Time evolution of expectation values

Consider an observable $A$ and its expectation value in the (normalized) state $|\psi\rangle$:

$$\langle A \rangle = \langle \psi | A | \psi \rangle$$

$$\frac{d}{dt} \langle A \rangle = \langle \frac{\partial \psi}{\partial t} | A | \psi \rangle + \langle \psi | \frac{\partial A}{\partial t} | \psi \rangle +$$

$$+ \langle \psi | A | \frac{\partial \psi}{\partial t} \rangle = \langle \psi | (i\hbar)^{-1} H \psi | A | \psi \rangle +$$

$$+ \langle \psi | \frac{\partial A}{\partial t} | \psi \rangle + \langle \psi | A | (i\hbar)^{-1} H \psi \rangle =$$

$$= \langle \psi | \frac{\partial A}{\partial t} | \psi \rangle - (i\hbar)^{-1} \langle \psi | HA | \psi \rangle + \langle \psi | AH | \psi \rangle$$

$$(+i\hbar)^{-1} = \langle \psi | \frac{\partial A}{\partial t} | \psi \rangle + (i\hbar)^{-1} \langle \psi | [A, H] | \psi \rangle$$

$$= \langle \frac{\partial A}{\partial t} \rangle - \frac{i}{\hbar} \langle [A, H] \rangle \Rightarrow$$
If $A$ does not depend explicitly on time $\Rightarrow$

$$\frac{d}{dt} \langle A \rangle = -\frac{i}{\hbar} \langle [A,H] \rangle \Rightarrow \text{if} \ [A,H] = C$$

$A$ is a constant of the motion

Example: Let $A = H \neq H(t)$

$$\frac{d}{dt} \langle H \rangle = -\frac{i}{\hbar} \langle [H,H] \rangle = 0 \Rightarrow \text{total energy is a constant of motion}$$

Note:
Consider an arbitrary observable $B$ such as $[B,H] \neq 0$ (generally).
Now find the expectation value of $B$ in the state $\psi_k$ which is an eigenstate of $H$:

$$\langle \psi_k | B | \psi_k(t) \rangle = \langle \psi_k | e^{i\frac{B}{\hbar}t} B e^{-i\frac{B}{\hbar}t} | \psi_k \rangle =$$

$$\langle \psi_k | B | \psi_k \rangle = \langle \psi_k | e^{i\frac{B}{\hbar}t} B e^{-i\frac{B}{\hbar}t} | \psi_k \rangle =$$

Consider $\langle [B,H] \rangle = 0$, the expectation value with respect to the energy eigenstate is time-independent.
energy eigenstate is a stationary state.

For an arbitrary state \( |\alpha, t_0 = 0\rangle = \sum_n c_n |\psi_n\rangle \),

\[
|\beta\rangle = \left( \sum_n c_n^* (0) \frac{e^{i E_n t}}{\sqrt{E_n}} \right) |\psi_n\rangle
\]

\[
|\alpha, t_0 = 0; t\rangle = \sum_n c_n (0) e^{-\frac{i}{\hbar} E_n t} |\psi_n\rangle
\]

\[
\langle \alpha, t_0 = 0; t | = \sum_n c_n^* (0) e^{\frac{i}{\hbar} E_n t} \langle \psi_n |\psi_m \rangle
\]

\[
C_n (0) e^{-\frac{i}{\hbar} E_n t} \left\{ \begin{array}{c}
\end{array} \right. \sum_{m,n} C_m^* (0) c_n (0) \langle \psi_m |\beta |\psi_n \rangle
\]

\[
e^{-\frac{i}{\hbar} (E_n - E_m)t} \uparrow \text{ in a general case of a nonstationary state} \Rightarrow \langle \beta | \text{ is a function of time} \rangle
\]

\[
\therefore \text{a collection of terms oscillating with Bohr frequency } \omega_{nm} = \frac{E_n - E_m}{\hbar}
\]
The Virial Theorem

Consider a particle of mass $M$ moving in a potential $\mathbf{V}(\mathbf{r}) \Rightarrow H = \frac{\mathbf{p}^2}{2m} + \mathbf{V}(\mathbf{r})$

Consider a time-independent operator $A = \mathbf{r} \cdot \mathbf{p}$

Then, for the stationary states of $H \Rightarrow$

$$\frac{d}{dt} \langle \Psi \mid A \mid \Psi \rangle = 0 \Rightarrow \mathbf{H} \mid \Psi \rangle = E \mid \Psi \rangle \quad \langle [A, H] \rangle = 0$$

Let's find $[A, H] = [r \cdot p, H] = [r \cdot p, \frac{\mathbf{p}^2}{2m} + \mathbf{V}(x, y, z)]$

$$= \left[ xp_x + yp_y + zp_z, \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) \right] = 2i\hbar \mathbf{T} - i\hbar \mathbf{r} \cdot \nabla \mathbf{V}, \text{ where } T = \frac{\mathbf{p}^2}{2m} < \text{kinetic energy operator}$$

Show at homework!

