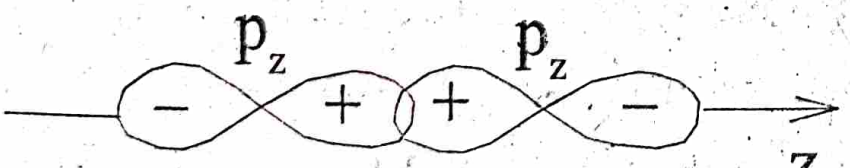
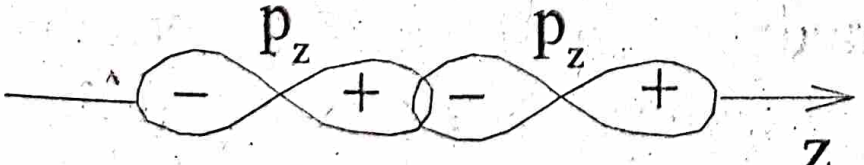
4.5. Valence bond theory

The main assumptions in valence bond theory are:

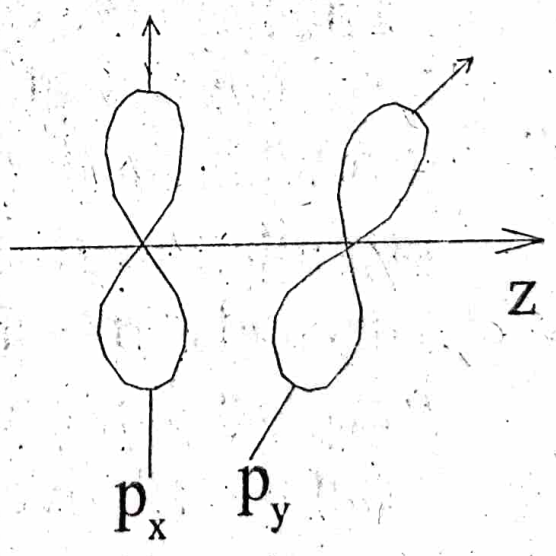
- Covalent bond is formed by the partial overlapping of atomic orbitals which results in the pairing of electrons.
- The extent of overlap decides the strength of a covalent bond.
- The overlap may be negative, positive or zero depending upon the properties of the overlapping atomic orbitals. (ഈ സിദ്ധാന്തമനു സരിച്ച് സഹസംയോജക ബന്ധനം ഉണ്ടാകുന്നത് അറ്റോമിക ഓർബിറ്റലുകൾ ഭാഗികമായി കൂടിച്ചേർന്നാണ്. ഇതുമൂലം ഇലക്ട്രോണുകൾ ജോടിയാക്കപ്പെടുന്നു. കൂടിച്ചേരലിന്റെ അളവാണ് ബന്ധനത്തിന്റെ ബലം കൂടാനും കുറയാനും കാരണമാകുന്നത്. കൂടിച്ചേരുന്ന ഓർബിറ്റലിന്റെ ഗുണങ്ങളുടെ വ്യതിയാനമനുസരിച്ച് കൂടിച്ചേരൽ പോസിറ്റീവോ, നെഗറ്റീവോ, സീറോയോ ആകാം).



Positive overlap



Negative overlap



Zero overlap

4.5.1. Orbital overlap concept

The partial merging of atomic orbitals is called overlapping of atomic orbitals which results in the pairingof electrons. According to orbital overlap concept, the formation of a covalent bond between two atoms results by pairing of electrons present in the valence shell having opposite spins.

4.5.2. Directional properties of bonds

The valence bond theory explains the shape, the formation and directional properties of bonds in polyatomic molecules like CH_4, NH_3 and H_2O, etc. in terms of overlap and hybridisation of atomic orbitals.

4.5.3. Overlapping of atomic orbitals

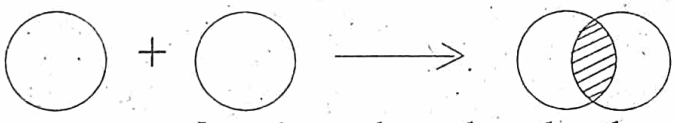
The criterion of overlap, as the main factor for the formation of covalent bonds applies uniformly to the homonuclear/heteronuclear diatomic molecules and polyatomic molecules. It would be therefore interesting to use VB theory to find out if these geometrical shapes can be explained in terms of the orbital overlaps.

