

Path Integrals in Quantum Mechanics

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Abstract

We present the path integral formulation of quantum mechanics and demonstrate its equivalence to the Schrödinger picture. We apply the method to the free particle and quantum harmonic oscillator, investigate the Euclidean path integral, and discuss other applications.

1 Introduction

A fundamental question in quantum mechanics is *how does the state of a particle evolve with time?* That is, the determination the time-evolution $|\psi(t)\rangle$ of some initial state $|\psi(t_0)\rangle$. Quantum mechanics is fully predictive [3] in the sense that initial conditions and knowledge of the potential occupied by the particle is enough to fully specify the state of the particle for all future times.¹

In the early twentieth century, Erwin Schrödinger derived an equation specifies how the instantaneous change in the wavefunction $\frac{d}{dt}|\psi(t)\rangle$ depends on the system inhabited by the state in the form of the Hamiltonian. In this formulation, the eigenstates of the Hamiltonian play an important role, since their time-evolution is easy to calculate (i.e. they are stationary). A well-established method of solution, after the entire eigenspectrum of $\hat{H}$ is known, is to decompose the initial state into this eigenbasis, apply time evolution to each and then reassemble the eigenstates. That is,

¹In the analysis below, we consider only the position of a particle, and not any other quantum property such as spin.

$$|\psi(t)\rangle = \sum_{n=0}^{n=\infty} \exp[-iE_n t/\hbar] \langle n|\psi(t_0)\rangle |n\rangle \quad (1)$$

This (Hamiltonian) formulation works in many cases. In classical mechanics, however, the Lagrangian formulation is known to be equivalent to the Hamiltonian one. Thus, we seek an answer to the above question that relies on some analogue of the *Lagrangian action*. In 1920, P.A.M. Dirac made a mysterious comment to this effect, which later inspired Richard Feynman. Consider a trajectory $x(t)$ between an initial point (x_0, t_0) and possible future point (x', t') . Let the *transition probability amplitude* $\langle\psi(x, t)|\psi(x_0, t_0)\rangle$ be the inner product of the wavefunction in the Schrödinger picture of the particle evaluated at these two points. Feynman hinted at the “equivalence” of the probability amplitude and the exponent of the classical action of the trajectory $\exp[iS[x(t)]/\hbar]$, where “equivalence” is not yet well-defined. It was not until 1948 that Feynman, as a post-doctoral student at Princeton, formalized this connection.

In his landmark paper [4], Feynman presented a formulation of quantum mechanics based on this principle. Let a given trajectory $x(t)$ be associated with a transition probability amplitude with the same form as that given by Dirac. Of course, by quantum mechanics, we cannot speak of the particle taking any well-defined trajectory between two points (x_0, t_0) and (x', t') . Instead, we can only speak of the probability of finding the particle at these locations, which is related to wavefunctions $|\psi(x_0, t_0)\rangle$ and $|\psi(x', t')\rangle$. That is, all that can be determined is the relative probability of the particle taking one path or another.

Feynman’s insight was this - the total transition probability amplitude can be obtained by summing the amplitudes of the particle having taken any individual path. If the quantity $\langle\psi(x', t')|\psi(x_0, t_0)\rangle$ can be calculated in the method suggested by Feynman, the time-evolution of the state can be determined by considering contributions from all possible future states, and the problem is solved. Below, the kets are eigenstates of the position operator, such that integration over all x spans the entire basis.

$$|\psi(x, t')\rangle = \int_{-\infty}^{\infty} \langle\psi(x', t')|\psi(x_0, t_0)\rangle dx' |\psi(x', t')\rangle \quad (2)$$

Known as the *path integral formulation* of quantum mechanics, this method gives the same results as those dictated by the Schrödinger picture, but also illuminates some of the deeper aspects of quantum mechanics. In this paper, we will present the method used by Feynman. Though it is pedagogically backward, we will then demonstrate

the use of the method before showing its equivalence to the Schrödinger picture. We will then investigate the method as applied to the harmonic oscillator. Following this, we will introduce the concept of Euclidean path integrals and discuss further uses of the path integral formulation in the field of statistical mechanics.

