Orbital: An Electric and Magnetic Field

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Abstract. Quantum mechanics is a non-intuitive subject which is very difficult to understand. Various investigations have been done on understanding the basic quantum mechanics. Nevertheless, many attempts have been made for understanding the appropriate techniques, which are known to help conceptual understanding of basics of orbital. As per the study the orbital is considered as an electric and magnetic field. The electric and magnetic field gets generated due to the continuous motion of electrons. So the orbital is nothing more than an electric and magnetic field. It is because of the electric and magnetic field of the orbital that it possesses electric and magnetic momentum. So taking all these points into consideration, it could be concluded that an orbital is no more than an electric and magnetic field.

1. Introduction
The orbital is defined as the place or space where there is probability to locate an electron. As a known fact the electrons are found only in these small spheres, without them there is no any place, space or an area where there is probability to find an electron. The idea of energy quantization was introduced in Atomic Physics in 1913 with the first explanation of the hydrogen electronic structure by the Dane Niels Bohr [1]. Inspired by Planck’s theory [2, 3] of black-body radiation, Bohr admitted that the electrons in hydrogen atom can only exist in stationary states with a well-defined energy. Transitions between these states occur by absorption or emission of energy. Bohr defended that electrons in such states follow classical circular orbits around the nucleus. The idea of orbitals as probability functions was still to come. Influenced by the interpretation of the Compton effect, the Frenchman Louis de Broglie [4] suggested, in 1924, that the accepted wave-particle duality for photons could be extended to any moving particle which would then have a wavelength associated with it. The somewhat mysterious wave of de Broglie was the predecessor of the wave function. The wave function contains all of the important properties of the electron: knowing it we can calculate the value of any measurable quantity. The probabilistic interpretation of the wave function was proposed, also in 1924, by the German Max Born. The wave function is simply related to the position of the electron in space. The square module of the wave function,

\[ |\psi(x, y, z)|^2 = \psi^*(x, y, z) \cdot \psi(x, y, z) \]  (1)

is the probability density for finding the particle at the(x, y, z) position. The sum of all probabilities in full space is unity since the particle should be anywhere. Helped by that interpretation, from 1925 to 1927, a pool of young physicists developed the complete theoretical machinery for getting the wave function and obtaining information from wave functions. An important step was given in 1925, when the Austrian Erwin Schrodinger, [5] inspired by the de Broglie theory [4], proposed a wave approach to quantum mechanics. For the simplest case of a free particle the Schrodinger equation is a
differential equation involving a second-order spatial derivative of the wave function, $\psi$ and the unknown energy $E$ (a real number),

$$\hat{H}\psi = E\psi \quad (2)$$

With

$$\hat{H} = -\frac{\partial^2}{\partial x^2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \quad (3)$$

An operator describing the kinetic energy which acts on the wave function (his Planck’s constant and $m$ the particle mass)? If the particle is confined to a limited region of space (box) the solution of the wave equation leads to a discrete set of energy values. Energy quantization appears, therefore, associated to the localization of the wave function. For a particle under a potential, the operator $\hat{H}$ has to include a potential term. Like the energy, any measurable physical quantity, or observable, has associated with it an operator, which acts on the wave function to yield the wave function multiplied by a real number, the value of the observable which should be measured.

In 1927, the German Werner Heisenberg [6] identified incompatible observables meaning that we could not measure with arbitrary precision on pair of observables. That is the case of (linear) momentum and position. This so-called uncertainty principle expresses therefore the impossibility of preparing a state for which both position and momentum can be determined with arbitrarily small uncertainties.

Still in 1927, with the first observations of electron diffraction by Clinton Davison and Lester Germer [7], in the United States, and by George Thompson [8], in Great Britain, the fundamental aspects de Broglie’s theory were confirmed. Further observations confirmed the validity of Bohr’s interpretation, the Schrödinger equation and Heisenberg’s uncertainty principle. Until now, none of the predictions of quantum mechanics have been contradicted by experiment.

When dealing with atomic systems and going beyond old quantum theory, the classical notion of particle trajectory has to be abandoned, since, in contrast to Newtonian Mechanics, a well-defined position and momentum are no longer possible at a given time. We can only describe the probability for the particle to be at a certain position, or the probability for it to have a certain momentum. Trajectories are replaced by diffuse spatial distributions. These distributions can be represented by surfaces on which all points have the same value of probability density $\psi^2$, the so-called isodensity surfaces.

Electrons surrounding atoms are concentrated in regions of space described by atomic orbitals. The boundaries of an atomic orbital are conventionally drawn by the surface of 90% probability, but they extend to infinity.

From the Schrödinger equation we can calculate the wave function of the hydrogen atom and therefore the probability for the position the electron can take [5]. For hydrogen the energy depends on the principal quantum number $n$, which is an integer ($n= 1, 2, \ldots$).

Angular momentum is also an observable. It is found that the angular momentum is quantized according to:

$$\hat{L}^2\psi = l(l+1)\hbar^2\psi \quad (4)$$

With $l$ the angular momentum quantum number ($l=0 \ldots n-1$).

The z-component of the angular momentum is given by

$$\hat{L}_z\psi = m_l\hbar\psi \quad (5)$$

Where $m_l$ is the magnetic quantum number ($m_l=-l \ldots +l$).