So, for a stationary state $\Rightarrow 2i\hbar \langle T \rangle = i\hbar \langle \mathbf{r} \cdot \nabla \mathbf{V} \rangle$

$$\langle T \rangle = \langle \mathbf{r} \cdot \nabla \mathbf{V} \rangle$$

virial theorem
Consider a quantum system in 1D with a time-independent potential $V(x)$. The system is described by a wave function $\psi(x,t)$, which doesn't have to be an eigenstate. Consider the expectation value $\langle x \rangle (t)$ and a term that depends on $V(x)$.

\[
\frac{d}{dt} \langle x \rangle = -i \frac{\hbar}{\langle x \rangle} \langle [xp, H] \rangle
\]

$H = \frac{p^2}{2m} + V(x)$

$[xp, H] = x[p, H] + [x, H]p$

$[p, H] = [p, \frac{p^2}{2m} + V(x)] = [p, V(x)] = -i \hbar \frac{d}{dx} V(x)$

$[i \hbar \frac{d}{dx}, V(x)] f(x) = -i \hbar \frac{d}{dx} (Vf) + V(x) \cdot i \hbar \frac{df}{dx} = -i \hbar (Vf + Vf') + i \hbar Vf' = -i \hbar \frac{d}{dx} V f(x)$

$[p, V(x)] = -i \hbar \frac{dV}{dx}$
\[
\{ x_1, H \} = \{ x_1, \frac{p^2}{2m} + V(x) \} = \{ x_1, \frac{p^2}{2m} \} = \frac{\hbar}{2m} \left( \{ x_1, p \} \right) = \frac{i \hbar}{m} p
\]

So,
\[
\{ xp, H \} = x \cdot \left( -i \hbar \frac{dV}{dx} \right) + \frac{i \hbar}{m} p^2
\]

Then,
\[
\frac{d}{dt} \langle xp \rangle = \langle \{ xp, H \} \rangle = \left( \frac{\hbar}{m} \right) \langle p^2 \rangle - \langle x \frac{dV}{dx} \rangle
\]

\[
= \left( \frac{\hbar}{m} \right) \langle p^2 \rangle - \langle x \frac{dV}{dx} \rangle
\]

\[
= \left( \frac{\hbar}{m} \right)^2 \langle T \rangle
\]

Note: if \( \psi(x,t) \) which describes the state of the system were an eigenstate of \( H \), then \( \frac{d}{dt} \langle xp \rangle = 0 \)

Consider a potential \( V(x) = V_0 x^n \) and assume that the system is in an eigenstate with energy \( E_j \). Find the expectation value of the potential in this state \( V_j = \langle V \rangle_j \)
Since we are in an eigenstate \( \Rightarrow \)
\[
\frac{d}{dt} \langle x p \rangle = 0 \Rightarrow 2 \langle T \rangle_j - \langle x \frac{dV}{dx} \rangle_j = 0
\]

\[
2 \langle T \rangle_j = \langle x \cdot hV_n x^{n-1} \rangle_j = \langle hV_n x^n \rangle_j = \langle hV(x) \rangle_j
\]

Since \( E_j = \langle T \rangle_j + \langle V \rangle_j \Rightarrow \)
\[
2 (E_j - \langle V \rangle_j) = h \langle V_{\phi} \rangle_j \Rightarrow
\]

\[
\langle V \rangle_j = \frac{2E_j}{h+2}
\]

Comp. exam problem in 10 min \( \Rightarrow \) solved!
Problem 7.

Consider a quantum system in one dimension, with a time independent potential $V(x)$. The system is described by a wave function $\psi(x, t)$, which does not have to be an eigenstate. Consider the expectation value of the product of position and momentum for this system, i.e. $\langle xp \rangle (t)$, as a function of time. The quantum virial theorem relates the time derivative of this quantity, $\frac{d}{dt} \langle xp \rangle (t)$, to expectation values of the kinetic energy and a term which depends on the potential. Derive such a relation.

Consider a potential $V(x) = V_n x^n$, and assume that the system is in an eigenstate $j$ with energy $E_j$. Show that in this case the expectation value of the potential is given by $\frac{2n}{n+2} E_j$. One may assume that $n$ is a positive, even number and that $V_n > 0$.

Problem 8.

One way to attempt nuclear fusion is to use magnetic confinement to raise the pressure of a hot plasma. Consider a modest model of this process, consisting of only a very thin-walled, hollow conducting tube of radius $R$ through which current $I$ is driven. When $I$ is sufficiently large, the tube can be crushed.

1. For a tube oriented along $\hat{z}$, find $\bar{E}(\rho, \phi, z)$ inside and outside the tube.

2. Determine the inward pressure on the tube. One approach to this problem is to orient the tube along $\hat{z}$ and calculate the total force in the $\hat{z}$ direction on one side of the tube.

3. How does the pressure change as the tube collapses?