Quantum Mechanics Formula Sheet

$E_{photon} = h\nu = \frac{1}{2}\ mv^2 + e\,\Gamma = \frac{1}{2}\ mv^2 + \Phi$ $\qquad \Delta E = h\nu = -\Re_h\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$

$e^{ix} = \cos x + i \sin x \qquad \frac{e^{i\phi} + e^{-i\phi}}{2} = \cos\phi \qquad \frac{e^{i\phi} - e^{-i\phi}}{2i} = \sin\phi \qquad \Psi = e^{ikx} \qquad k = \frac{p}{\hbar} = \frac{(2mE)^{1/2}}{\hbar}$

$E = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2} \qquad \Psi = \left(\frac{2}{a}\right)^{1/2}\sin\frac{n\pi x}{a} \qquad \Psi(x,y) = \left(\frac{4}{ab}\right)^{1/2}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{b} \qquad E = \frac{h^2}{8m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2}\right)$

$x \to \hat{x} \qquad p \to \frac{\hbar}{i}\left(\frac{\partial}{\partial x}\right) \qquad t \to \hat{t} \qquad E(t) \to \hat{E} = i\hbar\left(\frac{\partial}{\partial t}\right) \qquad E_k \to \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad [O_1, O_2] = \hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1$

$\Psi(x) = A\, e^{-\frac{1}{2} a^2 x^2} \qquad \alpha^2 = \frac{\sqrt{mk}}{\hbar} \qquad A = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \qquad \Psi(x) = \left(\frac{m\omega_o}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega_o x^2}{2\hbar}}$

$x = r\sin\theta\cos\phi \qquad y = r\sin\theta\sin\phi \qquad z = r\cos\theta \qquad d\tau = r^2\sin\theta\, dr\, d\theta\, d\phi$

$r^2 = x^2 + y^2 + z^2 \qquad \theta:\ 0 \le \theta \le \pi \qquad \phi:\ 0 \le \phi \le 2\pi \qquad r:\ 0 \le r \le \infty$

$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \qquad \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \qquad \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

$\nabla^2 = \frac{1}{r}\left(\frac{\partial^2}{\partial r^2}\right)r + \left(\frac{1}{r^2}\right)\Lambda^2 \qquad \Lambda^2 = \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right) + \left(\frac{1}{\sin\theta}\right)\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) \qquad |L| = \hbar\sqrt{\ell(\ell+1)}$

$L_z = \hbar m_\ell \qquad \Phi(\phi) = \left(\frac{1}{2\pi}\right)^{1/2} e^{im_\ell\phi} \qquad -\hbar^2\Lambda^2 Y_{\ell,m_\ell} = \ell(\ell+1)\hbar^2 Y_{\ell,m_\ell} \qquad E = \frac{\hbar^2}{2I}\ell(\ell+1)$

$\frac{-\hbar^2}{2m}\left(\frac{1}{r}\frac{d^2}{dr^2} r R\right) - \frac{Z e^2}{4\pi\varepsilon_o r} R = E R \qquad E_n = -\left(\frac{Z^2 e^4 m}{32\pi^2\varepsilon_o^2\hbar^2}\right)\frac{1}{n^2} \qquad a_o = \frac{4\pi\varepsilon_o\hbar^2}{me^2}$

$E_n = -\frac{Z^2\hbar^2}{2ma_o^2}\frac{1}{n^2} \qquad E_n = -13.6\ \text{eV}\frac{Z^2}{n^2} = -109{,}678\ \text{cm}^{-1}\frac{Z^2}{n^2} = -1312\ \text{kJ mol}^{-1}\frac{Z^2}{n^2} = -\frac{H}{2}\frac{Z^2}{n^2}$

$\Psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/a_o}$ $\qquad h = 6.626 \times 10^{-34}$ J s $\qquad \hbar = 1.055 \times 10^{-34}$ J s

$\Psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2}\left(2 - \frac{Zr}{a_o}\right) e^{-Zr/2a_o}$ $\qquad e = 1.602 \times 10^{-19}$ C

$\Psi_{2pz} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/2a_o}\frac{Zr}{a_o}\cos\theta$ $\qquad \varepsilon_o = 8.85 \times 10^{-12}\ J^{-1}c^2m^{-1}$

