An investigation of the theoretical and computational applications of Feynman's Path Integral.

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1 Brief overview

Until 1933, quantum mechanics was formulated almost entirely in terms of the Hamiltonian formalism — the operator representation of total energy. This changed when Paul Dirac proposed that the Lagrangian and the principle of least action might form a more fundamental basis for quantum theory [Dirac, 1933]. Richard Feynman realised this in 1948 [Feynman, 1948], when he first postulated the path integral, a new formulation of quantum mechanics. Instead of explicitly using operator notation or Heisenberg matrix mechanics, it considers all possible paths a particle could take when moving from one position to another in some time interval. By summing the probability amplitudes of all these different paths, we can find the "propagator" of a given system. The path integral can be manipulated into the partition function via a Wick rotation. This broadens the path integral's utility further, as will be demonstrated in this project. Since Feynman introduced the concept of the path integral, its conceptual advantages have been investigated and built upon. Today, it is still preferred by some researchers in condensed matter field theory and quantum chromodynamics (QCD), where the path integral formulation can be advantageous to work with.

2 Background information

The path integral formulation of quantum mechanics helps us find the probability amplitude that a particle will be at some point x_f at time t_f if is at a position x_i at time t_i. By taking $\hbar$ as our fundamental unit of action (setting $\hbar = 1$), this probability amplitude, often called the propagator or time-evolution kernel, can be written as

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-iHT} | x_i \rangle, \tag{1}$$

where $T = t_f - t_i$. If the Hamiltonian operator H takes its usual form of $H = \frac{p^2}{2m} + V(x)$, then we can find the configuration space path integral,

$$K = \int \mathscr{D}x(t) \exp\left(iS[x(t)]\right), \tag{2}$$

where $\mathscr{D}x$ represents integration over all paths with a prefactor included, and the action S is given by

$$S = \int_{t_i}^{t_f} dt \mathscr{L} = \int_{t_i}^{t_f} dt (T - V). \tag{3}$$

In certain systems (such as the quantum harmonic oscillator) we can find analytical solutions for (2), which are equivalent to solutions produced within the Schrödinger formulation. This expression is not always solvable analytically, instead the discretised form is often more useful,

$$K = \left(\frac{m}{2\pi i\delta}\right)^{N/2} \int \prod_{j=1}^{N-1} dx_j \exp\left[i\delta \sum_{j=0}^{N-1} \left(\frac{m\dot{x}_j^2}{2} - V(\bar{x}_j)\right)\right], \tag{4}$$

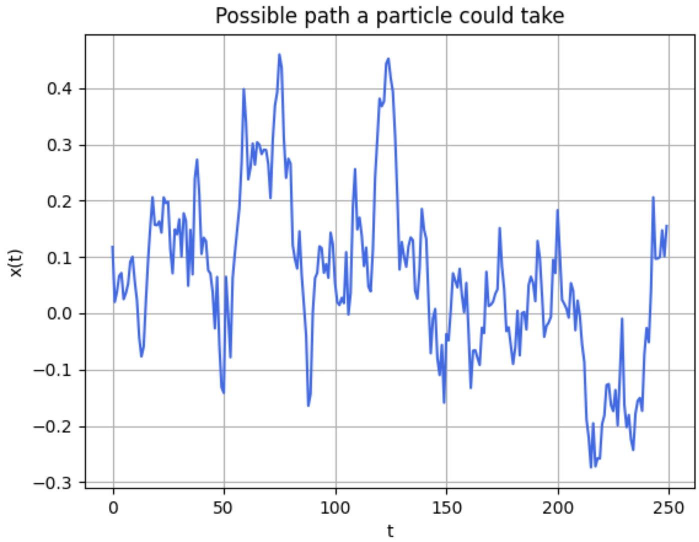

Figure 1: Representation of the path integral discretised by time interval δ, generated using python and a C++ Metropolis algorithm, with lattice size 250.

where the exact form is retrievable by taking the limit $N \to \infty$. Derivations of (2) and (4) can be found in [MacKenzie, 2000].