2 Path Integral Method

Define the *propagator* of a quantum system between two spacetime points (x', t') and (x_0, t_0) to be the probability transition amplitude between the wavefunction evaluated at those points.

$$U(x', t'; x_0, t_0) = \langle \psi(x', t') | \psi(x_0, t_0) \rangle \quad (3)$$

If the Hamiltonian carries no explicit time-dependence, we can relabel the first time-value $t_0 = 0$ and work only with elapsed time $t = t' - t_0$. We will often write (3) as $U(x', t; x_0)$ to illustrate this. The propagator above, along with an initial state ket, fully describes the evolution of a system over time. It is also customary, as is done in Sakurai [2], to use here the symbol K instead of U and refer to as the “kernel” or “Feynman kernel”. The path integral method, as we are about to see, is an explicit way to construct this propagator.

We consider possible trajectories $x(t)$ of a particle moving through a time-independent potential $V(x)$ with endpoints fixed at (x_0, t_0) and (x', t') .² An infinite continuum of such trajectories are possible, each with classical action $S[x(t)]$. Feynman [4] posits that the contribution to the propagator from a particular trajectory is $\exp[iS[x(t)]/\hbar]$. That is, every possible path contributes with equal amplitude to the propagator, but with a phase related to the classical action. Summing over all possible trajectories, we arrive at the propagator. The normalization constant $A(t)$ is independent of any individual path and therefore depends only on time.

$$U(x', t; x_0) = A(t) \sum_{\text{all trajectories}} \exp \left[\frac{i}{\hbar} S[x(t)] \right] \quad (4)$$

Equation (4) is the heart of the path integral formulation. How this summation (which has yet to be well-defined) is to arrive at the correct propagator is far from

²At this point, $x(t)$ could describe a trajectory through spacetime with any number of dimensions. For our purposes, however, the particle moves along one spatial dimension, though a generalization to more is straightforward.

obvious. We now discuss some salient features of (4) and dive into the technical details of a simple example.

2.1 The Classical Action

How can it be that the infinite sum above does not diverge? The different phases are the key to this. For trajectories between which the action differs by $\Delta S \approx \pi\hbar$, the corresponding contributions will cancel. Contributions to the propagator from possible trajectories through a region far away from the classical path would, in the aggregate, cancel.

Denote the *classical trajectory* $x_{cl}(t)$ as the trajectory with the minimum value of the action $S[x_{cl}]$, which is stationary to first order with regard to deviations. On the macroscopic system, this is the trajectory observed with very little uncertainty. Investigation of Equation (4) gives a reason for this. Trajectories close to the classical one cause no first-order deviation in the action, and contribute with coherent phase to the integral. Trajectories with action $\pi\hbar$ more than the classical action are out of phase, and interfere destructively with each other. Integrating over more and more such trajectories should cause their contribution to average out to zero.

In this way, the classical trajectory is qualitatively important. In general, the region of coherence is related to the “classical” nature of the system. On the (macroscopic) classical scale, $\pi\hbar$ is a frighteningly small amount, making the principal contributing trajectories those in a narrow band around the classical one. On the quantum scale, however, the action is small enough that $\pi\hbar$ is enough to allow significant quantum deviations from the classical trajectory. Intuitively, this corresponds to the fundamental uncertainty in the particle’s position at any given time. Shankar [3] briefly gives a more quantitative argument of the differences in the two cases.

2.2 Free Particle

For concreteness, we use the method above to determine the propagator for the simplest of systems - a particle moving in free space along one dimension. In this case, we will actually evaluate the integral given above “over all possible paths”, although, as MacKenzie [5] notes after a similar derivation, often much of the study of the path integral formulation is concerned with how to avoid just this.

