the time derivative, let us consider the integral of that expression

$$\begin{aligned}\int_{t_1}^{t_2}\mathrm{d}t\,(\mathbf{p}'\cdot\dot{\mathbf{x}}' - H') \;\approx\; & \int_{t_1}^{t_2}\mathrm{d}t\,(\mathbf{p}\cdot\dot{\mathbf{x}} - H) + (\mathbf{p}\cdot\delta\mathbf{x})\big|_{t_1}^{t_2} \\ & + \int_{t_1}^{t_2}\mathrm{d}t\,\left[(\dot{\mathbf{p}} + \nabla_{\mathbf{x}}H)\cdot\delta\mathbf{x} - (\dot{\mathbf{x}} - \nabla_{\mathbf{p}}H)\cdot\delta\mathbf{p}\right].\end{aligned} \tag{43}$$

Provided that $\delta\mathbf{x}$ vanishes at t_1 and t_2, the quantity $\int_{t_1}^{t_2}\mathrm{d}t\,(\mathbf{p}\cdot\dot{\mathbf{x}} - H)$ remains the same on-shell. This is pleasing but conflicting at the same time. We have argued that

$\delta\mathbf{x}$ and $\delta\mathbf{p}$ must vanish at t_1. This is equivalent to say that the equations are subject to initial conditions. But here, the equations have the "boundary" condition, i.e. $\mathbf{x}$ is given at t_1 and t_2 which are boundary points of the time interval. The specification of $\mathbf{p}$ at t_1 is translated to the specification of $\mathbf{x}$ at t_2. Can we solve the equations of motion with the "boundary" condition consistently? To illustrate that this is indeed possible, consider the $N = 1$ case with $\dot{p} = F(x)$ and $p = m\dot{x}$. Consider the time derivative of the equations and plug the equations into these expressions. We obtain

$$\ddot{p} = \frac{F'}{m}p, \quad F = m\ddot{x}. \tag{44}$$

Now we solve the equation of x, the equation that we start with! The particular solution is of the form $x(t) = c_1x_1(t) + c_2x_2(t)$. Since we know $x(t_1)$ and $x(t_2)$, we have a system

$$\begin{pmatrix} x(t_1) \\ x(t_2) \end{pmatrix} = \begin{pmatrix} x_1(t_1) & x_2(t_1) \\ x_1(t_2) & x_2(t_2) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}. \tag{45}$$

If the matrix is invertible, i.e. $x_1(t_1)x_2(t_2) - x_2(t_1)x_1(t_2) \neq 0$, we can solve the problem and use $p = m\dot{x}$ to give the expression for the momentum. For general case N the problem is solved provided that the corresponding matrix is invertible. Notice that E_1 is specified now after computing the form of $\mathbf{p}$ and evaluating it at t_1. Now, the fundamental point is to interpret the expression given in equation (43) to derive the equations of motion in another way. We define the action $S[\mathbf{x}, \mathbf{p}]$ as

$$S[\mathbf{x}, \mathbf{p}] = \int_{t_1}^{t_2} \mathrm{d}t\, (\mathbf{p}\cdot\dot{\mathbf{x}} - H(\mathbf{x}, \mathbf{p})). \tag{46}$$

The action is consider to be a functional and thus we make contact with the calculus of variations. Then, the virtual displacements corresponds to variations. Hence,

$$\begin{aligned} \delta S &= S[\mathbf{x} + \delta\mathbf{x}, \mathbf{p} + \delta\mathbf{p}] - S[\mathbf{x}, \mathbf{p}] \\ &= (\mathbf{p}\cdot\delta\mathbf{x})|_{t_1}^{t_2} + \int_{t_1}^{t_2} \mathrm{d}t\, \left[(\dot{\mathbf{p}} + \nabla_{\mathbf{x}}H)\cdot\delta\mathbf{x} - (\dot{\mathbf{x}} - \nabla_{\mathbf{p}}H)\cdot\delta\mathbf{p}\right]. \end{aligned} \tag{47}$$

Provided that $\delta\mathbf{x}(t_1) = 0 = \delta\mathbf{x}(t_2)$, by demanding $\delta S = 0$ we obtain $\dot{\mathbf{p}} = -\nabla_{\mathbf{x}}H$ and $\dot{\mathbf{x}} = \nabla_{\mathbf{p}}H$. This is known as Hamilton's principle. In words, the extremum of the action gives the equations of motion. Notice that we do not know if the extremum corresponds to a minimum or a maximum. In geometrical terms, among all the possible curves on Ω_{E_1} with $\mathbf{x}(t_1)$ and $\mathbf{x}(t_2)$ fixed, the curve that gives the solution is the one that extremize the action. The rest of curves then are virtual and thus unphysical.

We stress that we deal with a "boundary" problem for $\mathbf{x}$ rather than an initial value problem for $\mathbf{x}, \mathbf{p}$. There are no conditions on the momenta at any time.

Notice that with the Hamiltonian and the action, we have an off-shell language to define the theory. The action by itself, seems just a gadget like the Poisson bracket. In the following we will show that these objects lead us to a framework where we can discuss isometries (symmetries of phase space) and physical conserved quantities.

In order to do so let us study transformations of the form $\mathbf{X} = \mathbf{X}(\mathbf{x}, \mathbf{p}, t)$ and $\mathbf{P} = \mathbf{P}(\mathbf{x}, \mathbf{p}, t)$. If we demand that the transformations satisfy

$$\{X^i, X^j\} = 0, \quad \{P_i, P_j\} = 0, \quad \{X^i, P_j\} = \lambda \delta^i_j. \tag{48}$$

Then, for the functions $A(\mathbf{X}, \mathbf{P})$ and $B(\mathbf{X}, \mathbf{P})$ we find off-shell

$$\begin{aligned} \{A, B\}_{\mathbf{x},\mathbf{p}} &= \sum_{i,i'} \frac{\partial A}{\partial X^i} \frac{\partial B}{\partial X^{i'}} \{X^i, X^{i'}\} + \sum_{j,j'} \frac{\partial A}{\partial P_j} \frac{\partial B}{\partial P_{j'}} \{P_i, P_{j'}\} \\ &\quad + \sum_{i,j} \{X^i, P_j\} \left(\frac{\partial A}{\partial X^i} \frac{\partial B}{P_j} - \frac{\partial A}{\partial P_j} \frac{\partial B}{\partial X^i} \right), \\ &= \{A, B\}_{\mathbf{X},\mathbf{B}} \end{aligned} \tag{49}$$

We see that the transformation preserves or leave invariant (off-shell) the Poisson bracket. These transformations are refer as to canonical transformations. Now consider $\chi^A = (X^i, P_j)$, $\xi^a = (x^l, p_k)$. Then, equation (48) we can write $\{\chi^A, \chi^B\} = \lambda \epsilon^{AB}$ where $\epsilon^{ii'} = 0$, $\epsilon^{ij'} = \delta^i_{j'}$, $\epsilon^{ji'} = -\delta^{i'}_j$ and $\epsilon^{jj'} = 0$. Similarly we also consider ϵ^{ab} to obtain

$$\{\chi^A, \chi^B\} = \lambda \sum_{a,b} \epsilon^{ab} \frac{\partial \chi^A}{\partial \xi^a} \frac{\partial \chi^B}{\partial \xi^b}. \tag{50}$$

If we consider N particles moving in $\mathbb{R}^n$, all indices run from 1 to nN. Then, we have

$$\frac{1}{(nN)!} \sum_{A,B} \epsilon_{AB} \{\chi^A, \chi^B\} = \lambda \frac{1}{(nN)!} \sum_{A,B} \sum_{a,b} \epsilon_{AB} \epsilon^{ab} \frac{\partial \chi^A}{\partial \xi^a} \frac{\partial \chi^B}{\partial \xi^b} = \lambda \det J, \tag{51}$$

where J is the Jacobian matrix. This imply that $\det J = \frac{1}{(nN)!} \sum_{A,B} \epsilon_{AB} \epsilon^{AB} = 1$ and thus we conclude that transformation is invertible.

Consider the case on which $\mathbf{X} = \mathbf{X}(\mathbf{x}, \mathbf{p})$ and $\mathbf{P} = \mathbf{P}(\mathbf{x}, \mathbf{p})$, refer as to restricted canonical transformation. The trivial example of such transformation is the identity transformation $X^i = \sum_{l'} \delta^i_{l'} x^{l'}$, $P_j = \sum_k \delta^k_j p_k$. A no trivial transformation corresponds to global translations in phase space, i.e. $X^i = \sum_{l'} \delta^i_{l'} (x^{l'} + a^{l'})$, $P_j = \sum_k \delta^k_j (p_k + b_k)$, where $a^{l'}, b_k$ are constants. Now consider

$$X^i = \sum_{l'} R^i_{l'} x^{l'}, \quad P_j = \sum_k \bar{R}^k_j p_k. \tag{52}$$

In order to be a restricted canonical transformation we must have

$$\sum_{l,l'} R^i_{l'} \delta^{l'}_l \bar{R}^l_j = \delta^i_j. \tag{53}$$

In matrix notation we get $R\mathbb{I}\bar{R} = \mathbb{I}$. Then, $\det J = \det R \det \bar{R} = 1$. If we restrict ourselves to $\bar{R} = R^T$ we find that the transformations correspond to spatial rotations in phase space.

