Heisenberg's Equation of Motion

[Gottfried 2.4]

Consider TDSE (time-dependent Schrodinger's eq.):

$$i \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

Assuming $\hat{H}$ is independent of time, the solution is $|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(t=0)\rangle$.

This implies that the expectation value of an operator $\hat{O}$ at time t is:

$$\langle \hat{O} \rangle (t) = \langle \psi(t) | \hat{O} | \psi(t) \rangle$$

$$= \langle \psi(t=0) | \underbrace{e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t}}_{\hat{O}(t)} | \psi(t=0) \rangle$$

$$= \langle \psi(t=0) | \hat{O}(t) | \psi(t=0) \rangle.$$

The operator $\hat{O}(t) = e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t}$ is called "Heisenberg evolved operator", the same way as $|\psi(t)\rangle$ is called "Schrodinger-evolved state".

Therefore, there are two ways to calculate $\langle \hat{O} \rangle (t)$:

(a) Evolve $|\psi(t=0)\rangle$ to $|\psi(t)\rangle$ using TDSE and calculate $\langle \psi(t) | \hat{O} | \psi(t) \rangle$ where $\hat{O}$ is time-independent. This is called "Schrodinger's picture".

(b) Alternatively, don't evolve $|\psi\rangle$, and instead evolve the operator $\hat{O}$ as

$$\hat{O}(t) = e^{iHt} \hat{O} e^{-iHt}$$

and calculate

$$\langle \psi(t=0) | \hat{O}(t) | \psi(t=0) \rangle .$$

This is called "Heisenberg picture".

Of course, both methods give the same answer for any physical property (e.g. $\langle \hat{O} \rangle (t)$), but depending on the context, one method might be more convenient over other.

The Heisenberg evolution of operator can also be written in a differential form:

$$\frac{d\hat{O}(t)}{dt} = i\hat{H}\, e^{i\hat{H}t}\,\hat{O}(0)\, e^{-i\hat{H}t} + e^{i\hat{H}t}\,\hat{O}(0)\, e^{-i\hat{H}t}\,(-i\hat{H})$$

$$= i\hat{H}\,\hat{O}(t) - i\,\hat{O}(t)\,\hat{H}$$

$$= i\,[\hat{H}, \hat{O}(t)]$$

This is called <u>Heisenberg's eqn of motion</u>. (analog of TDSE for operators).

Since $\hat{H}$ commutes with itself $\Rightarrow$ $\hat{H}(t) = \hat{H}(t=0)$. Therefore, in the above equation one may replace $\hat{H}$ $(= \hat{H}(t=0))$ with $\hat{H}(t)$.

Let's consider a few examples...

(1) A non-relativistic particle in a potential

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

$$\frac{d\hat{x}(t)}{dt} = -i\left[\hat{x}(t), \frac{\hat{p}^2(t)}{2m} + V(\hat{x}(t))\right]$$

Importantly, the commutation relations are unchanged under the Heisenberg evolution:

$$[x(t), p(t)]$$

$$= e^{iHt} x(0) e^{-iHt} \; e^{iHt} p(0) e^{-iHt}$$

$$- e^{iHt} p(0) e^{-iHt} \; e^{iHt} x(0) e^{-iHt}$$

$$= e^{iHt} (x(0) p(0) - p(0) x(0)) e^{-iHt}$$

$$= e^{iHt} \, i \, e^{-iHt} = i$$

Therefore :

$$\frac{d\hat{x}(t)}{dt} = -i\left[\hat{x}(t), \frac{\hat{p}^2}{2m}\right] - i\,\cancelto{0}{\left[\hat{x}(t), V(\hat{x}(t))\right]}$$

$$= \frac{\hat{p}(t)}{m}$$

(note that this resembles velocity $= \frac{\text{momentum}}{\text{mass}}$)

Similarly,

$$\frac{d\hat{p}(t)}{dt} = -i\,\cancelto{0}{\left[\hat{p}(t), \frac{\hat{p}^2(t)}{2m}\right]} - i\left[\hat{p}(t), \hat{V}(\hat{x}(t))\right]$$

$$= -i \cdot -i \frac{\partial \hat{V}(\hat{x}(t))}{\partial \hat{x}(t)} = -\frac{\partial \hat{V}(\hat{x}(t))}{\partial \hat{x}(t)}$$

Combining the two equations,

$$m\frac{d^2\hat{x}}{dt^2} = \frac{d\hat{p}(t)}{dt} = -\frac{\partial \hat{V}(\hat{x}(t))}{\partial \hat{x}(t)}$$

which resembles Newton's equation of motion since $-\frac{\partial \hat{V}}{\partial x} \sim$ force.

However, this parallel with Newton's laws is somewhat misleading, because classical equations of motion would be

$$m\frac{d^2 x(t)}{dt^2} = -\frac{\partial V(x(t))}{\partial x(t)}$$

where $x(t)$ is a <u>number</u> and not an operator. To make correspondence with Heisenberg's equation, the most natural meaning of $x(t)$ would be

$x(t) = \langle \psi(0) | \hat{x}(t) | \psi(0) \rangle$ i.e. the expectation value of $\hat{x}$ operator at time t. Therefore lets consider taking expectation value w.r.t. $|\psi(0)\rangle$ in

$$m\frac{d^2 \hat{x}}{dt^2} = -\frac{\partial \hat{V}(\hat{x}(t))}{\partial \hat{x}(t)}$$

The LHS is $\langle\psi(0)|\, m\dfrac{d^2\hat{x}(t)}{dt^2}\,|\psi(0)\rangle$

$= m\dfrac{d^2x(t)}{dt^2}$ where $x(t) = \langle\psi(0)|\hat{x}(t)|\psi(0)\rangle$

The RHS is $\langle\psi(0)|\, -\dfrac{\partial\hat{V}(\hat{x}(t))}{\partial\hat{x}(t)}\,|\psi(0)\rangle$.