Let $x(t)$ describe a potential trajectory from (x_a, t_a) to (x_b, t_b) . We discretize the trajectory by dividing it into chunks of time $\Delta t = \frac{(t_b - t_a)}{N}$, such that the intermediate

points are $(x_1, t_1), \dots, (x_{N-1}, t_{N-1})$. We do this with the hope that in the limit as $N \rightarrow \infty$, this models a continuous path.³ As $V(x) = 0$ for a free particle, the action depends only on the velocity, which between any t_i and $t_{i+1} = t_i + \Delta t$ is a constant. We denote the action between t_i and t_{i+1} by

$$S_i = \int_{t_i}^{t_{i+1}} \frac{m}{2} \dot{x}(t)^2 dt = \frac{m}{2} \left(\frac{x_{i+1} - x_i}{t_{i+1} - t_i} \right)^2 (t_{i+1} - t_i) = \frac{m}{2\Delta t} (x_{i+1} - x_i)^2 \quad (5)$$

To describe every path from (x_0, t_0) to (x_N, t_N) , we simply vary each intermediate point x_i at each t_i over the entire domain. As the $\{x_i\}$ each take on a continuum of values from $-\infty$ to ∞ , the sum of the contributions from every path is

$$\langle \psi(x_N, t_N) | \psi(x_0, t_0) \rangle = A(t) \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp \left[\frac{i}{\hbar} \frac{m}{2\Delta t} \sum_{i=1}^{i=N} (x_i^2 - x_{i-1}^2) \right] dx_1 \cdots dx_{N-1} \quad (6)$$

Here $A(t)$ is the normalization constant that depends only on the elapsed time $t_N - t_0$. We can evaluate (6) by integrating over one variable at a time. For convenience, let $k = \frac{im}{2\hbar\Delta t}$. Integration over the first variable yields

$$\int_{-\infty}^{\infty} \exp [k(x_2^2 - x_1^2) + k(x_1^2 - x_0^2)] dx_1 \quad (7)$$

$$= \int_{-\infty}^{\infty} \exp [2kx_1^2 + kx_1(-2x_2 - 2x_0) + k(x_2^2 + x_0^2)] dx_1 \quad (8)$$

$$= \frac{\sqrt{\pi}}{\sqrt{2\sqrt{k}}} \exp \left[\frac{k}{2} (x_2 - x_0)^2 \right] \quad (9)$$

We ignore the constant term, since it is absorbed into the normalization constant A . After a few more integrations, a pattern emerges which Feynman and Hibbs [1] illustrate more explicitly: integrating over the first n spacetime points leaves a factor of $\frac{k}{n+1} (x_n - x_0)^2$ in the exponent after evaluation. We evaluate $N-2$ more integrations after the first one, and use the fact that $N\Delta t = (t_N - t_0)$ to rewrite expression (6) concisely as

³Note that the constructed acceleration is a discontinuous impulse train of instantaneous jumps in the velocity. Since the Lagrangian does not vary explicitly with $\ddot{x}$, and that in the limit this value is continuous anyway, we ignore this.

$$U(x_N, t_N; x_0, t_0) = A(t_N - t_0) \exp \left[\frac{k}{N} (x_N - x_0)^2 \right] \quad (10)$$

$$U(x, t; x_0) = A(t) \exp \left[\frac{im}{2t\hbar} (x - x_0)^2 \right] \quad (11)$$

The value for A is obtained by normalizing (11) over all x while holding t constant. The final result is

$$U(x, t; x_0) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp \left[\frac{im}{2t\hbar} (x - x_0)^2 \right], \quad (12)$$

which is in fact the propagator for a free particle. A fascinating feature of this result is that U is composed of the contribution from the classical path alone. This is not always the case, and we will discuss this phenomenon in Section 3.

