It's The Least We Could Do: The Principle of Least Action From Classical Physics To Quantum Mechanics

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Abstract

The Path Integral formulation of Quantum Mechanics is a novel and revolutionary approach to studying the dynamics of particle physics via variational principles. While the familiar Hamiltonian is often used to give a complete picture of the interaction energies of a quantiesed system, the path integral approach utilises Lagrangian mechanics to explore and understand the dynamics of particle physics. The path integral approach has its origins in the works of fundamental post-Newtonian classical physicists who sought to understand the behaviour of physical quantities without reliance upon well-known equations, but rather on known observable boundary conditions. From these modest beginnings a powerful expressive device has emerged in the form of the path integral. The principle of least action begins with formative studies of the behaviour of light and its interaction with matter, the mathematics of canonical systems, and leading up until the quantum revolution of the early 20th century. Our discussion will cover some simple computational implementations as toy model of these concepts, realised through stochastic Monte-Carlo methods, briefly concluding with a consideration of further, and more advanced avenues of work.

1 The Classical Principle of Least Action

1.1 Fermat's Principle

The physical properties of a system are most often expressed in terms of local extrema such as minima, maxima, and points of inflection which characterise the physical system[8]. For example, we can consider the path of a ray of photons traveling a distance from known points α to β in terms of an integral:

$$t = \int_{\alpha}^{\beta} dt = \int_{\alpha}^{\beta} \frac{d\ell}{v}, \tag{1}$$

where $dt = \frac{d\ell}{v}$ is the derivative of the length of travel over velocity of light. The observation that these photons follow the minimum possible time is referred to as Fermat's principle. Since the solution of this integral is an extremum, small changes in the parameters of it will not change the final value. Hence, we can use variational principles from true path I to derive the neighbouring path δI. This is best observed when we consider the difference in the path of light as it traverse one medium of index of refraction n_1 to a second medium of index of refraction n_2 with boundary point P. We define $v = \frac{c}{n_i}$, giving:

$$t = t_\alpha + t_\beta = \int_{\alpha}^{P} \frac{n_1}{c} d\ell + \int_{P}^{\beta} \frac{n_2}{c} d\ell = \frac{n_1}{c}\sqrt{s^2 + h_1^2} + \frac{n_2}{c}\sqrt{(w-s)^2 + h_2^2},$$

where h_i is the height of a given medium with s, the distance from the edge of the boundary to the point of refraction at the boundary, and w, the horizontal displacement from the initial point α to the final point β. If we compute the minute change in $\delta t = 0$, we have that:

$$\delta t = \frac{\partial t}{\partial s}\delta s = \left(\frac{n_1}{c}\frac{s}{\sqrt{s^2 + h_1^2}} - \frac{n_2}{c}\frac{w-s}{\sqrt{(w-s)^2 + h_1^2}} \right) \delta s = 0.$$

As this change is equally zero for all δs, one may then derive the notorious relationship between the angles of transmission and refraction of light through varying media known as Snells' law:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2. \tag{2}$$

Thus the total time for a ray of photons to travel from a point α to the boundary P is a straight line with constant slope $y'(x)$:

$$t_\alpha = \frac{n_1}{c}\int_\alpha^P \sqrt{1+\left(\frac{dy}{dx}\right)}dx, \tag{3}$$

which holds equally true for the time it takes the light to travel the second path from the boundary to point β. It is from these humble roots that we find the original formulation of a physical law expressing what would come to be known as the least action principle[5].

1.2 Lagrangian Mechanics

D'Alembert's principle states that the forces of constraint vanish for virtual work in conservative systems. Building upon this, Lagrange discovered that, for a system of Cartesian coordinates in which the kinetic energy can be described as $T(x) = \sum_i \frac{1}{2}m_i v_i(x)^2$ and in which the potential energy $V(x)$ does not explicitly depend on time, a new function $\mathcal{L}$ can be defined as:

$$\mathcal{L}(q_j, \dot{q}_j) = T - V,$$

for which the relationship,

$$\frac{d}{dt}\left(\frac{\mathcal{L}}{\partial \dot{q}_j}\right) - \frac{\mathcal{L}}{\partial q_j} = 0,$$

vanishes with respect to virtual displacements $\partial \dot{q}_j$ and ∂q_j. Referred to as the Lagrangian, these equations describe the dynamical motion of all conservative systems.

