# Lecture 6, Jan 24, 2022

## Hydrogen Atom

- In our infinite well there is only 1 degree of freedom so we only have $E_n$; in higher dimensions, more degrees of freedom create more quantum numbers, so we have $E_{n,m}$, etc
- In 3D the TISE becomes $-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)=-\frac{\hbar^2}{2m}\nabla^2\psi+V=E\psi$
  - $\nabla^2$ is the Laplacian
  - $-\frac{\hbar^2}{2m}\nabla^2+V$ is the total energy operator or *Hamiltonian* $\hat{H}$
- In a hydrogen atom electrons have Coulomb potential $V(r)=-\frac{e^2}{4\pi\varepsilon_0 r}$
- Use spherical coordinates $(r,\theta,\phi)$ ($\theta$ is angle from $z$ axis, $\phi$ is rotation in the $x$-$y$ plane)
  - We also need to transform the Laplacian $\nabla^2=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\csc^2\theta\frac{\partial^2}{\partial\phi^2}\right)$
- Again use separation of variables; assume wavefunction is a product of $\phi(\boldsymbol{r})=\phi(r,\theta,\phi)=R(r)Y(\theta,\phi)$
  - This allows us to take advantage of radial symmetry for the hydrogen atom since Coulomb potential only depends on $r$
  - This gives us two equations; do this a second time, $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$
  - Azimuthal equation: $\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}+B=0$
    * This is easy to solve with trial solution $Ke^{im\phi}$ where $B=-m^2$
  - Solving for the energy eigenvalues gives the Bohr model
- Takeaway: the wavefunction is defined by 3 quantum numbers $n,l,m$ for the 3 spacial degrees of freedom, and one $m_s$ quantum number for the spin of the electron
  - $n$ – Principal quantum number: Gives the Bohr model solution, for a spherical model it is the solution
    * $n=1,2,3,\cdots$
    * Designation: $K,L,M,N$ shells corresponding to $n=1,2,3,\cdots$
    * Distance from the nucleus
  - $l$ – (Subsidiary) Orbital angular momentum quantum number
    * $l=0,1,2,\cdots,n-1$
    * $s\to 0, p\to 1, d\to 2, f\to 3$
    * Distribution/shape of electron density
  - $m_l$ – Magnetic quantum number
    * $m_l=-l,-l+1,\cdots,0,\cdots,l-1,l$
    * This and $l$ describe orientation
  - $m_s$ – Spin quantum number (quantized either up or down)
    * $m_s=\pm\frac{1}{2}$ for each $m_t$