2.3 Equivalence to Schrödinger Picture

But is this new formulation really an equivalent picture of non-relativistic quantum mechanics? Schrödinger's equation in differential form defines the time-derivative of a given initial state $|\psi(x_0, t_0)\rangle$.

$$i\hbar \frac{d}{dt} |\psi(x_0, t_0)\rangle = \hat{H} |\psi(x_0, t_0)\rangle = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x_0) \right) |\psi(x_0, t_0)\rangle \quad (13)$$

We attempt to recreate this differential equation using the path integral formulation. Consider an initial state $|\psi(x_0, t_0)\rangle$. Some infinitesimal time α later⁴, and at some infinitesimal position γ away, the state can be described as follows.

$$|\psi(x, t_0 + \alpha)\rangle = \int_{-\infty}^{\infty} d\gamma |\psi(x_0 + \gamma, t_0 + \alpha)\rangle U(x_0 + \gamma, \alpha; x_0) \quad (14)$$

To calculate the propagator $U = \langle \psi(x_0 + \gamma, t_0 + \alpha) | \psi(x_0, t_0) \rangle$, we need to determine the action. For a given position coordinate $x_0 + \gamma$ at time α , the particle's velocity and position can be approximated as $\frac{1}{\alpha}(\gamma)$ and $x + \frac{\gamma}{2}$, respectively. The propagator is

⁴Our eventual intention is to allow $\alpha \rightarrow 0$ to recreate the instantaneous derivative. Thus, we feel no qualm making any justifying assumptions that are exact in the limit.

$$U(x_0 + \gamma, \alpha; x_0) = A(\alpha) \exp \left[\frac{i}{\hbar} \int_0^\alpha dt \left(\frac{m}{2} \dot{x}(t)^2 - V(x(t)) \right) \right] \quad (15)$$

$$\approx A(\alpha) \exp \left[\frac{i}{\hbar} \left(\frac{m}{2\alpha} \gamma^2 - V \left(x_0 + \frac{\gamma}{2} \right) \alpha \right) \right] \quad (16)$$

In the limit as α (and therefore γ) become zero, the approximation above becomes exact. Therefore, we expand several of the quantities in (16) in powers of α and γ . The exponential of the potential energy, and the potential energy itself are

$$\frac{i\alpha}{\hbar} \exp \left[-V \left(x_0 + \frac{\gamma}{2} \right) \right] = 1 - \frac{i\alpha}{\hbar} V \left(x_0 + \frac{\gamma}{2} \right) + \dots \quad (17)$$

$$V \left(x_0 + \frac{\gamma}{2} \right) = V(x_0) + \gamma \frac{d}{d\gamma} V(x_0) + \dots \quad (18)$$

We keep the first two terms of (17) and only the first term of (18), which has the effect of discarding all terms second order in (α, γ) and higher. Additionally, we can expand the ket in the integrand $|\psi(x_0 + \gamma, t)\rangle$ around x_0 . The first and third terms are significant, but the second term results in an odd function within the (symmetric) integrand, so we discard it as in [1].

$$|\psi(x_0 + \gamma, t_0)\rangle = |\psi(x_0, t_0)\rangle + \gamma \frac{d|\psi(x_0, t_0)\rangle}{dx} + \frac{1}{2} \gamma^2 \frac{d^2|\psi(x_0, t_0)\rangle}{dx^2} + \dots \quad (19)$$

The approximate expression for (14) becomes

$$|\psi(x, t_0 + \alpha)\rangle = A(\alpha) \left[1 - \frac{i\alpha}{\hbar} V(x_0) \right] \int_{-\infty}^{\infty} d\gamma \left[|\psi\rangle + \frac{1}{2} \gamma^2 \frac{d^2|\psi\rangle}{dx^2} \right] \exp \left[\frac{i}{\hbar} \frac{m}{2\alpha} \gamma^2 \right] \quad (20)$$

