Alan Robledo

11/14/19

1 Introduction

1.1 Quantum Harmonic Oscillator Partition Function

Similar to the classical harmonic oscillator, we have a particle that is subject to a harmonic potential so that the 1D Hamiltonian looks like

$$\hat{H} = \hat{K} + \hat{U} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{1}$$

where m is the particle's mass and ω is the angular frequency of the oscillator. We know that we can derive the properties of the harmonic oscillator from the canonical ensemble. To do this, we start with the canonical partition function,

$$Q = \sum_k e^{-\beta E_k} \tag{2}$$

where the sum is performed over all possible states of the system, which are discrete. We know from introductory quantum mechanics that the energies of a harmonic oscillator are

$$E_n = \hbar\omega(n + \frac{1}{2}) \tag{3}$$

This can be derived from solving Schrödinger's equation with the hamiltonian in equation (1). Alternatively, the energies can be derived using Dirac's ladder operators, $\hat{a}$ and $\hat{a}^\dagger$. The "raising operator" $\hat{a}$ and "lowering operator" $\hat{a}^\dagger$ can be defined in terms of the position and momentum operators as

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$
$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \tag{4}$$

where the prefactors are such that they allow the math to work out nicely when deriving the energies for a harmonic oscillator. The Hamiltonian can then be expressed in terms of the ladder operators.

$$\hat{H} = \hbar\omega(\hat{a}\hat{a}^\dagger + \frac{1}{2}) \tag{5}$$

1.2 Path Integral Derivation

As always, we will start with the case of a single quantum particle moving in one dimension. So our Hamiltonian is the same as in equation (1). We consider the amplitude of a path that the particle can take when going from x to x' over some time t as the propagator written in position space.

$$A = \langle x'|e^{-iHt/\hbar}|x\rangle \tag{6}$$

This is useful to know because the probability of the particle choosing a particular path would simply be $|A|^2$. In terms of state vectors, the initial state of our particle can be represented as $|\Psi(0)\rangle$, so the state of our particle can be represented as the inital state vector being acted upon by the propagator

$$|\Psi(t)\rangle = e^{-iHt/\hbar}|\Psi(0)\rangle \tag{7}$$

And we can project the coordinate basis onto our state vectors to give us a meaningful representation of our state vector

$$
\begin{aligned}
\langle x' | \Psi(t) \rangle = \Psi(x', t) &= \langle x' | e^{-iHt/\hbar} | \Psi(0) \rangle \\
&= \langle x' | e^{-iHt/\hbar} \int dx |x\rangle \langle x | \Psi(0) \rangle \\
&= \int dx \, \langle x' | e^{-iHt/\hbar} | x \rangle \langle x | \Psi(0) \rangle \\
&= \int dx \, \langle x' | e^{-iHt/\hbar} | x \rangle \, \Psi(x, 0)
\end{aligned}
\tag{8}
$$

where we introduced the resolution of identity $\int dx \, |x\rangle \langle x| = 1$.

So now we have a more mathematical representation of our problem; we want to know how to go from $\Psi(x, 0)$ to $\Psi(x', t)$. The physical representation of our problem is that we have a particle at some point x in space, and we want to be able to detect our particle at some other point x' in space after some time t passes.

By going to imaginary time, which is done by substituting $it/\hbar = \beta$, we can express the coordinate-space quantum propagator as the canonical density matrix,

$$
\rho(x, x') = \langle x' | e^{-\beta \hat{H}} | x \rangle
\tag{9}
$$

The motive behind doing this is so that we can deal with a damped exponential as opposed to a complex exponential. Therefore, we can derive the path integral form of the density matrix and simply resubstitute time in place of β to obtain the path integral form of the time propagator.

We would like to separate the hamiltonian into its kinetic and potential energy components, $\hat{H} = \hat{K} + \hat{U}$. However, we cannot split the exponentials because for two operators that do not commute $\exp(\hat{H}) \neq \exp(\hat{K})\exp(\hat{U})$. To get around this we employ the trotter decompositon

$$
e^{-\beta \hat{H}} = e^{-\beta(\hat{K}+\hat{U})} = \lim_{P \to \infty} \left[e^{-\beta \hat{U}/2P} e^{-\beta \hat{K}/P} e^{-\beta U/2P} \right]^P.
\tag{10}
$$

Substituting this into equation (9) gives us,

$$
\rho(x, x') = \lim_{P \to \infty} \langle x' | \left[e^{-\beta \hat{U}/2P} e^{-\beta \hat{K}/P} e^{-\beta U/2P} \right]^P | x \rangle
\tag{11}
$$

which can be condensed by defining another operator Ω as

$$
\Omega = e^{-\beta \hat{U}/2P} e^{-\beta \hat{K}/P} e^{-\beta \hat{U}/2P}.
\tag{12}
$$

