

Title: The Simplest Time Dependent Case - QHO

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Traditionally, the Hamiltonian for the 1-D time-independent quantum harmonic oscillator is written as:

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

The general time-independent 1-D Hamiltonian produces the following eigenvalue-eigenstate pairs:

$$\begin{aligned} E_n &= \hbar\omega \left(n + \frac{1}{2} \right) \\ \psi_n(x) &= \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) \end{aligned} \quad (2)$$

The generality of the eigenvalue-eigenstate pair in terms of the oscillator frequency is very useful for the case of testing time-dependent theory with a concrete example, since for any time-dependent frequency function $\omega(t)$, the instantaneous eigenstate and eigenvalues remain of the same form:

$$\begin{aligned} \hat{H}(t) &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(t) x^2 \\ E_n(t) &= \hbar\omega(t) \left(n + \frac{1}{2} \right) \\ \psi_n(x, t) &= \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega(t)}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega(t)x^2}{2\hbar}} H_n \left(\sqrt{\frac{m\omega(t)}{\hbar}} x \right) \end{aligned} \quad (3)$$

where $H_n(x)$ is the n th Hermite polynomial. The equation defining the orthonormal basis of Hermite polynomials is:

$$\frac{1}{2^n n!} \int_{-\infty}^{\infty} dx H_n(x) H_p(x) e^{-x^2} = \sqrt{\pi} \delta_{np} \quad (4)$$

Now, the critical quantity to express is $\langle \psi_p(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle$. To start:

$$\begin{aligned} \frac{\partial}{\partial t} \psi_n(x, t) &= \frac{\psi_n(x, t)}{4\omega(t)} \frac{\partial \omega(t)}{\partial t} - x^2 \psi_n(x, t) \frac{m}{2\hbar} \frac{\partial \omega(t)}{\partial t} + \frac{x \psi_n(x, t)}{2\sqrt{\frac{\hbar\omega(t)}{m}}} \frac{H'_n \left(\sqrt{\frac{m\omega(t)}{\hbar}} x \right)}{H_n \left(\sqrt{\frac{m\omega(t)}{\hbar}} x \right)} \frac{\partial \omega(t)}{\partial t} \\ \frac{\partial}{\partial t} \psi_n(x, t) &= \frac{\psi_n(x, t)}{4\omega(t)} \frac{\partial \omega(t)}{\partial t} - x^2 \psi_n(x, t) \frac{m}{2\hbar} \frac{\partial \omega(t)}{\partial t} + \frac{x \psi_{n-1}(x, t)}{\sqrt{\frac{2\hbar\omega(t)}{nm}}} \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (5)$$

which, while tending towards more algebra, is still well within the realm of standard mathematics. The following mathematical identities are useful:

$$H'_n(x) = 2nH_{n-1}(x), \quad n \geq 1 \quad (6)$$

$$I_{np\ell} = \sqrt{\frac{1}{2^n n!}} \sqrt{\frac{1}{2^p p!}} \int_{-\infty}^{\infty} dx H_n(x) H_p(x) H_\ell(x) e^{-x^2} = \frac{2^{\frac{\ell}{2}} \ell! \sqrt{p! n! \pi}}{\left(\frac{\ell+p-n}{2}\right)! \left(\frac{n+p-\ell}{2}\right)! \left(\frac{\ell+n-p}{2}\right)!} \delta_{\text{condition}} \quad (7)$$

where the conditions to be met for $\delta_{\text{condition}} = 1$ are:

$$\begin{aligned} \frac{n+p+\ell}{2} &\in \mathbb{Z}_+ \\ \ell+p-n &\geq 0 \\ n+p-\ell &\geq 0 \\ \ell+n-p &\geq 0 \end{aligned} \quad (8)$$

else $\delta_{\text{condition}} = 0$. These conditions can be shortened if we specify p to be the largest of the three integers, without loss of generality:

$$\begin{aligned} \frac{n+p+\ell}{2} &\in \mathbb{Z}_+ \\ n+\ell &\geq p \end{aligned}$$

as the triangle inequality with sum of integers even. Of course, all integers are ≥ 0 . Then, we can calculate the inner product $\langle \psi_p(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle$ of Equation 5 as:

$$\begin{aligned} \frac{\partial}{\partial t} | \psi_n(x, t) \rangle &= \frac{\psi_n(x, t)}{4\omega(t)} \frac{\partial \omega(t)}{\partial t} + \sqrt{\frac{\hbar}{m\omega(t)}} \frac{H_1\left(\sqrt{\frac{m\omega(t)}{\hbar}} x\right)}{2\sqrt{\frac{2\hbar\omega(t)}{nm}}} \psi_{n-1}(x, t) \frac{\partial \omega(t)}{\partial t} \\ &\quad - \frac{1}{4} \frac{\hbar}{m\omega(t)} \left(H_2\left(\sqrt{\frac{m\omega(t)}{\hbar}} x\right) + 2H_0\left(\sqrt{\frac{m\omega(t)}{\hbar}} x\right) \right) \psi_n(x, t) \frac{m}{2\hbar} \frac{\partial \omega(t)}{\partial t} \\ \langle \psi_p(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle &= \frac{\delta_{np}}{4\omega(t)} \frac{\partial \omega(t)}{\partial t} + \frac{1}{2} \sqrt{\frac{n\hbar}{2m\omega(t)}} \frac{I_{n-1,p,1} \delta_{np}}{\omega(t)} \sqrt{\frac{m\omega(t)}{\pi\hbar}} \frac{\partial \omega(t)}{\partial t} \\ &\quad - \frac{1}{8} \sqrt{\frac{\hbar}{m\omega(t)}} \frac{I_{np2}}{\omega(t)} \sqrt{\frac{m\omega(t)}{\pi\hbar}} \frac{\partial \omega(t)}{\partial t} - \frac{\delta_{np}}{4\omega(t)} \frac{\partial \omega(t)}{\partial t} \\ \langle \psi_p(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle &= \frac{1}{2} \sqrt{\frac{n}{2\pi}} \frac{I_{n-1,p,1} \delta_{np}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} - \frac{1}{8\sqrt{\pi}} \frac{I_{np2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (9)$$

where:

$$\begin{aligned} x^2 &= \frac{1}{4} (H_2(x) + 2H_0(x)) \\ x &= \frac{1}{2} H_1(x) \end{aligned}$$

and:

$$I_{n-1,n,1} = \sqrt{2\pi n}$$

$$I_{nn2} = 4n\sqrt{\pi}, \text{ and } I_{n,n+2,2} = 2\sqrt{(n+1)(n+2)}\sqrt{\pi}$$

These results imply that:

$$\begin{aligned} \langle \psi_n(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle &= 0 \\ \langle \psi_{n+2}(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle &= -\frac{1}{4} \frac{\sqrt{(n+1)_2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (10)$$

where $(n+1)_2$ is the rising Pochhammer symbol. The first result is as expected, since we know that $\langle \psi_n(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle$ must be imaginary, and since the eigenstates are all purely real, it must follow that the only possible imaginary solution is the value $0 = 0i$. Then, the only surviving matrix element is the expectation value $\langle \psi_{n+2}(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle$. Then, we can exactly relate this quantity to the matrix elements of $\frac{\partial \hat{H}(t)}{\partial t}$ in the basis of the energy eigenstates by:

$$\begin{aligned} \langle \psi_p(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_n(x, t) \rangle &= (E_n(t) - E_p(t)) \langle \psi_p(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle \\ \implies \langle \psi_p(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_n(x, t) \rangle &= \frac{\delta_{p,n+2}}{4} \hbar (p-n) \sqrt{(p-1)_2} \frac{\partial \omega(t)}{\partial t} \\ \implies \langle \psi_{n+2}(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_n(x, t) \rangle &= \frac{\hbar}{2} \sqrt{(n+1)_2} \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (11)$$

as the only off-diagonal elements that are non-vanishing are the $(n, n+2)$ and $(n+2, n)$ rows-columns. The diagonal matrix elements can be calculated by Hellmann-Feynman theorem:

$$\begin{aligned} \langle \psi_n(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_n(x, t) \rangle &= \frac{\partial E_n(t)}{\partial t} \\ \implies \langle \psi_n(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_n(x, t) \rangle &= \frac{\hbar}{2} (2n+1) \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (12)$$

Equation 11 calculates the off-diagonal elements for the $(n+2)$ th row and n th column. To calculate the n th row and $(n+2)$ th column, we take the Hermitian conjugate of Equation 10:

$$\begin{aligned} \left(\langle \psi_{n+2}(x, t) | \frac{\partial}{\partial t} | \psi_n(x, t) \rangle \right)^\dagger &= \langle \psi_n(x, t) | \left(-\frac{\partial}{\partial t} \right) | \psi_{n+2}(x, t) \rangle = -\frac{1}{4} \frac{\sqrt{(n+1)_2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \\ \implies \langle \psi_n(x, t) | \frac{\partial}{\partial t} | \psi_{n+2}(x, t) \rangle &= \frac{1}{4} \frac{\sqrt{(n+1)_2}}{\omega(t)} \frac{\partial \omega(t)}{\partial t} \\ \implies \langle \psi_n(x, t) | \frac{\partial \hat{H}(t)}{\partial t} | \psi_{n+2}(x, t) \rangle &= \frac{\hbar}{2} \sqrt{(n+1)_2} \frac{\partial \omega(t)}{\partial t} \end{aligned} \quad (13)$$

Now, in the last post, it was found that for short change in time δt ,

$$\frac{\partial^2 \hat{H}(t + \delta t)}{\partial t^2} \approx \frac{i}{\hbar} \left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t} \right]$$