In the lowest-energy state (ground-state) of the hydrogen atom the electron has a spherical distribution in space since the wave function has spherical symmetry. At higher energy the orbitals may take other shapes. Spence et al. [9, 10] also claim that it is acceptable to use words like “orbital” in different senses, provided that this does not lead to confusion. However, it was precisely because that the conflation of the terms orbital and charge density does cause confusion that there is currently some theoretical interest directed at performing orbital-free density functional calculations [11]. But in
order not to seem too dogmatic, it must be said that some alternative interpretations of quantum mechanics, such as Bohm’s theory, do regard electrons as having definite trajectories. However, this theory has not yet received any experimental evidence that might lead one to prefer it to the currently accepted Copenhagen interpretation [12].

2. Results and Discussion

As usual an orbital may be defined as the place or space where there is maximum probability to find an electron. Definitely electrons could be found only within these small spheres, without them there is no any place, space or an area where there is probability to find an electron. First there is probability in finding an electron; no any exactness is there in the location of an electron. But the point to be considered over here is, why do electrons exist only in spheres, the answer is simple that in multi-electron system, there occurs some boundary for a particular set of electrons, which doesn’t allow another set of electrons to collapse in an isolated atom. In actual sense after studying various phenomenon’s it could be concluded that an orbital is nothing other than a field (Both electric as well as magnetic) which gets generated around an electron, due to the circulation of an electron around its own axis. As electrons being negatively charged body is always under motion as per Bohr’s theory. Any moving body develops some sort of field either electric or magnetic as per Columbia law [13]. So what about a negatively charged moving electron, which could develop much more intense field than the neutral body, so in actual sense, an orbital is nothing less than a field developed due to the motion of an electron (Fig: 1). Also an electric field can be felt only when another field is being brought in-contact with the first field.

Figure 1. the shape of an Orbital developed due circulation of an electron.

The other mechanism which could support, that an orbital is actually a field is that an orbital posses an orbital angular momentum. If we simply consider an orbital as a place or space how it could be in such a situation that it could develop angular momentum. So while considering orbital as a field, it does posses momentum- i.e. orbital angular momentum. All it had been shown that orbital does posses some sort of shape like- S- orbital as spherical, i.e. the field developed due to the circulation of an electron in s- orbital is same along all sides, or electric or magnetic flux is same along all the three axis from the point of its origin. In case of p-orbital having dumble shape, meaning thereby is that the alignment of the field is only along one axis at once, it could be along X, Y or Z axis, or it could follow the entire three axis at once depending upon the presence of electrons in the respective orbitals. Same trend goes for the electrons which are located in the (d) and (f) sub shell orbitals respectively (Fig: 2).
Figure 2. The 1s orbital, the 2p orbitals, the 3d orbitals and the 4f orbitals are contrasted.

While discussing the probability of finding an electron, two important concepts are being taken into consideration, radial wave probability and angular wave probability. It is by the utilisation of these two concepts that it had been found that \( (\psi^2) \) does possess a value else \( (\psi) \) does have any value. A single \( (\psi) \) could give information about the distance of electron from the nucleus, or the angle at which the electron is located from the nucleus, so the total \( (\psi^2) \) could give information about the distance or the angle at which the electron is located. So by taking distance factor and the angle factor into consideration, it had been mentioned that single \( (\psi) \) doesn’t possess any value, but \( (\psi^2) \) bears a value.

An electron always remains in circular motion, is because of the fact that it had to develop some force which could kept the electron on its own tract or orbit. The force that kept the electron under motion and aligned without any support is the centripetal and centrifugal force which gets developed due to the circular motion of an electron. During the course of motion of an electron, the electron looses energy in order to maintain pace and to remain in a circular way. The energy released is acting as a barrier which also does have circular direction so is simply acting as an orbital. So an orbital is simply the field developed due to the circulation of an electron, which kept this electron to behave like a magnet.

During the course of bond formation as per the valence bond theory and the molecular orbital theory it is simply mentioned that the nuclear pull of one atom attracts the electron pairs from the another atom leading to the formation of molecular orbitals. All though there are so many mathematical proofs regarding the bonding and anti-bonding molecular orbital formation on the basis of the interaction between the electronic cloud and the nuclear portion of the concerned atoms leading to the formation of the molecules. But the main point of formation could be due to the orbital-orbital interactions, i.e., the field generated from one atom in the form of orbital interacts with the field of another atom (but only those atoms interact which may have comparable field strength, orbitals having same energy and this could be the reason that every atom in the periodic table doesn’t interact with every other atom in the periodic table, besides some other chemical properties, so only those atoms interact which have comparable energy). The orbitals of the concerned atoms also interact on the basis of the direction of the orbitals, either clockwise or anticlockwise, if the orbital direction of the connecting atoms is same either both clockwise or both anticlockwise a bonding orbital gets formed, and if the direction of the connecting atoms is in such a way that one atom have clockwise direction and another atom anticlockwise direction, an anti-bonding molecular orbital formation may take place.
3. Conclusion
So, on the basis of the above results it could be concluded that a bond formation is because of the orbital interaction meaning thereby that these are actually the fields which get connected. Total bond formation is only up to the involvement of orbitals, although their generation is totally because of the circulation of the electrons both on their own axis as well as round the nucleus. Electrons are simply the sources for the generation of field, which acts as an orbital. So in total it could be concluded that an orbital is nothing than a field- either electric or magnetic.

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