It is straightforward to evaluate this Gaussian. Integrating, and keeping the first order terms in the infinitesimals gives

$$|\psi(x_0, t_0 + \alpha)\rangle = A(\alpha) \sqrt{\frac{2\hbar\pi\alpha}{im}} \left[1 - \frac{i\alpha}{\hbar} V(x_0) + \frac{\hbar\alpha}{2mi} \frac{d^2}{dx^2} \right] |\psi(x_0, t_0)\rangle \quad (21)$$

For small α , we see that the first term on the right must equal the expression on the left, and that the normalization constant is necessarily $A(\alpha) = \sqrt{\frac{m}{2\pi\hbar i\alpha}}$. To recover the time derivative, we can rearrange (21) and take the limit as $\alpha \rightarrow 0$ of $i[|\psi(x, t_0 + \alpha)\rangle - |\psi(x, t_0)\rangle] / (\hbar\alpha)$.

$$i\hbar \frac{d}{dt} |\psi(x, t_0)\rangle = \left(V(x_0) - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) |\psi(x_0, t_0)\rangle \quad (22)$$

This is just (13), the time-dependent Schrödinger Equation, derived from a path integral formulation of quantum mechanics. There are other ways to show this equivalence. For example, MacKenzie [5] begins with the Schrödinger picture and shows that it can be massaged into the Feynman formulation. Our direction, which is the same as that of Feynman and Hibbs [1], is to show that the standard quantum theory can be reconstructed from the “first principles” of the path integral method.

3 Harmonic Oscillator

Now let the particle be in a potential given by $V(x) = \frac{1}{2}m\omega^2 x^2$. In principle, we could explicitly compute the propagator by considering a generic initial state and applying time-evolution to each of the eigenstates. This way is algebraically brutal, requiring the summation of an infinite series of expressions involving Hermite polynomials.

Using the tools we have developed above, we will derive the propagator for the one-dimensional harmonic oscillator with a surprising lack of intense computation, relying instead on the theoretical basis of the path integral formulation.

3.1 Derivation of the Propagator

We approach the problem in a slightly different manner. Let $x_{cl}(t)$ and $\dot{x}_{cl}(t)$ be the classical path and its velocity, respectively. We can represent any other path as a deviation from this one, $x_{cl}(t) + y(t)$ and $\dot{x}_{cl}(t) + \dot{y}(t)$, with the correct boundary conditions (y and $\dot{y}$ are zero at the endpoints of the path). Let’s rewrite the Lagrangian for a generic path in a way that isolates the classical Lagrangian. We relax the time dependence, since it is implicit.

$$\begin{aligned} L(x_{cl} + y, \dot{x}_{cl} + \dot{y}) &= \frac{1}{2}m(\dot{x}_{cl} + \dot{y})^2 + \frac{1}{2}m\omega^2(x_{cl} + y)^2 \\ &= \left(\frac{1}{2}m\dot{x}_{cl}^2 + \frac{1}{2}m\omega^2 x_{cl}^2 \right) + (m\dot{x}_{cl}\dot{y} + m\omega x_{cl}y) + \left(\frac{1}{2}m\dot{y}^2 + \frac{1}{2}m\omega^2 y^2 \right) \end{aligned} \quad (23)$$

The first term in (23) is just the Lagrangian for the classical trajectory. The second term is zero by the Euler-Lagrange equations (since on a stationary path x_{cl} , this

term must be zero for any well-behaved deviation y). We will return to this later. The third term is the Lagrangian for the deviation. The action is separable in the sense that the propagator has the following form:

$$U = A(t) \exp \left[\frac{i}{\hbar} S[x_{cl}] \right] \int_{\text{all paths}} \exp \left[\frac{i}{\hbar} \int_{t=t_0}^{t=t_N} \left(\frac{1}{2} m \dot{y}^2 + \frac{1}{2} m \omega^2 y^2 \right) \right] \quad (24)$$

