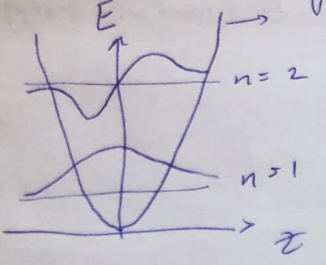
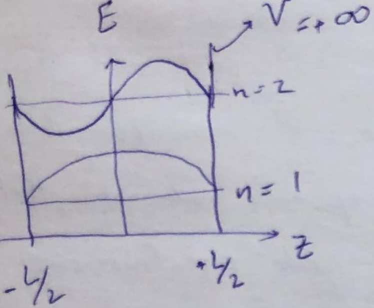
L10: review



$\rightarrow V(z) = \frac{1}{2} k z^2$

$$E_n = \hbar \sqrt{\frac{k}{m}} \left(n - \frac{1}{2}\right)$$

$n = 1, 2, \cdots$



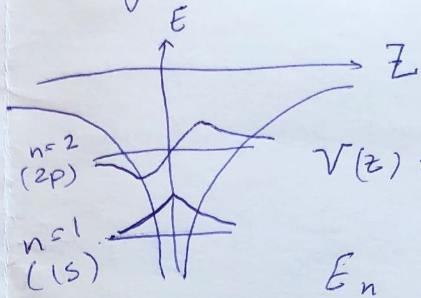
$$E_n = \frac{h^2 n^2}{8 m L^2}$$

$n = 1, 2, \cdots$

* the spring model provides a good approximation of diatomic bonds;

* the particle in box model provides a good approximation of energy states (and thus the absorption wavelength) of π electrons in conjugated systems.

today: H atom

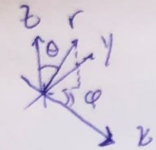


$$V(z) = \frac{e^2}{4\pi \varepsilon_0} \cdot \frac{1}{z}$$

$$E_n \propto \frac{-1}{n^2}$$

* note that the dependence of $V(z)$ of H atom on z at high Z values is much softer than that of spring model or box model, that is $V(z)$ does not change significantly by changing z at high $|z|$ values $\Rightarrow$ energy of H atom changes much less steeply for higher quantum numbers ($E_n \propto \frac{-1}{n^2}$ for H atom vs $E_n \propto n$ for spring model)

The main difference today: 3D vs 1D



* there is one quantum number per coordinate.

$r = \sqrt{x^2 + y^2 + z^2}$

CM: $E = \frac{1}{2m_e}(p_x^2 + p_y^2 + p_z^2) - \frac{e^2}{4\pi\varepsilon_0 r}$

QM: $\hat{H}\Psi = E_{nlm_l}\Psi$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - \frac{e^2}{4\pi\varepsilon_0 r}$$

the three quantum numbers are n, l, and m_l:

$$\begin{cases} n = 1, 2, 3, \dots \\ l = 0, 1, \dots, n-1 \\ m_l = -l, -l+1, \dots, l-1, l \end{cases}$$

Some examples of Ψ_{nlm_l}:

① $\Psi_{2,1,1} \sim r e^{-r/a_0} \sin\theta (\cos\varphi + i \sin\varphi)$ ($2 \to n$, $1 \to l$, $1 \to m_l$)

② $\Psi_{2,1,-1} \sim r e^{-r/a_0} \sin\theta (\cos\varphi - i \sin\varphi)$

③ $\Psi_{2,1,0} \sim r e^{-r/a_0} \cos\theta$

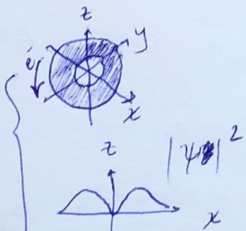
$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e \cdot e^2} \approx 0.529\ \text{Å} \text{ (Bohr length)}$$

! Plug the above Ψ examples in the Schrödinger equation and show that they are indeed valid eigenfunctions.

Now let's talk about how some of thesse functions look like...

CM

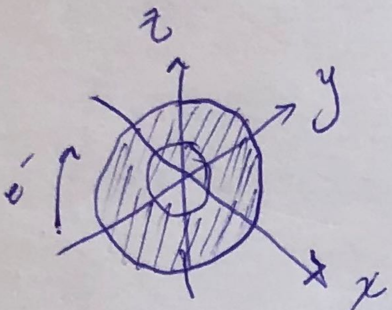
① $\Psi_{2,1,1}$



$\cos\varphi + i \sin\varphi = e^{i\varphi}$

$|\Psi|^2 \sim |e^{i\varphi}|^2 = 1$

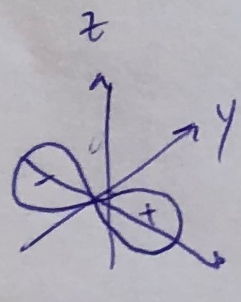
② $\psi_{2,1,\underset{\rightarrow m_l}{-1}}$



m_l dictates the angular momentum of electron, i.e the direction of electron's orbit.

the $\overbrace{\text{more convenient}}^{\text{real (not imaginary)}}$ solutions of H model are formed by linear combination of the wavefunctions:

(1) + (2) : $\psi_{p_x} \sim r e^{-r/a_0} \cdot \sin\theta \cdot \cos\varphi$



(1) − (2) : $\psi \sim r e^{-r/a_0} \sin\theta \sin\varphi$