One reason why the path integral is such an important formalisation of quantum mechanics is that it can be mutated into the partition function,

$$Z = \sum_j \exp\left(-\frac{H_j}{k_B T}\right), \tag{5}$$

where H is the Hamiltonian or total energy. The technique used to remove the oscillatory behaviour from the propagator is the Wick rotation. Using the convention $t \mapsto -i\tau$, the factor

$$\exp\left(i \int dt \mathscr{L}\right) \tag{6}$$

maps to

$$\exp(-S_E) \quad \text{with} \quad S_E = \int d\tau \mathscr{L}_E, \tag{7}$$

where for a particle with $\mathscr{L} = \frac{1}{2}m\dot{x}^2 - V(x)$ we obtain the Euclidean Lagrangian

$$\mathscr{L}_E = \frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 + V(x). \tag{8}$$

The Euclidean propagator then becomes

$$\begin{aligned} K &= \left(\frac{m}{2\pi\delta}\right)^{N/2} \int \prod_{j=1}^{N-1} dx_j \exp\left[-\delta \sum_{j=0}^{N-1} \left(\frac{m\dot{x}_j^2}{2} + V(\bar{x}_j)\right)\right] \\ &= \int \mathscr{D}x(t) \exp\left(-S_E[x(t)]\right), \end{aligned} \tag{9}$$

with $(\delta = (\tau_f - \tau_i)/N$. This derivation is formally executed in [Creutz and Freedman, 1981].

One use of this formulation is find the ground-state energy of the quantum harmonic oscillator. This is performed by constructing a lattice of discretised positions at different times, and evolving the particle using the Metropolis algorithm. We use the Euclidean propagator (9) as an analogous form of the partition function. Further information about simulating the quantum harmonic oscillator on a lattice can be found

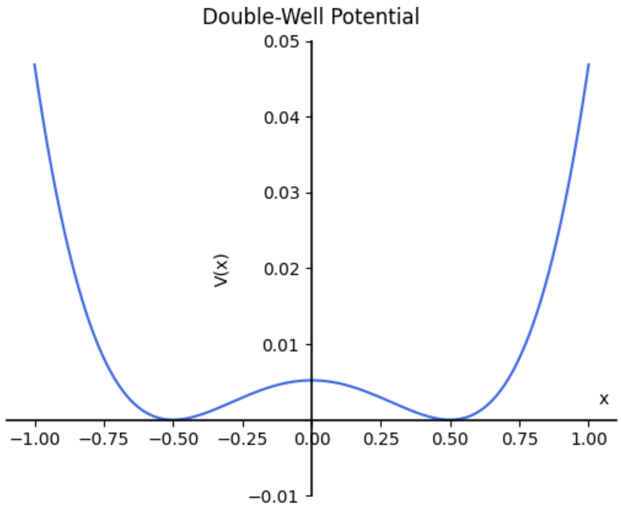

Figure 2: Double-Well Potential, $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$, generated in python with $\lambda = 5$, $a = 0.5$, with 1000 points.

in [Lepage, 2005]. A C++ program emulating the path integral of a quantum harmonic oscillator has been written, one frame of the path integral can be seen in Figure 1.
The Metropolis algorithm is the method of evolving the Feynman path integral in simulations. It is an example of an MCMC (Markov Chain Monte Carlo) method, where small random changes to the path are suggested and then tested with a probability that depends on the change in the action. This process is repeated, which generates a sequence of paths that emulates the path space of the path integral.
When we change the potential present in the Lagrangian to that of the double-well potential (see Figure 2), we can investigate an interesting physical phenomena. The double-well potential will have two ground state energies at $-a$ and a. If the particle subject to this potential is in its ground state energy at position $x_i = -a$, then in theory it could (in the infinite time limit) move to $x = 0$. At this point it could roll back down to the other ground state energy at $x_f = a$ and then stay there at rest. This process would happen in an instant, hence the name of the phenomena, instantons.