It can be shown that the integral over all paths depends only on elapsed time t and not on $x(t_0)$ or $x(t_N)$. Shankar [3] argues that this must be true since every deviation has no knowledge of the endpoints of the trajectory (since y and $\dot{y}$ are zero there). We therefore absorb this time-dependent function into the normalization factor, and are left with just the classical action.⁵ Normalizing this expression is not trivial. Feynman and Hibbs [1] consider the decomposition of a deviation $y(t)$ into its Fourier series with period $t_N - t_0$, and then integrate over the components. We use their result, though there are other methods.

$$U = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega t}} \exp \left[\frac{im\omega}{2\hbar \sin \omega t} [(x^2 + x_0^2) \cos \omega t - 2xx_0] \right] \quad (25)$$

This is the correct answer. Later, when we investigate the connection between the path integral formulation and statistical mechanics, we will use this result to recover the energy eigenvalues.

3.2 Separable Lagrangians

We have discovered that in some cases, only the classical trajectory contributes to the summation in (4). There is a straightforward reason for this. The Lagrangian for any generic path can be expressed as a two-dimensional Taylor expansion about the Lagrangian of the classical action.

$$\begin{aligned} L(x_{cl} + y, \dot{x}_{cl} + \dot{y}) &= L_{cl} + \sum_{n=1}^{\infty} \frac{1}{n!} \left[y \frac{d}{dx} + \dot{y} \frac{d}{d\dot{x}} \right]^n L_{cl} \\ &= L_{cl} + \left(y \frac{dL_{cl}}{dx} + \dot{y} \frac{dL_{cl}}{d\dot{x}} \right) + \left(y^2 \frac{d^2 L_{cl}}{dx^2} + 2y\dot{y} \frac{d}{dx} \frac{dL_{cl}}{d\dot{x}} + \dot{y}^2 \frac{d^2 L_{cl}}{d\dot{x}^2} \right) + \dots \end{aligned} \quad (26)$$

⁵This is a known result, so we do not derive it here.

The Euler-Lagrange equations on the classical (stationary) trajectory dictate that the $n = 1$ term is zero. In a non-relativistic framework, the kinetic energy term in the Lagrangian contributes a $\frac{m}{2}\dot{y}^2$ term. Additionally, in a potential is quadratic in x and $\dot{x}$ (as in the case of the harmonic oscillator and many other elementary potentials), the Lagrangian separates exactly. Relation (26) shows that in these cases, the propagator is simply related to the imaginary exponent of the classical action divided by the quantum of action.

$$U \approx A(t) \exp \left[\frac{i}{\hbar} S[x_{cl}] \right] \quad (27)$$

Thus, there are many problems which can be reduced to determining the classical action, once the relation above is shown to be true for the system. After this, the normalization of the propagator becomes the only challenging task.

Although (27) is often a good approximation (and is even exact in some important systems), we must be aware of its limitations and uses. Third or higher powers of x or $\dot{x}$ in the Lagrangian will annul it. However, it works readily if the Lagrangian depends on more than one trajectory, and can even be solved in the case of a time-dependent input into the system $f(t)$. Feynman and Hibbs [1] provide a more in depth discussion of this solution method and where it is applicable.

4 Euclidean Path Integrals

Our approach in the following section is pragmatic, focusing more on the functionality of a method than on a rigorous justification. In previous sections, we have related the transition probability amplitude of the wavefunction between two points in spacetime. This next section concerns revising not the method but the sense of *spacetime*.

Far from the classical trajectory, the rapidly oscillating terms in (2) can cause convergence issues and are generally unpleasant to deal with. Observe that in Minkowski spacetime with one physical coordinate, the proper distance σ^2 goes as the negative square of the time $-t^2$. However, in Euclidean spacetime, the sign of the t^2 term is positive; they differ by a phase factor i . Consider what would happen if we introduced a factor of i into the exponentials - the oscillating terms would turn into decaying exponentials, which have an entirely different physical meaning.