For a system of spacial displacements x_j, we can define the action of a given system as:

$$S = \int_{t_\alpha}^{t_\beta} \mathcal{L}(x, \dot{x}, t)dt, \tag{4}$$

such that S is an invariant. For a small variation in S, we have that:

$$\begin{aligned}\delta S &= \int_{t_\alpha}^{t_\beta} \delta\mathcal{L}(x,\dot{x},t)dt = \int_{t_\alpha}^{t_\beta}\left[\frac{\mathcal{L}}{\partial x_j}\delta x_j + \frac{\mathcal{L}}{\partial \dot{x}_j}\delta \dot{x}_j\right]dt \\ &= \int_{t_\alpha}^{t_\beta}\left[\frac{\mathcal{L}}{\partial x_j}\delta x_j - \frac{d}{dt}\left(\frac{\mathcal{L}}{\partial \dot{x}_j}\right)\delta x_j\right]dt = \int_{t_\alpha}^{t_\beta}\delta x_j\left[\frac{\mathcal{L}}{\partial x_j} - \frac{d}{dt}\left(\frac{\mathcal{L}}{\partial \dot{x}_j}\right)\right]dt = 0\end{aligned}$$

It is from this fundamental relationship of quantities that we find a very important characteristic description of conservative physical systems:

$$\frac{d}{dt}\left(\frac{\mathcal{L}}{\partial \dot{x}_j}\right) = \frac{\mathcal{L}}{\partial x_j}, \tag{5}$$

which are referred to as the Euler-Lagrange equations of motion. From this important result one may derive the classical principle of least action as:

$$\delta \int_{t_\alpha}^{t_\beta} \mathcal{L}\, dt = 0, \tag{6}$$

for which the Lagrangian is defined as the minimal action per unit of time.

2 Classical Least Action for a Particle (Java)

The basic utility of our program is to qualitatively and ⟨hopefully⟩ quantitatively describe the principle of least action in a classical particle trajectory. As previously noted, we should be able to graphically depict the trajectory of a free particle under the influence of a field potential (generally, gravity) using on the initial and final boundary conditions, a fixed duration of time, and a maximum spatial displacement value. This simulation can be used to model simple particle behaviours such as the path of a projectile.

We will find the solution to our classical action minimisation with the help of a simple Monte Carlo algorithm for the generation of random y-coordinate values graphed against this fixed time, t, with the individual segments corresponding to the piecewise continuous components of the action. We will initially plot a straight line with an appropriate slope to connect the boundary points linearly, and then vary the segments to find the minimal action across the entire time duration to arrive at the correct particle trajectory.

2.1 The Action Integral

Fixing the initial and final positions of the particle at given times y_i and y_f we can randomly select coordinates such that we can minimise the action if the Lagrangian[6]. Discretely, the 1-D version of this integral can be represented for time $t_i = t_0 + \Delta t$ as roughly equivalent to the Riemann sum:

$$\mathcal{S} \approx \sum_{i=1}^{N-1} \mathcal{L}(t_i)(t_i - t_0). \tag{7}$$

The sum over these path segments is represented graphically in our program to give the total action. In the presence of an external potential, $u(y_i)$, the Lagrangian can be further discretised as roughly:

$$\mathcal{L}(t_i) \approx \frac{m}{2}\left(\frac{y_{i+1}-y_i}{t_{i+1}-t_i}\right)^2 - u(y_i), \tag{8}$$

where the usual quantity $v_i(y)^2 = \left(\frac{\Delta y}{\Delta t}\right)^2 \approx \left(\frac{y_{i+1}-y_i}{t_{i+1}-t_i}\right)^2$ has been factored out by algebraically. In our code, this is defined as:

$$Lagrangian = (m/2.0) * Math.pow(((y[j+1]-y[j])/\Delta t), 2) - u(s,j),$$

where $u(s,j)$ corresponds to one of a set of four defined potentials selected by the user. Additionally, the user specifies the boundary conditions y_i and y_f, the fixed time duration, a maximal displacement factor, and has free choice of potential coefficients.

