The Quantum Path Integral and its Applications to Statistical Mechanics

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The quantum path integral is a powerful formulation of quantum mechanics identical to the Schrödinger equation. It is especially useful in fields like quantum field theory, quantum statistical mechanics, and the study of systems with many degrees of freedom.

This paper provides a derivation of the path integral and the related Feynman-Kac formula, giving analogies to simpler stochastic processes like Brownian motion. We will then explore some applications to quantum statistical mechanics, such as analytically computing ensemble averages or simulating equilibrium thermodynamics.

I. INTRODUCTION AND BACKGROUND

I.1. Stochastic processes

A continuous time stochastic process $(X)_{t\geq 0}$ is a collection of random variables indexed by non-negative times t. A trajectory of the process is one possible outcome of evaluating the process at each time (see Fig. 1 for an example).

I.2. Brownian motion definition

The most commonly studied continuous-time stochastic process is the Wiener process (also known as Brownian motion) A continuous-time stochastic process $(B)_{t\geq 0}$ is a Brownian motion if it has the following properties [1]:

1. **Started from zero:** $B_0 = 0$
2. **Continuous sample paths:** realizations of the process are continuous functions
3. **Independent increments:** for any sequence of increasing times $t_{n\in\mathbb{N}}$, the set of random variables $\{B_{t_{i+1}} - B_{t_i} | i \in \mathbb{N}\}$ is independent
4. **Gaussian increments:** $B_t - B_s \sim \mathcal{N}(0, t-s)$ for any $t \geq s \geq 0$.

Shown in Figure 1 are several simulated trajectories of Brownian motion.

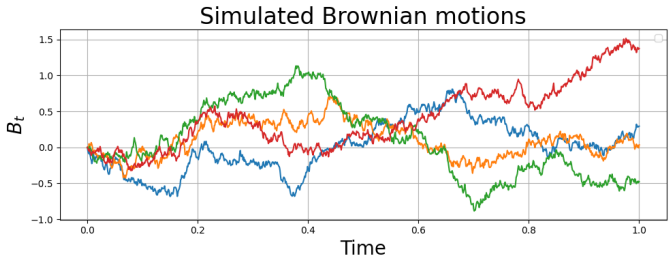

FIG. 1. Four simulated trajectories of Brownian motion.

Brownian motion has many special properties that make it very useful for studying stochastic calculus.

It is also extremely important in physics: examples of physical Brownian motion include pollen in water (where it was originally observed), dust in air, or electrons in a conductor. We will now examine another special physical property of Brownian motion.

I.3. Brownian motion satisfies the diffusion equation

By properties (1) and (4), we see that

$$B_t - B_0 = B_t \sim \mathcal{N}(0, t)$$

$$B_t \sim \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}} =: P(x,t) \tag{1}$$

This is the probability distribution of a Brownian motion at time t. Now we can compute

$$\partial_x^2 P(x,t) = \frac{x^2 - t}{t} P(x,t)$$

$$\partial_t P(x,t) = \frac{x^2 - t}{2t} P(x,t) = \frac{1}{2}\partial_x^2 P(x,t)$$

This satisfies the diffusion equation

$$\partial_t P(x,t) = D\partial_x^2 P(x,t) \tag{2}$$

with diffusion constant $D = 1/2$. Thus, Brownian motion solves the diffusion equation with initial condition $P(x,0) = \delta(x)$.

Using stochastic processes to solve partial differential equations (PDEs) is a very powerful technique, and we will explore using this idea to solve the Schrödinger equation.

I.4. Path integral background

The path integral for quantum mechanics was developed by Richard Feynman in 1948, but in general path

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integrals can be used to solve a much wider variety of PDEs. In fact, the method we used in I.3 was a basic path integral, although much of the complexity was hidden since Brownian motion is such a simple process.

Qualitatively, given an initial condition and a PDE describing the evolution of a system, a path integral computes a future state as a weighted sum of all possible paths from the initial state. The weights are computed using a functional, which in our case will be the classical action of the system.

Path integrals are a natural way of representing quantum mechanics since they can easily encode concepts like superposition and time evolution.

II. DERIVATION OF THE PATH INTEGRAL

In order to derive the form of the path integral that is most commonly used in physics, we will start by deriving a more general version known as the Feynman-Kac formula. Feynman developed this formula along with a mathematician named Mark Kac, who mainly studied probability theory, in an attempt to formalize his quantum path integral.