This opens the beautiful door of using symmetries as guidance principle. For example consider the hamiltonian for free particles and with any loss of generality we set their masses set to unity. Then,

$$H(\mathbf{x}, \mathbf{p}) = \sum_{k,k'} \frac{1}{2} \delta^{kk'} p_k p_{k'}. \tag{54}$$

The equations of motion are

$$\frac{\mathrm{d}x^l}{\mathrm{d}t} = \sum_k \delta^{lk} p_k, \quad \frac{\mathrm{d}p_k}{\mathrm{d}t} = 0. \tag{55}$$

It is straightforward to check that the Hamiltonian and the equations of motion are invariant under global spatial translations $X^i = \sum_{l'} \delta^i_{l'} (x^{l'} + a^{l'})$, $P_j = \sum_k \delta^k_j p_k$. The equations for the momenta tells us that $\sum_k p_k$ is a constant of motion, i.e. the total momenta is conserved. An equivalent statement of this is that $\sum_k p_k a^k$ is conserved. Hence, we see that invariance of the hamiltonian, realized off-shell, gives a conserved quantity after going on-shell. On the other hand, since $\sum_{ij} \delta^{ij} P_j \dot{X}^i$ is invariant we see that the action is also invariant off-shell.

Now consider the rescaling transformation

$$X^i = \alpha \sum_{l'} \delta^i_{l'} x^{l'}, \quad P_j = \alpha \sum_k \delta^k_j p_k, \tag{56}$$

where $\alpha \neq 1$. The Hamiltonian and the action are not invariant but the equations of motion are invariant. This is not a surprise since the transformation is not a canonical transformation (unless $\alpha = 1$) but it shows us that invariance of the equations of motion not necessarily implies invariance of the off-shell quantities. If the action and Hamiltonian are indeed invariant, then it is insured that the equations of motion are invariant.

The action shows us how to find the conserved quantity. First we use the action with arbitrary variations and the respective boundary condition to derive the equations. Then we consider the promotion of the $a^{l'}$ to be functions of time. Since $X^i = \sum_{l'} \delta^i_{l'} (x^{l'} + a^{l'})$, the variation is taken to be $\delta x^l = a^l$ with a^l small. The variations for the momenta are zero. For this particular variations and Hamiltonian we obtain

$$\delta S = S[\mathbf{X} = \mathbf{x} + \delta\mathbf{x}, \mathbf{P} = \mathbf{p} + \delta\mathbf{p}] - S[\mathbf{x}, \mathbf{p}] = \int_{t_1}^{t_2} \mathrm{d}t\, \mathbf{p} \cdot \dot{\mathbf{a}}. \tag{57}$$

We can write the expression as

$$\delta S = \mathbf{p}\cdot\mathbf{a}|_{t_1}^{t_2} + \int_{t_1}^{t_2} \mathrm{d}t\, \dot{\mathbf{p}}\cdot\mathbf{a}. \tag{58}$$

If we now consider the equations of motion we obtain

$$\delta S|_{\text{on-shell}} = \mathbf{p}\cdot\mathbf{a}|_{t_1}^{t_2}\,. \tag{59}$$

We see that $\mathbf{p}\cdot\mathbf{a} = \sum_k p_k a^k$ must be conserved.

Let us now consider spatial rotations $X^i = \sum_{l'} R^i_{l'} x^{l'}, \quad P_j = \sum_k (R^T)^k_j p_k$. We write $R = \mathrm{e}^{\omega}$ where ω is another matrix. The action and the hamiltonian are invariant. Since $\det R = 1$ we use $\det R = \mathrm{e}^{\mathrm{Tr}\ln\exp(\omega)}$ to conclude that $\mathrm{Tr}\omega = 0$ and $\omega^T = -\omega$. Let the coefficient of the traceless matrix be small and time dependent. Then, we have $R \approx \mathbb{I} + \omega$. The variations are now taken to be $\delta x^l = \sum_{l'} \omega^l_{l'} x^{l'}$ and $\delta p_k = \sum_{k'} (\omega^T)^{k'}_k p_{k'}$. We find

$$\delta S|_{\text{on-shell}} = \sum_{l,k} p_k \omega^k_l x^l \Big|_{t_1}^{t_2}\,, \tag{60}$$

And thus $\sum_{l,k} p_k \omega^k_l x^l$ must be conserved. Notice that the quantity can be written as $\sum_{l,k} \omega_{kl} x^l p^k$ and since $\omega^T = -\omega$, we need to antisymmetrized the product $x^l p^k$ to obtain a non-zero result. Then

$$\sum_{l,k} \omega_{kl} x^l p^k = \frac{1}{2}\sum_{l,k} \omega_{kl}(x^l p^k - x^k p^l). \tag{61}$$

Hence we conclude, that

$$L^{lk} = x^l p^k - x^k p^l, \tag{62}$$

must be conserved. We can corroborate by computing $\dot{L}^{lk}$. This is the conservation of angular momentum.

The variations consider so far can be written as

$$\delta x^l = \frac{1}{\lambda}\{x^l, \sum_k p_k a^k\}, \quad \delta x^l = \frac{1}{\lambda}\{x^l, \frac{1}{2}\sum_{l',k} \omega_{kl'} L^{l'k}\}. \tag{63}$$

Thus, we see that the momenta and angular momenta are the generators of infinitesimal spatial translations and rotations respectively.

We know, by construction, that the energy is a conserved quantity. How do we see it from the action point of view? Notice that space transformations are embedded in the formalism in a natural way but time does not. This should be clear that the action is an integral over time.

Let us consider $X^i(t')$ where $t' = t + f(t)$. Let $f(t)$ be small and thus

$$X^i(t') \approx X^i(t) + \left.\frac{\mathrm{d}X^i}{\mathrm{d}t'}\right|_{t'=t} f(t). \tag{64}$$

If X^i is related to a canonical transformation (not restricted) of x^l then we identify $X^i(t) = \sum_l \delta^i_l x^l(t)$. Then,

$$X^i(t') \approx \sum_l \delta^i_l (x^l(t) + \dot{x}^l f(t)). \tag{65}$$

The variation of the transformation is $\delta x^l = \dot{x}^l f(t)$ and for the momenta is defined analogously as $\delta p_k = \dot{p}_k g(t)$. On-shell, they can be written as

$$\delta x^l = \{x^l, f(t)H\}, \quad \delta p_k = \{p_k, g(t)H\}. \tag{66}$$

Hence, the Hamiltonian is the generator of time translations. For the action, we consider the variations $\delta x^l = \dot{x}^l f(t)$ and $\delta p_k = \dot{p}_k g(t)$ to obtain

$$\delta S|_{\mathrm{on-shell}} = \mathbf{p} \cdot \dot{\mathbf{x}} f(t)|_{t_1}^{t_2} = \mathbf{p} \cdot \mathbf{p} f(t)|_{t_1}^{t_2} = 2E f(t)|_{t_1}^{t_2}. \tag{67}$$

We have seen have transformations that leave invariant the action and that also are canonical transformations are related to conserved quantities. The language of these invariances is off-shell but the conserved quantities we need to use the equations of motion. We see that symmetries of the action and hamiltonian are powerful and thus may serve to construct theories. Of course, one has to first postulate the symmetry and through experiment (i.e. solutions of the equations of motion) check if they are physical. For example, we can study potentials V that are invariant under spatial translations and rotations.

We discussed three types of transformations that indeed are realized in nature that also are canonical transformations. This is not a rule. The fundamental quantities are the action and the hamiltonian. Therefore, we can have symmetries that are not related to canonical transformations at all. On the other hand, not every symmetry of the hamiltonian is symmetry of the action and not every symmetry of the action leads to a conserved quantity. For the former consider the hamiltonian of the free particles with the transformation $\mathbf{p} \to -\mathbf{p}$ with $\mathbf{x}$ unchanged. For the later consider $\mathbf{p} \to -\mathbf{p}$ and $\mathbf{x} \to -\mathbf{x}$. The problem with this case is that we cannot write an infinitesimal version of it, i.e. the identity transformations plus the variation.

