Karlsruhe Institute of Technology (KIT) SS 2010
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Boundary and Eigenvalue Problems: 14th problem sheet

Preliminaries: Associated Legendre and Laguerre Polynomials

- One family of solutions of the differential equations

  $$xz'' + (k+1-x)z' + nz = 0, \qquad k,n \in \mathbb{N}_0,\ k \le n$$

  is given by the so-called *associated Laguerre polynomials*

  $$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x)$$

  where $L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})$ denote the *Laguerre polynomials.*

- One family of solutions of the differential equations

  $$(1-x^2)y'' - 2xy' + \Big(l(l+1) - \frac{m^2}{1-x^2}\Big)y = 0, \qquad m,l \in \mathbb{N}_0,\ m \le l$$

  is given by the so-called *associated Legendre polynomials*

  $$P_n^{(m)}(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_n(x)$$

  where $P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n$ denote the *Legendre polynomials.*

Our aim is to determine nontrivial classical solutions of the linear time-independent Schrödinger equation

$$\frac{\hbar^2}{2m_e}\Delta u + V(x)u = \lambda u \tag{LS}$$

for the hydrogen atom with potential $V(x) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|x|}$. Here, $\hbar$ is the Planck constant, e the charge of an electron, m_e its mass and λ describes the energy level of an electron. We will use separation of variables.

Exercise:

a) Define $\tilde{u}, \tilde{\lambda}$ in such a way that (LS) becomes $\Delta\tilde{u} + \big(\frac{1}{|x|} - \tilde{\lambda}\big)\tilde{u} = 0$ for $x \in \mathbb{R}^3$.

b) Assume $\tilde{u}(x, y, z) = R(r)\Theta(\theta)T(t)$ in 3D polar coordinates (r, θ, t) as defined on exercise sheet 11. Show that there are constants $\mu, \sigma \in \mathbb{R}$ such that

$$R'' + \frac{2}{r}R' + \big(-\tilde{\lambda} + \frac{1}{r} - \frac{\mu}{r^2}\big)R = 0 \qquad \text{(Radial equation)}$$

$$\Theta''(\theta) + \cot\theta\,\Theta'(\theta) + \mu\Theta(\theta) - \frac{\sigma}{\sin^2\theta}\Theta(\theta) = 0 \qquad \text{(Colatitude equation)}$$

$$T''(t) + \sigma T(t) = 0 \qquad \text{(Azimuthal equation)}$$

In the following let

$$\tilde{\lambda} = \frac{1}{4n^2}, \quad \mu = l(l+1), \quad \sigma = m^2 \qquad \text{where}$$

$n \in \mathbb{N}$, $m, l \in \mathbb{N}_0$ such that $0 \le m \le l \le n-1$.

c) Show that the functions

$$R_{nl}(r) = e^{-\frac{2}{n}r} r^l w\big(\tfrac{r}{n}\big)$$

solve the *Radial equation* if w is a suitable associated Laguerre polynomial.

d) Show that $\Theta_{ml}(\theta) = P_l^{(m)}(\cos\theta)$ solves the *Colatitude equation.*

e) Solve the *Azimuthal equation.*

f) Collect your results and write down all solutions of the Schrödinger equation (LS) obtained by the above procedure. Find the correponding energy levels λ.

Note: In quantum physics the parameters n, l, m of the three parameter family of solutions obtained in f) are referred to as the

- principal quantum number $n \in \mathbb{N}$,
- orbital quantum number $l \in \mathbb{N}_0$, $0 \le l \le n-1$,
- magnetic quantum number $m \in \mathbb{N}_0$, $0 \le m \le l$.