Alan Robledo

11/14/19

1 Derivation of Path Integral for 1D Harmonic Oscillator

As always, we will start with the case of a single quantum particle moving in one dimension. So the Hamiltonian looks like,

$$H = \frac{p^2}{2m} + U(x) \tag{1}$$

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.

$$A = \langle x'|e^{-iHt/\hbar}|x\rangle \tag{2}$$

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

$$|\Psi(t)\rangle = e^{-iHt/\hbar}|\Psi(0)\rangle \tag{3}$$

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

$$\begin{aligned}
\langle x'|\Psi(t)\rangle = \Psi(x',t) &= \langle x'|e^{-iHt/\hbar}|\Psi(0)\rangle \\
&= \langle x'|e^{-iHt/\hbar}\int dx|x\rangle\langle x|\Psi(0)\rangle \\
&= \int dx\,\langle x'|e^{-iHt/\hbar}|x\rangle\langle x|\Psi(0)\rangle \\
&= \int dx\,\langle x'|e^{-iHt/\hbar}|x\rangle\,\Psi(x,0)
\end{aligned} \tag{4}$$

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,

$$\rho(x,x') = \langle x'|e^{-\beta\hat{H}}|x\rangle \tag{5}$$

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

$$e^{-\beta\hat{H}} = e^{-\beta(\hat{K}+\hat{U})} = \lim_{P\to\infty}\left[e^{-\beta\hat{U}/2P}e^{-\beta\hat{K}/P}e^{-\beta U/2P}\right]^P. \tag{6}$$

Substituting this into equation (5) gives us,

$$\rho(x,x') = \lim_{P\to\infty}\langle x'|\left[e^{-\beta\hat{U}/2P}e^{-\beta\hat{K}/P}e^{-\beta U/2P}\right]^P|x\rangle \tag{7}$$

which can be condensed by defining another operator Ω as

$$\Omega = e^{-\beta\hat{U}/2P} e^{-\beta\hat{K}/P} e^{-\beta\hat{U}/2P}. \tag{8}$$

So our density matrix becomes,

$$\rho(x, x') = \lim_{P\to\infty} \langle x'|\Omega^P|x\rangle \tag{9}$$

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

$$\rho(x, x') = \lim_{P\to\infty} \int\cdots\int dx_P \cdots dx_2 \,\langle x'|\Omega|x_P\rangle \langle x_P|\Omega|x_{P-1}\rangle \langle x_{P-1}|\cdots|x_3\rangle \langle x_3|\Omega|x_2\rangle \langle x_2|\Omega|x\rangle \tag{10}$$

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,

$$\langle x_{k+1}|\Omega|x_k\rangle = \langle x_{k+1}|e^{-\beta\hat{U}/2P} e^{-\beta\hat{K}/P} e^{-\beta\hat{U}/2P}|x_k\rangle \tag{11}$$

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 $\hat{U}$.

$$e^{-\beta\hat{U}/2P} = \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n} \hat{U}^n}{n!} \tag{12}$$

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

$$\begin{aligned} e^{-\beta\hat{U}/2P} |x_k\rangle &= \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n}}{n!} \hat{U}^n |x_k\rangle \\ &= \sum_{n=0}^{\infty} \frac{\beta^n (2P)^{-n}}{n!} (U(x_k))^n |x_k\rangle \\ &= e^{-\beta U(x_k)/2P} |x_k\rangle \end{aligned} \tag{13}$$

So equation (11) simplifies to

$$\langle x_{k+1}|\Omega|x_k\rangle = e^{-\beta U(x_{k+1})/2P} \langle x_{k+1}|e^{-\beta\hat{K}/P}|x_k\rangle e^{-\beta U(x_k)/2P}. \tag{14}$$

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

$$\begin{aligned} \langle x_{k+1}|\Omega|x_k\rangle &= \int e^{-\beta U(x_{k+1})/2P} \langle x_{k+1}|\, e^{-\beta\hat{K}/P}\, |p\rangle \langle p|x_k\rangle\, e^{-\beta U(x_k)/2P} \\ &= \int e^{-\beta U(x_{k+1})/2P} e^{-\beta p^2/2mP} \langle x_{k+1}|p\rangle \langle p|x_k\rangle\, e^{-\beta U(x_k)/2P} dp \end{aligned} \tag{15}$$

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,

$$\hat{p}\,|p\rangle = p\,|p\rangle \tag{16}$$

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

$$\langle x|\hat{p}|p\rangle = p\,\langle x|p\rangle \quad\Rightarrow\quad \langle \hat{p}x|p\rangle = p\,\langle x|p\rangle \quad\Rightarrow\quad -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle = p\,\langle x|p\rangle \tag{17}$$

