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Quantum Chemistry

- The Eleventh Lecture -

Stage 4

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Pastulate for Quantum (Mechanics Hypotheses)

The first hypothesis pastulate

This hypothesis means any case of the dynamic system consisting of N particles by function (ψ) which is called the state function or wave function of a system so if we have particles (n_1, n_2, n_3) and their locations (r_1, r_2, r_3) be comprehensive ($n_1, n_2, n_3, \dots, n_n$) Described as function so it can be written as follows

$$(\psi_{r_1, r_2, r_3, \dots, r_n})$$

That is, the function contains all the information that can be obtained experimentally from the system so to study which system should

- 1 A dynamic equation is formulated for the movement of its particles
- 2 Solve the equation to get the function that represents the system
- 3 Find a way to extract information from the function

The function that is orbital is characterized by chemistry is a set of quantum numbers on which the function depends and

symbolizes (n, m, L) where the quantum setting describes a case of dynamic system so

Main quantum number (energy) n :

Number of magnetic quantum (permelectron) m :

Number of quantum(energy shape) L :

So the function can be expected by

a) Schrödinger Schrodinger representation

$$\int \psi_{n,m,l}^* \psi_{n,m,l} dx = 1$$

b) Representation of Dirace representation

bra $\langle n, m, l | n, m, l \rangle$ *ket*

$$\langle n, m, l | n, m, l \rangle = 1$$

That ψ is, the probability of the presence of the particle described by the case function $n(r)$ represents the location (r) is $(\psi_{n(r)}^* \psi_{n(r)} dr)$

Scientist Max Bourne gave another description of the probability of the particle being within the size (τ) so the function becomes:

$$\Psi_{n(r)}^* \Psi_{n(r)} d\tau$$

c) The possibility of the particle being present in all space is written as follows

$$\int_{-\infty}^{+\infty} \Psi_{n(r)}^* \Psi_{n(r)} d\tau = 1$$

And when the equation is expressed in the form of Dirac

$$\langle n|n \rangle = 1$$

2) Second Hypothesis Second Postulate

Observable Note

(Physical property that can be observed in practice such as time, temperature represents the amounts observed by the effects)

1) Linear (Sin)

This is a characteristic that represents the result of the damage to the system b. complete it itself if the A. is solitary on the components and when the results are collected

2) Hermetime

In this capacity, the properties of the pyramids are generally studied.

Therefore, these effects are formulated according to general rules in which the information contained in the case function of that function (ψ) contains physical information (energy, time, location, momentum)

So the relationship between the traditional variable and the quantum mechanics effect can be found as in the table

Property	Classic change	Quantum Mechanics Influencer
1) Energy Energy	E	$i\hbar = \frac{\partial}{\partial t} \text{ or } E$ $i\hbar = \frac{\hbar}{i}$ $E = \frac{\hbar \partial}{i \partial t}$
2) Time Time	t	It's a hit product, so it doesn't produce anything new.
3) Site Position	X ,Y ,Z	x,y,z represents a multiplication product so it does not affect the function that follows
4) Momentum Moment	Px , py , pz	$\frac{\hbar \partial}{i \partial x}$ $\frac{\hbar \partial}{i \partial y}$ $\frac{\hbar \partial}{i \partial z}$

Therefore, classical physics laws can be transformed into quantum mechanics by formulating quantitative effects as follows:

- 1) And the traditional change of property in the alternative of coordinates and linear zakum only
- 2) Compensation for coordinates and the same in quantum mechanics. as in the previous table.

One of the most important qualities of the old influencer is:

The influencer is said to be hermit by the function of any function (Ψ_M, Ψ_N) if the following is achieved:

$$\begin{aligned}\int \psi_m \hat{A} \psi_n d\tau &= \int (\hat{A} \psi_m^*) \psi_n d\tau \\ &= \int (\psi_m^* \hat{A} \psi_n)^* \psi_n d\tau \\ &= \int \psi_m \hat{A} \psi_m^* \\ \langle m | \hat{A} | n \rangle &> \text{ or } \langle n | \hat{A} | m \rangle\end{aligned}$$

So you should note the functions that are in the fore.

