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

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

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

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

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

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

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

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

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

Atomic Units

Unit of length is the Bohr radius:

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

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

$v_0 = \alpha c = 2.18710^6$ m s$^-1$ Bohr velocity

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

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

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

R $= N_A k_B$

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

$\mu_B = 0.579\ 10^{-4}$ eV (Tesla)$^{-1}$ 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

$P_0\,(cos\theta) = 1$ $P_1\,(cos\theta) = cos\theta$

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