So our density matrix becomes,

$$
\rho(x, x') = \lim_{P \to \infty} \langle x' | \Omega^P | x \rangle
\tag{13}
$$

We can insert the resolution of identity in terms of the position basis P-1 times between each of the omegas, remembering that $\Omega^P = \Omega\Omega \cdots \Omega$,

$$
\rho(x, x') = \lim_{P \to \infty} \int \cdots \int dx_P \cdots dx_2 \, \langle x' | \Omega | x_P \rangle \langle x_P | \Omega | x_{P-1} \rangle \langle x_{P-1} | \cdots | x_3 \rangle \langle x_3 | \Omega | x_2 \rangle \langle x_2 | \Omega | x \rangle
\tag{14}
$$

The integration over a coordinate x_i can be thought of as integrating over a possible path that your particle can take because we can obtain integrations over all possible paths when P $\to \infty$. If we consider an element of the matrix,

$$
\langle x_{k+1} | \Omega | x_k \rangle = \langle x_{k+1} | e^{-\beta \hat{U}/2P} e^{-\beta \hat{K}/P} e^{-\beta \hat{U}/2P} | x_k \rangle
\tag{15}
$$

we can recognize that the set of $|x_k\rangle$ are eigenvectors of $e^{-\beta \hat{U}/2P}$ with eigenvalue $e^{-\beta U(x_k)}/2P$ because $\hat{U} = U(\hat{x})$ is a function of the coordinate operator. This can be shown easily by writing the exponential as a power series in $\hat{U}$.

$$
e^{-\beta \hat{U}/2P} = \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n} \hat{U}^n}{n!}
\tag{16}
$$

2

and if we operate on an eigenvector $|x_k\rangle$, we get

$$
\begin{aligned}
e^{-\beta \hat{U}/2P} |x_k\rangle &= \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n}}{n!} \hat{U}^n |x_k\rangle \\
&= \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n}}{n!} (U(x_k))^n |x_k\rangle \\
&= e^{-\beta U(x_k)/2P} |x_k\rangle
\end{aligned}
\tag{17}
$$

So equation (15) simplifies to

$$
\langle x_{k+1}|\Omega|x_k\rangle = e^{-\beta U(x_{k+1})/2P} \langle x_{k+1}|e^{-\beta \hat{K}/P}|x_k\rangle e^{-\beta U(x_k)/2P}.
\tag{18}
$$

We know that $\hat{K}$ is a function of the momentum operator, $\hat{K} = \hat{p}^2/2m$, so we can use the same technique as we did with $\hat{U}$ and the position eigenvectors by introducing the resolution of identity in terms of the momentum basis

$$
\begin{aligned}
\langle x_{k+1}|\Omega|x_k\rangle &= \int e^{-\beta U(x_{k+1})/2P} \langle x_{k+1}| e^{-\beta \hat{K}/P} |p\rangle \langle p|x_k\rangle e^{-\beta U(x_k)/2P} \\
&= \int e^{-\beta U(x_{k+1})/2P} e^{-\beta p^2/2mP} \langle x_{k+1}|p\rangle \langle p|x_k\rangle e^{-\beta U(x_k)/2P} dp
\end{aligned}
\tag{19}
$$

where $\langle x_{k+1}|p\rangle$ is the momentum wavefunction expressed in the coordinate x_{k+1}, and $\langle p|x_k\rangle$ is the complex conjugate of the momentum wavefunction expressed in the coordinate x_k basis, i.e. $\langle p|x_k\rangle = \langle x_k|p\rangle^*$.

We can obtain a functional form of these wavefunctions by recalling the eigenvalue problem for the momentum operator,

$$
\hat{p}|p\rangle = p|p\rangle
\tag{20}
$$

If we project this equation on the coordinate basis, we can make use of the hermitian property of the momentum operator to obtain

$$
\langle x|\hat{p}|p\rangle = p\langle x|p\rangle \quad \Rightarrow \quad \langle \hat{p}x|p\rangle = p\langle x|p\rangle \quad \Rightarrow \quad -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle
\tag{21}
$$

