Quantum Mechanics PHYS2B22
Problem Sheet 4

Work in by Monday March 21st <u>AT THE LATEST</u>

NB: This is an absolute deadline because I have to get final marks in before the end of term.

1) From the definition of a Hermitian operator $\hat{O}$, show that the quantity $I = \int_{-\infty}^{\infty} dx\ \psi^*(\hat{O}\psi)$ is real for any function $\psi(x)$. [**5**]

2) By considering how it acts on an arbitrary function, show that the commutator of the momentum and potential energy operators in 1D is [**3**]

$$\left[\hat{p}, \hat{V}(x)\right] = -i\hbar \frac{dV}{dx}.$$

Hence, if the Hamiltonian is $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, show that the time evolution of the expectation value of the momentum satisfies [**5**]

$$\frac{d\langle \hat{p}\rangle}{dt} = -\left\langle \frac{dV}{dx} \right\rangle.$$

How does this result relate to the motion of the particle that you would expect in classical physics? [**2**]

3) What is the atomic unit of time? Give an expression for it in terms of fundamental constants and a value in seconds. [**5**]

4) Show, starting from the series solution derived in the lectures, that in atomic units the radial part of the solution to the time-independent Schrödinger equation for the 2p state of hydrogen ($Z = 1$, $n = 2$, $l = 1$) is

$$R_{21}(r) = cr\exp(-r/2)$$

where c is a constant. [**3**] Use the normalization condition to show that $|c|^2 = 1/24$. [**5**]

Hence write down the probability per unit length of finding the electron at a distance r from the nucleus. [**2**] At what value of r is the electron *most likely* to be found? [**4**] At what distance will it be found *on average* (i.e. what is $\langle r\rangle$)? [**4**] Compare your results with the distance from the nucleus of the $n = 2$ orbit in the Bohr model. [**2**]

[Hint: You may use the result $\int_0^{\infty} r^p \exp(-ar)dr = p!/a^{p+1}$.]

PTO

5) **For discussion only (no marks)**. In atomic units, the effective potential for radial motion in a hydrogenic atom with angular momentum quantum number l is

$$V_{\text{eff}}(r) = -\frac{Z}{r} + \frac{l(l+1)}{2r^2}$$

Except for $l = 0$, this potential has a well-defined minimum value V_{min}. What is this minimum value and at what distance r from the origin does it occur? Compare V_{min} with the energy of the lowest energy eigenfunction having angular momentum quantum number l. Hence give a reason why the principal quantum number n must satisfy $n > l$.