4.5.4. Types of overlapping and nature of covalent bonds

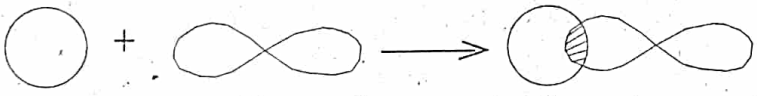
A covalent bond is formed by the overlapping of two half-filled atomic orbitals. Depending on the type and the extent of overlapping covalent bonds may be divided into sigma (σ) and pi (π) bonds.

Sigma bond (σ): The axial overlapping of atomic orbitals resulting in the formation of σ bond. The electrons involved in σ bond are called σ electrons.

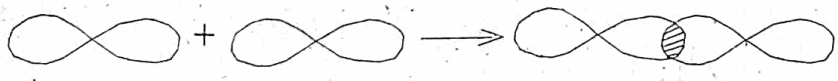
s –s overlapping takes place by the mutual overlapping of two half filled s - orbitals



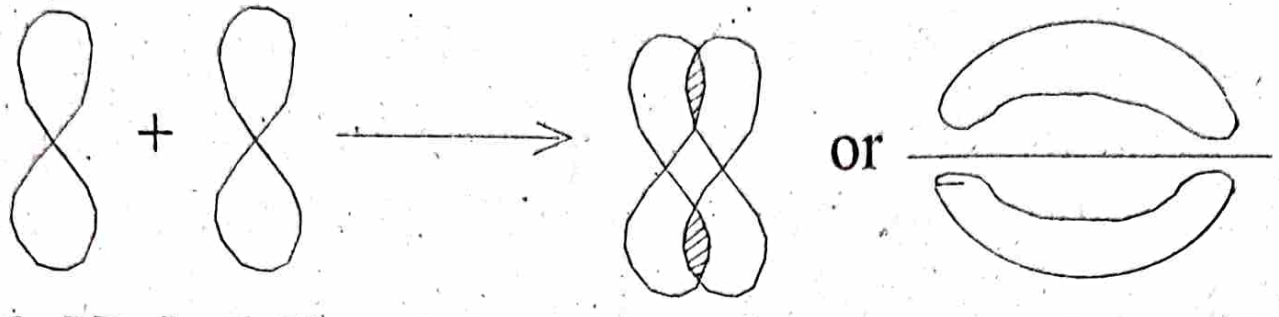
s – p overlapping takes place by the mutual overlapping of a half filled s orbital and a half filled p orbital of two atoms.



p – p overlapping involves the axial overlapping of two half filled p - orbitals of two atoms.



Pi - bond (π): The lateral or sidewise overlapping leads to the formation of a π bond. If there are more than one bond between two atoms, the first bond formed will be σ bond; and the additional bonds are π bonds. π bond formation is represented as.



4.6. Hybridisation

Hybridisation is defined as the phenomenon of intermixing of atomic orbitals of different energies and shapes to get an equal number of orbitals of equivalent energies and identical shapes. (വ്യത്യസ്ത ഊർജവും ആകൃതിയുമുള്ള അറ്റോമിക ഓർബിറ്റലുകൾ കൂടിച്ചേർന്ന്, ഒരേ ഊർജവും ആകൃതിയുമുള്ള അതേ എണ്ണം ഓർബിറ്റലുകൾ ഉണ്ടാകുന്ന പ്രക്രിയയാണ് ഹൈബ്രിഡൈസേഷൻ).

4.6.1. Types of hybridisation

There are many types of hybridisations. The three major types of hybridisation are sp^3, sp^2 and sp. The process of mixing up of one 's' orbital and three 'p' orbitals to get four orbitals of equivalent energy, which are directed to the four corners of a regular tetrahedron is called sp^3 hybridisation. The process of mixing up of one 's' orbital with two 'p' orbital to form three equivalent orbitals which are coplanar is called sp^2 hybrid orbitals. The bond angle is 120^0. The process of mixing up of one 's' orbital and one p orbital to get two orbitals of same energy which are directed along a line is called sp hybridisation. The bond angle is 180^0.