3 Research ideals

This project focuses primarily on the theoretical foundations and practical applicability of the path integral formulation of quantum mechanics. While not directly aligned with the main research goals of the department, the techniques explored — including propagator analysis and partition function methods — overlap with theoretical and computational tools used within the department.
The analytical study of path integrals relates to the interests of my supervisor, Dr. Francesca Caloro, particularly in the context of quantum chromodynamics. Here the path integral is used as an alternative (and often advantageous) formalisation of quantum mechanics.
Additionally, analytical and computational calculations in condensed matter field theory are often conducted via a Wick-rotated propagator. This results in a Euclidean partition function which is currently being used in research by post doctorates who use the path integral to find effective actions.
Although the project does not sit within a specific departmental research programme, it contributes to the theoretical foundation of many active areas of physics. It is essentially an investigation into the utility of the path integral as a formulation of quantum mechanics, providing conceptual and methodological insight rather than advancing a particular research objective.

4 Aims and Objectives

4.1 Project Aim

This project begins with analytical foundations and advances toward numerical simulation and quantum phenomena such as instantons. We start by verifying the computational methods by comparing the extracted ground-state energy of the quantum harmonic oscillator with the known analytical value. Building on this established method, the project now transitions to studying instantons in the double-well potential, aiming to derive analytical tunnelling predictions and verify them numerically via lattice path integral methods. This approach ensures theoretical consistency, computational reliability, and allows extension to a similar system, such as the two spin system.

4.2 Objectives

1. **Read literature about the path integral formulation.**
   Before any derivations or computations can be performed, an understanding of the path integral as a formulation of quantum mechanics was acquired. This included learning about the propagator and its equivalent derivation in the Schrödinger formulation.

2. **Derive the propagator for the general quadratic Lagrangian analytically.**
   Within the first 4 weeks of the project, the propagator for the general quadratic Lagrangian form of a particle was derived fully. This established an analytical foundation for later comparison with numerical methods.

3. **Develop Monte-Carlo Metropolis simulation for the quantum harmonic oscillator.**
   The purpose of this objective is to create a strong foundation for the computational methods to be used throughout the project. We will construct a framework in **C++** for simulating systems with different potentials using the path integral formalism of the partition function. By comparing theoretical results with the extractable ground-state energy of the quantum harmonic oscillator, the numerical framework can be verified for later simulations.

4. **Derive analytic instanton solutions and tunnelling observables in the 1D double-well.**
   We will analytically study the instantons as a system using the path integral formalism of quantum mechanics. By obtaining expressions for the instantons, this allows us to compare numerical approximations with theoretical solutions.

5. **Extend existing Monte-Carlo code to simulate instanton tunnelling.**
   By adapting the lattice simulation to the double-well potential, we can simulate the behaviour of instantons. This builds directly onto the quantum harmonic oscillator simulation, using the familiar Monte-Carlo Metropolis algorithm.

6. **Extension: Investigate more uses of the path integral.**
   If the instanton tunnelling investigation is completed on time, a possible extension could be to the two-level spin system.

7. **Contingency plans.**

   (a) In the case that the instanton analysis or computations prove impractical, one possible contingency plan is to investigate the Aharonov-Bohm effect using the path integral. This system can also be simulated with a computational model, so analytical answers can still be compared against numerical ones.

   (b) Another contingency plan is to adapt our computational framework for the quantum harmonic oscillator to simulate an anharmonic potential (where the potential varies with position to the order of 4). This should also be solvable analytically, allowing comparison between methods.

To make sure that we have enough time to complete the project, one of these contingency plans should be started no later than the 16th week.

8. **Complete project report, analysis, and viva preparation.**
   The final stages of the project should be finalising the report and preparing for the viva. All other analyses and computations must be complete before this.

