# Useful Formulae

## Harmonic oscillator

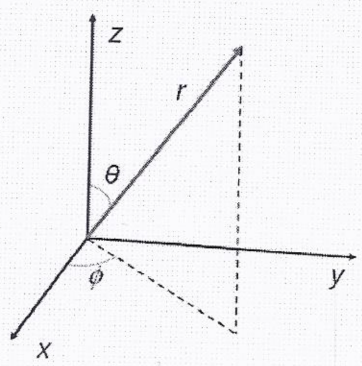
$$u_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}, \qquad E_0 = \tfrac{1}{2}\hbar\omega$$

$$u_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}}\, x e^{-m\omega x^2/2\hbar}, \qquad E_1 = \tfrac{3}{2}\hbar\omega$$

$$u_2 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}} \left(\frac{2m\omega}{\hbar}x^2 - 1\right) e^{-m\omega x^2/2\hbar}, \qquad E_2 = \tfrac{5}{2}\hbar\omega$$

$$u_3 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{m\omega}{3\hbar}}\, x \left(\frac{2m\omega}{\hbar}x^2 - 3\right) e^{-m\omega x^2/2\hbar}, \qquad E_3 = \tfrac{7}{2}\hbar\omega$$

## Spherical coordinates




$$r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$$

$$x = r \sin\theta \cos\phi$$
$$y = r \sin\theta \sin\phi$$
$$z = r \cos\theta$$

$$\nabla_{sph} = \frac{\partial}{\partial r}\hat{r} + \frac{\partial}{\partial\theta}\frac{\hat{\theta}}{r} + \frac{\partial}{\partial\phi}\frac{\hat{\phi}}{r sin\theta}$$

$$\nabla^2_{sph} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$\int d^3r\, f(r) = \int_0^\infty dr\, r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi\, f(r,\theta,\varphi)$$

## Angular momentum

$$\hat{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2\, Y_{lm}(\theta,\varphi)$$
$$\hat{L}_z Y_{lm}(\theta,\varphi) = m\hbar\, Y_{lm}(\theta,\varphi)$$

### Component commutation relation

$$i\hbar\,\hat{\boldsymbol{L}} = \hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}}$$

# Hydrogenic atom

## Energies

$$E_n = -\frac{E_h}{2}\frac{Z^2}{n^2}, \quad E_h = \frac{\hbar^2}{m_e a_0^2} = 27.2\ \text{eV}$$

## Wavefunctions

$$\psi_{nlm}(\mathbf{r},t) = u_{nlm}(\mathbf{r})\,\mathrm{e}^{-iE_n t/\hbar}$$

$$u_{nlm}(\mathbf{r}) = R_{nl}(r)\,Y_{lm}(\theta,\varphi)$$

## Radial equation

$$\hat{H}\chi = E\chi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V'(r)$$

$$V'(r) = -\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} + l(l+1)\frac{\hbar^2}{2mr^2}$$

$$\chi = \chi_{nl}(r) = rR_{nl}$$

## Radial functions

$$R_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-(Zr/a_0)}$$

$$R_{20}(r) = 2\left(\frac{Z}{2a_0}\right)^{3/2}\left(1-\frac{Zr}{2a_0}\right) e^{-(Zr/2a_0)}$$

$$R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right) e^{-(Zr/2a_0)}$$

$$R_{30}(r) = 2\left(\frac{Z}{3a_0}\right)^{3/2}\left(1-\frac{2Zr}{3a_0}+\frac{2Z^2r^2}{27a_0^2}\right) e^{-(Zr/3a_0)}$$

$$R_{31}(r) = \frac{4\sqrt{2}}{9}\left(\frac{Z}{3a_0}\right)^{3/2}\left(1-\frac{Zr}{6a_0}\right)\left(\frac{Zr}{a_0}\right) e^{-(Zr/3a_0)}$$

$$R_{32}(r) = \frac{4}{27\sqrt{10}}\left(\frac{Z}{3a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-(Zr/3a_0)}$$

## Spherical harmonics

$$Y_{00} = \sqrt{\frac{1}{4\pi}}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{2\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi}$$

$$Y_{2\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi}$$

## Parity

$$Y_{lm}(\pi-\theta,\varphi+\pi) = (-1)^l Y_{lm}(\theta,\varphi)$$

## Photon wavelength and energy

$$\lambda E = 1240\ \text{nm}\cdot\text{eV}$$

## Atomic units

| Physical quantity | Name of unit | Symbol for unit | Value of unit in SI |
|---|---|---|---|
| mass | electron rest mass | $m_e$ | $9.109\,3897(54) \times 10^{-31}$ kg |
| charge | elementary charge | $e$ | $1.602\,177\,33(49) \times 10^{-19}$ C |
| action | Planck constant/2π[1] | $\hbar$ | $1.054\,572\,66(63) \times 10^{-34}$ J s |
| length | bohr[1] | $a_0$ | $5.291\,772\,49(24) \times 10^{-11}$ m |
| energy | hartree[1] | $E_h$ | $4.359\,7482(26) \times 10^{-18}$ J |
| time | | $\hbar/E_h$ | $2.418\,884\,3341(29) \times 10^{-17}$ s |
| velocity[2] | | $a_0E_h/\hbar$ | $2.187\,691\,42(10) \times 10^{6}$ m s$^{-1}$ |
| force | | $E_h/a_0$ | $8.238\,7295(25) \times 10^{-8}$ N |
| momentum, linear | | $\hbar/a_0$ | $1.992\,8534(12) \times 10^{-24}$ N s |
| electric current | | $eE_h/\hbar$ | $6.623\,6211(20) \times 10^{-3}$ A |
| electric field | | $E_h/ea_0$ | $5.142\,2082(15) \times 10^{11}$ V m$^{-1}$ |
| electric dipole moment | | $ea_0$ | $8.478\,3579(26) \times 10^{-30}$ C m |
| magnetic flux density | | $\hbar/ea_0^2$ | $2.350\,518\,08(71) \times 10^{5}$ T |
| magnetic dipole moment[3] | | $e\hbar/m_e$ | $1.854\,803\,08(62) \times 10^{-23}$ J T$^{-1}$ |