There is another quantity that it will be fundamental for quantum mechanics. Let us define the function

$$\mathcal{S}(\mathbf{x}, t) \equiv \int_{t_1}^{t} \mathrm{d}t' \left(\mathbf{p} \cdot \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t'} - H(\mathbf{x}, \mathbf{p}) \right). \tag{68}$$

By definition we must have $\mathcal{S}(\mathbf{x}(t_1), t_1) = 0$ and $\mathcal{S}(\mathbf{x}, t)$ is known as Hamilton's principal function. From

$$\dot{\mathcal{S}} = \mathbf{p} \cdot \dot{\mathbf{x}} - H(\mathbf{x}, \mathbf{p}) = \nabla_{\mathbf{x}} \mathcal{S} \cdot \dot{\mathbf{x}} + \frac{\partial \mathcal{S}}{\partial t}. \tag{69}$$

Provided that

$$\nabla_{\mathbf{x}} \mathcal{S} = \mathbf{p}, \tag{70}$$

we find

$$-\frac{\partial \mathcal{S}}{\partial t} = H\left(\mathbf{x}, \nabla_{\mathbf{x}} \mathcal{S}\right). \tag{71}$$

The above is known as the Hamilton-Jacobi equation and suggest that $\mathcal{S}$ should be of the form

$$\mathcal{S}(\mathbf{x}, t) = W(\mathbf{x}) - W(\mathbf{x}(t_1)) - C(t - t_1), \tag{72}$$

where C is a constant and now $\nabla_{\mathbf{x}} W = \mathbf{p}$. Then, we obtain

$$H\left(\mathbf{x}, \nabla_{\mathbf{x}} W\right) = C. \tag{73}$$

On-shell we find that $C = E$. Let us consider the Hamiltonian for the free particles . Then,

$$\frac{1}{2} \nabla_{\mathbf{x}} W \cdot \nabla_{\mathbf{x}} W = E, \quad \mathcal{S}(\mathbf{x}, t) = W(\mathbf{x}) - W(\mathbf{x}(t_1)) - E(t - t_1). \tag{74}$$

The solution of the remaining equation is $W(\mathbf{x}) = \pm \mathbf{p} \cdot \mathbf{x}$. Thus,

$$\mathcal{S}(\mathbf{x}, t) = \pm \mathbf{p} \cdot (\mathbf{x} - \mathbf{x}(t_1)) - E(t - t_1). \tag{75}$$

The function $\mathcal{S}(\mathbf{x}, t)$ computes the on-shell action without using the equations of motions for $\mathbf{x}$ and $\mathbf{p}$ after setting $t = t_2$.The equation that we solve is an equation for the function $W(\mathbf{x})$. Let us see this more clearly for the harmonic oscillator. We have

$$H(x, p) = \frac{1}{2m} p^2 + \frac{1}{2} m \omega^2 x^2. \tag{76}$$

The equations of motion are

$$p = m\dot{x}, \quad \dot{p} = -m\omega^2 x. \tag{77}$$

Taking a derivative of the equations and using them we find

$$\ddot{x} + \omega^2 x = 0, \quad \ddot{p} + \omega^2 p = 0. \tag{78}$$

Then, we solve for x with $x(t_1)$ and $x(t_2)$ given. Using $p = m\dot{x}$ we obtain the solution for the momentum. In general we can write the solutions as

$$x(t) = c_1 \cos(\omega t) + c_2 \sin(\omega t), \quad p = -m\omega c_1 \sin(\omega t) + m\omega c_2 \cos(\omega t), \tag{79}$$

where A and B are functions of $x(t_1)$ and $x(t_2)$. Then, $E = \frac{1}{2}m\omega^2(c_1^2 + c_2^2)$. The on-shell action gives

$$S|_{\text{on-shell}} = m\omega \int_{t_1}^{t_2} \mathrm{d}t[(c_2^2 - c_1^2)\cos(\omega t)\sin(\omega t) + c_2 c_1(2\cos^2(\omega t) - 1)] - E(t_2 - t_1). \tag{80}$$

It remains to solve the integrals and then write the answer in terms of $x(t_1)$ and $x(t_2)$. Using $\mathcal{S}(x,t)$ we just need to solve

$$W(x) = \pm\sqrt{2mE} \int_{x(t_1)}^{x} \mathrm{d}x' \sqrt{1 - \frac{m\omega^2}{2E}x'^2}. \tag{81}$$

For this case the integral can be performed. Hence, we see that the function $\mathcal{S}(x,t)$ it is useful for computing the equations of motion provided that $W(x)$ can be computed.

On the conceptual point of view, off-shell $\mathcal{S}(\mathbf{x},t)$ corresponds to the action with the end point free. Moreover, it also indicates that the momentum is not an independent variable as the in the case of the Hamiltonian. On the other hand, let us consider a free particle with mass m moving in $\mathbb{R}^3$. We have

$$\mathcal{S}(\mathbf{x},t) = \pm\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}(t_1)) - E(t - t_1). \tag{82}$$

Let us now consider the dimensionfull constant λ and consider the dimensionless quantity

$$\bar{\mathcal{S}}(\mathbf{x},t) = \frac{1}{\lambda}\mathcal{S}(\mathbf{x},t). \tag{83}$$

Then we can write

$$\bar{\mathcal{S}}(\mathbf{x},t) = \pm\mathbf{k}\cdot(\mathbf{x} - \mathbf{x}(t_1)) - \omega(t - t_1), \tag{84}$$

with

$$\mathbf{p} = \lambda\mathbf{k}, \quad E = \lambda\omega, \tag{85}$$

where $[\mathbf{k}] = 1/L$ and $[\omega] = 1/T$. Since we now that $E = \frac{1}{2m}\mathbf{p}^2$ then $\omega = \frac{\lambda}{2m}\mathbf{k}^2$. Therefore,

$$\bar{\mathcal{S}}(\mathbf{x},t) = \pm\mathbf{k}\cdot(\mathbf{x} - \mathbf{x}(t_1)) - \omega(\mathbf{k})(t - t_1). \tag{86}$$

We can relate, mathematically, $\bar{\mathcal{S}}(\mathbf{x},t)$ to a wavepacket

$$\Psi(\mathbf{x},t) = \int \mathrm{d}\mathbf{k}\,\mathcal{A}(\mathbf{k})\,\mathrm{e}^{i\bar{\mathcal{S}}(\mathbf{x},t)}. \tag{87}$$

In order to reproduce $\omega = \frac{\lambda}{2m}\mathbf{k}^2$, the wavepacket must satisfy

$$i\lambda\frac{\partial}{\partial t}\Psi = -\frac{\lambda^2}{2m}\nabla_{\mathbf{x}}^2\Psi. \tag{88}$$

This is the birth of quantum mechanics as a matter-wave theory. We see how λ plays a fundamental role, it corresponds to $\hbar$. Following Dirac, the canonical quantization procedure is to consider x^l, p_k as operators $\hat{x}^i$, $\hat{p}_k$ that satisfy

$$\frac{1}{i\hbar}[\hat{x}^l, \hat{p}_k] = \delta^l_k \hat{1}, \quad \frac{1}{i\hbar}[\hat{x}^l, \hat{x}^{l'}] = 0, \quad \frac{1}{i\hbar}[\hat{p}_k, \hat{p}_{k'}] = 0, \tag{89}$$

where $[\hat{x}^l, \hat{p}_k] = \hat{x}^l \hat{p}_k - \hat{p}_k \hat{x}^l$. We have the replacement

$$\frac{1}{\lambda}\{\cdot, \cdot\} \to \frac{1}{i\hbar}[\cdot, \cdot]. \tag{90}$$

With this rule we, in the Schrödinger picture, we consider Ψ to be an eigenfunction of the position operator $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}} = -i\hbar\nabla_{\mathbf{x}}$. Then, we quantize the Hamiltonian. Notice that the later can achieved without ambiguities for Hamiltonians that not include terms such as $\mathbf{x} \cdot \mathbf{p}$. After taking the above rules and considerations, we finally write the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \quad \hat{H} = H(\hat{\mathbf{x}}, \hat{\mathbf{p}}). \tag{91}$$

In order to solve this equation, let us consider $\Psi(\mathbf{x}, t) = \psi_E(\mathbf{x})\mathrm{e}^{-i\frac{E}{\hbar}(t-t_1)}$. Then, we obtain the time-independent Schrödinger equation

$$\hat{H}\psi_E(\mathbf{x}) = E\psi_E(\mathbf{x}). \tag{92}$$

Notice then that $\psi_E(\mathbf{x})$ is a eigenfunction of the position operator and the quantized Hamiltonian. Moreover, the Hamiltonian must satisfy $\hat{H}^\dagger = \hat{H}$ in order to obtain real energies E. The key point is that once, we solve the above equation we will find that the energy is quantized, i.e. $E \to E_n$. Then the full solution is of the form

$$\Psi(\mathbf{x}, t) = \sum_n \psi_{E_n}(\mathbf{x})\mathrm{e}^{-i\frac{E_n}{\hbar}(t-t_1)}. \tag{93}$$

This gives a superposition of solutions with energy E_n. Together with the Born rule, we find that quantum mechanics is radically different from classical mechanics. For the rules that are not going to be discussed, we refer to the reader to any serious textbook in quantum mechanics. Here, we only emphasize that equation (92) is the quantum analog of the on-shell condition for the classical Hamiltonian.

We see how the Hamiltonian, λ and the Poisson brackets play a fundamental role as advertised. What about the action? In some sense we already took into account the action by writing the wavepacket. But in the following section will show that it drives another quantization method, the path integral approach. For the moment notice that the action is compatible with the uncertainty principle. The boundary conditions are set on the initial and final positions and there is no condition on the momenta.