II.1. Feynman-Kac formula

The Feynman-Kac formula is a way of writing solutions to certain PDEs in terms of expected values of stochastic processes. It can solve PDEs of the form [2]

$$\frac{\partial u}{\partial t} + \mu(x,t)\frac{\partial u}{\partial x} + \frac{1}{2}\sigma^2(x,t)\frac{\partial^2 u}{\partial x^2} = V(x,t)u \tag{3}$$

with the terminal condition $u(x,T) = f(x)$.

In order to solve this, we will introduce two stochastic processes:

$$(X)_{\mathbb{R}^+}: \quad dX_t = \mu(X_t,t)dt + \sigma(X_t,t)dB_t \tag{4}$$

$$(Y)_{\mathbb{R}^+}: \quad Y_s = u(X_s,s)\exp\left(-\int_t^s V(X_r)dr\right) \tag{5}$$

Using results from stochastic calculus known as Itô product rule and Itô's lemma on Y [1], we get

$$dY_s = e^{-\int_t^s V(X_r)dr}\cdot du + u\cdot d\left(e^{-\int_t^s V(X_r)dr}\right)$$

$$d\left(e^{-\int_t^s V(X_r)dr}\right) = -V(X_s)\left(e^{-\int_t^s V(X_r)dr}\right)ds$$

$$du = \left(\frac{\partial u}{\partial s} + \mu\frac{\partial u}{\partial x} + \frac{1}{2}\sigma^2\frac{\partial^2 u}{\partial x^2}\right)ds$$

Combining these, we see that

$$dY_s = e^{-\int_t^s V(X_r)dr}\cdot\left(F(x,t)\cdot ds + \sigma\frac{\partial u}{\partial x}dB_s\right) \tag{6}$$

where

$$F(x,t) = \frac{\partial u}{\partial s} + \mu\frac{\partial u}{\partial x} + \frac{1}{2}\sigma^2\frac{\partial^2 u}{\partial x^2} - Vu \tag{7}$$

Since we assumed that u evolves according to (3), we have $F(x,t) = 0$. Therefore,

$$\mathbb{E}Y_t = \mathbb{E}Y_T$$

Noticing that $u(x,t) = \mathbb{E}[u(X_t,t)|X_t = x]$ and $Y_t = u(X_t,t)$, we see that $u(x,t) = \mathbb{E}Y_T$. With our terminal condition on u, we finally obtain the Feynman-Kac formula:

$$u(x,t) = \mathbb{E}[f(X_T)e^{-\int_t^T V(X_r)dr}|X_t = x] \tag{8}$$

This equation solves for all past u (at times earlier than T). However, in most problems we would like to solve for future u. However, simply changing variables to reverse time does not work here because it requires Y to be a time-homogeneous Markov process [1]. This is not satisfied since so far, we have treated μ and σ as functions of x and t. However, if we restrict them to be only functions of x, a symmetry argument shows that

$$v(x,t) = \mathbb{E}[\psi(X_t)e^{-\int_0^t V(X_r)dr}|X_0 = x] \tag{9}$$

where $v(x,t)$ satisfies the transformed PDE

$$-\frac{\partial v}{\partial t} + \mu(x)\frac{\partial v}{\partial x} + \frac{1}{2}\sigma^2(x)\frac{\partial^2 v}{\partial x^2} = V(x,t)v \tag{10}$$

with the initial condition $v(x,0) = \psi(x)$. Notice that (10) is very similar to the Schrödinger equation. With some slight modifications, we will be able to solve the Schrödinger equation with Feynman-Kac to obtain the quantum mechanical path integral.

II.2. Quick simulations with Feynman-Kac

By generating Brownian motion trajectories at each x and weighting them according to (9), we can simulate wavefunctions of any potential. Since the imaginary time evolution operator $e^{-t\hat{H}}$ decreases the amplitude of higher energy states more quickly, we have $\lim_{t\to\infty} v(x,t) = \psi_0(x)$, the ground state solution of the system.

As a validation for our formula, Figure 2 shows excellent agreement between the simulated and analytic ground state solution of a harmonic oscillator.

