$$H = T_1 + V_1 + T_2 + V_2 + +V_{12}$$

$$H = T_1(\mathbf{r}_1) + V_1(\mathbf{r}_1) + T_2(\mathbf{r}_2) + V_2(\mathbf{r}_2) + V_{12}(\mathbf{r}_2, \mathbf{r}_2)$$

$$T_1(\mathbf{r}_1) \longrightarrow -\frac{\hbar^2}{2m_e}\nabla_{r_1}^2 \qquad T_2(\mathbf{r}_1) \longrightarrow -\frac{\hbar^2}{2m_e}\nabla_{r_2}^2$$

$$V_1(\mathbf{r}_1) = -\frac{Z\,e^2}{|\mathbf{r}_1|} \longrightarrow -\frac{Z\,e^2}{r_1} \qquad V_2(\mathbf{r}_2) = -\frac{Z\,e^2}{r_2}$$

$$V_{12}(\mathbf{r}_2, \mathbf{r}_2) = +\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \longrightarrow +\frac{e^2}{r_{12}}$$

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2\right)$$

$$H = T_1(\mathbf{r}_1) \ + \ V_1(\mathbf{r}_1) \ + \ T_2(\mathbf{r}_2) \ + \ V_2(\mathbf{r}_2) \ + \ V_{12}(\mathbf{r}_2, \mathbf{r}_2)$$

$$[T_1(\mathbf{r}_1) \ + \ V_1(\mathbf{r}_1) \ + \ T_2(\mathbf{r}_2) \ + \ V_2(\mathbf{r}_2) \ + \ V_{12}(\mathbf{r}_2, \mathbf{r}_2)] \, \Psi(\mathbf{r}_1, \mathbf{r}_2) \ = \ E \, \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

$$\left[-\frac{\hbar^2}{2m_e}\nabla_{r_1}^{\ 2} \ - \ \frac{Z \, e^2}{r_1} \ - \ \frac{\hbar^2}{2m_e}\nabla_{r_2}^{\ 2} \ - \ \frac{Z \, e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \right] \Psi(\mathbf{r}_1, \mathbf{r}_2) \ = \ E \, \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

Atomic Units

Unit of length is the Bohr radius:

$$a_0 = \frac{\hbar^2}{m_e e^2} \left(\quad = 4\pi\epsilon_0 \frac{\hbar^2}{m_e e^2} \quad \right)$$

The first is in atomic units, second in SI-units. This quantity can be remembered by recalling the virial theorem, i.e. that in absolute value, half of the potential energy is equal to the kinetic energy. This gives us

$$\frac{1}{2} \frac{e^2}{a_0} = \frac{\hbar^2}{2m_e a_0{}^2}$$

and if we accept this relation, we have the above value of a_0.

The so called fine structure constant

$$\alpha = \frac{e^2}{\hbar c}$$

expresses in general the *weakness* of electromagnetic interaction.

Some Constants and Quantities

$$v_0 = \alpha c = 2.187 \cdot 10^6 \text{ m s}^{-1} \qquad \text{Bohr velocity}$$

$$a_0 = 0.529177 \cdot 10^{-10} \text{ m} \qquad \text{Bohr radius}$$

$$\hbar = 0.6582 \cdot 10^{-15} \text{ eV s} \qquad \text{Planck's constant}$$

$$k_B = 0.8625 \cdot 10^{-4} \text{ eV } {}^\circ\text{K}^{-1} \qquad \text{Boltzmann constant}$$

$$\text{R} = N_A k_B$$

$$N_A = 6.0222 \cdot 10^{23} \qquad \text{Avogadro's number}$$

$$\mu_B = 0.579 \cdot 10^{-4} \text{ eV (Tesla)}^{-1} \qquad \text{Bohr magneton}$$

Plank's formula

$$\rho(\omega_{ba}) \;=\; \frac{\hbar \omega_{ba}^3}{\pi^2 c^3} \; \frac{1}{e^{\hbar\omega/kT} - 1}$$

Useful formulae and informations

$$P_0\left(\cos\theta\right) = 1 \qquad\qquad P_1\left(\cos\theta\right) = \cos\theta$$

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