We end this discussion by considering the wavefunction of the form

$$\Psi(\mathbf{x}, t) = \mathrm{e}^{\frac{i}{\hbar}\mathfrak{S}(\mathbf{x},t)}. \tag{94}$$

The Schrödinger equation for the free particle becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}, t) = \frac{1}{2m}\hat{\mathbf{p}}^2\Psi(\mathbf{x}, t). \tag{95}$$

Notice that

$$\hat{\mathbf{p}}\Psi(\mathbf{x}, t) = (\nabla_{\mathbf{x}}\mathfrak{S})\Psi(\mathbf{x}, t). \tag{96}$$

Then, we have

$$-\frac{\partial}{\partial t}\mathfrak{S} = -\frac{i\hbar}{2m}\nabla^2_{\mathbf{x}}\mathfrak{S} + \frac{1}{2m}(\nabla_{\mathbf{x}}\mathfrak{S})^2. \tag{97}$$

In the limit $\hbar \to 0$ we find

$$\lim_{\hbar\to 0}\mathfrak{S} = \mathcal{S}, \quad \lim_{\hbar\to 0}\nabla_{\mathbf{x}}\mathfrak{S} = \mathbf{p}. \tag{98}$$

Hence, the semiclassical behavior of the wavefunction is of the form

$$\lim_{\hbar\to 0}\Psi(\mathbf{x}, t) = \mathrm{e}^{\frac{i}{\hbar}\mathcal{S}(\mathbf{x},t)}. \tag{99}$$

2 Path integral in quantum mechanics

We now that a classical theory can be defined off-shell from the action

$$S[\mathbf{x}, \mathbf{p}] = \int_{t_1}^{t_2} \mathrm{d}t\,(\mathbf{p}\cdot\dot{\mathbf{x}} - H(\mathbf{x}, \mathbf{p})). \tag{100}$$

The equations of motion follow from Hamilton's principle $\delta S = 0$. The equations for the position are subject to boundary conditions and the momenta have no conditions. The solution corresponds to a curve over the hypsersurface at constant energy Ω_E. In general, there will be infinitely many virtual curves for $\mathbf{x}(t_1)$ and $\mathbf{x}(t_2)$. Classically they have no meaning except only the one that corresponds to the solution. Time corresponds to the parameter of the curves. Let us consider the curves projected to the position space and we will referred to them as paths. Thus, there are infinitely many virtual paths for $\mathbf{x}(t_1)$ and $\mathbf{x}(t_2)$ and the classical path satisfy the equations of motion for $\mathbf{x}$. Of course there are infinitely many virtual paths in momentum space but their endpoints are deduced not given.

In the las section we saw that the semiclassical behavior of the wavefunction is of the form $\mathrm{e}^{\frac{i}{\hbar}\mathcal{S}}$, where $\mathcal{S}$ corresponds to the action with the end point not specified. Now let us consider

$$\mathrm{e}^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}. \tag{101}$$

Since the action is a function over all possible paths, then also $\mathrm{e}^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}$. Consider now the sum over all possible paths weighted by the factor $\mathrm{e}^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}$, i.e.

$$\sum_{\substack{\text{paths in position space} \\ \text{with } \mathbf{x}(t_1) \text{ and } \mathbf{x}(t_2) \text{ given}}} \; \sum_{\text{paths in momentum space}} \mathrm{e}^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}. \tag{102}$$

Let us assume that the above quantity exists. At this point, we can only interpret that this quantity is related to the time evolution of the system and thus it has to be directly related to quantized Hamiltonian. This seems to be naive but notice that among all the paths there is a the classical path, the one that corresponds to a solution of the classical equations of motion, and we know that the classical Hamiltonian is the generator of time evolution.

With the goal of interpreting sum over all paths, let us consider a particle moving in $\mathbb{R}$. Then, we have the position operator $\hat{x}$ and the continuous basis $|x\rangle$ with

$$\hat{x}|x\rangle = x|x\rangle, \quad \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x\, |x\rangle\langle x| = \hat{1}, \quad \langle x'|x\rangle = \ell\delta(x'-x), \tag{103}$$

where ℓ is introduced so that the vector $|x\rangle$ are dimensionless. Due to the properties of δ, we have

$$\ell\delta(x'-x) = \delta(x'/\ell - x/\ell). \tag{104}$$

On the other hand we have the momentum operator $\hat{p}$ and the continuous basis $|p\rangle$ with

$$\hat{p}|p\rangle = p|p\rangle, \quad \frac{1}{\kappa}\int_{-\infty}^{\infty} \mathrm{d}p\, |p\rangle\langle p| = \hat{1}, \quad \langle p'|p\rangle = \kappa\delta(p'-p), \tag{105}$$

where κ is also introduced so that the vector $|p\rangle$ are dimensionless. The basis are related by

$$|p\rangle = \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x\, |x\rangle\langle x|p\rangle, \quad |x\rangle = \frac{1}{\kappa}\int_{-\infty}^{\infty} \mathrm{d}p\, |p\rangle\langle p|x\rangle. \tag{106}$$

The quantity $\langle x|p\rangle$ corresponds to the transition function and we denoted as $f(x,p)$ and $\langle p|x\rangle = f^*(x,p)$. From

$$\langle p'|p\rangle = \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x\, \langle p'|x\rangle\langle x|p\rangle, \quad \langle x'|x\rangle = \frac{1}{\kappa}\int_{-\infty}^{\infty} \mathrm{d}p\, \langle x'|p\rangle\langle p|x\rangle, \tag{107}$$

we find

$$\int_{-\infty}^{\infty} \mathrm{d}(x/\ell)\, f^*(x,p')f(x,p) = \delta(p'/\kappa - p/\kappa), \quad \int_{-\infty}^{\infty} \mathrm{d}(p/\kappa)\, f^*(x,p)f(x',p) = \delta(x'/\ell - x/\ell). \tag{108}$$

Due to the integral representation of δ, we find that $f(x,p) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{+i\frac{px}{\kappa\ell}}$. Demanding $\hat{p}f = pf$, with $\hat{p} = -i\hbar\partial_x$, we find that $\ell\kappa = \hbar$ as expected. Hence

$$f(x,p) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{+i\frac{px}{\hbar}}, \tag{109}$$

and

$$|p\rangle = \frac{1}{\ell} \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \, |x\rangle \mathrm{e}^{+i\frac{px}{\hbar}}, \quad |x\rangle = \ell \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{\sqrt{2\pi}\hbar} \, |p\rangle \mathrm{e}^{-i\frac{px}{\hbar}}. \tag{110}$$

Then, a general state $|\psi\rangle$ can be expressed in term of these basis

$$|\psi\rangle = \frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x \, |x\rangle\langle x|\psi\rangle, \quad |\psi\rangle = \ell \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{\hbar} \, |p\rangle\langle p|\psi\rangle. \tag{111}$$

In order to have a probabilist interpretation we demand $\langle\psi|\psi\rangle$ must by finite, i.e.

$$\frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x \, |\langle x|\psi\rangle|^2 < \infty, \quad \ell \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{\hbar} \, |\langle p|\psi\rangle|^2 < \infty. \tag{112}$$

From these we see the wavefunctions $f(x,p)$ satisfy

$$\int_{-\infty}^{\infty} \mathrm{d}x \, f^*(x,p')f(x,p) = \hbar\delta(p'-p), \quad \int_{-\infty}^{\infty} \mathrm{d}p \, f^*(x,p)f(x',p) = \hbar\delta(x'-x), \tag{113}$$

and thus, alone, they are not suitable to describe a state.

The time evolution of a state is given by the time evolution operator $\hat{U}$. For time-independent Hamiltonians, as in our case, it takes the form

$$\hat{U}(t,t_1) = \mathrm{e}^{-\frac{i}{\hbar}(t-t_1)\hat{H}}. \tag{114}$$

Let us assume that at t_1 the state of the system is given by the superposition

$$|i,t_1\rangle = \frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x' \, |x'\rangle\langle x'|i,t_1\rangle, \quad \frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x' \, |\langle x'|i,t_1\rangle|^2 < \infty. \tag{115}$$

The state evolves to a final state at t_2 as

$$|f,t_2\rangle = \mathrm{e}^{-\frac{i}{\hbar}(t_2-t_1)\hat{H}}|i,t_1\rangle, \tag{116}$$

This state also have the expression

$$|f,t_2\rangle = \frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x'' \, |x''\rangle\langle x''|f,t_2\rangle, \quad \frac{1}{\ell} \int_{-\infty}^{\infty} \mathrm{d}x'' \, |\langle x''|f,t_2\rangle|^2 < \infty. \tag{117}$$

We find that

$$\langle x''|f,t_2\rangle = \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x' \, \langle x''|\hat{U}(t_2,t_1)|x'\rangle\langle x'|i,t_1\rangle. \tag{118}$$

For

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x}), \tag{119}$$

we have

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \langle x''|\mathrm{e}^{-\frac{i}{\hbar}(t_2-t_1)\left(\frac{1}{2m}\hat{p}^2+V(\hat{x})\right)}|x'\rangle. \tag{120}$$

The above can be expressed as

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \ell\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar}\,\mathrm{e}^{\frac{i}{\hbar}(p(x''-x')-H(x',p)(t_2-t_1))}. \tag{121}$$

We see the first hint of the action after looking the argument of the exponential in the momentum integral.