With this as our motivation, let us analytically extend the time parameter into the complex numbers $\mathbb{C}$. In particular, let time have no real component, and identify

$t = -i\tau$ with a real parameter τ called *imaginary time*. This is formally known as a *Wick rotation*, and rigorous justification of this step is not trivial. The fruit of such a gambit will hopefully soon be made clear. Nevertheless, let us examine the form propagator over a small time interval $-i\tau$.

$$U(x', -i\tau; x) \approx \sum_{\text{all paths}} \exp \frac{i}{\hbar} \left[\frac{m}{2} \frac{(x' - x)^2}{-i\tau} - i\tau V \left(\frac{x + x'}{2} \right) \right] \quad (28)$$

We see that the potential energy has flipped sign relative to the kinetic energy term! We redefine the *Euclidean action* $S_E[x(\tau)]$ of a trajectory in imaginary time $x(\tau)$ below.

$$S_E[x(\tau)] = \int_{\tau_1}^{\tau_2} \left(\frac{m}{2} \dot{x}^2(\tau) + V(x(\tau)) \right) \quad (29)$$

The Euclidean action is a value related to the quantum tunneling process. We will not enter into more detail on this; both Grosche [6] and MacKenzie [5] give a more in-depth treatment. With this, we can define the *imaginary time propagator* $U(x', \tau; x)$ as well.

$$U(x', \tau; x) = A(\tau) \int_{\text{all paths}} \exp \left[-\frac{1}{\hbar} S_E[x(\tau)] \right] \quad (30)$$

Though the physical meaning behind this new propagator is still not obvious, we can gain some sense of its interesting properties. What sort of value can the sum over all paths in (30) have? No longer does the classical action cause the contribution to the summation to oscillate; each path is now given a negative exponential weight based on its Euclidean action. The classical path has the largest contribution, since the action is a minimum there. Trajectories far away from the classical one see an exponentially decreased contribution as S_E grows. A particle obeying the Euclidean equations of motion experiences the potential in the other direction, which is intuitively correct - a path through a region of high potential dampens the contribution of that path through the negative exponential dependence of the action.

4.1 Statistical Mechanics

We briefly explore the connection between the Euclidean path integral and statistical mechanics. Consider an ensemble system at thermodynamic equilibrium with ordered

energy microstates $\{E_n\}$ for $n = 1, 2, \dots$. The *partition function* Z of statistical mechanics encodes probabilistic information about the system.

$$Z = \sum_{n=1}^{\infty} e^{-\beta E_n} \quad (31)$$

Above, $\beta = 1/k_b T$ be the *inverse temperature* of the system at a given temperature T with Boltzmann's constant k_b . The form of (31) is reminiscent of the time-evolution constructed from energy eigenstates back in (1), which we have shown has an equivalent expression as the integral over propagators to all possible points in (2). The natural question is whether we can derive the partition function from a path integral standpoint. It would seem that replacing the time variable t with the quantity $-i\beta$ would be a good first step. As we have seen above, this moves us into the realm of Euclidean path integrals.

The analysis below is based on that of Grosche [6] and Feynman and Hibbs [1]. Consider a quantum system with the discrete energy spectrum given above. We rewrite the imaginary time propagator between x' and x by decomposing the bra and ket into a basis of eigenstates and applying time-evolution to each one.

$$U(x', \tau; x) = \sum_n \langle x' | n \rangle e^{-iE_n(-i\tau)/\hbar} \langle n | x \rangle = \sum_n \langle n | x \rangle e^{-iE_n(-i\tau)/\hbar} \langle x' | n \rangle \quad (32)$$

Now, setting $x' = x$ and $\tau = \beta\hbar$ and integrating over all x yields

$$\int dx U(x, \beta\hbar; x) = \sum_n \langle n | \int dx e^{-\beta E_n} | x \rangle \langle x | n \rangle = \sum_n e^{-\beta E_n} = Z \quad (33)$$

