Advanced Atomic and Molecular Physics 2017-05-08 Prof. Heyne 2. assignment

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Deadline: lecture next Monday (2017-05-15)

1. For the harmonic oscillator, for $n = 1, 2, \ldots$, it is

$$a^+ a\psi_n = -2n\psi_n$$

   (a) (2 points) Show that for quadratically integrable functions ψ and φ that

$$\int \left(a^+\varphi\right)^* \psi \mathrm{d}y = -\int \varphi^* a\psi \mathrm{d}y$$

   by partial integration and

$$\int \left(a^+\psi_n\right)^* \left(a^+\psi_n\right) \mathrm{d}y = 2(n+1) \int \psi_n^* \psi_n \mathrm{d}y$$

   (b) (2 points) Use the results of a) for normalized ψ_n to show

$$\psi_{n+1} = \frac{1}{\sqrt{2(n+1)}} a^+\psi_n \quad \text{and} \quad a\psi_n = -\sqrt{2n}\psi_{n-1}.$$

   (c) (3 points) Show that the transition probability from $\psi_n \to \psi_m$ is proportional to the square of the matrix element

$$\int \psi_m^* x \psi_n \mathrm{d}y = \sqrt{\frac{\hbar}{m\omega}} \int \psi_m^* y \psi_n \mathrm{d}y = \sqrt{\frac{\hbar}{m\omega}} \int \psi_m^* \left(\frac{a - a^+}{2}\right) \psi_n \mathrm{d}y.$$

   Use b) to prove that the transition probability is only unequal zero for $m = n \pm 1$ (selection rule) and that

$$\left|\int \psi_{n+1}^* x \psi_n \mathrm{d}y\right|^2 = \frac{(n+1)\hbar}{2m\omega}$$
$$\left|\int \psi_{n-1}^* x \psi_n \mathrm{d}y\right|^2 = \frac{n\hbar}{2m\omega}$$

2. (a) (2 points) Calculate the 5 spherical harmonics of Y_{lm} using the L_- operator starting at Y_{22} and determine the normalization constants.

   (b) (2 points) Calculate the expectation value $\langle r \rangle$ in the state $n = 3$ and $l = 2$ of the hydrogen atom.

   (c) (3 points) Use the variational method with the test function $e^{-\alpha r}$ to estimate the energy E_0 of the hydrogen atom. Show for the solution $\langle T \rangle = -1/2 \langle V \rangle$.