It is also possible to simulate an excited state using symmetries of the system. For example, if we let the initial wavefunction be $\Psi(x,0) = x$, which has a single node at $x = 0$, we obtain the first excited state instead (shown in Figure 3). This is because we begin with an odd wavefunction with a node at the same place as the first excited QHO state.

Finally, we can apply this technique to a more complicated potential that we do not know how to solve. For

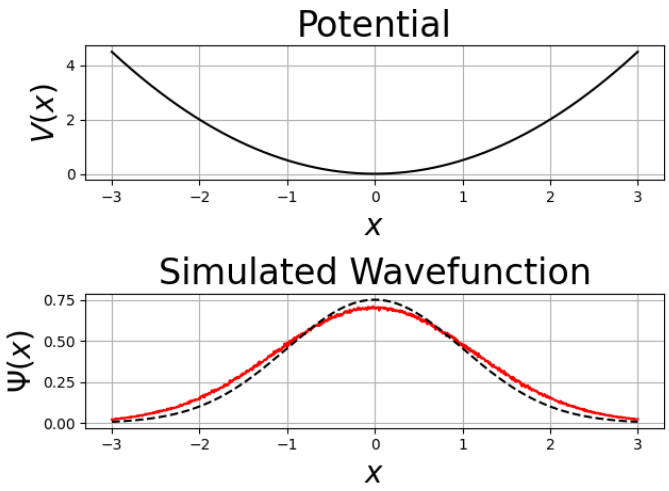

FIG. 2. Simulated and analytic ground state solution of QHO

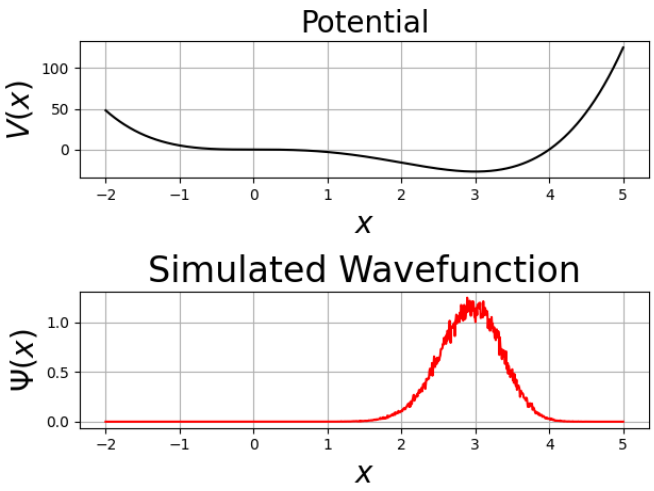

FIG. 4. Simulated ground state solution of $x^4 - 4x^3$ potential

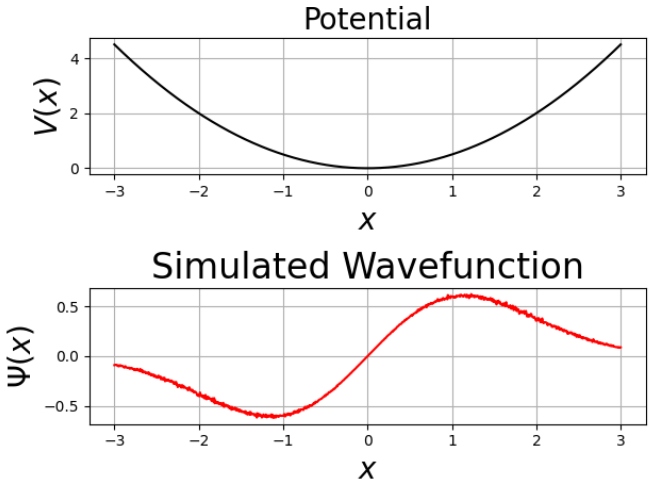

FIG. 3. Simulated first excited state solution of QHO

example, we could solve for $V(x) = x^4 - x^3$, as shown in Figure 4.

As expected for this complicated potential, the wavefunction peaks at the minimum of the potential and appears roughly Gaussian since the local minimum of the potential can be approximated by a harmonic oscillator. The left tail is also slightly larger due to the shallower potential on the left side.