Let us focus in the free particle, we obtain

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \ell\sqrt{\frac{m}{2\pi\hbar i(t_2-t_1)}}\mathrm{e}^{\frac{i}{\hbar}(t_2-t_1)\frac{m}{2}\left(\frac{x''-x'}{t_2-t_1}\right)^2}. \tag{122}$$

Notice that the on-shell action for the free particle is

$$S_{\mathrm{free}}[x,p]|_{\mathrm{on-shell}} = \frac{m}{2}\frac{(x''-x')^2}{t_2-t_1}, \quad x'' = x(t_2), \quad x' = x(t_1). \tag{123}$$

This is intriguing since we have recover a semiclassical result without taking a semiclassical limit. Moreover, the expression suggests that the square root pre-factor must take into account non classical behavior only.

Since no measurement has been taken into account, there is no position state preferred at t_1 and t_2, i.e. we have infinitely many matrix elements $\langle x''|\hat{U}(t_2,t_1)|x'\rangle$. In the Copenhagen interpretation we consider a measurement and the initial state "collapse" or "reduced" to a specific position. Let us assume that it reduces to $|i,t_1\rangle \to |x_1\rangle\langle x_1|i,t_1\rangle$, i.e the position at t_1 is x_1. Then, the final state takes the form

$$|f,t_2\rangle = \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x''\,|x''\rangle\langle x''|\hat{U}(t_2,t_1)|x_1\rangle. \tag{124}$$

We then only can compute the probabilities of finding the free particle at t_2 between the region x'' and $x''+\mathrm{d}x''$, i.e. $\frac{1}{\ell}|\langle x''|\hat{U}(t_2,t_1)|x_1\rangle|^2\mathrm{d}x''$. Among infinitely many positions, let us consider $x''=x_2$. Thus

$$\frac{1}{\ell}|\langle x_2|\hat{U}(t_2,t_1)|x_1\rangle|^2\mathrm{d}x_2 = \frac{m}{2\pi\hbar(t_2-t_1)}\mathrm{d}x_2, \tag{125}$$

corresponds to the probability of a free particle that was initially located at x_1 at t_1 will be located in a region $[x_2, x_2+\mathrm{d}x_2]$ at the instant t_2. This is actually a conditional probability trivially realized. In fact, if no measurement is consider we have

$$P(x_1 \leq x' \leq x_1 + \mathrm{d}x_1)\mathrm{d}x' = \frac{1}{\ell}|\langle x'|i, t_1\rangle|^2 \mathrm{d}x', \tag{126}$$

$$P(x_2 \leq x'' \leq x_2 + \mathrm{d}x_2)\mathrm{d}x'' = \frac{1}{\ell}|\langle x''|f, t_2\rangle|^2 \mathrm{d}x''. \tag{127}$$

These corresponds to unconditional probabilities if $|f, t_2\rangle$ and $|i, t_1\rangle$ are not related. This is not true for our case since $|f, t_2\rangle = \hat{U}(t_2, t_1)|i, t_1\rangle$, i.e. the probability amplitudes are related by

$$\langle x''|f, t_2\rangle = \frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x' \,\langle x''|\hat{U}(t_2, t_1)|x'\rangle\langle x'|i, t_1\rangle. \tag{128}$$

Without any measurement at t_1 we can only have the conditional probability that the free particle will be located in a region $[x_2, x_2 + \mathrm{d}x_2]$ at the instant t_2 given the probability that it was initially located at x_1 at t_1. The measurement removes the uncertainty at t_1 by telling us that the probability that the particle is located at x_1 is 1. Hence, we conclude that $\frac{1}{\ell}|\langle x''|\hat{U}(t_2, t_1)|x_1\rangle|^2 \mathrm{d}x''$ is in reality a conditional probability. To enforce this interpretation we see that the sum of all conditional probabilities

$$\frac{1}{\ell}\int_{-\infty}^{\infty} \mathrm{d}x'' \,|\langle x''|\hat{U}(t_2, t_1)|x'\rangle|^2 = \langle x'|x'\rangle = \ell\delta(0), \tag{129}$$

diverges. For the free particle we have $|\langle x''|\hat{U}(t_2, t_1)|x'\rangle|^2 = \frac{m}{2\pi\hbar(t_2-t_1)}$ and thus divergence is due to the integral for finite time interval.

From the evidence of the free particle we consider

$$\langle x''|\hat{U}(t_2, t_1)|x'\rangle = \frac{\displaystyle\sum_{\substack{\text{paths in position space}\\ \text{with } x(t_1)=x' \text{ and } x(t_2)=x'' \text{ given}}}}{\displaystyle\sum_{\text{paths in position space}}} \mathrm{e}^{\frac{i}{\hbar}S[x,p]}. \tag{130}$$

If the above is true, we see that the right hand side corresponds to a conditional probability amplitude. From the direct result, it is reasonable to consider the splitting

$$x = \bar{x} + \hbar\eta, \quad p = \bar{p} + \hbar\zeta, \tag{131}$$

where η and ζ are considered as quantum fluctuations and $\bar{x}, \bar{p}$ classical terms. The later must be the responsible of the phase factor. With this splitting the action becomes

$$S_{\text{free}}[x, p] = S_{\text{free}}[\bar{x}, \bar{p}] + \hbar\,(\bar{p}\eta)|_{t_1}^{t_2} + \hbar\int_{t_1}^{t_2} \mathrm{d}t\,\left[(\dot{\bar{x}} - \bar{p}/m)\zeta - \dot{\bar{p}}\eta\right] + \hbar^2 S_{\text{free}}[\eta, \zeta]. \tag{132}$$

Let $\bar{x}, \bar{p}$ satisfy classical equations of motion with $\bar{x}(t_2) = x''$ and $\bar{x}(t_1) = x'$ and no condition for $\bar{p}$. Then, we must have $\eta(t_2) = 0 = \eta(t_1)$ and no condition for ζ. The expression reduces to

$$S_{\rm free}[x,p] = S_{\rm free}[\bar{x},\bar{p}]|_{\rm on-shell} + \hbar^2 S_{\rm free}[\eta,\zeta]. \tag{133}$$

and therefore

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \left[\sum_{\substack{\text{paths in position space}\\ \text{with } \zeta(t_1)=0 \text{ and } \zeta(t_2)=0 \text{ given}}} \sum_{\text{paths in momentum space}} \mathrm{e}^{i\hbar S_{\rm free}[\eta,\zeta]}\right] \times \mathrm{e}^{\frac{i}{\hbar} S_{\rm free}[\bar{x},\bar{p}]|_{\rm on-shell}}. \tag{134}$$

Notice that $S_{\rm free}[\eta,\zeta]$ is purely off-shell quantity and we see that the virtual paths contribute at the quantum level. In fact we must have

$$\sum_{\substack{\text{paths in position space}\\ \text{with } \eta(t_1)=0 \text{ and } \eta(t_2)=0 \text{ given}}} \sum_{\text{paths in momentum space}} \mathrm{e}^{i\hbar S_{\rm free}[\eta,\zeta]} \propto \ell\sqrt{\frac{m}{2\pi\hbar i(t_2-t_1)}}. \tag{135}$$

It remains to give a mathematical meaning to the sum over paths of the above expression. Let us divide the time interval into N equal intervals ϵ. Then,

$$t_2 - t_1 = N\epsilon, \tag{136}$$

and

$$\int_{t_1}^{t_2} \mathrm{d}t = \int_{t_1}^{t_1+\epsilon} \mathrm{d}t + \int_{t_1+\epsilon}^{t_1+2\epsilon} + \ldots + \int_{t_1+(N-1)\epsilon}^{t_1+N\epsilon} \mathrm{d}t = \sum_{n=0}^{N-1} \int_{t_1+n\epsilon}^{t_1+(n+1)\epsilon} \mathrm{d}t\,. \tag{137}$$

Now we approximate the paths to polygonal paths. Consider the expansions

$$\begin{aligned} \eta(t) &= \eta|_{t_1+n\epsilon} + \dot{\eta}|_{t_1+n\epsilon}(t-t_1-n\epsilon) + \frac{1}{2!}\ddot{\eta}|_{t_1+n\epsilon}(t-t_1-n\epsilon)^2 + \ldots, \\ \zeta(t) &= \zeta|_{t_1+n\epsilon} + \dot{\zeta}\Big|_{t_1+n\epsilon}(t-t_1-n\epsilon) + \frac{1}{2!}\ddot{\zeta}\Big|_{t_1+n\epsilon}(t-t_1-n\epsilon)^2 + \ldots, \end{aligned} \tag{138}$$

For $t = t_1 + (n+1)\epsilon$, ϵ small and N large we obtain

$$\dot{\eta}|_{t_1+n\epsilon} \equiv \frac{\Delta\eta_n}{\epsilon} = \frac{\eta|_{t_1+(n+1)\epsilon} - \eta|_{t_1+n\epsilon}}{\epsilon}, \tag{139}$$

and

$$\mathrm{e}^{i\hbar S_{\rm free}[\eta,\zeta]} = \prod_{n=0}^{N-1} \mathrm{e}^{\frac{i\epsilon}{\hbar}\left(\hbar\zeta|_{t_1+n\epsilon}\frac{\hbar\Delta\eta_n}{\epsilon} - \frac{(\hbar\zeta|_{t_1+n\epsilon})^2}{2m}\right)} \tag{140}$$

