Title: Quantum Operator Time Expansions
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As derived in a previous post, Heisenberg's Equation of Motion is:

$$\frac{\mathrm{d}\hat{A}\left(t\right)}{\mathrm{d}t} = \frac{i}{\hbar}\left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right] + \frac{\partial \hat{A}\left(t\right)}{\partial t} \tag{1}$$

The Taylor Series of such a quantum operator $\hat{A}\left(t\right)$ expanded fully in terms of the time variable can be written as:

$$\hat{A}\left(t\right) = \sum_{n=0}^{\infty} \frac{\mathrm{d}^n\hat{A}\left(t_0\right)}{\mathrm{d}t^n}\frac{\left(t-t_0\right)^n}{n!} \tag{2}$$

Combining Equation 1 and Equation 2, and keeping the operator $\hat{A}\left(t\right)$ as general as possible (with both implicit and explicit time dependence), we find for the first two derivatives:

$$\begin{aligned}
\frac{\mathrm{d}^2\hat{A}\left(t\right)}{\mathrm{d}t^2} &= \frac{i}{\hbar}\left[\hat{H}\left(t\right), \frac{\mathrm{d}\hat{A}\left(t\right)}{\mathrm{d}t}\right] + \frac{\partial \frac{\mathrm{d}\hat{A}(t)}{\mathrm{d}t}}{\partial t} \\
&= \frac{i}{\hbar}\left[\hat{H}\left(t\right), \frac{i}{\hbar}\left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right] + \frac{\partial \hat{A}\left(t\right)}{\partial t}\right] + \frac{i}{\hbar}\frac{\partial\left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right]}{\partial t} + \frac{\partial^2 \hat{A}\left(t\right)}{\partial t^2} \\
&= -\frac{1}{\hbar^2}\left[\hat{H}\left(t\right), \left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right]\right] + \frac{2i}{\hbar}\left[\hat{H}\left(t\right), \frac{\partial \hat{A}\left(t\right)}{\partial t}\right] + \frac{i}{\hbar}\left[\frac{\partial \hat{H}\left(t\right)}{\partial t}, \hat{A}\left(t\right)\right] + \frac{\partial^2 \hat{A}\left(t\right)}{\partial t^2} \\
\frac{\mathrm{d}^3\hat{A}\left(t\right)}{\mathrm{d}t^3} &= \frac{i}{\hbar}\left[\hat{H}\left(t\right), \frac{\mathrm{d}^2\hat{A}\left(t\right)}{\mathrm{d}t^2}\right] + \frac{\partial \frac{\mathrm{d}^2\hat{A}(t)}{\mathrm{d}t^2}}{\partial t} \\
&= \left(\frac{i}{\hbar}\right)^3\left[\hat{H}\left(t\right), \left[\hat{H}\left(t\right), \left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right]\right]\right] + 2\left(\frac{i}{\hbar}\right)^2\left[\hat{H}\left(t\right), \left[\hat{H}\left(t\right), \frac{\partial \hat{A}\left(t\right)}{\partial t}\right]\right] \\
&+ \left(\frac{i}{\hbar}\right)^2\left[\hat{H}\left(t\right), \left[\frac{\partial \hat{H}\left(t\right)}{\partial t}, \hat{A}\left(t\right)\right]\right] + \frac{i}{\hbar}\left[\hat{H}\left(t\right), \frac{\partial^2 \hat{A}\left(t\right)}{\partial t^2}\right] + \frac{\partial^3 \hat{A}\left(t\right)}{\partial t^3} \\
&+ \left(\frac{i}{\hbar}\right)^2\left[\frac{\partial \hat{H}\left(t\right)}{\partial t}, \left[\hat{H}\left(t\right), \hat{A}\left(t\right)\right]\right] + \left(\frac{i}{\hbar}\right)^2\left[\hat{H}\left(t\right), \left[\frac{\partial \hat{H}\left(t\right)}{\partial t}, \hat{A}\left(t\right)\right]\right] \\
&+ \left(\frac{i}{\hbar}\right)^2\left[\hat{H}\left(t\right), \left[\hat{H}\left(t\right), \frac{\partial \hat{A}\left(t\right)}{\partial t}\right]\right] + \frac{3i}{\hbar}\left[\frac{\partial \hat{H}\left(t\right)}{\partial t}, \frac{\partial \hat{A}\left(t\right)}{\partial t}\right] + \frac{i}{\hbar}\left[\frac{\partial^2 \hat{H}\left(t\right)}{\partial t^2}, \hat{A}\left(t\right)\right] \\
&+ \frac{2i}{\hbar}\left[\hat{H}\left(t\right), \frac{\partial^2 \hat{A}\left(t\right)}{\partial t^2}\right]
\end{aligned} \tag{3}$$