II.3. Derivation of the path integral

We begin by transforming the Schrödinger equation (in units where $\hbar = m = 1$):

$$i\frac{\partial \Psi}{\partial t} + \frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2} - V(x)\Psi = 0 \tag{11}$$

into a form that more closely resembles (10). Performing a Wick rotation (mapping $it \to t$) gives us

$$-\frac{\partial \Psi}{\partial t} + \frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2} - V(x)\Psi = 0 \tag{12}$$

This matches (10) with $\mu = 0$, $\sigma = 1$, so by Feynman-Kac we have

$$\Psi(x,t) = \mathbb{E}[\Psi(X_t, 0)e^{-\int_0^t V(X_r)dr}] \tag{13}$$

$$X_t = x + \int_0^t dB_s = x + B_t \tag{14}$$

For intuition, since Brownian motion trajectories are continuous real functions, the trajectories of X_t are continuous functions with $f(0) = x$. Also, note that (13) is already a path integral since the expected value is an integral over trajectories of X_t. However, in its current form it is difficult to work with for physical applications. We will work on converting this to a form that makes the physics more apparent.

Since we are working with physical wavefunctions, we can assume Ψ and V are continuous almost everywhere. Therefore we can use a Riemann integral along with the properties of Brownian motion to compute the expected value over the trajectories.

For each $n \in \mathbb{N}$, partition $[0, t]$ into a sequence of times $\{t_i = \frac{i}{n}t | 0 \le i \le n\}$, and define $\epsilon = \frac{t}{n}$. Then by (14) the corresponding values of X_t are $\{x_n = x + B_{t_i} | 0 \le i \le n\}$ (given a particular realization of the Brownian motion term B_t, we can compute the position x_i of the path at each t_i). Notice that

$$\exp\left[-\sum_{i=0}^{n-1}\int_{t_i}^{t_{i+1}} V(X_r)dr\right] \sim \prod_{i=0}^{n-1}\exp\left[-\epsilon V(x_i)\right]$$

for small ϵ. Additionally, the independent Gaussian increments of Brownian motion give us

$$\mathbb{P}[x_{i+1}|x_i] = \frac{1}{\sqrt{2\pi\epsilon}} \exp\left[\frac{-(x_{i+1}-x_i)^2}{2\epsilon}\right]$$

Combining these results, we can write the joint density of the path integral as

$$\Psi(x_i, 0) \prod_{i=0}^{n-1} \exp\left[-\epsilon V(x_i)\right] \mathbb{P}[x_{i+1}|x_i] \tag{15}$$

Now we can approximate (13) with an n-dimensional Euclidean integral:

$$\int \Psi(x_i, 0) \prod_{i=0}^{n-1} \exp\left[-\left(\frac{(x_{i+1}-x_i)^2}{2\epsilon^2}\epsilon + V(x_i)\epsilon\right)\right] dx_i \tag{16}$$

which converges to $\Psi(x,t)$ in the limit where $n \to \infty$. Note that the factor $(\frac{1}{2\pi\epsilon})^{n/2}$ has been dropped since we will need to normalize again later anyway.

In the limit where $n \to \infty$ we can also approximate the quadratic term in x. Taking $dt = \epsilon$, we get

$$\lim_{\epsilon \to 0} \left(\frac{(x_{i+1}-x_i)^2}{2\epsilon^2}\right) = \frac{1}{2}\dot{x}^2(t_i) \tag{17}$$

We should note that this step was not completely justified, since Brownian motion trajectories are almost surely not differentiable (the probability that a trajectory is differentiable is 0), meaning that $\dot{x}(t)$ does not exist. However, this problem is resolved when computing the integral by using small finite time intervals, on which the discrete time approximation to $\dot{x}^2$ is used. With this notation, (16) becomes

$$\lim_{n\to\infty} \int \Psi(x_i, 0) \prod_{i=0}^{n-1} \exp\left[-\frac{t}{n}\left(\frac{1}{2}\dot{x}^2(t_i) + V(x_i)\right)\right] dx_i$$

$$= \lim_{n\to\infty} \int \Psi(x_i, 0) \exp\left[-\frac{t}{n}\sum_{i=0}^{n-1}\left(\frac{1}{2}\dot{x}^2(t_i) + V(x_i)\right)\right] \prod_{i=0}^{n-1} dx_i$$

$$= \lim_{n\to\infty} \int \Psi(x_i, 0) \exp\left[-\int_0^t \left(\frac{1}{2}\dot{x}^2(s) + V(x(s))\right) ds\right] \prod_{i=0}^{n-1} dx_i$$

