

Structuur der Materie: Atoms and Molecules

werkcollege-opgaven

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Gebruik Mathematica op je computer !

Numerical treatment of the Schrödinger wave functions for the hydrogen atom and calculation of spectral line intensities in the framework of quantum mechanics

The general solution for the wave function of the hydrogen atom is:

$$\Psi_{n\ell m}(r, \theta, \phi) = \frac{u_{n,\ell}(r)}{r} Y_{\ell m}(\theta, \phi)$$

With the radial part (You may choose to fill in $Z=1$ and $a=a_0$), the general solution from the radial Schrödinger equation:

$$u_{n\ell}(r) = \sqrt{\frac{2Z}{na}} \sqrt{\frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{-Zr/na} \left(\frac{2Zr}{na}\right)^{\ell+1} L_{n-\ell-1}^{2\ell+1}\left(\frac{2Zr}{na}\right)$$

Find and define representations in the framework of Mathematica of the **Spherical harmonics** $Y_{\ell m}$, the **Laguerre functions** L , and the radial functions $u_{n\ell}$, or the functions $R_{n\ell}=u_{n\ell}/r$. Note that in Mathematica several forms of Laguerre polynomial functions are defined; you will need the generalized ones (with a superscript, a subscript and an argument).

Reduce this representation to find a radial wave functions for $u(1s)$.

Verify (in between) also that $u(1p)$ is not a valid representation.

Construct a general radial wave function for $u(np)$, so for arbitrary n quantum number.

Hint p means $l=1$ (a p -wave function).

You may include in these wave functions also the angular part by multiplying with the appropriate $Y_{\ell m}$. But as you will find out the intensities of the $1s \rightarrow np$ (Lyman) series in hydrogen are not affected by this (if you simply stick to the z -operator, which physically can be interpreted as linear polarization of the absorbing electromagnetic field).

Calculate the intensity of the Lyman series in hydrogen. Those are transitions originating in the $1s$ ground state of the atom (hence choose, $n=1$, $l=0$, $m=0$) and the levels np .

You may choose linear polarization along the z -axis, hence (n is kept as a variable in the excited state, $l=1$, and $m=0$). By this means you can simplify the equation by fixing the angular part to a constant.

The intensity in quantum mechanics is given by the so-called matrix element of the transition electric dipole moment:

$$I \propto \left| \langle \Psi_{1s} | z | \Psi_{np} \rangle \right|^2$$

The writing of this matrix element requires some explanation. It means:

$$\langle \Psi_f | f(\vec{r}) | \Psi_i \rangle = \int_{space} \Psi_f^* f(\vec{r}) \Psi_i d\Omega$$

Note that the integral must be taken over all space, for which we give a hint and a warning:

Hint: do not forget the Jacobian if you use a certain coordinate system.

Warning: the radial coordinate in spherical coordinates extends only over $[0, \infty)$, while a vector \mathbf{r} extends over $(-\infty, \infty)$ in three dimensions.

Go as far as possible in simplifying your result. Try to establish the intensity behavior at large n values. Hint: Do not forget to take the square of the matrix element.

Verify that this result scales approximately as $I \propto n^{-3}$

Good luck !!!