And if we write $\langle x|p\rangle = \psi_p(x)$, then we just have a first order differential equation. The solution to this equation can easily be found

$$
-i\hbar\frac{\partial}{\partial x}\psi_p(x) = p\psi_p(x) \quad \Rightarrow \quad \int \frac{d\psi_p}{\psi_p} dx = \int \frac{ip}{\hbar} dx \quad \Rightarrow \quad \ln \psi_p(x) = \frac{ipx}{\hbar} + C_1 \quad \Rightarrow \quad \psi_p(x) = C_2 e^{ipx/\hbar}
\tag{22}
$$

where C_2 is a normalization constant. With proper normalization, the momentum wavefunction looks like

$$
\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.
\tag{23}
$$

And it's complex conjugate looks like,

$$
\langle x|p\rangle^* = \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}
\tag{24}
$$

We can use this to rewrite our matrix elements of Ω as

$$
\begin{aligned}
\langle x_{k+1}|\Omega|x_k\rangle &= \int e^{-\beta U(x_{k+1})/2P} e^{-\beta p^2/2mP} \langle x_{k+1}|p\rangle \langle p|x_k\rangle e^{-\beta U(x_k)/2P} dp \\
&= \frac{1}{2\pi\hbar} \int e^{-\beta p^2/2mP} e^{-\beta(U(x_{k+1})+U(x_k))/2P} e^{ip(x_{k+1}-x_k)/\hbar} dp
\end{aligned}
\tag{25}
$$

We can move the exponential without the momenta outside of the integral and combine the exponentials with the momenta to obtain

$$
\langle x_{k+1}|\Omega|x_k\rangle = \frac{1}{2\pi\hbar} e^{-\beta(U(x_{k+1})+U(x_k))/2P} \int e^{-\beta p^2/2mP + ip(x_{k+1}-x_k)/\hbar} dp
\tag{26}
$$

Since our momentum basis extends from $+\infty$ to $-\infty$, we end up having an integral of a gaussian if we complete the square,

$$
\begin{aligned}
\frac{-\beta p^2}{2mP} + \frac{(x_{k+1} - x_k)ip}{\hbar} &= \frac{-\beta}{2mP}\left[p^2 - \frac{2imP(x_{k+1} - x_k)}{\beta\hbar}\right] \\
&= \frac{-\beta}{2mP}\left[\left(p - \frac{mP(x_{k+1} - x_k)i}{\beta\hbar}\right)^2 - \left(\frac{imP(x_{k+1} - x_k)}{\beta\hbar}\right)^2\right] \\
&= \frac{-\beta}{2mP}\left[\left(p - \frac{imP(x_{k+1} - x_k)}{\beta\hbar}\right)^2 + \frac{m^2P^2(x_{k+1} - x_k)^2}{\beta^2\hbar^2}\right] \\
&= \frac{-\beta}{2mP}\left(p - \frac{imP(x_{k+1} - x_k)}{\beta\hbar}\right)^2 - \frac{mP(x_{k+1} - x_k)^2}{2\beta\hbar^2}
\end{aligned}
\tag{27}
$$

and make a variable substitution,

$$
u = p - \frac{imP(x_{k+1} - x_k)}{\beta\hbar}.
\tag{28}
$$

Our integral is now,

$$
\langle x_{k+1}|\Omega|x_k\rangle = \frac{1}{2\pi\hbar}\exp\left[\frac{-\beta(U(x_{k+1}) + U(x_k))}{2P}\right]\exp\left[\frac{-mP(x_{k+1} - x_k)^2}{2\beta\hbar^2}\right]\int e^{\frac{-\beta u^2}{2mP}}\,du
\tag{29}
$$

which evaluates to,

$$
\begin{aligned}
\langle x_{k+1}|\Omega|x_k\rangle &= \frac{1}{2\pi\hbar}\exp\left[-\frac{\beta}{2P}(U(x_{k+1}) + U(x_k))\right]\exp\left[-\frac{mP}{2\beta\hbar^2}(x_{k+1} - x_k)^2\right]\left(\frac{2\pi mP}{\beta}\right)^{1/2} \\
&= \left(\frac{mP}{2\pi\beta\hbar^2}\right)^{1/2}\exp\left[\frac{mP}{2\beta\hbar^2}(x_{k+1} - x_k)^2 - \frac{\beta}{2P}(U(x_{k+1}) + U(x_k))\right]
\end{aligned}
\tag{30}
$$

Plugging in our matrix elements into equation (14) P times for each element gives us the discretized path integral representation of our density matrix.

$$
\rho(x, x') = \lim_{P\to\infty}\left(\frac{mP}{2\pi\beta\hbar^2}\right)^{P/2}\int\cdots\int dx_P\cdots dx_2 \quad \exp\left(\sum_{k=1}^{P}\left[\frac{mP}{2\beta\hbar^2}(x_{k+1} - x_k)^2 - \frac{\beta}{2P}(U(x_{k+1}) + U(x_k))\right]\right)
\tag{31}
$$

where $x_1 = x$ and $x_P = x'$.