2.2 Minimising the Action

The basic Monte Carlo algorithm is described by the following steps:

1) Choose an arbitrary y_{trial} value given by a sum of the previous y_j value plus the product of twice the maximum displacement value and a psuedo-randomly generated real number on the unit interval.

2) Define the $previousLagrangian$ as the sum of the left and right components of the Lagrangians of $y[j]-y[j-1]$ and $y[j+1]-y[j]$, respectively.

3) Replace $y[j]$ with y_{trial} and define $trialLagrangian$ as the sum of the left and right components of the Lagrangians of $y_{trial}-y[j-1]$ and $y[j+1]-y_{trial}$, respectively.

4) Compare the values of $previousLagrangian$ and $trialLagrangian$, changing $y[j]$ to y_{trial} if the latter is smaller than the former.

5) Repeat until the total action is minimised over all intervals of time.

Allowing this algorithm to run for several hundreds or perhaps thousands steps will eventually solve the trajectory from which the equations of motion for the given physical system could easily be derived.

3 The Path Integral of Quantum Mechanics

3.1 Feynman's Dreams

The great revolution in physics at the turn of the 20th century was the growing awareness of probabilistic interpretations of the underlying physical foundations of the laws of particle interaction and their respective dynamical equations. Feynman himself remarked upon the emerging theories of his day[3]:

> "It is a curious historical fact that modern quantum mechanics began with two quite different mathematical formulations: the differential equation of Schroedinger, and the matrix algebra of Heisenberg. The two apparently dissimilar approaches, were proved to be mathematically equivalent. ... a third formulation of non-relativistic quantum theory ... was suggested by some of Dirac's remarks concerning the relation of classical action to quantum mechanics. A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time.

As it turned out, Feynman was speaking specifically about a rather obscure comment by Dirac concerning the physical significance of the probability amplitude, $e^{i\frac{S}{\hbar}}$[4].

3.2 Theoretical Underpinnings

A deep relationship between quantum field theory and classical statistical mechanics is revealed through the examination of the path integral formulation[2]. For the duration of our study, we will concern ourselves with the imaginary time Euclideanised sum-over-histories approach to the Feynman path integral:

$$Z_{fi} = \langle x_f | e^{i\frac{S}{\hbar}} | x_i \rangle \sim \int [dx] e^{i\frac{S[x]}{\hbar}}. \tag{9}$$

Here the Euclidean action of S is defined over $\tau = it$ as:

$$S = \int_{x_i(\tau)}^{x_f(\tau)} d\tau \left[\frac{1}{2} m_0 \left[\frac{dx}{d\tau} \right]^2 + V(x) \right], \tag{10}$$

from which we can define the propagator $G(x, x_0, \tau)$ as[6]:

$$G(x, x_0, \tau) = A \sum_{\text{paths}} e^{i\frac{S}{\hbar}}, \tag{11}$$

with a normalisation constant, A. Similarly to the previous approximation of the Lagrangian(8), we can approximate the total action as[10]:

$$S \approx \sum_{j=1}^{N-1} \left(\frac{m_0}{2(\Delta\tau)^2}(x_j - x_{j-1})^2 - V(x_j) \right) \Delta\tau. \tag{12}$$

Dividing time into N intervals from τ_0 to τ_n, we express $G(x, \tau; x_0, \tau_0)$ as:

$$G(x, \tau; x_0, \tau_0) = \lim_{N\to\infty} dx_i \cdots dx_{N-1} \prod_{j=0}^{N-1} G(x_{j+1}, x_j, \Delta\tau),$$

which is evaluated for small $\Delta\tau$. As our computation involves oscillatory integrals, we can finally express $G(x, x_0, N\Delta\tau)$ as[12]:

$$G(x, x_0, N\Delta\tau) = \left(\frac{m_0}{2\pi\hbar\Delta\tau}\right)^{N/2} \int dx_i \cdots dx_{N-1} e^{-\frac{\Delta\tau}{\hbar}\sum_{j=1}^{N}\left[\frac{m_0}{2}\left(\frac{x_j - x_{j-1}}{\Delta\tau}\right)^2 + V(x_j)\right]}, \tag{13}$$

for N virtual atoms on a ring.