The above can be written as

$$e^{i\hbar S_{\text{free}}[\eta,\zeta]} \approx \prod_{n=0}^{N-1} e^{-\frac{i}{2m\hbar}\epsilon(\hbar\zeta|_{t_1+n\epsilon}-m\frac{\hbar\Delta\eta_n}{\epsilon})^2} \prod_{n'=0}^{N-1} e^{\frac{im}{2\hbar}\epsilon\left(\frac{\hbar\Delta\eta_{n'}}{\epsilon}\right)^2}. \tag{141}$$

The sum over all the paths in momentum space translates to the sum over the possible values of $\zeta|_{t_1+n\epsilon}$ per each polygon. This of course corresponds to a integral over $\zeta|_{t_1+n\epsilon}$. Since $\hbar\,\zeta|_{t_1+n\epsilon}$ has dimensions of momentum, the integrals must be accompanied with a factor $\ell/\hbar$. Therefore

$$\begin{aligned}\sum_{\text{paths in momentum space}} e^{i\hbar S_{\text{free}}[\eta,\zeta]} \approx & \prod_{n'=0}^{N-1} e^{\frac{im}{2\hbar}\epsilon\left(\frac{\hbar\Delta\eta_{n'}}{\epsilon}\right)^2} \\ & \times \prod_{n=0}^{N-1} \frac{\ell}{\hbar} \int_{-\infty}^{\infty} d(\hbar\,\zeta|_{t_1+n\epsilon}) e^{-\frac{i}{2m\hbar}\epsilon(\hbar\zeta|_{t_1+n\epsilon}-m\frac{\hbar\Delta\eta_n}{\epsilon})^2}.\end{aligned} \tag{142}$$

The integrals that we need to solve are

$$\int_{-\infty}^{\infty} dy\, e^{i\alpha(y-b)^2} = e^{i\text{sgn}(\alpha)\frac{\pi}{4}} \sqrt{\frac{\pi}{|\alpha|}}, \tag{143}$$

and thus

$$\sum_{\text{paths in momentum space}} e^{i\hbar S_{\text{free}}[\eta,\zeta]} \approx \prod_{n'=0}^{N-1} e^{\frac{im}{2\hbar}\epsilon\left(\frac{\hbar\Delta\eta_{n'}}{\epsilon}\right)^2} \times e^{-iN\frac{\pi}{4}} \left(\frac{2\pi m\ell^2}{\hbar\epsilon}\right)^{\frac{N}{2}}. \tag{144}$$

For the remaining, we have

$$\begin{aligned}\prod_{n'=0}^{N-1} e^{\frac{im}{2\hbar}\epsilon\left(\frac{\hbar\Delta\eta_{n'}}{\epsilon}\right)^2} = & e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+\epsilon}-\hbar\,\eta|_{t_1}\right)^2}{\epsilon}} e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+2\epsilon}-\hbar\,\eta|_{t_1+\epsilon}\right)^2}{\epsilon}} \times \cdots \\ & \times e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+(N-1)\epsilon}-\hbar\,\eta|_{t_1+(N-2)\epsilon}\right)^2}{\epsilon}} e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+N\epsilon}-\hbar\,\eta|_{t_1+(N-1)\epsilon}\right)^2}{\epsilon}}.\end{aligned} \tag{145}$$

Since $\eta(t_2) = 0 = \eta(t_2)$, we obtain

$$\begin{aligned}\prod_{n'=0}^{N-1} e^{\frac{i}{2m\hbar}\epsilon\left(\frac{\hbar\Delta\eta_{n'}}{\epsilon}\right)^2} = & e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+\epsilon}\right)^2}{\epsilon}} e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+2\epsilon}-\hbar\,\eta|_{t_1+\epsilon}\right)^2}{\epsilon}} \times \cdots \\ & \times e^{\frac{im}{2\hbar}\frac{\left(\hbar\,\eta|_{t_1+(N-2)\epsilon}-\hbar\,\eta|_{t_1+(N-1)\epsilon}\right)^2}{\epsilon}} e^{\frac{im}{2\hbar}\frac{(\hbar\,\eta|_{t_1+(N-1)\epsilon})^2}{\epsilon}}.\end{aligned} \tag{146}$$

Performing $N-1$ integrals we obtain

$$\sum_{\substack{\text{paths in position space}\\ \text{with } \eta(t_1)=0 \text{ and } \eta(t_2)=0 \text{ given}}} \sum_{\text{paths in momentum space}} \mathrm{e}^{i\hbar S_{\text{free}}[\eta,\zeta]} \approx (2\pi)^N \sqrt{N}\ell \sqrt{\frac{m}{2\pi\hbar i(t_2-t_1)}}. \tag{147}$$

This is promising because we recover the desired facto with the drawback is that in the limit $N \to \infty$ the constant $(2\pi)^N \sqrt{N}$ diverges. We formally define a measure

$$[\delta x \delta p] = \mathcal{N} \prod_{n=0}^{N-1} \frac{\ell}{\hbar} \mathrm{d}\delta p \prod_{n=1}^{N-1} \frac{1}{\ell} \mathrm{d}\delta x, \tag{148}$$

where $\mathcal{N}$ is an inifnite normalization constant that cancels the divergent term $(2\pi)^N \sqrt{N}$. Hence, the sum over paths then can be written as

$$\sum_{\substack{\text{paths in position space}\\ \text{with } \eta(t_1)=0 \text{ and } \eta(t_2)=0 \text{ given}}} \sum_{\text{paths in momentum space}} = \int_{\delta x(t_1)=0}^{\delta x(t_2)=0} \int [\delta x \delta p]. \tag{149}$$

Since for the free case, the action of the quantum fluctuations is the same as the action of the classical solution, we see that we can undo the linear splitting to obtain

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \int_{x(t_1)=x'}^{x(t_2)=x''} [\mathrm{d}x\mathrm{d}p]\, \mathrm{e}^{\frac{i}{\hbar}S[x,p]}. \tag{150}$$

Instead of using the symbol $[\mathrm{d}x\mathrm{d}p]$ it is used $\mathcal{N}\mathcal{D}x(t)\mathcal{D}p(t)$, we the final form is

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle = \mathcal{N} \int_{x(t_1)=x'}^{x(t_2)=x''} \mathcal{D}x(t) \int \mathcal{D}p(t)\, \mathrm{e}^{\frac{i}{\hbar}S[x,p]}. \tag{151}$$

This is the path integral representation of the matrix elements $\langle x''|\hat{U}(t_2,t_1)|x'\rangle$. Notice that the path integral by no means is a well define mathematical quantity. Nevertheless gives the desire physical results. The above expression applies for classical Hamiltonians of the form

$$H(x,p) = \frac{1}{2m}p^2 + V(x), \tag{152}$$

and the generalization to a system of N particles moving in $\mathbb{R}^n$ is straightforward. Let us compute the path integral for the above Hamiltonian. We have

$$\mathcal{N} \int_{x(t_1)=x'}^{x(t_2)=x''} \mathcal{D}x(t) \int \mathcal{D}p(t)\, \mathrm{e}^{\frac{i}{\hbar}\int_{t_1}^{t_2} \mathrm{d}t \left(p\dot{x} - \frac{1}{2m}p^2 - V(x)\right)}, \tag{153}$$

which can be written as

$$\mathcal{N}\int\limits_{x(t_1)=x'}^{x(t_2)=x''}\mathcal{D}x(t)\int\mathcal{D}p(t)\,\mathrm{e}^{-\frac{i}{2m\hbar}\int\limits_{t_1}^{t_2}\mathrm{d}t\,(p-m\dot{x})^2}\,\mathrm{e}^{\frac{i}{\hbar}\int\limits_{t_1}^{t_2}\mathrm{d}t\,\left(\frac{m}{2}\dot{x}^2-V(x)\right)}. \tag{154}$$

The momentum integral can be perform and its result is absorb into $\mathcal{N}$ to obtain another $\mathcal{N}'$ and

$$\langle x''|\hat{U}(t_2,t_1)|x'\rangle=\mathcal{N}'\int\limits_{x(t_1)=x'}^{x(t_2)=x''}\mathcal{D}x(t)\,\mathrm{e}^{\frac{i}{\hbar}\int\limits_{t_1}^{t_2}\mathrm{d}t\,\left(\frac{m}{2}\dot{x}^2-V(x)\right)}. \tag{155}$$

In the last section we deliberately avoid to mention the Lagrangian function. Here, we see that emerges naturally and has the form

$$L(x,\dot{x})=\frac{m}{2}\dot{x}^2-V(x). \tag{156}$$

Quantum mechanics was founded with the Hamiltonian function and the appearance of the Lagrangian is solely due to the path integral approach. After defining the momentum as

$$p=\frac{\partial L}{\partial\dot{x}}, \tag{157}$$

the equations of motion derived from the action, with $\delta x(t_1)=0=\delta x(t_2)$, is the Euler-Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{x}}=\frac{\partial L}{\partial x}\to\frac{\mathrm{d}p}{\mathrm{d}t}=-V'(x). \tag{158}$$

There is not obstacle for deriving the Hamiltonian for the Lagrangian given in equation (156). Thus, it seems that nothing profound is happening. However, if we consider relativity, it is the Lagrangian the quantity that is best suited.