This <u>does not</u> equal $-\dfrac{\partial\hat{V}(x(t))}{\partial x(t)}$ where

$x(t) = \langle\psi(0)|\hat{x}(t)|\psi(0)\rangle$ generically.

Only when the "force operator" $-\dfrac{\partial V(\hat{x})}{\partial\hat{x}}$

is <u>linear</u> in $\hat{x}$ (e.g. simple harmonic

oscillator), $\langle\psi(0)|\, -\dfrac{\partial\hat{V}(\hat{x}(t))}{\partial\hat{x}(t)}\,|\psi(0)\rangle = -\dfrac{\partial V(x(t))}{\partial x(t)}$

To see the deviation from Newton's

laws, let's Taylor expand $-\dfrac{\partial\hat{V}(\hat{x}(t))}{\partial\hat{x}(t)}$

around $\hat{x}(t) = x(t)\,\mathbb{1} \equiv x(t)$

$= \langle\psi(0)|\hat{x}(t)|\psi(0)\rangle\,\mathbb{1}$.

$$\hat{F}(\hat{x}(t)) \left(= -\frac{\partial \hat{V}(\hat{x}(t))}{\partial \hat{x}(t)} \right)$$

$$= \underbrace{\hat{F}(x(t))}_{=F(x(t))} + \frac{\partial \hat{F}(\hat{x}(t))}{\partial \hat{x}(t)}\bigg|_{\hat{x}(t)=x(t)} (\hat{x}(t) - x(t))$$

$$+ \frac{1}{2} \frac{\partial^2 \hat{F}(\hat{x}(t))}{\partial \hat{x}^2(t)}\bigg|_{\hat{x}(t)=x(t)} [\hat{x}(t) - x(t)]^2 + \dots$$

Again taking the expectation value of Heisenberg eq.

$$\langle \psi(0) | \, m \frac{d^2 \hat{x}(t)}{dt^2} | \psi(0) \rangle = \langle \psi(0) | \hat{F}(\hat{x}(t)) | \psi(0) \rangle$$

and using the above Taylor expansion for $\hat{F}(\hat{x}(t))$ $\Rightarrow$

$$m \frac{d^2 x(t)}{dt^2} = \langle \psi(0) | F(x(t)) | \psi(0) \rangle$$

$$+ \frac{\partial \hat{F}(\hat{x}(t))}{\partial \hat{x}(t)}\bigg|_{\hat{x}(t)=x(t)} \cancelto{0}{[\langle \psi(0) | \hat{x}(t) | \psi(0) \rangle - x(t)]}$$

$$+ \frac{1}{2} \frac{\partial^2 \hat{F}(\hat{x}(t))}{\partial \hat{x}^2(t)}\bigg|_{\hat{x}(t)=x(t)} \langle \psi(0) | (\hat{x}(t) - x(t))^2 | \psi(0) \rangle$$

$$= F(x(t)) + \underbrace{\frac{1}{2}\frac{\partial^2 F(x(t))}{\partial x(t)^2}}_{\text{a number}} \langle\psi(0)|(\hat{x}(t) - x(t))^2|\psi(0)\rangle$$

Therefore if $\frac{\partial^2 F(x)}{\partial x^2}$ is not zero, one obtains corrections to Newton's laws of motion.

Let's study the case of SHO (simple harmonic oscillator) explicitly. Based on above discussion, here we expect that expectation value of operators satisfy Newton's laws.

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

$$\Rightarrow \quad \frac{d\hat{a}(t)}{dt} = i\left[a^\dagger(t)\, a(t) + \frac{1}{2} , a(t) \right]$$

$$= i\, a(t)$$

$$\Rightarrow \quad \hat{a}(t) = e^{-it}\, \hat{a}(t=0)$$

Using $\hat{a}(t) = [\hat{x}(t) + i\,\hat{p}(t)]/\sqrt{2}$,

$$\Rightarrow \quad \hat{x}(t) = \hat{x}(0)\cos(t) + \hat{p}(0)\sin(t)$$

$$\hat{p}(t) = \hat{p}(0)\cos(t) - \hat{x}(0)\sin(t)$$

Putting back units of m, ω :

$$\hat{x}(t) = \hat{x}(0)\cos(\omega t) + \frac{\hat{p}(0)}{m\omega}\sin(\omega t)$$

$$\hat{p}(t) = \hat{p}(0)\cos(\omega t) - m\omega\,\hat{x}(0)\sin(\omega t).$$

Taking expectation value w.r.t. $|\psi(0)\rangle \Rightarrow$

$$x(t) = \langle\psi(0)|\,\hat{x}(t)\,|\psi(0)\rangle$$

$$= x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t)$$

$$p(t) = p(0)\cos(\omega t) - m\omega\, x(0)\sin(\omega t)$$

Therefore, expectation values satisfy Newton's laws as expected (since

$$\underset{\text{operator}}{\text{Force}} = -\frac{\partial V(\hat{x})}{\partial \hat{x}} = -\hat{x} \text{ is linear in } \hat{x}).$$

However, quantum mechanics still matters. For example, $[\hat{x}(t), \hat{x}(0)] \neq 0$.

In particular, using above result,

$$[\hat{x}(t), \hat{x}(0)] = \frac{[\hat{p}(0), \hat{x}(0)]}{m\omega}\sin(\omega t) = \frac{\hbar}{i}\frac{\sin(\omega t)}{m\omega}$$

where we have put back $\hbar$ to show that this is a quantum effect.