Ehrenfest's Theroem

In the lecture notes for the harmonic oscillator we derived the expressions for $\langle\hat{x}\rangle(t)$ and $\langle\hat{p}_x\rangle(t)$ using standard approaches – integrals involving Hermite polynomials (see pages 17 and 18, Lecture Summary 12-15). The calculations are algebraically intensive, but showed that $\langle\hat{x}\rangle(t)$ and $\langle\hat{p}_x\rangle(t)$ oscillate at the vibrational frequency. The results were as follows:

$$\langle x\rangle(t) = (2\alpha)^{-1/2}\cos(\omega_{vib}t) = \left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\cos(\omega_{vib}t)$$

and

$$\langle p\rangle(t) = \frac{1}{2}\left[i\hbar\left(\frac{\alpha}{2}\right)^{1/2}\left(e^{i\omega_{vib}t} - e^{-i\omega_{vib}t}\right)\right] = -\left(\frac{\hbar\mu\omega}{2}\right)^{1/2}\sin(\omega_{vib}t)$$

The issue considered here is an approach to calculate $\langle x\rangle(t)$ and $\langle p\rangle(t)$ in a more straightforward manner.

Classically, (we use *m* instead of μ since we are dealing with a free particle)

$$p = mv = m\frac{dx}{dt}$$

So, quantum mechanically we might expect

$$\langle p\rangle(t) = m\frac{d\langle x\rangle(t)}{dt}.$$

But, is this expression valid ? We can show that in fact it is with the following argument.

For $\frac{d\langle x\rangle(t)}{dt}$ our original expression was ...

$$\frac{d\langle x\rangle(t)}{dt} = \frac{d}{dt}\left\{\int_{-\infty}^{\infty}\psi^*\hat{x}\psi\,dx\right\} = \int_{-\infty}^{\infty}\frac{d\psi^*}{dt}\hat{x}\psi\,dx + \int_{-\infty}^{\infty}\psi^*\hat{x}\frac{d\psi}{dt}dx$$

Recall the time dependent Schrödinger equation is

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \qquad or \qquad \frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}H\psi$$

Inserting these results into the expression above yields

$$\frac{d\langle x\rangle(t)}{dt} = -\frac{1}{i\hbar}\int_{-\infty}^{\infty}\left(\hat{H}\psi\right)^{*}\hat{x}\psi\,dx + \frac{1}{i\hbar}\int_{-\infty}^{\infty}\psi^{*}\hat{x}\left(\hat{H}\psi\right)dx$$

$$= \frac{1}{i\hbar}\int_{-\infty}^{\infty}\psi^{*}\left(\hat{x}\hat{H}-\hat{H}\hat{x}\right)\psi\,dx \;= \frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^{*}\left(\hat{H}\hat{x}-\hat{x}\hat{H}\right)\psi\,dx$$

Evaluating the commutator (assuming that H is the HO Hamiltonian) we find …

$$\left(\hat{H}\hat{x}-\hat{x}\hat{H}\right)f(x) = \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+U(x)\right)\hat{x}\,f(x) - \hat{x}\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+U(x)\right)f(x)$$

$$= -2\frac{\hbar^2}{2\mu}\frac{df}{dx} = -\frac{\hbar^2}{\mu}\left(\frac{i}{\hbar}\hat{p}_x\right) = -\frac{i\hbar}{\mu}\hat{p}_x$$

And therefore

$$\frac{d\langle x\rangle(t)}{dt} = \frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^{*}\left(\hat{H}\hat{x}-\hat{x}\hat{H}\right)\psi\,dx = \frac{1}{m}\int_{-\infty}^{\infty}\psi^{*}\hat{p}_x\,\psi\,dx$$

Which is the result that is desired

$$\boxed{\langle\hat{p}_x\rangle(t) = \mu\frac{d\langle x\rangle(t)}{dt}}$$

Thus, we can now obtain $\langle\hat{p}_x\rangle(t)$ without the lengthy calculation contained in the HO lecture notes.

$$\langle\hat{p}_x\rangle(t) = \mu\frac{d\langle x\rangle(t)}{dt} = \mu\frac{d}{dt}\left\{\left(\frac{\hbar}{2\mu\omega}\right)^{1/2}\cos(\omega t)\right\} = -\left(\frac{\mu\omega\hbar}{2}\right)^{1/2}\sin(\omega t)$$

$$\boxed{\langle\hat{p}_x\rangle(t) = -\left(\frac{\mu\omega\hbar}{2}\right)^{1/2}\sin(\omega t)}$$

which is the result with which we started initially.

The equations above are a specific illustration of a more general result due to Paul Ehrenfest (an Austrian physicst who later resided in Leiden, The Netherlands) and known as *Ehrenfest's Theorem*. In particular, for any dynamical variable *F*

$$\frac{d\langle F\rangle(t)}{dt}=\frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^{*}\left(\hat{H}\hat{F}-\hat{F}\hat{H}\right)\psi\,dx$$

For further information see McQuarrie Problems 4-43 and 4-44, p 187-188.