# USEFUL CONSTANTS AND FORMULAS

## Physical constants and common integrals

$h = 6.63\times10^{-34}\,\text{J s}$ $\quad \hbar = 1.06\times10^{-34}\,\text{J s}$ $\quad m_e = 9.11\times10^{-34}\,\text{kg}$ $\quad c = 3.0\times10^{8}\,{}^{\text{m}}\!/\!_{\text{s}}$

$E = h\nu = hc/\lambda$ $\quad \Delta x\,\Delta p \ge \hbar/2$ $\quad \lambda = h/p$ $\quad \lambda\nu = c$

$$\int_0^\infty e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \qquad \int_0^\infty x\,e^{-ax^2}dx = \frac{1}{2a} \qquad \int_0^\infty x^2\,e^{-ax^2}dx = \frac{\sqrt{\pi}}{4a^{3/2}} \qquad \int_0^\infty x^n\,e^{-ax}dx = \frac{n!}{a^{n+1}}$$

valid for $n > -1$, $a > 0$

## Fundamental equations

Time Dependent Schrödinger's Equation $\quad i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\,\Psi(x,t)$

Time Independent Schrödinger's Equation $\quad \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\,\psi(x)$

Canonical Commutation Relation $\quad [\hat{x}, \hat{p}] = i\hbar$

Heisenberg Uncertainty Principle $\quad \sigma_x\sigma_p \ge \frac{\hbar}{2}$

Fermi's Golden Rule $\quad W_{fi} = \frac{2\pi}{\hbar}\left|V_{fi}\right|^2\left[\delta\left(E_f - E_i - \hbar\omega\right) + \delta\left(E_f - E_i + \hbar\omega\right)\right]$

$$\hat{V}(t) = \hat{V}\cos(\omega t) \qquad V_{fi} = \int d^3\mathbf{r}\,\psi_f^*(\mathbf{r})\hat{V}\psi_i(\mathbf{r})$$

## Particle in a box

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \qquad V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{everywhere else} \end{cases}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \psi(0 \le x \le a) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

## Separable systems

$$\hat{H}(x,y) = \hat{H}_x(x) + \hat{H}_y(y) \qquad \Psi_{m,n}(x,y) = \psi_m(x)\psi_n(y) \qquad E_{m,n} = E_m + E_n$$

## Harmonic oscillator

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}k\,x^2 = \hat{a}_+\hat{a}_+ + \frac{\hbar\omega}{2}$$

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right); \quad \omega = \sqrt{\frac{k}{\mu}}$$

$$\hat{a}_\pm = \frac{1}{\sqrt{2m\hbar\omega}}\left(m\omega\hat{x} \mp i\hat{p}\right)$$

$$\left[\hat{a}_-, \hat{a}_+\right] = 1$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_+ + \hat{a}_-\right)$$

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}\left(\hat{a}_+ - \hat{a}_-\right)$$

$$\hat{a}_+\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}(x)$$

$$\hat{a}_-\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x)$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\alpha}{\pi}\right)^{1/4} H_n\left(\alpha^{1/2}x\right)e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_1(x) = \frac{1}{\sqrt{2}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(2\alpha^{1/2}x\right)e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_2(x) = \frac{1}{\sqrt{8}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(4\alpha x^2 - 2\right)e^{-\frac{1}{2}\alpha x^2}$$

$$\psi_3(x) = \frac{1}{\sqrt{48}}\left(\frac{\alpha}{\pi}\right)^{1/4}\left(8\alpha^{3/2}x^3 - 12\alpha^{1/2}x\right)e^{-\frac{1}{2}\alpha x^2}$$

## Angular momentum operators and spherical harmonics

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$\hat{L}_z = i\hbar\frac{\partial}{\partial\phi}$$

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z$$

$$\left[\hat{L}^2, \hat{L}_i\right] = 0$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

$$\hat{L}^2 Y_l^m = \hbar^2 l(l+1)Y_l^m$$

$$\hat{L}_z Y_l^m = \hbar m Y_l^m$$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^{\pm1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

## Rigid rotor

$$\hat{H} = \frac{\hat{J}^2}{2I}; \quad I = \mu R^2\left(\text{diatomic}\right)$$

$$\hat{H}\,Y_j^{j_z} = E_j Y_j^{j_z}; \qquad E_j = \hbar^2 j\left(j+1\right)$$

$$j = 0,1,2,3,\ldots \qquad j_z = -j, -j+1, \ldots, j-1, j$$

## Hydrogenic atom

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{r};$$

in atomic units, $\hbar = m_e = e = 4\pi\varepsilon_0 = a_0 = 1$.

$$E_n = -\frac{Z^2e^2}{8\pi\varepsilon_0 a_0 n^2} = \frac{Z^2}{2n^2}\left(\text{a.u.}\right)$$

## Hydrogenic atom wavefunctions

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\,Y_l^m(\theta,\phi)$$

$n=1 \quad l=0 \quad m=0$

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma} = \psi_{1s}$$

$n=2 \quad l=0 \quad m=0$

$$\psi_{200}(r,\theta,\phi) = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)\,e^{-\frac{\sigma}{2}} = \psi_{2s}$$

$l=1 \quad m=0$

$$\psi_{210}(r,\theta,\phi) = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \cos\theta = \psi_{2p_z}$$

$l=1 \quad m=\pm 1$

$$\psi_{21\pm1}(r,\theta,\phi) = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin\theta\, e^{i\phi}$$

$$\frac{1}{\sqrt{2}}\left(\psi_{21+1} + \psi_{21-1}\right) = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin\theta\cos\phi = \psi_{2p_x}$$

$\sigma = \dfrac{Z\,r}{a_0}$

$$\frac{1}{\sqrt{2}i}\left(\psi_{21+1} - \psi_{21-1}\right) = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\frac{\sigma}{2}} \sin\theta\sin\phi = \psi_{2p_y}$$

## Spin ½ Matrices

$$\mathbf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathbf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \mathbf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## Independent Particle Model

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = \begin{vmatrix} \psi_1(\mathbf{x}_1) & \psi_1(\mathbf{x}_2) & \psi_1(\mathbf{x}_2) \\ \psi_2(\mathbf{x}_1) & \psi_2(\mathbf{x}_2) & \psi_2(\mathbf{x}_2) \\ \psi_3(\mathbf{x}_1) & \psi_3(\mathbf{x}_2) & \psi_3(\mathbf{x}_3) \end{vmatrix}$$

$$E_{avg} = \sum_i \varepsilon_i + \sum_i \sum_{j<i} \tilde{J}_{ij} - \tilde{K}_{ij} \quad \text{where } \tilde{J}_{ij} = J_{ij} \text{ and } \tilde{K}_{ij} = \begin{matrix} K_{ij} & \text{if } \sigma_i = \sigma_j \\ 0 & \text{if } \sigma_i \neq \sigma_j \end{matrix}$$

## Variational method and M.O. theory

$$\mathbf{Hc} = E_{avg}\mathbf{Sc} \qquad \mathbf{H} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$$

$$\psi(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \qquad H_{ij} = \int d^3r\, \phi_i^*(\vec{r})\,\hat{H}\,\phi_j(\vec{r}) \qquad S_{ij} = \int d^3r\, \phi_i^*(\vec{r})\,\phi_j(\vec{r})$$