Finally, we define the measure $\mathcal{D}[x(t)]$ as follows:

$$\mathcal{D}[x(t)] := \lim_{n\to\infty} \prod_{i=0}^{n-1} dx_i$$

By (14) and $B_0 = 0$ we see that $X_0 = x$. Therefore, since Brownian motion has continuous sample paths, we can interpret $\mathcal{D}[x(t)]$ as a measure over continuous paths $x(s) : [0,t] \to \mathbb{R}$ with $x(0) = x$. Using our new measure to pass back into continuous time, we get

$$\int \Psi(x(t), 0) \exp\left[-\int_0^t \left(\frac{1}{2}\dot{x}^2(t) + V(x(t))\right) dt\right] \mathcal{D}[x(t)] \tag{18}$$

Finally, recall that in (12) we performed a Wick rotation to allow us to use the Feynman-Kac formula. We now undo this by mapping back $t \to it$, which changes the form of the integral in the exponential:

$$-\int_0^t \left(\frac{1}{2}\dot{x}^2(t) + V(x(t))\right) dt \to i\int_0^t \left(\frac{1}{2}\dot{x}^2(t) - V(x(t))\right) dt \tag{19}$$

Notice that the right side of (19) is exactly $i\mathbf{S}(x, \dot{x})$, where

$$\mathbf{S}(x, \dot{x}) = \int_0^t \left(\frac{1}{2}\dot{x}^2(t) - V(x(t))\right) dt \tag{20}$$

is the classical action of our system. Combining all these results, we finally obtain the path integral formulation of quantum mechanics:

$$\Psi(x,t) = \int \Psi(x(t), 0) \exp\left[i\mathbf{S}(x(t), \dot{x}(t)\right] \mathcal{D}[x(t)] \tag{21}$$

III. QUANTUM STATISTICAL MECHANICS

III.1. Introduction

In classical statistical mechanics, many thermodynamic properties of a system at equilibrium can be obtained from its *partition function*. In the canonical ensemble, where a system exchanges energy with a heat bath of constant temperature T, the partition function is

$$Z(\beta) = \sum_n e^{-\beta E_n} \tag{22}$$

Here, n labels indices of the microstates of the system, E_n is the energy of each microstate, and $\beta = \frac{1}{k_B T}$. The probability to find this system in a given microstate is

$$\mathbb{P}(n; \beta) = \frac{1}{Z(\beta)} e^{-\beta E_n} \tag{23}$$

and the expected energy of the system is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z(\beta) \tag{24}$$

In quantum mechanics, the partition function becomes [3]

$$Z(\beta) = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \tag{25}$$

where $\hat{H}$ is the Hamiltonian of the system. Combining this with (23), we get the density matrix of the system:

[3]

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z(\beta)} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}\left(e^{-\beta \hat{H}}\right)} \tag{26}$$

Using the density matrix, we can compute $\rho(x, x; \beta)$, the probability to find the system at position x:

$$\rho(x, x; \beta) = \langle x|\hat{\rho}|x\rangle = \frac{\langle x|e^{-\beta \hat{H}}|x\rangle}{Z(\beta)} \tag{27}$$

Therefore we can compute the position space probability distribution of the system by computing $\langle x|e^{-\beta \hat{H}}|x\rangle$ for each x and normalizing by $Z(\beta)$.

III.2. Density matrices with Feynman-Kac

In our derivation of the path integral, we showed that the Feynman-Kac formula in (13) solves the imagniary time Schrödinger equation $|\Psi, t\rangle = e^{-t\hat{H}}|\Psi, 0\rangle$. If we take $t = \beta$ and $|\Psi, 0\rangle = |\Psi, t\rangle = |x\rangle$, we see that

$$\langle x|e^{-\beta \hat{H}}|x\rangle = \mathbb{E}\left[e^{-\int_0^\beta V(X_r)dr} \middle| X_0 = X_\beta = x\right] \tag{28}$$

$$Z(\beta) = \int \mathbb{E}\left[e^{-\int_0^\beta V(X_r)dr} \middle| X_0 = X_\beta = x\right] dx \tag{29}$$

$$\rho(x, x; \beta) = \frac{\mathbb{E}\left[e^{-\int_0^\beta V(X_r)dr} \middle| X_0 = X_\beta = x\right]}{Z(\beta)} \tag{30}$$

The conditional expectation in (28) imposes the condition that X_t is a Brownian bridge, meaning that it starts and ends at the same value (see Fig. 5). By simulating Brownian bridge trajectories and taking a weighted expectation, we can obtain the position-space probability distribution of the system.