This is the relation between the imaginary time propagator and the partition function that we are looking for. As a vivid illustration of this equality, we return to the case of the harmonic oscillator, whose propagator we derived in Section 3.1.

$$U(x, \beta\hbar; x) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh \beta\hbar\omega}} \exp \left[-\frac{m\omega x^2}{\hbar \sinh \beta\hbar\omega} (\cosh \beta\hbar\omega - 1) \right] \quad (34)$$

The partition function for the harmonic oscillator Z is the integral of (34) over all x , which is easy to evaluate since the function is a Gaussian.

$$Z = \int dx U(x, -i\beta; x) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh \beta\hbar\omega}} \int dx \exp \left[-\frac{x^2}{\left(\frac{\hbar \sinh \beta\hbar\omega}{m\omega(\cosh \beta\hbar\omega - 1)} \right)} \right] \quad (35)$$

$$= \sqrt{\frac{m\omega}{2\pi\hbar \sinh \beta\hbar\omega}} \sqrt{\pi} \sqrt{\frac{\hbar \sinh \beta\hbar\omega}{m\omega(\cosh \beta\hbar\omega - 1)}} = \frac{1}{\sqrt{2(\cosh \beta\hbar\omega - 1)}} \quad (36)$$

Expanding this hyperbolic function gives the desired result.

$$(\sqrt{2(\cosh \beta\hbar\omega - 1)})^{-1} = (\sqrt{e^{\beta\hbar\omega} - 2 + e^{-\beta\hbar\omega}})^{-1} = (e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2})^{-1} \quad (37)$$

$$= e^{-\beta\hbar\omega/2} \frac{1}{1 - e^{-\beta\hbar\omega}} = \sum_{n=0} \exp \left[-\beta \left(n + \frac{1}{2} \right) \hbar\omega \right] \quad (38)$$

This is the expected partition function, complete with the energy eigenvalues of the harmonic oscillator!

5 Discussion

This manuscript has been intended as a brief introduction; the literature is richer in application, scope and rigor. Feynman and Hibbs' [1] textbook classic introduces all of quantum theory from this perspective. MacKenzie [5] notes that a path integral formulation naturally leads to an investigation of the Aharonov-Bohm effect using these methods, and goes on to present stationary perturbation theory using Feynman kernels. Shankar [3] delves into path integrals through phase space and coherent state space, and applies them to a number of sophisticated topics such as the Berry phase. Sakurai [2] writes more generally about Green's functions. Grosche [6] presents a paper startling in its rigor and thoroughness on the topic. Other sources even demonstrate the use of path integrals in quantum field theory.

Still, we have managed to cover quite a bit of ground on the topic of path integrals in quantum mechanics. Our formulation of quantum mechanics has been driven by two key principles. Starting from the principle that a particle takes no well-defined trajectory between two points at which it is observed, we define the transition probability amplitude between two points as a summation over all paths. This was Feynman's insight. Then, we connect the contribution to the amplitude from any given path with the corresponding classical action along the path in the manner suggested by Dirac.

We have derived the free particle propagator in a manner that fully demonstrating the “integrate over all possible paths” principle. We have shown equivalence to the standard Schrödinger formulation of quantum mechanics. Then, taking advantage of the restrictions that the classically observed Lagrangian action provides, we have derived the harmonic oscillator propagator, and discussed potentials for which the propagator is easily solvable. After this, we have defined the path integral in Euclidean spacetime, and showed how it is related to the partition function in statistical mechanics. From this, we have recovered the energy eigenvalues of the harmonic oscillator.

It is said that Richard Feynman could not allow believe any physics he had not rederived for himself. Though our analysis has been brief, and with less emphasis on straightforward rigor than on pragmatism, it is clear that the scope and success of Feynman’s method is truly remarkable.

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