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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,

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

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.

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

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 initial state vector being acted upon by the propagator

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

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

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

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

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,

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

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 decomposition

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

Substituting this into equation (5) gives us,

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

which can be condensed by defining another operator Ω as

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

So our density matrix becomes,

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

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

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

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 $P \rightarrow \infty$. If we consider an element of the matrix,

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

we can recognize that the set of $|x_k\rangle$ are eigenvectors of $e^{-\beta \hat{U}/2P}$ with eigenvalue $e^{-\beta U(\hat{x}_k)/2P}$ 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} .

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

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

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

So equation (11) simplifies to

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

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.

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

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,

$$\hat{p} |p\rangle = p |p\rangle \quad (16)$$

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

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

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

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

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

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

And it's complex conjugate looks like,

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

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

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

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

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

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

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

and make a variable substitution,

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

Our integral is now,

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

which evaluates to,

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

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

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

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