4 Path Integral Monte Carlo (Java)

Taking some inspiration from our aforementioned implementation of the principle of least action for Classical Mechanics we have sought to develop a reasonably qualitatively accurate representation of the Path Integral formulation of QM. For this, we have chosen to use similar stochastic approaches as we had in the previous demonstration. This particular approach is referred to as the Path Integral Monte Carlo (PIMC); chiefly for its usage of pseudo-random number generation for finding the minimal distribution of points in x[9]. For estimating these x-coordinates in time we make usage of two variations of the Metropolis algorithm. We then graph these changes in the coordinates over a fixed time period. Herein we will describe with some detail the overall structure and functionality of the PIMC program.

4.1 Path Segment Generation

Using the Metropolis-Hastings algorithm, we seek to minimise the distribution of x-coordinates necessary to ensure the correct wave function probability density of our simulated quantum path integral. Since we are no longer in the realm of deterministic particle behaviours we are unable to simulate an exact trajectory for any given particle, however we are able to compute some examples of an infinite number of physically possible quantum paths. The overall algorithm is described as follows:

1) Initially, we must choose a pseudo-random x_{trial} defined as:

$$x_{trial} = x[j] + \delta * (2 * r_1 - 1),$$

where r_1 is a pseudo-random number on the unit interval and δ is the maximum atomic displacement on the order of $(\hbar/m\omega)^{1/2}$.

2) Calculate ΔE, where $x_0 = x_N$ to satisfy the condition that our virtual atoms are displaced on a ring, in terms of:

$$\begin{aligned}\Delta E = (1/2.0)&\\ &* (Math.pow(((x[j+1] - x_{trial}/\Delta\tau), 2)\\ &+ Math.pow(((x_{trial} - x[j-1])/\Delta\tau), 2) + V_{trial}(s, xt)\\ &- Math.pow(((x[j+1] - x[j])/\Delta\tau), 2)\\ &- Math.pow(((x[j] - x[j-1])/\Delta\tau), 2) - V(s, j)),\end{aligned}$$

3) Calculate the probability $p = e^{-\Delta\tau\Delta E}$ and generate a second pseudo-random number r_2. If $\Delta E < 0$ or if $r_2 \leq p$ then replace $x[j]$ with x_{trial}.

4) Repeat this procedure until the Path Integral Monte Carlo reaches equilibrium (this may take up to 10^5 steps).

4.2 Ground State Probability Distribution

Since we have already found the x-coordinates, it is now possible to generalise them in terms of probability distribution using a simple Metropolis algorithm. The process is described as follows.

1) Divide the coordinates x_i into a finite number of bins of width Δx.

2) Using the numerical value of the selected potential and $M < N$ randomly generated walkers, compare the value of the calculate difference in product of the probability and time differentials, $dp\,dt$, against a randomly generated number, r on the unit interval.

3)If the number of walkers $M > 0$ and $dp\,dt > r$ then reduce the number of walkers by one and decrease the potential sum by the value of the potential $V(x)$ at that point. Otherwise, if $r < -dp\,dt$ then increase the number of walkers by one and increase the value of the potential sum by the value of the potential $V(x)$ at that point.

4) Repeat until the probability distribution has reached equilibrium.