IV. SIMULATION: THERMODYNAMICS OF A QUANTUM HARMONIC OSCILLATOR

As an application of this technique, let us simulate a quantum harmonic oscillator (potential $V(x) = \frac{1}{2}x^2$) at finite temperature. We will first use the path integral derived in II.3 to obtain the analytic solutions to the energy and partition function of the QHO.

We will then use the Feynman-Kac formula to simulate the density matrix of the equilibrium system, from which we obtain information like the position distribution and expected energy.

IV.1. Analytic solution for partition function

Combining (29) with our derivation of the path integral in II.3, we see that

$$Z(\beta) = \int \exp\left[-\frac{1}{2}\int_0^\beta \dot{x}^2(t) + x^2(t)dt\right] \mathcal{D}[x(t)] \tag{31}$$

where we integrate over periodic paths $x(0) = x(\beta)$. Since the paths are periodic, we may write them as a Fourier series:

$$x(t) = \sum_{n=-\infty}^{\infty} c_n e^{i\omega_n t} \tag{32}$$

where $\omega_n = \frac{2\pi n}{\beta}$. Substituting, we obtain

$$Z(\beta) = \int \exp\left[-\frac{1}{2}\int_0^\beta \sum_n (1+\omega_n^2)|c_n|^2 ds\right] \prod_{n=-\infty}^{\infty} dc_n \tag{33}$$

$$= \int \prod_{n=-\infty}^{\infty} \exp\left[-\frac{\beta(1+\omega_n^2)|c_n|^2}{2}\right] dc_n \tag{34}$$

This becomes an infinite product of Gaussian integrals, where the integral of each one is proportional to $\frac{1}{\sqrt{1+\omega_n^2}}$. Therefore in total,

$$Z(\beta) = \prod_{n=-\infty}^{\infty} \left(1+\omega_n^2\right)^{-\frac{1}{2}} \tag{35}$$

We can then use the Weierstrass factorization of $\frac{\sinh x}{x}$ to simplify this:

$$\frac{\sinh x}{x} = \prod_{n=1}^{\infty}\left(1 + \frac{x^2}{\pi^2 n^2}\right) \tag{36}$$

$$\prod_{n=-\infty}^{\infty}\left(1+\omega_n^2\right) = \left(\prod_{n=1}^{\infty}\left(1+\omega_n^2\right)\right)^2 = \left(\frac{\sinh\frac{\beta}{2}}{\frac{1}{2}}\right)^2 \tag{37}$$

$$Z(\beta) = \left(\frac{\sinh\frac{\beta}{2}}{\frac{1}{2}}\right)^{-1} = \frac{1}{2\sinh\frac{\beta}{2}} \tag{38}$$

This is the analytic canonical partition function of the quantum harmonic oscillator. From this, we can use the expected energy relation in (24) to compute:

$$\langle E(\beta)\rangle = -\frac{\partial}{\partial\beta}\log Z(\beta) = \frac{1}{2} + \frac{1}{e^\beta - 1} \tag{39}$$

We have now obtained analytic relations for the expected energy and partition function of the system, which we will use to validate our simulation method. In general, it is not possible to compute these analytically for more complicated potentials, which makes simulations essential for studying more complex systems.

IV.2. Feynman-Kac simulation strategy

We simulate many Brownian bridge trajectories starting at each value of x. We then take the weighted expected value of these trajectories (according to (28)) to obtain $Z(\beta)$ and $\rho(x, x; \beta)$. Repeating this procedure for many values of β, we will see the dependence of the expected energy $\langle E(\beta)\rangle$ on β.

IV.2.1. Generating Brownian bridges

From the definition of Brownian motion, it is straightforward to verify that given a Brownian motion B_t, the process $X_t = x + B_t - \frac{t}{T}B_T$ is also a Brownian motion (shifted by x). Furthermore, X_t is a Brownian bridge on $[0, T]$ because $X_0 = X_T = x$. We use this procedure to generate many Brownian bridges at each x. Several simulated trajectories for $x = 0$ are shown in Figure 5.