a. Normalized Function

If we have two functions (ψ_m, ψ_n) with a general complaint where $m=n$ or if we have functions (ψ_m, ψ_n) to achieve both characteristics you must meet the following condition

$$\int \psi_m \psi_n d\tau = 1$$

$$\int \psi_n \psi_m d\tau = 1$$

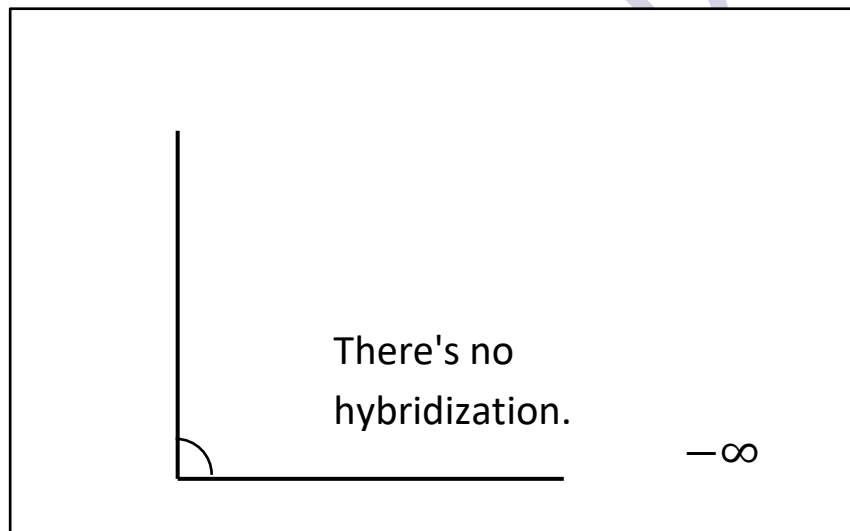
$$\langle n | |n \rangle = 1$$

b) orthogonal Function

If we have two functions (ψ_n, ψ_m) where $n \neq m$

The two functions are perpendicular if the following condition is met.

$$\int \psi_m \psi_n d\tau = 0$$



c) Normalized function

If the functions are perpendicular and consistent, this condition is called a harmonic perpendicular and symbolizes it and δ_{nm} is called kroniker delta.

$$\int \psi_m \psi_n d\tau = \delta_{nm} = \begin{cases} n = m, & \int \psi_m \psi_n d\tau = 1 \quad \delta = 1 \\ n \neq m, & \int \psi_m \psi_n d\tau = 0 \quad \delta = 0 \end{cases}$$

Q/ Prove that the op of the position by X the hermetion (op)

$$\int \psi_m^* \hat{A} \psi_n d\tau \quad \text{where } \hat{A} = x$$

$$\int \psi_m^* \hat{A} \psi_n dx = \int (\psi_m^* \hat{x} \psi_n)^* dx$$

$$= \psi_m \hat{x}^* \psi_n^* dx$$

$$x^n = x^{n*}$$

Q/ Prove that the linear momentum op \hat{P}^1 by dx the hermetion (op)

$$\int \psi_m^* \hat{A} \psi_n d\tau \quad \hat{A} = \hat{P}_x$$

$$\int \psi_m^* \hat{P} \psi_n d\tau = \int \psi_m^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_n d\tau$$

$$= \frac{\hbar}{i} \int \psi_m^* \frac{\partial}{\partial x} \psi_n dx, dy, dz$$

Takeretail integration

$$= \frac{\hbar}{i} \left[\int \psi_m^* \psi_n dx, dy, dz \right]_{x = -\infty}^{x = +\infty} - \left[\int \psi_m^* \psi_n dx, dy, dz \right]_{-\infty}^{+\infty}$$

The first limit = zero if the wave function is approaching infinity and the function value must be limited so that the equation can be written in the form of

$$\begin{aligned} -\frac{\hbar}{i} &= \int \psi_m^* \frac{\partial}{\partial x} \psi_n dx, dy, dz \quad x-1 \\ &= \int \psi_m^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_n d\tau \\ &= \int \psi_m^* \hat{P}_x \psi_n d\tau \end{aligned}$$