With the notion of spacetime, the time coordinate is on equal footing of spatial coordinates. Notice the Hamiltonian necessarily breaks this since on-shell it corresponds to the energy of the system and thus is Lorentz co-variant rather than invariant.

To clarify this point consider a free relativistic particle. We know that the particle trajectory generate a curve (or worldline) in Minwkoski spacetime. The action is proportional to the lenght of such curve. If the particle has mass m we have

$$S[x]=-mc\int\limits_{u_1}^{u_2}\mathrm{d}u\,\sqrt{-\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}},\quad\mu,\nu=0,1,\ldots,D-1,\quad x^0=ct, \tag{159}$$

where c is the speed of light and $\eta_{\mu\nu}$ are the components of the metric of D-dimensional Minwkoski spacetime $\mathbb{R}^{1,D-1}$ with $\eta_{\mu\nu} = \mathrm{diag}(-,+,\ldots,+)$. Notice that we consider $D-1$ space directions and we are using Einstein's summation convention, i.e. $\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}$ stands for

$$\sum_{\mu\nu}\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}. \tag{160}$$

In the action, u parametrized all possible worldlines and the action is actually invariant under reparametrizations. More important, the action is explicitly Lorentz invariant. Consider $u = x^0$, then

$$S[x] = -mc^2\int_{t_1}^{t_2}\mathrm{d}t\,\sqrt{1-\frac{1}{c^2}\dot{\mathbf{x}}^2}, \tag{161}$$

and thus

$$\mathbf{p} = \frac{m\dot{\mathbf{x}}}{\sqrt{1-\frac{1}{c^2}\dot{\mathbf{x}}^2}}. \tag{162}$$

Since $H = \mathbf{p}\cdot\dot{\mathbf{x}} - L$ and $\dot{\mathbf{x}}^2 = \frac{\mathbf{p}^2c^2}{\mathbf{p}^2+m^2c^2}$ we obtain

$$H = \sqrt{\mathbf{p}^2c^2+m^2c^4}. \tag{163}$$

On-shell we find

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = 0, \quad E = \sqrt{\mathbf{p}^2c^2+m^2c^4}. \tag{164}$$

So far, everting looks good. Now consider the action

$$S[\mathbf{x},\mathbf{p}] = \int_{t_1}^{t_2}\mathrm{d}t\,(\mathbf{p}\cdot\mathbf{x} - H(\mathbf{x},\mathbf{p})), \quad H = \sqrt{\mathbf{p}^2c^2+m^2c^4}. \tag{165}$$

This action gives the same physical on-shell quantities but is not manifestly Lorentz invariant. Moreover, if we want to consider its quantization, the Hamiltonian will be

$$\hat{H} = \sqrt{-\hbar^2\nabla^2+m^2c^2}. \tag{166}$$

Now, let us return the action given in (159) and now define the $(D-1)$-momentum as

$$p_\mu = \frac{\partial L}{\partial\frac{\mathrm{d}x^\mu}{\mathrm{d}u}} = \frac{mc\,\eta_{\mu\rho}\frac{\mathrm{d}x^\rho}{\mathrm{d}u}}{\sqrt{-\eta_{\rho\sigma}\frac{\mathrm{d}x^\rho}{\mathrm{d}u}\frac{\mathrm{d}x^\sigma}{\mathrm{d}u}}}. \tag{167}$$

Then we will find that

$$H = p_\mu\frac{\mathrm{d}x^\mu}{\mathrm{d}u} - L = 0, \quad p_\mu p^\mu + m^2c^2 = 0. \tag{168}$$

From the second expression we derive

$$p^0 = \sqrt{\mathbf{p}^2 + m^2c^2}. \tag{169}$$

This is the usual Hamiltonian but our actual Hamiltonian vanishes off-shell. The second off-shell expressions $p_\mu p^\mu + m^2c^2 = 0$ plays a role of a constraint. In order to incorporate this constraint off-shell, let us consider now the Lorentz invariant and reparametrization invariant action

$$S[x,p,N] = \int_{u_1}^{u_2} \mathrm{d}u \left(p_\mu \frac{\mathrm{d}x^\mu}{\mathrm{d}u} - N\mathcal{C} \right), \quad \mathcal{C} = p_\mu p^\mu + m^2c^2, \tag{170}$$

We see that N under the reparametrization $u' = u'(u)$ transforms as

$$N'(u') = \frac{\mathrm{d}u}{\mathrm{d}u'} N(u), \tag{171}$$

in order to leave the action invariant. $x^\mu(u)$ and $p_\mu(u)$ transform a scalars, i.e. $x'^\mu(u') = x^\mu(u)$ and $p'_\mu(u') = p_\mu(u)$. The equations of motion are

$$p_\mu p^\mu + m^2c^2 = 0, \quad \frac{\mathrm{d}p_\mu}{\mathrm{d}u} = 0, \quad \frac{\mathrm{d}x^\mu}{\mathrm{d}u} = 2Np^\mu. \tag{172}$$

We see that N is dot dynamical and its equation gives $\mathcal{C} = 0$. N corresponds to a Lagrange multiplier. On-shell we find

$$-\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u} = -4N^2 p_\mu p^\mu = 4N^2m^2c^2. \tag{173}$$

which imply

$$2N = \frac{1}{mc}\sqrt{-\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}}. \tag{174}$$

Then from the equation for x^μ we recover the $(D-1)$-momentum

$$p_\mu = \frac{mc\,\eta_{\mu\rho}\frac{\mathrm{d}x^\rho}{\mathrm{d}u}}{\sqrt{-\eta_{\rho\sigma}\frac{\mathrm{d}x^\rho}{\mathrm{d}u}\frac{\mathrm{d}x^\sigma}{\mathrm{d}u}}}. \tag{175}$$

The key point now is that we can canonical quantize the theory by demanding $\hat{\mathcal{C}}|\psi\rangle = 0$.

So we have seen the advantage of the use of the Lagrangian over the Hamiltonian when we want to incorporate relativity and quantized the theory. However the action given in (159) involves a square root and thus seems impossible to compute the path integrals. For this reason consider the action

$$S[x,e] = \frac{1}{2}\int_{u_1}^{u_2} \mathrm{d}u \left(\frac{1}{e}\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u} - m^2c^2e \right), \tag{176}$$

where e is not dynamical as in the case of N and also makes the action reparametrization invariant. Its equation of motion is

$$\frac{1}{e^2}\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}+m^2c^2=0. \tag{177}$$

If we insert this into the action we find

$$S[x,e_{\text{on-shell}}]=\int_{u_1}^{u_2}\mathrm{d}u\,\left(\frac{1}{e}\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}\right)=-mc\int_{u_1}^{u_2}\mathrm{d}u\,\sqrt{-\eta_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}u}\frac{\mathrm{d}x^\nu}{\mathrm{d}u}}, \tag{178}$$

Under parametrization, x^μ again transform as a scalar and

$$e'(u')=\frac{\mathrm{d}u}{\mathrm{d}u'}e(u). \tag{179}$$

Notice that e is not a Lagrange multiplier as N but rather an auxiliary field. In both cases they are not physical and its presence is to realized reparametrization invariance. Since we have seen that demanding Lorentz invariance lead us to reparametrization invariance one may think that the later is a fundamental symmetry. It is not a real symmetry but rather a gauge symmetry, i.e. it is a redundancy in our description. One can think of it as the price to keep the theory manifestly Lorentz invariant.

The $(D-1)$-momentum and Hamiltonian result

$$p_\mu=\frac{1}{e}\eta_{\mu\nu}\frac{\mathrm{d}x^\nu}{\mathrm{d}u},\quad H=e(p_\mu p^\mu+m^2c^2). \tag{180}$$

The equation for e implies again that $H=0$. Hence, we conclude that reparametrization invariance implies that on-shell: $H=0$ and $p_\mu p^\mu+m^2c^2=0$ appears as a constraint. On the other hand, since the action is now quadratic, in principle we can perform the path integral and after considering e it must be of the form

$$\int_{x^\mu(u_1)=x_1^\mu}^{x^\mu(u_2)=x_2^\mu}\mathcal{D}x^\mu(u)\int\mathcal{D}e(u)\,\mathrm{e}^{\frac{i}{\hbar}S[x,e]}. \tag{181}$$

However, we do not know clearly what it stands for and how to deal with the redundancies introduced by e. We will return to this point later.

We have discussed in detail, for a relativistic free particle, how the Lagrangian is enters in a natural way to incorporate special relativity. Moreover, with the Lagrangian one can easily study different theories like non-relativistic particles, relativistic p-dimensional membranes ($p=0$ is a particle, $p=1$ is a string, etc...) and fields.

The main goal of the next section is to discuss the path integral for fields but before we end with a discussion of the ground state of a non-relativistic particle. Let us assume that for a Hamiltonian of the form

$$\hat{H}=\frac{1}{2m}\hat{p}^2+V(\hat{x}), \tag{182}$$

There is also the basis $\hat{H}|n\rangle = E_n|n\rangle$ with $\sum_n |n\rangle\langle n| = \hat{1}$ and $\langle n'|n\rangle = \delta_{n'n}$. Then

$$\langle x''|\hat{U}(t_2, t_1)|x'\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-i\frac{E_n}{\hbar}\Delta t}\langle x''|n\rangle\langle n|x'\rangle, \tag{183}$$

with $\Delta t = t_2 - t_1$. The wave function $\psi_n(x) = \langle x|n\rangle$ is a solution of the time-independent Schröndiger equation and we assume that $E_n > E_0$ for $n > 0$.