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

$$-i\hbar\frac{\partial}{\partial x}\psi_p(x) = p\psi_p(x) \quad\Rightarrow\quad \int\frac{d\psi_p}{\psi_p}dx = \int\frac{ip}{\hbar}dx \quad\Rightarrow\quad \ln\psi_p(x) = \frac{ipx}{\hbar} + C_1 \quad\Rightarrow\quad \psi_p(x) = C_2 e^{ipx/\hbar} \tag{18}$$

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

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}. \tag{19}$$

And it's complex conjugate looks like,

$$\langle x|p\rangle^* = \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \tag{20}$$

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

$$\begin{aligned} \langle x_{k+1}|\Omega|x_k\rangle &= \int e^{-\beta U(x_{k+1})/2P} e^{-\beta p^2/2mP} \langle x_{k+1}|p\rangle \langle p|x_k\rangle \, e^{-\beta U(x_k)/2P} dp \\ &= \frac{1}{2\pi\hbar} \int e^{-\beta p^2/2mP} e^{-\beta(U(x_{k+1})+U(x_k))/2P} e^{ip(x_{k+1}-x_k)/\hbar} dp \end{aligned} \tag{21}$$

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

$$\langle x_{k+1}|\Omega|x_k\rangle = \frac{1}{2\pi\hbar} e^{-\beta(U(x_{k+1})+U(x_k))/2P} \int e^{-\beta p^2/2mP + ip(x_{k+1}-x_k)/\hbar} dp \tag{22}$$

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

$$\begin{aligned} \frac{-\beta p^2}{2mP} + \frac{(x_{k+1}-x_k)ip}{\hbar} &= \frac{-\beta}{2mP}\Big[p^2 - \frac{2imP(x_{k+1}-x_k)}{\beta\hbar}\Big] \\ &= \frac{-\beta}{2mP}\Big[\Big(p - \frac{mP(x_{k+1}-x_k)i}{\beta\hbar}\Big)^2 - \Big(\frac{imP(x_{k+1}-x_k)}{\beta\hbar}\Big)^2\Big] \\ &= \frac{-\beta}{2mP}\Big[\Big(p - \frac{imP(x_{k+1}-x_k)}{\beta\hbar}\Big)^2 + \frac{m^2P^2(x_{k+1}-x_k)^2}{\beta^2\hbar^2}\Big] \\ &= \frac{-\beta}{2mP}\Big(p - \frac{imP(x_{k+1}-x_k)}{\beta\hbar}\Big)^2 - \frac{mP(x_{k+1}-x_k)^2}{2\beta\hbar^2} \end{aligned} \tag{23}$$

and make a variable substitution,

$$u = p - \frac{imP(x_{k+1}-x_k)}{\beta\hbar}. \tag{24}$$

Our integral is now,

$$\langle x_{k+1}|\Omega|x_k\rangle = \frac{1}{2\pi\hbar}\exp\Big[\frac{-\beta(U(x_{k+1})+U(x_k))}{2P}\Big]\exp\Big[\frac{-mP(x_{k+1}-x_k)^2}{2\beta\hbar^2}\Big]\int e^{\frac{-\beta u^2}{2mP}} du \tag{25}$$

which evaluates to,

$$\begin{aligned} \langle x_{k+1}|\Omega|x_k\rangle &= \frac{1}{2\pi\hbar}\exp\Big[-\frac{\beta}{2P}(U(x_{k+1})+U(x_k))\Big]\exp\Big[-\frac{mP}{2\beta\hbar^2}(x_{k+1}-x_k)^2\Big]\Big(\frac{2\pi mP}{\beta}\Big)^{1/2} \\ &= \Big(\frac{mP}{2\pi\beta\hbar^2}\Big)^{1/2}\exp\Big[\frac{mP}{2\beta\hbar^2}(x_{k+1}-x_k)^2 - \frac{\beta}{2P}(U(x_{k+1})+U(x_k))\Big] \end{aligned} \tag{26}$$

Plugging in our matrix elements into equation (10) P times for each element gives us the discretized path integral representation of our density matrix.

$$\rho(x,x') = \lim_{P\to\infty}\Big(\frac{mP}{2\pi\beta\hbar^2}\Big)^{P/2}\int\cdots\int dx_P\cdots dx_2 \quad \exp\Big(\sum_{k=1}^{P}\Big[\frac{mP}{2\beta\hbar^2}(x_{k+1}-x_k)^2 - \frac{\beta}{2P}(U(x_{k+1})+U(x_k))\Big]\Big) \tag{27}$$

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