Ministry of Higher Education
and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- The Fifteenth lecture-

Stage 4

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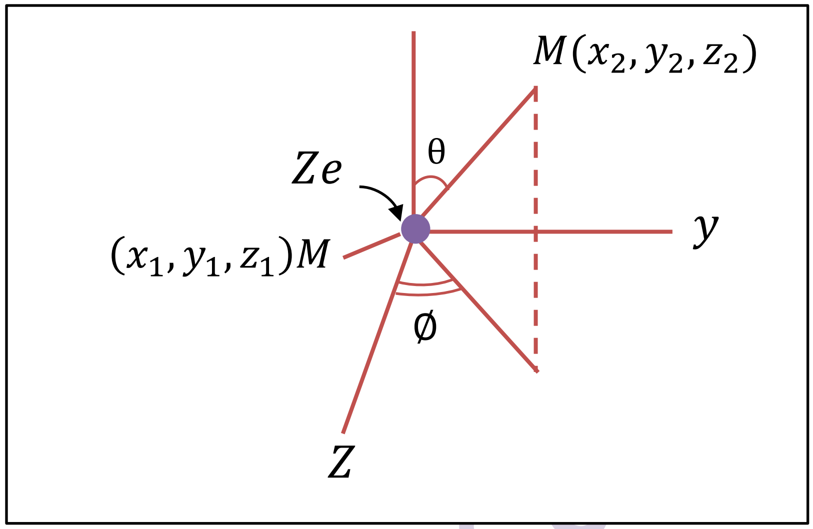
Hydrogen atom and hydrogen-like atoms

Hydrogen atom and hydrogen-like ions interact as a single group (Li, He) because they are different from each other only by nuclear charge.. note the table

	Nucleus	electron
charge	Ze (nuclear charge)	e
mass	M (mass reduce)	m

a) Coordinate coordinate:- Because the nucleus is heavier than the electron and it has to assume that the electrons are in a state of motion and the nucleus is fixed and thus will approach the state of the particle in the box



B. Hamilton Influencer:- $\hat{H} = T + N$ ____(1)

The underlying energy is the energy of attracting the electron with the nucleus and calculating from

$$V = -\frac{Ze^2}{r} \qquad \text{\_\_\_\_\_\_\_\_\_\_(2)}$$

$$\hat{H} = \frac{\hbar}{2m}\nabla^2 - \frac{Ze^2}{r} \qquad \text{\_\_\_\_\_\_\_\_\_\_(3)}$$

The proton mass (nucleus) is 1,846 times larger than the electron mass, so the reduced mass mass can be replaced by the electron mass.

C. Hamilton influenced by polar spherical coordinates: -

The situation is similar around the center, it is better to use polar spherical coordinates and the expression (∇^2)in polar spherical coordinates is:-

$$\nabla^2 = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{diagonal\ part} + \frac{1}{r^2}\underbrace{\frac{\partial}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\theta^2}}_{angular\ part} \rightarrow 1$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r} + \underbrace{\Lambda^2}_{L(op)}\right) \qquad \_\_\_\_\_\_\_(2)$$

- *Country part: - The dimension from the nucleus to the electron $\bar{e}$*
- Λ^2:- Influencer Leagendrian operator

So when you use it for compensation in the general equation and rearrangement we get the following:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial(r,\theta,\emptyset)}{\partial r} + \frac{1}{r^2}\frac{\partial}{\sin\theta}\frac{\partial}{\partial\emptyset}\right)\left(\sin\frac{\partial(r,\theta,\emptyset)}{\partial\emptyset}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\psi(r,\theta,\emptyset)}{\partial\emptyset^2} + \frac{2m}{\hbar^2}\left(E + \frac{Ze^2}{r}\right)\psi = 0$$

............(3) ((Schrodenker equation for h atom))

From the equation (3) in the way variables are separated we get: -

$$\psi(r,\theta,\emptyset) = R_{(r)} \cdot \theta_{\theta} \cdot \emptyset_{\emptyset} \qquad \_\_\_\_\_\_\_\_\_\_(4)$$

Compensate (4) in (3) (then divide by 4 with order and abbreviation)

$$\frac{1}{R_{(r)}} \cdot \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} R_{(r)} + \frac{2mr^2}{\hbar}\right)\left(E + \frac{Ze^2}{r}\right) + \left[\frac{1}{sin\theta} \cdot \frac{1}{\theta_{\theta}} \cdot \frac{\partial}{\partial \theta}\left(sin\frac{\partial}{\partial \theta}\theta_{\theta}\right)\right] + \left[\left(\frac{1}{sin^2\theta} \cdot \frac{1}{\emptyset_{\emptyset}} \cdot \frac{\partial^2}{\partial^2 \emptyset}\right)\emptyset_{\emptyset}\right] = 0$$

So we conclude.

1) *The R-based part of equation 5 is called the theoretical part and contains information on the electron radius in various Europeans.*

$$R_{(r)} = Redecal\ part$$

2) Angular part angular part

$$y_{\theta,\emptyset} = \theta_\theta \cdot \emptyset_\emptyset$$

Depends on two variables. The function determines the shape of orbital in the atom by the $\emptyset, \theta\theta$L,m,n quantum numbering allowance, either determines the $\emptyset$direction of each orbital in space as follows:

$$\therefore \psi = R_{(n,L)} \cdot \theta_{(L,m)} \cdot \emptyset_m = R(\, n, L \cdot y(\theta, \emptyset)\,) \_\_\_(6)$$

Theories Approximation

Rounding methods: - In quantum chemistry two ways

1) Perturbation theory jamming theory

This case or theory is used when the case to be resolved is similar to another case that has a precise solution. For example, the Schrodenker equation of hydrogen atom can be solved in a stable state, i.e. we can impose its function, so the theory of confusion helps to know the subjective function of the atom when exposed, for example,to a small electric field(if it is large, ionization occurs).

If we had a stable system that represented the following equation,

Original $H^\circ\ \psi^\circ = E^\circ\ \psi^\circ$ ______(1)

But if we have a confused system that issimilar to the first, but it is so different from it that theSchrodnker equation cannot be solved. So...

Confused system $H\psi = E\ \psi$ _______(2)

$\because\ H = H^\circ + \lambda\ H'$ ______(3)

$\because\ \psi = \psi^\circ + \lambda\ \psi'$ ______(4)

$\because\ E = E^\circ + \lambda\ E'$ ______(5)

We compensate (3) (4) (5) in (2) conclude

$$\because\ (H^\circ + \lambda\, H')(\psi^\circ + \lambda\, \psi') = (\, E^\circ + \lambda\, E') \cdot (\psi^\circ + \lambda\, \psi')$$

2) Variation theory

There is no statute here, but it has changed, we try tochange our system with another system of change based on guesswork and to interpret this function we use when there is no experimental function close to the real function containing more than one variable and then change these variables to reach the best evidence is the one that possesses the lowest self-value.