It's clear that we need a more concise way to represent these terms. We can choose not to use the product derivative rule to the commutators. As well, we may be interested in looking at strictly simultaneous eigenstates (where $\left[\hat{H}(t), \hat{A}(t)\right] = 0$), such that we attain a more straightforward expression:

$$\begin{aligned}
\frac{\mathrm{d}^2 \hat{A}(t)}{\mathrm{d}t^2} &= \frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{A}(t)}{\partial t}\right] + \frac{\partial^2 \hat{A}(t)}{\partial t^2} \\
\frac{\mathrm{d}^3 \hat{A}(t)}{\mathrm{d}t^3} &= \left(\frac{i}{\hbar}\right)^2 \left[\hat{H}(t), \left[\hat{H}(t), \frac{\partial \hat{A}(t)}{\partial t}\right]\right] \\
&\quad + \frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial^2 \hat{A}(t)}{\partial t^2}\right] + \frac{i}{\hbar}\frac{\partial\left[\hat{H}(t), \frac{\partial \hat{A}(t)}{\partial t}\right]}{\partial t} + \frac{\partial^3 \hat{A}(t)}{\partial t^3}
\end{aligned} \tag{4}$$

This model is particularly applicable to the time evolution of the Hamiltonian, since $\left[\hat{H}(t), \hat{H}(t)\right] = 0$ trivially. Note that this very specific notation ensures that the Hamiltonian always commutes with itself when the instant is the same (i.e. it is possible for the Hamiltonian to not commute with itself when evaluated at different times). Now imagine a very slowly changing Hamiltonian (which I will broadly classify as "adiabatic change"), such that $\frac{\partial \hat{H}(t)}{\partial t} \sim \lim_{a \to 0} af(at)$, where $f(t)$ is a smooth function. For this model, we shall take $\frac{\mathrm{d}^{\geq 3}\hat{H}(t)}{\mathrm{d}t^{\geq 3}} \approx 0$. It would also be feasible (and albeit, even more restrictive) to apply this same logic to particularly small changes in time. Then:

$$\begin{aligned}
\hat{H}(t+\delta t) &\approx \lim_{\delta t \to 0} \hat{H}(t) + \frac{\mathrm{d}\hat{H}(t)}{\mathrm{d}t}\delta t + \frac{1}{2}\frac{\mathrm{d}^2 \hat{H}(t)}{\mathrm{d}t^2}\delta t^2 \\
\lim_{\delta t \to 0} \frac{\hat{H}(t+\delta t) - \hat{H}(t)}{\delta t} &\approx \lim_{\delta t \to 0} \frac{\partial \hat{H}(t)}{\partial t} + \frac{1}{2}\left(\frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right] + \frac{\partial^2 \hat{H}(t)}{\partial t^2}\right)\delta t \\
\lim_{\delta t \to 0} \frac{\frac{\partial \hat{H}(t+\delta t)}{\partial t} - \frac{\partial \hat{H}(t)}{\partial t}}{\delta t} &\approx \lim_{\delta t \to 0} \frac{1}{2}\left(\frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right] + \frac{\partial^2 \hat{H}(t)}{\partial t^2}\right) \\
\frac{\partial^2 \hat{H}(t)}{\partial t^2} &\approx \frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right] \implies \frac{\mathrm{d}^2 \hat{H}(t)}{\mathrm{d}t^2} \approx \frac{2i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right] \\
\implies \left\langle \frac{\partial^2 \hat{H}(t)}{\partial t^2} \right\rangle &\approx \left\langle \frac{i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right]\right\rangle \text{ and } \left\langle \frac{\mathrm{d}^2 \hat{H}(t)}{\mathrm{d}t^2} \right\rangle \approx \left\langle \frac{2i}{\hbar}\left[\hat{H}(t), \frac{\partial \hat{H}(t)}{\partial t}\right]\right\rangle
\end{aligned} \tag{5}$$

where the fourth line is a particularly interesting expression since though it is only true for $\delta t \to 0$, it is not explicitly dependent on δt. Now we can write a particularly simple approximation for the higher derivatives in the Taylor Series:

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

Now we can begin to examine the expectation value formula in the energy eigenbasis:

$$\begin{aligned}
\langle\psi_m(\mathbf{r},t)|\frac{\partial^2\hat{H}(t)}{\partial t^2}|\psi_n(\mathbf{r},t)\rangle &\approx \frac{i}{\hbar}\langle\psi_m(\mathbf{r},t)|\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]|\psi_n(\mathbf{r},t)\rangle \\
\langle\psi_m(\mathbf{r},t)|\frac{\partial^2\hat{H}(t)}{\partial t^2}|\psi_n(\mathbf{r},t)\rangle &\approx \frac{i}{\hbar}\left((E_m(t)-E_n(t))\langle\psi_m(\mathbf{r},t)|\frac{\partial\hat{H}(t)}{\partial t}|\psi_n(\mathbf{r},t)\rangle\right) \\
\implies \frac{\langle\psi_m(\mathbf{r},t)|\frac{\partial^2\hat{H}(t)}{\partial t^2}|\psi_n(\mathbf{r},t)\rangle}{E_n(t)-E_m(t)}i\hbar &\approx \langle\psi_m(\mathbf{r},t)|\frac{\partial\hat{H}(t)}{\partial t}|\psi_n(\mathbf{r},t)\rangle,\ n\neq m \\
\implies \frac{\langle\psi_m(\mathbf{r},t)|\frac{\partial^2\hat{H}(t)}{\partial t^2}|\psi_n(\mathbf{r},t)\rangle}{(E_n(t)-E_m(t))^2}[\hat{\mathbf{r}},\hat{\mathbf{p}}] &\approx \langle\psi_m(\mathbf{r},t)|\frac{\partial}{\partial t}|\psi_n(\mathbf{r},t)\rangle,\ n\neq m \\
\implies \langle\psi_n(\mathbf{r},t)|\frac{\partial^2\hat{H}(t)}{\partial t^2}|\psi_n(\mathbf{r},t)\rangle &= 0,\ n=m
\end{aligned} \tag{6}$$