$\Psi_{211} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/2a_o}\frac{Zr}{a_o}\sin\theta\, e^{i\phi}$ $\qquad a_o = 0.0529$ nm $= 0.529$Å

$\Psi_{21-1} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/2a_o}\frac{Zr}{a_o}\sin\theta\, e^{-i\phi}$ $\qquad 1H = 2625.5\ \text{kJ mol}^{-1}$

$\Psi_{2px} = \frac{\Psi_{211} + \Psi_{21-1}}{2} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/2a_o}\frac{Zr}{a_o}\sin\theta\cos\phi$ $\qquad m_e = 9.11 \times 10^{-31}$ kg

$\Psi_{2py} = \frac{\Psi_{211} - \Psi_{21-1}}{2i} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/2a_o}\frac{Zr}{a_o}\sin\theta\sin\phi$ $\qquad \Re_h = 109{,}678\ \text{cm}^{-1}$

ℓ	m_ℓ	Y_{ℓ,m_ℓ}
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2}\cos\theta$
	±1	$\pm(3/8\pi)^{1/2}\sin\theta\, e^{\pm i\phi}$
2	0	$(5/16\pi)^{1/2}(3\cos^2\theta - 1)$
	±1	$\pm(15/8\pi)^{1/2}\cos\theta\sin\theta\, e^{\pm i\phi}$
	±2	$\pm(15/32\pi)^{1/2}\sin^2\theta\, e^{\pm i2\phi}$

$y = \alpha x$ $\quad\quad$ $\Psi_\upsilon(y) = H_\upsilon e^{-\frac{1}{2}y^2}$

υ	$H_\upsilon(y)$	$H_\upsilon(\alpha x)$
0	1	1
1	$2y$	$2\alpha x$
2	$4y^2 - 2$	$4\alpha^2x^2 - 2$
3	$8y^3 - 12y$	$8\alpha^3x^3 - 12\alpha x$

$$\frac{d^2H_\upsilon}{dy^2} - 2y\frac{dH_\upsilon}{dy} + 2\upsilon H_\upsilon = 0$$

$$H_{\upsilon+1} = 2y H_\upsilon - 2\upsilon H_{\upsilon-1}$$

$$\int_{-\infty}^{\infty} H_{\upsilon'} e^{-\frac{1}{2}y^2} H_\upsilon e^{-\frac{1}{2}y^2}\, dy = 0 \quad \text{if } \upsilon' \neq \upsilon$$

$$= \pi^{1/2} 2^\upsilon \upsilon! \quad \text{if } \upsilon' = \upsilon$$

$$\int \sin^2(x)\,dx = -\tfrac{1}{2}\sin(x)\cos(x) + \tfrac{1}{2}x$$

$$\int \cos^2(x)\,dx = \tfrac{1}{2}\sin(x)\cos(x) + \tfrac{1}{2}x$$

$$\int \sin(x)\cos(x)\,dx = \tfrac{1}{2}\sin^2(x)$$

$$\int_0^{\pi/2} \sin^2(x)\,dx = \int_0^{\pi/2} \cos^2(x)\,dx = \frac{\pi}{4}$$

$$\int_0^{\pi/2} \sin^3(x)\,dx = \int_0^{\pi/2} \cos^3(x)\,dx = \frac{2}{3}$$

$$\int_0^{\pi} \sin^2(ax)\,dx = \int_0^{\pi} \cos^2(ax)\,dx = \frac{\pi}{2}$$

$$\int_0^{\pi/a} \cos(ax)\sin(ax)\,dx = \int_0^{\pi} \cos(ax)\sin(ax)\,dx = 0$$

$$\int_0^{\pi} \sin(ax)\sin(bx)\,dx = \int_0^{\pi} \cos(ax)\cos(bx)\,dx = 0 \quad (a \neq b;\ a,b \text{ integers})$$

$$\int_0^{\pi} \sin(ax)\cos(bx)\,dx = \frac{2a}{a^2-b^2} \quad \text{if a-b is odd, or zero if a-b is even}$$

$$\int_0^{\pi} \cos(ax)\sin(ax)\,dx = 0$$

$$\int_0^{n\pi} x^2\sin^2(x)\,dx = \frac{n^3\pi^3}{6} - \frac{n\pi}{4}$$