5 Programme of work

The project progresses from analytical derivation, to computational implementation, to data extraction and validation. The path integral propagator for quadratic systems has already been derived analytically, and a Monte-Carlo Metropolis simulation has been created. It remains to validate this simulation, along with extending these methods to instanton physics.

5.1 Timeline of Tasks

- In the first week of the project, a brief recap of quantum mechanics from previous studies was conducted. Following this, the next 2 weeks were spent reading papers on the path integral formulation of quantum mechanics, including [Dirac, 1933], [Feynman, 1948], and [MacKenzie, 2000]. A derivation of the propagator for a particle subject to a general quadratic potential from [Schulman, 1981] was followed and reproduced in the fourth week. This concluded the introductory analytical period of the project, and we started setting up an environment to simulate the quantum harmonic oscillator computationally.

- From the fifth to eighth week, literature regarding the statistical methods of modelling the quantum harmonic oscillator are being read. This includes learning about Wick rotations and simulation techniques in [Lepage, 2005], then further understanding of the Metropolis algorithm being developed by reading [Creutz and Freedman, 1981] and [MacKeown, 1985].

- In the ninth week of the project, there should be a focus on preparation for the oral examination. This will involve writing slides and further familiarisation with the path integral through reading.

- From the tenth to twelfth week, the theory surrounding instantons should be read about. Resources that are available for learning about instantons include the latter pages in [MacKenzie, 2000] and examples in [Altland and Simons, 2010]. To conclude this, some derivation for computable values involving instantons should be completed. Following the theoretical research into instantons, our existing computational model should be adapted to simulate the instantons. Once the model is functional, data that was derived analytically should be extracted. This will occupy weeks 13 to 18.

- This schedule leaves six weeks to either advance with extensional tasks or catch up where time constraints might have been underestimated. In the case that analysing or computing instantons is not completable within the time frame, eight weeks should be made available to swap to one of the contingency plans. Therefore, on the 9th of March, whether the project is completable within the time frame should be considered.