(1) $\hbar = h/2\pi$; $a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$; $E_h = \hbar^2/m_e a_0^2$.
(2) The numerical value of the speed of light, when expressed in atomic units, is equal to the reciprocal of the fine structure constant $\alpha$; $c$/(au of velocity) $= c\hbar/a_0E_h = \alpha^{-1} \approx 137.035\,9895(61)$.
(3) The atomic unit of magnetic dipole moment is twice the Bohr magneton, $\mu_B$.

$$m_e = \frac{\hbar^2}{E_h a_0^2} \qquad E_h = \frac{e^2}{4\pi\varepsilon_0\, a_0}$$

### Electric field amplitude vs. intensity in an EM wave

$$F = \sqrt{\frac{8\pi}{c4\pi\varepsilon_0}}\sqrt{I} \quad \text{(SI)}$$

$$F = \sqrt{8\pi/c}\sqrt{I} \quad \text{(atomic units)}$$

$$1\,\text{a.u. intensity} = \frac{E_h^2}{a_0^2\hbar} = 6.436\times10^{15}\ \text{W/cm}^2$$

$$\equiv 22.02\times10^{10}\ \text{V/m} = 0.4283\ E_h/(ea_0)$$

$$F\Big/\frac{\text{V}}{\text{cm}} = 27.48\sqrt{I\Big/\frac{\text{W}}{\text{cm}^2}}$$

$$F\Big/\frac{E_h}{ea_0} = 5.338\times10^{-9}\sqrt{I\Big/\frac{\text{W}}{\text{cm}^2}}$$

## Dirac notation

$$\psi(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi\rangle$$

$$\langle\varphi|\psi\rangle = \int \varphi^*(\boldsymbol{r})\,\psi(\boldsymbol{r})\,\mathrm{d}^3r$$

$$\langle\varphi|\hat{Q}|\psi\rangle = \int \varphi^*(\boldsymbol{r})\,\hat{Q}\,\psi(\boldsymbol{r})\,\mathrm{d}^3r$$

$$\langle\varphi|\hat{Q}|\psi\rangle^* = \langle\psi|\hat{Q}^\dagger|\varphi\rangle$$

$$\hat{\boldsymbol{r}}|\boldsymbol{r}\rangle = \boldsymbol{r}|\boldsymbol{r}\rangle$$

$$Y_{lm}(\theta,\varphi) = \langle\theta\varphi|l\,m\rangle$$

$$u_{nlm}(\boldsymbol{r}) = \langle\boldsymbol{r}|n\,l\,m\rangle$$

$$u_i(\boldsymbol{r}) = \langle\boldsymbol{r}|i\rangle$$

$$\langle i|j\rangle = \delta_{ij} \qquad \langle\boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')$$

$$\sum_i |i\rangle\langle i| = \hat{1} \qquad \int \mathrm{d}^3r\,|\boldsymbol{r}\rangle\langle\boldsymbol{r}| = \hat{1}$$

## Interaction with electromagnetic radiation

$$\mathbf{F} = \boldsymbol{\varepsilon} F_0 \cos(\omega t)$$

$$\mu = -e\langle 2|\boldsymbol{\varepsilon}\cdot\mathbf{r}|1\rangle$$

$$\Omega = -\frac{\mu F_0}{2\hbar}$$

$$I = \frac{c\varepsilon_0}{2} F_0^2$$

$$I_{\text{indoor}} \approx 1\ \text{W/m}^2$$

$$I_{\text{sunlight}} \approx 1\ \text{kW/m}^2$$

$$T_{\text{Sun surface}} \approx 5800\,K$$

$$A_{21} = \frac{\hbar\omega^3}{\pi^2 c^3} B_{21}$$

$$B_{12} = \frac{\pi\mu^2}{\varepsilon_0 \hbar^2}$$

$$I(\omega) = c\,\rho(\omega)$$

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

## Spin

$$\hat{\boldsymbol{S}} = \frac{\hbar}{2}\boldsymbol{\sigma} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## Helium-like systems

### Ionisation and detachment energies

$$\text{He} + 24.4\ \text{eV} \to \text{He}^+ + \text{e}^-$$

$$\text{H}^- + 0.8\ \text{eV} \to \text{H} + \text{e}^-$$

### Coulomb integral for the ground state

$$J = \langle 1s|\langle 1s|\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_{12}}|1s\rangle|1s\rangle = \frac{5}{8}E_{\text{h}}Z$$

## Pilot wave theory

$$\psi = R e^{iS/\hbar}$$

$$\boldsymbol{v} = \frac{\nabla S}{m}$$

$$Q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) = 0$$

## Mathematics

$$\int_{-\infty}^{\infty} e^{-x^2}\,\mathrm{d}x = \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} x^2 e^{-x^2}\,\mathrm{d}x = \frac{\sqrt{\pi}}{2}$$

$$\int_{-\infty}^{\infty} x^4 e^{-x^2}\,\mathrm{d}x = \frac{3\sqrt{\pi}}{4}$$

### Dirac delta

$$\int \mathrm{d}^3 r'\, f(\boldsymbol{r}')\,\delta(\boldsymbol{r}-\boldsymbol{r}') = f(\boldsymbol{r})$$

$$\delta(-\boldsymbol{r}) = \delta(\boldsymbol{r})$$

*8 March 2011*