QUANTUM MECHANICS 2 - WORKSHOP 6

Q1: In terms of the Hamiltonian operator H Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi.$$

Now, consider the rate of change of the expectation value of some measurable quantity Q

$$\frac{d\langle Q\rangle}{dt} \equiv \frac{d}{dt}\int \psi*(x)Q\psi(x)\,dx = \int \left(\left(\frac{\partial\psi^*}{\partial t}\right)Q\psi + \psi^*\frac{\partial Q}{\partial t}\psi + \psi^* Q\left(\frac{\partial\psi}{\partial t}\right)\right)\,dx$$

(we use partial time derivatives $\partial/\partial t$ to remind us that if, e.g., we are considering the motion of a 1D particle in x, we are only differentiating with respect to t, and not with respect to the coordinate x — however in expectation values, x is no longer "there" as it has already been integrated over, and we use ordinary time derivatives d/dt).[1]

(a) By taking the complex conjugate of Schrödinger's equation and making use of the fact that H is Hermitian , i.e.

$$\int H^* f(x)^* g(x)\,dx = \int f(x)^* H g(x)\,dx$$

show that

$$\frac{d\langle Q\rangle}{dt} = \frac{i}{\hbar}\langle [H,Q]\rangle + \left\langle \frac{\partial Q}{\partial t}\right\rangle.$$

(b) Set $Q = x$ and $H = p^2/2m + V(x)$. Show that $[H,x] = -i\hbar p/m$, and therefore that the expression in (b) implies $d\langle x\rangle/dt = \langle p\rangle/m$. This is what we expect from classical physics (Ehrenfest theorem — see lecture 3).

(c) Set $Q = xp$ and $H = p^2/2m + V(x)$. Show that $[H,xp] = -(i\hbar/m)p^2 + x(i\hbar dV/dx)$, and therefore that the expression in (b) implies $d\langle xp\rangle/dt = 2\langle T\rangle - \langle x dV/dx\rangle$.

(d) In steady state $d\langle xp\rangle/dt = 0$. Find a relation for $\langle T\rangle$ in terms of dV/dx. This is the *virial theorem* in 1D Cartesian coordinates, and is useful, as calculating dV/dx is typically more straightforward than calculating $\langle T\rangle$, which by default involves integrating over an expression involving a second order differential operator.

[1] Surprising though it may sound, the notational choice of whether to use ordinary derivatives (d/dt) or partial derivatives ($\partial/\partial t$) is quite variable in practice. Probably more usual, in fact, is

$$i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle; \qquad \frac{d\langle Q\rangle}{dt} \equiv \frac{d}{dt}\langle\psi|Q|\psi\rangle = \left(\frac{d\langle\psi|}{dt}\right)Q|\psi\rangle + \langle\psi|\frac{\partial Q}{\partial t}|\psi\rangle + \langle\psi|Q\left(\frac{d|\psi\rangle}{dt}\right).$$

With regard to $|\psi\rangle$ or $\langle\psi|$, the rationale (beyond the scope of the course) is that no representation involving another continuous variable is specified in Dirac notation, and so partial derivatives are unnecessary. With regard to the operator Q (again beyond the scope of the course), the partial derivative emphasises that the only relevant time dependence is in the operator's *definition*, e.g., if $Q = x\sin(\omega t)$, $\partial Q/\partial t = \omega x\sin(\omega t)$, but x itself is not considered to change (at least not in the *Schrödinger picture*, which we are assuming in this course).