To test this hypothesis, we calculate the resultant commutator matrix. First:

$$\hat{H}(t) \frac{\partial \hat{H}(t)}{\partial t} = \begin{bmatrix} \frac{\hbar \omega(t)}{2} & 0 & 0 & \dots \\ 0 & \frac{3\hbar \omega(t)}{2} & 0 & \dots \\ 0 & 0 & \frac{5\hbar \omega(t)}{2} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} \frac{\hbar \frac{\partial \omega(t)}{\partial t}}{2} & 0 & \frac{\hbar \frac{\partial \omega(t)}{\partial t}}{2} \sqrt{2} & \dots \\ 0 & \frac{3\hbar \frac{\partial \omega(t)}{\partial t}}{2} & 0 & \dots \\ \frac{\hbar \frac{\partial \omega(t)}{\partial t}}{2} \sqrt{2} & 0 & \frac{5\hbar \frac{\partial \omega(t)}{\partial t}}{2} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (14)$$

This calculation yields the following elements:

$$\left(\hat{H}(t) \frac{\partial \hat{H}(t)}{\partial t} \right)_{ij} = (H)_{ii} \left(\frac{\partial H}{\partial t} \right)_{ij} \quad (15)$$

Conversely, the second term yields the following elements:

$$\left(\frac{\partial \hat{H}(t)}{\partial t} \hat{H}(t) \right)_{ij} = \left(\frac{\partial H}{\partial t} \right)_{ij} (H)_{jj} \quad (16)$$

Thus, the matrix elements of the commutator are:

$$\left(\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t} \right] \right)_{ij} = \left(\frac{\partial H}{\partial t} \right)_{ij} \left((H)_{ii} - (H)_{jj} \right) \quad (17)$$

Clearly, the diagonal elements of the commutator vanish, such that only the $(n, n+2)$ and $(n+2, n)$ elements stand to remain. Since $\left(\frac{\partial H}{\partial t} \right)_{ij} = \left(\frac{\partial H}{\partial t} \right)_{ji}$, we find:

$$\left(\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t} \right] \right)_{ij} = - \left(\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t} \right] \right)_{ji}$$

It is clear from this calculation the resulting commutator is non-Hermitian, and that the approximation given in the previous post must be not correct, since the diagonal terms of $\frac{\partial^2 \hat{H}(t)}{\partial t^2}$ will not be 0. An important distinction (and indeed where I made my mistake) is mixing the Heisenberg and Schrodinger pictures. First off, I believe I have made the following mistakes:

- In the Schrodinger picture:

$$\frac{\partial \hat{H}_S(t)}{\partial t} = \lim_{\delta t \rightarrow 0} \frac{\hat{H}_S(t + \delta t) - \hat{H}_S(t)}{\delta t}$$

In the Heisenberg picture:

$$\frac{d\hat{H}_H(t)}{dt} = \lim_{\delta t \rightarrow 0} \frac{\hat{H}_H(t + \delta t) - \hat{H}_H(t)}{\delta t}$$

The bridge between them is through:

$$\hat{H}_H(t) = U^\dagger \hat{H}_S(t) U$$

where U is the unitary time-evolution operator (where $U^\dagger = U^{-1}$). The unitary time evolution operator will be discussed in more detail in the next post, where we will define the general Dyson series after examining the case of a Hamiltonian with no explicit time dependence. To be clear, U can have explicit time dependence.

- Due to the distinction of the operator in Heisenberg vs. Schrodinger pictures, the action of writing the truncated Taylor series crucially depends on which picture we are working in. For example in many physical systems (such as Hamiltonians with the time-dependent potential $V(x, t)$), the Taylor series in Schrodinger picture would be governed by:

$$\frac{d^q \hat{H}_S}{dt^q} = \frac{\partial^q \hat{H}_S}{\partial t^q}$$

which is markedly different from the relations between operators in the Heisenberg picture from:

$$\frac{d\hat{A}_H}{dt} = \frac{i}{\hbar} [\hat{H}_H, \hat{A}_H] + \frac{\partial \hat{A}_H}{\partial t}$$

while noteably that when the unitary time evolution operator commutes with the time derivative operator (only has implicit time dependence), we get:

$$\frac{\partial \hat{H}_H}{\partial t} = \frac{\partial \hat{H}_S}{\partial t}$$

Though I'm still trying to get to the bottom of what is specifically wrong with writing the Taylor series as I had in the previous post (I suspect something to do with the way the Heisenberg and Schrodinger picture derivatives are defined), it is clear that the relation found in the last post is *wrong*. One simple trick to think about it is to take derivatives with respect to δt and see exact alignment of Taylor series coefficients with the derivatives of the left side common in the theory of Taylor series mathematical definition. This concludes this blog post.