where $[\hat{\mathbf{r}},\hat{\mathbf{p}}]=i\hbar$ is the canonical commutation relation that holds at all instances. Thus, under the short time approximation, for well behaved Hamiltonians, the partial second time derivative of the Hamiltonian has vanishing diagonal elements. An interesting inquiry is what other conclusions can be drawn from this approximation. From the previous simple approximation:

$$\begin{aligned}
\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3} &\approx \frac{2i}{\hbar}\left[\hat{H}(t),\frac{\mathrm{d}^2\hat{H}(t)}{\mathrm{d}t^2}\right] = \left(\frac{2i}{\hbar}\right)^2\left[\hat{H}(t),\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right] \\
\frac{\mathrm{d}^4\hat{H}(t)}{\mathrm{d}t^4} &\approx \frac{2i}{\hbar}\left[\frac{\mathrm{d}\hat{H}(t)}{\mathrm{d}t},\frac{\mathrm{d}^2\hat{H}(t)}{\mathrm{d}t^2}\right]+\frac{2i}{\hbar}\left[\hat{H}(t),\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3}\right] \\
&\approx \left(\frac{2i}{\hbar}\right)^2\left[\frac{\partial\hat{H}(t)}{\partial t},\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right]+\left(\frac{2i}{\hbar}\right)^3\left[\hat{H}(t),\left[\hat{H}(t),\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right]\right] \\
\frac{\mathrm{d}^5\hat{H}(t)}{\mathrm{d}t^5} &\approx 2\frac{2i}{\hbar}\left[\frac{\mathrm{d}\hat{H}(t)}{\mathrm{d}t},\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3}\right]+\frac{2i}{\hbar}\left[\hat{H}(t),\frac{\mathrm{d}^4\hat{H}(t)}{\mathrm{d}t^4}\right] \\
&\approx 2\left(\frac{2i}{\hbar}\right)^3\left[\frac{\partial\hat{H}(t)}{\partial t},\left[\hat{H}(t),\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right]\right] \\
&\quad+\left(\frac{2i}{\hbar}\right)^3\left[\hat{H}(t),\left[\frac{\partial\hat{H}(t)}{\partial t}\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right]\right] \\
&\quad+\left(\frac{2i}{\hbar}\right)^4\left[\hat{H}(t),\left[\hat{H}(t),\left[\hat{H}(t)\left[\hat{H}(t),\frac{\partial\hat{H}(t)}{\partial t}\right]\right]\right]\right]
\end{aligned} \tag{7}$$

From these approximations, we can deduce by starting with $\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3}$:

$$\begin{aligned}
\langle\psi_m(\mathbf{r},t)|\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3}|\psi_n(\mathbf{r},t)\rangle &\approx \frac{2i}{\hbar}(E_m(t)-E_n(t))\langle\psi_m(\mathbf{r},t)|\frac{\mathrm{d}^2\hat{H}(t)}{\mathrm{d}t^2}|\psi_n(\mathbf{r},t)\rangle \\
&\approx \left(\frac{2i}{\hbar}\right)^2(E_m(t)-E_n(t))^2\langle\psi_m(\mathbf{r},t)|\frac{\partial\hat{H}(t)}{\partial t}|\psi_n(\mathbf{r},t)\rangle \\
\implies \langle\psi_m(\mathbf{r},t)|\frac{\partial}{\partial t}|\psi_n(\mathbf{r},t)\rangle &\approx -\left(\frac{\hbar}{2}\right)^2\frac{\langle\psi_m(\mathbf{r},t)|\frac{\mathrm{d}^3\hat{H}(t)}{\mathrm{d}t^3}|\psi_n(\mathbf{r},t)\rangle}{(E_n(t)-E_m(t))^3},n\neq m
\end{aligned} \tag{8}$$

This is an interesting investigation, as we can see that there will ultimately be an approximation for the $\langle\psi_m(\mathbf{r},t)|\frac{\partial}{\partial t}|\psi_n(\mathbf{r},t)\rangle$ for every total derivative of the Hamiltonian. This analysis can be further complemented by considering the following Jacobi commutator identity:

$$[A,[B,C]]+[C,[A,B]]+[B,[C,A]]=0 \tag{9}$$

In the next post, I intend to find ways to test these formulas for a slowly changing time dependent Hamiltonian, or at least for a time-dependent Hamiltonian at short time (like in perturbation theory). In fact, it may be worthwhile to solve a simple time-dependent system in full, and then compare the exact results to the approximation. This concludes this blog post.