12) States of the 3D Coulomb Potential

Estimate of the relevant velocities in the Bohr model:

$$E_n = -\frac{1}{n^2}\frac{mZ^2e^4}{2(4\pi\varepsilon_0)^2\hbar^2} = \frac{1}{2}mv^2 - \frac{Ze^2}{4\pi\varepsilon_0 r} \rightarrow \frac{v}{c} = \frac{1}{n}\frac{Ze^2}{4\pi\varepsilon_0\hbar c} = \frac{Z}{n}\alpha$$

Fine-structure constant: $\alpha \approx \frac{1}{137}$

Relativistic effects can become important on the order of $(\frac{v}{c})^2 \approx 10^{-4}$

One can still use the non-relativistic Schrödinger equation and consider relativistic effects as small corrections (except for very large Z).

$$V(r)\Phi(r,\vartheta,\varphi) + \frac{1}{2m}(\hat{p}_r^2 + \frac{1}{r^2}\hat{\vec{L}}^2)\Phi(r,\vartheta,\varphi) = E\Phi(r,\vartheta,\varphi)$$

Coulomb potential: $V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$

$$\hat{p}_r^2\Psi = -\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\Psi)$$

$$\hat{\vec{L}}^2\Psi = -\hbar^2\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial}{\partial\vartheta}\Psi) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\Psi\right]$$

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The basis of 3D stationary states

$$V(r)\Phi(r,\vartheta,\varphi)+\tfrac{1}{2m}(\hat{p}_r^2+\tfrac{1}{r^2}\hat{\vec{L}}^2)\Phi(r,\vartheta,\varphi)=E\Phi(r,\vartheta,\varphi)$$

Choose simultaneous eigenstates to L^2:

$$\hat{\vec{L}}^2\Phi(r,\vartheta,\varphi)=\hbar^2 l(l+1)\Phi(r,\vartheta,\varphi)$$

This leads to a one dimensional Schrödinger equation

$$[V(r)+\tfrac{\hbar^2}{2mr^2}l(l+1)]\Phi(r,\vartheta,\varphi)+\tfrac{1}{2m}\hat{p}_r^2\Phi(r,\vartheta,\varphi)=E\Phi(r,\vartheta,\varphi)$$

Were the set of eigenfunctions depends on l:

$$\Phi(r,\vartheta,\varphi)=R_{nl}(r)f(\vartheta,\varphi)\,,\quad E=E_{nl}$$

But there are many eigenstates of L^2, e.g. all linear combinations

$$\Phi=R_{nl}(r)\sum_{m=-l}^{l}A_m Y_{lm}(\vartheta,\varphi)$$

One therefore arbitrarily chooses that the basis states are also eigenstates of L_z

$$L_z\Phi=\hbar m\Phi\quad\rightarrow\quad\Phi=R_{nl}(r)Y_{lm}(\vartheta,\varphi)$$

$$\Psi(r,\vartheta,\varphi)=\sum_{\text{all }n}\sum_{\text{all }l}\sum_{m=-l}^{l}A_{nlm}R_{nl}(r)Y_{lm}(\vartheta,\varphi)$$

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