5. **Calculation of partial ionic character of a covalent bond.** The ionic character in a covalent bond between two atoms, say, A and B, is due to the difference in the electronegativities of A and B. Greater the difference in the electronegativities, greater would be the ionic character and consequently the higher would be the stability of the resulting bond.

Pauling suggested the following correlation between the electronegativity difference $\chi_A - \chi_B$ and the per cent ionic character of the covalent bond:

$$\text{Per cent ionic character} = [1 - e^{-0.25(\chi_A - \chi_B)}] \times 100$$

Let us calculate the per cent ionic character in HF molecule using Pauling's equation. Electronegativity values (Alfred-Rochow) of H and F are 2.2 and 4.1 respectively.

According to Pauling's equation,

$$\left.\begin{array}{c}\text{Per cent ionic character}\\ \text{of H} - \text{F bond}\end{array}\right] = [1 - e^{-0.25(1.9)}] \times 100$$

$$= 37.77$$

Pauling suggested an alternative empirical equation also for calculating the per cent ionic character, according to which

$$\text{Per cent ionic character} = 18\,(\chi_A - \chi_B)^{1.4}$$

According to this equation, the per cent ionic character of HF comes out to be 44.12. This value is quite close to the one (*viz.*, 44.8) obtained by Pauling from dipole moment of HF.

2.6 EFFECTIVE NUCLEAR CHARGE AND SCREENING EFFECT

The relation between energy and energy shell for an electron in hydrogen atom is given by expression

$$E = -R\frac{Z^2}{n^2} \qquad \text{... (2.9)}$$

For hydrogen atom ($Z = 1$, $n = 1$), the energy of the outermost electron calculated from equation (2.9) agrees with the observed I.E. 1312 kJ mole^{-1}. However the calculated and observed value for atom with $Z > 1$ do not agree fairly. The observed ionization energy of say Li is considerably lower than that calculated from equation (2.9) because of following reasons:

(*i*) The expression does not hold good for multi-electron atom because it does not take interelectronic repulsions into account.

(*ii*) The $2s^1$ electron does not face the nuclear charge directly. There are intervening $1s^2$ electrons which not only shield the nucleus but also repel the $2s^1$ electron resulting in removal of the electron.

Thus the inner core of electrons shield or screen the nucleus from outer electron. Consequently the outer electrons experience only a part of the nuclear charge or the effective nuclear charge faced by the outer electron is lower than that expected from total nuclear charge. In case of Li, the effective nuclear charge faced by $2s^1$ electron is not 3 but between 1 and 2 (actual value is 1.59). However if we recall the radical probability distribution curve of 2*s* orbital in hydrogen like atoms, it is apparent that 2*s* electron has definite probability of finding itself near the nucleus and hence would penetrate the inner 1*s* orbital core. This means that although 2*s* electron is shielded by the 1*s* core yet 2*s* electron penetrates it to some extent and experiences somewhat higher nuclear charge. In fact the energy of outer electron is determined by the effective nuclear charge (Z_{eff}) which is less than Z (nuclear charge) by an amount shielding constant (*S*) of the intervening core of the electrons

$$Z_{eff} = Z - S$$

Due to greater penetration, *s*-electrons tend to shield the nucleus more effectively than *p*-electrons which in turn shield the nucleus more effectively than *d*-electrons. That is, for a given *n*, the screening or shielding effect varies as

$$s > p > d > f$$