

two separate equations are obtained by solving equation (6) after equation being:

$$-\sum_{i=1}^N \frac{\hbar^2}{8\pi^2 M_i} \nabla_i^2 \Psi_N(R) + E(R) \Psi_N(R) = E_T \Psi_N(R) \quad (7)$$

$$\left[ \hat{T}_N + E(R) \right] \Psi_N(R) = E_T \Psi_N(R) \quad (8)$$

Equation (8) is the nuclear Schrödinger Equation in which  $\hat{T}_N = -\sum_{i=1}^N \frac{\hbar^2}{8\pi^2 M_i} \nabla_i^2$  is Kinetic energy operator and  $E(R)$  is potential energy operator, making  $\hat{H}_N$  the nuclear Hamiltonian

$$\text{Similarly } -\sum_{j=1}^N \frac{\hbar^2}{8\pi^2 m_j} \nabla_j^2 \psi_e(r, R) + V(r, R) \psi_e(r, R) = E(R) \psi_e(r, R)$$

$$\left[ \hat{T}_e + V(r, R) \right] \psi_e(r, R) = E(R) \psi_e(r, R)$$

$$\hat{H}_e \psi_e(r, R) = E(R) \psi_e(r, R) \quad (9)$$

This is the electronic Schrödinger Equation.

Solution of equation (9) gives the electronic energy  $E(R)$  and the wave function  $\psi_e(r, R)$  for a particular value of  $R$ . Such separation of nuclear and electronic functions describes Born-Oppenheimer approximation, according to which the true wave functions of systems of moving electrons and nuclei will differ very slightly from those calculated assuming nuclei to be stationary.

The approximation holds good for ground state of molecules and may break down for excited states