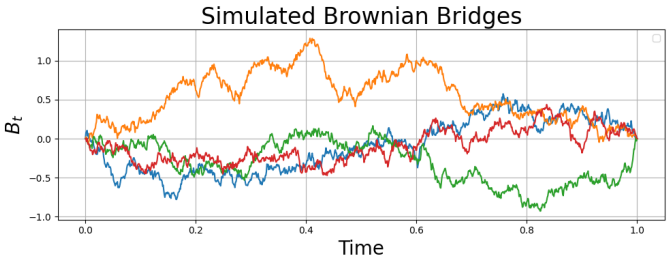

FIG. 5. Four Brownian bridge trajectories on [0, 1].

IV.2.2. Taking the conditional expectation

We use our simulated trajectories along with (28) to approximate the values of $\langle x|e^{-\beta\hat{H}}|x\rangle$ for each x.

However, we must be careful to remember that the expectation is over all Brownian motion trajectories, conditioning on Brownian bridge paths. Since we directly generated only Brownian bridges, we must account for the nonzero probability that a Brownian motion is not a Brownian bridge.

To correct for this we consider the simplest case of a free particle, which has $\rho_{free}(x, x; \beta) = \mathbb{E}[1|X_0 = X_\beta = x]$. This is just the probability that a Brownian motion satisfies $B_0 = B_\beta = 0$. From the gaussian increments of Brownian motion we see that $\rho_{free}(x, x; \beta) = \frac{1}{\sqrt{2\pi\beta}} \exp\left(\frac{(x-x)^2}{2\beta}\right) = \frac{1}{\sqrt{2\pi\beta}}$, which is what we should get from our simulation. However, since we only generated Brownian bridges, the simulated value would be 1. Therefore we are missing a factor $\frac{1}{\sqrt{2\pi\beta}}$, which we account for in the code. (It is interesting to note that this factor comes from the *free particle propagator* $K(x, x', \beta) = \frac{1}{\sqrt{2\pi\beta}} \exp \frac{-(x-x')^2}{2\beta}$, but that we obtained it using only the properties of Brownian motion).

IV.3. Obtaining the energy as a function of β

We use the result of the previous section to compute $Z(\beta)$ through the relation in (29). Recall our analytic solution for the partition function:

$$Z(\beta) = \frac{1}{2\sinh\frac{\beta}{2}} \tag{40}$$

The Feynman-Kac simulation provides excellent agreement with this solution, as shown in Figure 6. Also recall

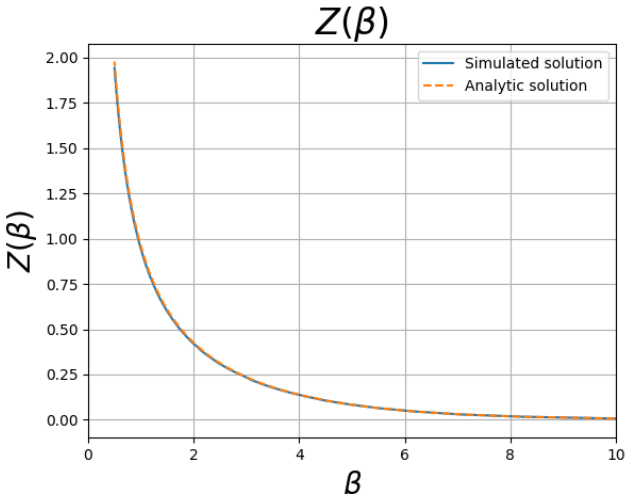

FIG. 6. Simulated and analytic partition functions for QHO. The agreement is perfect; the two lines overlap so well that they are hard to distinguish.

the analytic solution for the energy of our system:

$$\langle E(\beta)\rangle = \frac{1}{2} + \frac{1}{e^\beta - 1} \tag{41}$$

for which we again have good agreement between the analytic and simulated solutions, as shown in Fig. 7.

Notice that at low temperatures the energy is $\frac{1}{2}$ (which is precisely the energy of the ground state of the QHO), while at high temperatures the energy scales linearly with T. This is as expected: classically, the energy of the system at equilibrium should be $k_B T$, but at low temperatures it can never drop below the ground state energy.