Now let us consider the complex time

$$z = \tau + it, \tag{184}$$

and

$$W(z_2, x'', z_1, x') = \sum_{n=0} \mathrm{e}^{-\frac{E_n}{\hbar}(z_2 - z_1)}\psi_n(x'')\psi_n^*(x'), \tag{185}$$

with z_1, z_2 fixed. Let us further consider a contour γ defined in the complex time plane with end points at z_1 and z_2 and

$$\gamma = \begin{cases} \tau + it_1 & \tau_1 \leq \tau \leq \tau_2 \\ \tau_2 + it & t_1 \leq t \leq t_2 \end{cases}. \tag{186}$$

This is depicted in figure I. Then, we see that

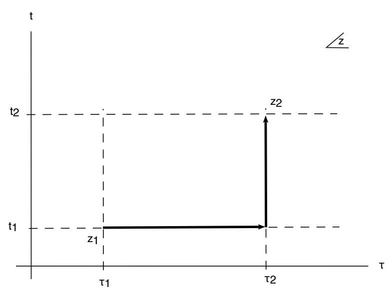

Figure I: Contour γ.

$$W(z_2, x''; z_1, x') = \sum_{n=0} \mathrm{e}^{-\frac{E_n}{\hbar}\Delta\tau}\mathrm{e}^{-i\frac{E_n}{\hbar}\Delta t}\psi_n(x'')\psi_n^*(x'). \tag{187}$$

The sum now is regulated for $\Delta\tau > 0$. Moreover for large values of $\Delta\tau$ we find that the only relevant term in the sum is $E_0\Delta\tau$. Hence, for $\Delta\tau \gg 0$ we find

$$W(z_2, x''; z_1, x') \approx \mathrm{e}^{-\frac{E_0}{\hbar}\Delta\tau}\mathrm{e}^{-i\frac{E_0}{\hbar}\Delta t}\psi_0(x'')\psi_0^*(x'). \tag{188}$$

The introduction of complex time serves as a regulator and also allow us to extract the ground state $\psi_0(x'')$.

Now consider the complex-time evolution operator

$$\hat{\mathcal{U}}(z_2, z_1) \equiv \mathrm{e}^{-\frac{1}{\hbar}(z_2 - z_1)\hat{H}}. \tag{189}$$

For a path integral representation of the matrix elements

$$W(z_2, x''; z_1, x') = \langle x''|\hat{\mathcal{U}}(z_2, z_1)|x'\rangle, \tag{190}$$

we need to consider the following Euclidean action

$$S_E[\chi]|_\gamma = \int_\gamma \mathrm{d}z \left(\frac{m}{2}\left(\frac{\mathrm{d}\chi}{\mathrm{d}z}\right)^2 + V(\chi)\right), \tag{191}$$

where now $\chi(z_1) = x'$, $\chi(z_2) = x''$ and in general χ is complex. Notice that the contour γ has nothing to do with the classical and virtual paths and in general the Euclidean action is complex. Then, we consider

$$W(z_2, x''; z_1, x') = \int\limits_{\chi(z_1)=x'}^{\chi(z_2)=x''} \mathcal{D}\chi(z)\, \mathrm{e}^{-\frac{1}{\hbar} S_E[\chi]|_\gamma}. \tag{192}$$

In order to extract the ground state, we see that only $\chi(z_2) = x''$ corresponds to a physical requirement and we should think $\chi(z_1) = x'$ as the condition that will lead us to the ground state. Stating differently, we need to find the initial condition that reproduces the ground state. Thus, $\chi(z_1) = x'$ is not a physical condition but rather a mathematical one. We can see this from

$$W(z_2, x''; z_1, x') \approx \mathrm{e}^{-\frac{E_0}{\hbar}\Delta\tau}\mathrm{e}^{-i\frac{E_0}{\hbar}\Delta t}\psi_0(x'')\psi_0^*(x'), \quad \Delta\tau \gg 0. \tag{193}$$

The contribution of x' enters from $\psi_0^*(x')$ and since want to extract $\psi_0(x'')$, it has no physical relevance.

Hence, we write

$$W(z_2, x; z_1) = \int\limits_{\chi(z_1)}^{\chi(z_2)=x} \mathcal{D}\chi(z)\, \mathrm{e}^{-\frac{1}{\hbar} S_E[\chi]|_\gamma}. \tag{194}$$

Notice that the only way to incorporate $\Delta\tau \gg 0$ in the path integral is via the contour γ. Therefore we finally consider the prescription

$$\psi_0(x) = \int\limits_{\chi(z_1)}^{\chi(z_2)=x} \mathcal{D}\chi(z)\, \mathrm{e}^{-\frac{1}{\hbar} S_E[\chi]|_{\gamma|_{\Delta\tau\gg 0}}}. \tag{195}$$

Let us test the above for the harmonic oscillator. We now that $\psi_0(x) \sim \mathrm{e}^{\frac{m\omega}{2}x^2}$. In spite that we can actually compute the full path integral, we will assume the limit

$1/m \to 0$. The reason behind this limit comes from the fact that the action can be written as

$$S_E[\chi]|_\gamma = \frac{1}{2g}\int_\gamma \mathrm{d}z \left(\left(\frac{\mathrm{d}\chi}{\mathrm{d}z}\right)^2 + \omega^2\chi^2\right) \equiv \frac{1}{2g}\, I_E[\chi]|_\gamma\,, \tag{196}$$

with $g = 1/m$. Then,

$$\frac{1}{\hbar}\, S_E[\chi]|_\gamma = \frac{1}{2g\hbar}\, I_E[\chi]|_\gamma\,, \tag{197}$$

and thus we can interchange the semiclassical limit $\hbar \to 0$ with the $g \to 0$ limit. This implies that only need to compute the action on-shell. The classical equations of motion are

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}z^2} = \omega^2\chi, \tag{198}$$

and thus we obtain

$$S_E[\chi]|_\gamma\Big|_{\mathrm{on-shell}} = \frac{1}{2g}\left(\chi\frac{\mathrm{d}\chi}{\mathrm{d}z}\right)\Big|_{z_1}^{z_2}. \tag{199}$$

Now we turn to the difficult part. The general solution of the equations is

$$\chi(z) = A_+\mathrm{e}^{\omega z} + A_-\mathrm{e}^{-\omega z}, \tag{200}$$

and therefore

$$\begin{aligned} S_E[\chi]|_\gamma\Big|_{\mathrm{on-shell}} &= \frac{\omega}{2g}\left(A_+^2\mathrm{e}^{2\omega z} - A_-^2\mathrm{e}^{-2\omega z}\right)\Big|_{z_1}^{z_2}, \\ &= \frac{\omega}{2g}(\chi^2(z_2)^2 - \chi^2(z_1)), \\ &= \frac{m\omega}{2}(x^2 - \chi^2(z_1)). \end{aligned} \tag{201}$$

Along the contour we see that the solution is of the form

$$\chi(z) = \begin{cases} A_+\mathrm{e}^{\omega\tau} + A_-\mathrm{e}^{-\omega\tau} & \tau_1 \le \tau \le \tau_2 \\ A_+\mathrm{e}^{\omega\tau_2}\mathrm{e}^{i\omega t} + A_-\mathrm{e}^{-\omega\tau_2}\mathrm{e}^{-i\omega t} & t_1 \le t \le t_2 \end{cases}. \tag{202}$$

where for convenience we have set $t_1 = 0$. We must have

$$\begin{aligned} \chi(z_1) &= A_+\mathrm{e}^{\omega\tau_1} + A_-\mathrm{e}^{-\omega\tau_1}, \\ x &= A_+\mathrm{e}^{\omega\tau_2}\mathrm{e}^{i\omega t_2} + A_-\mathrm{e}^{-\omega\tau_2}\mathrm{e}^{-i\omega t_2}. \end{aligned} \tag{203}$$

and $(\tau_2 - \tau_1) \to \infty$. Let us fix τ_2 and consider $\tau_1 \to -\infty$. For a finite value of $\chi(z_1)$ we must set $A_- = 0$ such that $\chi(z_1) = 0$. We also obtain $x = A_+\mathrm{e}^{\omega\tau_2}\mathrm{e}^{i\omega t_2}$ which imply that $A_+ = \mathrm{e}^{-i\omega t_2}$. Hence, the find a complex solution that gives

$$S_E[\chi]|_\gamma\Big|_{\mathrm{on-shell}} = \frac{m\omega}{2}x^2. \tag{204}$$

This means that $\psi_0(x) \propto \mathrm{e}^{-\frac{m\omega}{2\hbar}x^2}$. This example was enlightening. The domain of applicability of the prescription is quantum strong coupling systems or semiclassical ground state wavefunctions. In quantum cosmology, the Hartley-Hawking state a.k.a the wavefunction of the universe, is calculated in this way.