4.3 Ground State Wave Function Probability Density

Using the value of the probability distribution $P(x)$, normalised by dividing it by the product of the total number of Monte Carlo steps, mcs, and the total number of path segments, N, it is possible to calculate the wave density:

$$|\Psi_0(x)|^2 = \sqrt{P(x)}/\Delta x$$

4.4 Ground State Energy

The normalised ground state probability density is also used to calculate the ground state energy, E_0:

$$E_0 = \sum_x P(x)[T(x) + V(x)],$$

where $T(x)$ is derived from the virial formula:

$$\langle T(x)\rangle = \left\langle \frac{x}{2}\frac{dV}{dx} \right\rangle,$$

which results in lower statistical variance than calculating $T(x)$ from the averages over $(x_j - x_{j-1})^2$. We then graph the value of E_0 against the number of Monte Carlo steps, effectively over time, t.

5 Conclusion

5.1 Unfinished Business

While we have achieved many of our computational and theoretical objectives via the aforementioned Java programs described in the previous sections, it should go without saying that certain features and capacities were overlooked due to constraints of both time and space. This project was originally conceived as an opportunity to implement theories of quantised gravity in a computational model. However, as time went on and the realities of the temporal limitations of this project became more apparent, these ambitions had to be temporarily abandoned in favour of the more concrete examples of the PIMC that you have seen herein.

The theory of Causal Dynamical Triangulations is a view of quantised gravity which sees spacetime as a discrete, connected non-abelian linear construction of chaotically generated foliations of spin-network topologies, based upon the limitations of irreducible Planckian distances and doubly special relativity. At the core of CDT is the notion of the Einstein-Hilbert action as the generator of a path integral view of quantisable spacetime. This theory lends itself well to the viewpoint of computational physics as one can produce a discretised 4D gravitational worldline from a finite set of two dimensional triangulations. Much work has been done in this regard, such that it is not infeasible to accomplish a limited demonstration of the concept with consumer-grade hardware and open-source software[7], such as C++ or even Python.

Along these lines, an early proposal of this project would have also included the representation of relativistic path integrals in curved space. Once again, due to certain unforeseen temporal constraints these ambitions were not able to be realised within the scope of this completed project. However, the next logical step in this work would be to adapt this work for the support of special relativistic spacetime geometries, which could themselves be extended towards Euclidean approximations of path integrals on curved manifolds[1]. With some optimism, with our efforts in the near future we will further our studies in this area.

In addition to some of these shortcomings, there were also certain problems encountered in our implementation of the Path Integral Monte Carlo. Some of these unexpected difficulties included the calculation of accurate magnitudes for the total probability and the wave function. Even though

the values were normalised by dividing the each value by the product of the number of segments multiplied by the number of Monte Carlo steps they were still at least an order of magnitude greater than the expected values. We have attenuated the values of the probability distribution $P(x)$ by dividing by an additional factor of 0.1, but this has not completely mitigated the numerical inaccuracy, rather it has only slightly masked the problem æsthetically. In light of this glaring calculational inadequacy, this program is best viewed as a qualitative representation rather than a numerically accurate vision of the path integral formulation of QM[2]. It is possible to implement a moving window to calculate the average of E_0 over this period, but for our purposes the streaming value offers an appropriately qualitative sensation of the overall energetic behaviour of our simulated Path Integral Monte Carlo.

5.2 Closing Thoughts

Despite the drawbacks of our implementation, these toy models offer a satisfactory and mathematically interesting view into computational methods in statistical quantum mechanics. Further study into functional approaches in mathematical physics is a rich and interesting area in which the author wishes to focus an increasingly continual effort. While certain aspects of the path integral formulation of QM have only been superficially considered there is a clear attractive quality to the expressive potential of Path Integral Monte Carlo methods, both heuristically and theoretically.

As seen in Euclideanised approaches to quantised gravity theories such as CDT and quantum causal sets, the central notion of the sum-over-histories viewpoint remains a fundamental approach to generalising non-commutative geometrical relationships of edgewise connected topologies. It is our hope that a near-future avenue of novel research into computational aspects of these topics avails itself to us. Until then we will continue to examine the existing corpus of work in this domain with the intention of remaining on the cutting edge of published theoretical material. The path integral formulation of QM remains one of the most deep and powerful expressions in all of physics. We owe it to ourselves to examine it closely: after all, it's the very least we could do.

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