IV.4. Position distribution at finite temperature

Using the partition function that we obtained, it is simple to obtain $\rho(x, x; \beta)$ through equation (30). Shown in Figure 8 are plots of the position distribution for several values of β.

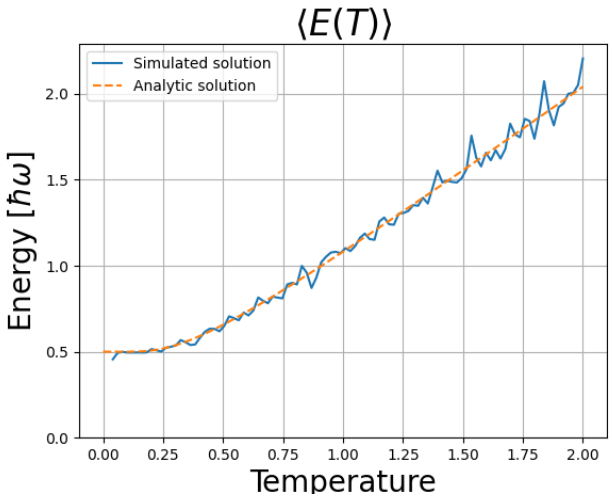

FIG. 7. Simulated and analytic energies as a function of temperature, taking $k_B = 1$. Agrees with ground state energy at $T = 0$ and classical prediction $E = k_B T$ for $T \gg 1$.

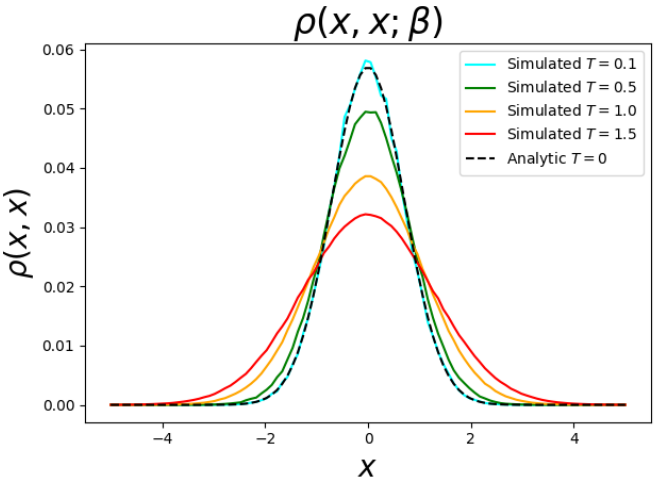

FIG. 8. Simulated position distributions at several temperatures, along with analytic ground state distribution at $T = 0$.

As expected, the distributions spread out as T increases. This is due to the higher energy of the system (seen in Figure 7), which increases the probability of reaching a higher potential.

IV.5. Limitations of Feynman-Kac simulation

As we have seen in the preceding sections, the Feynman-Kac formula is an excellent method of simulating the thermodynamics of a quantum system at equilibrium. Although we applied it to a very simple system where we already know the analytic solution, we could have applied it just as easily to a more complicated potential.

Recall that in section III.2, we drew an analogy between the Boltzmann factor $e^{-\beta \hat{H}}$ and the imaginary time evolution operator $e^{-t\hat{H}}$. It was this connection to imaginary time evolution that allowed us to apply the Feynman-Kac formula, which solves the imaginary time Schrödinger equation. For this reason, Feynman-Kac is very well-suited to treating equilibrium statistical mechanics problems.

However, imaginary time works against us when we consider dynamics of systems that are out of equilibrium. Since these systems evolve, simulating them requires us to use real time. For such systems, it would likely be easier to directly use the time-dependent Schrödinger equation to evolve the wavefunction.

V. CONCLUSION

The quantum mechanical path integral is an extremely useful formulation of quantum mechanics that allows us to study some very complex systems.

While the quantum harmonic oscillator system we studied in this paper was simple enough to do analytically, the simulation code that I wrote works with almost any potential, making the path integral capable of simulating far more complicated systems.

Finally, the Feynman-Kac formula is surprisingly elegant, allowing us to derive many seemingly unrelated results using only probability theory. Recall that we used it to obtain the form of the kinetic energy in the classical action, as well as the free particle propagator correction factor in the simulation. I greatly enjoyed many of these derivations!

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