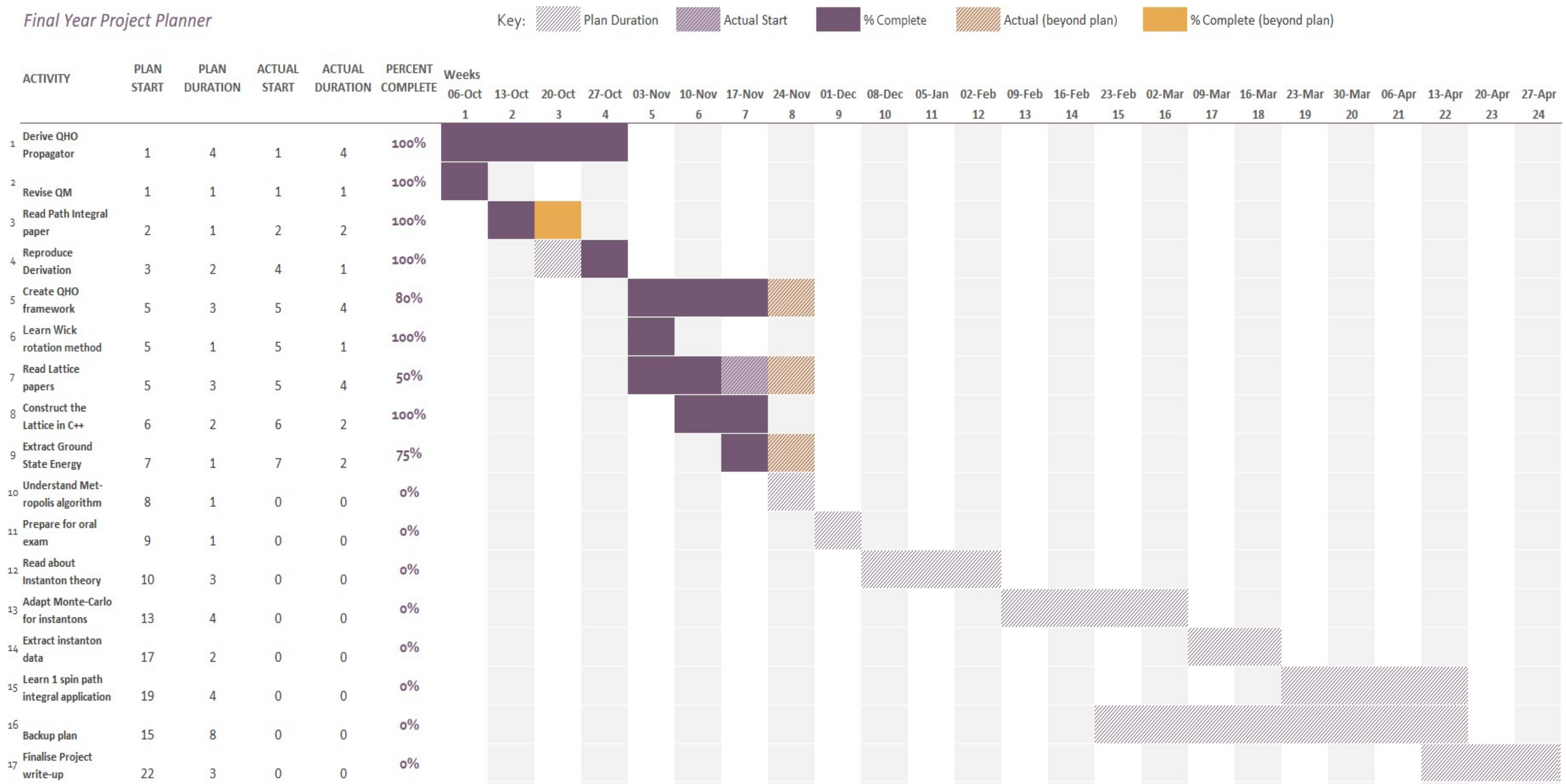

Figure 3: Timeline overview of the project, produced using Microsoft Excel.

5.2 Project Risks and Mitigation Strategies

The primary risks relate to numerical convergence, statistical scaling, and computational feasibility rather than conceptual barriers. Risks are categorised by *Likelihood (L)* and *Impact (I)* on a scale of 1-10, and *Overall Score (O)*, which is their product on a scale of 1-100.

Risk	**L**	**I**	**O**	**Mitigation Strategy**	**Contingency Plan**
Monte-Carlo simulation fails for the instanton case	3	8	24	Ensure that the Monte-Carlo method is well understood	Switch to a contingency plan by Week 15
Analysis of the instantons proves overly difficult	2	9	18	Leave enough time to fully digest instantons literature	Switch to a contingency plan by Week 15
Contingency plans are left too late to execute	3	10	30	Keep track of the time frame of the project using the Gantt chart	Not applicable
Computation becomes too slow	3	7	21	Enable parallel computation and optimise update steps	Reduce lattice size, or lessen the repeats taken for averages

Table 1: Risk assessment with mitigation and contingency planning.

6 Resources, Health and Safety, and ethics

6.1 Health and Safety

This project is purely theoretical, and so the major concerns of health and safety in experimental projects are not of concern. The most relevant concern for health and safety is to ensure an ergonomic work environment, which has already been completed.

6.2 Ethics and Data Management

This project does not cause harm to any humans or animals, and does not use any data from humans. To ensure ethical practices are upheld, any knowledge from external resources (such as papers or journal entries) are to be referenced appropriately.

6.3 Resources

Throughout the project, there are many books, articles, and papers which are used to gain insight into path integrals and their applications. A full list of the resources included in this paper follows, and any further resources accessed will be properly referenced in the final project. Other than these literary resources, there is also the computational resources used. However these are also of minimal concern as calculations are not expected to be very intensive.

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