Constants and units

$$c = 2.998 \times 10^{8}\,\mathrm{m\,s^{-1}}$$
$$h = 6.626 \times 10^{-34}\,\mathrm{J\,s}$$
$$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34}\,\mathrm{J\,s}$$
$$N_A = 6.022 \times 10^{23}\,\mathrm{mol^{-1}}$$
$$k_B = 1.381 \times 10^{-23}\,\mathrm{J\,K^{-1}}$$
$$R = 8.3145\,\mathrm{J\,K^{-1}\,mol^{-1}}$$
$$= 0.082\,06\,\mathrm{L\,atm\,mol^{-1}\,K^{-1}}$$
$$m_{e^-} = 9.109 \times 10^{-31}\,\mathrm{kg}$$
$$e = 1.602 \times 10^{-19}\,\mathrm{C}$$
$$m_{p^+} = 1.673 \times 10^{-27}\,\mathrm{kg}$$
$$m_{n^0} = 1.675 \times 10^{-27}\,\mathrm{kg}$$
$$a_0 = 0.5292 \times 10^{-10}\,\mathrm{m}$$
$$\varepsilon_0 = 8.8542 \times 10^{-12}\,\mathrm{C^2\,N^{-1}\,m^{-2}}$$
$$R_H = 1.097 \times 10^{5}\,\mathrm{cm^{-1}}$$
$$1\,\mathrm{N} = 1\,\mathrm{kg\,m\,s^{-2}}$$
$$1\,\mathrm{J} = 1\,\mathrm{N\,m} = 1\,\mathrm{kg\,m^2\,s^{-2}}$$
$$1\,\mathrm{eV} = 1.602 \times 10^{-19}\,\mathrm{J}$$
$$1\,\mathrm{cm^{-1}} = 1.986 \times 10^{-23}\,\mathrm{J}$$
$$1\,\mathrm{u} = 1.661 \times 10^{-27}\,\mathrm{kg}$$

Kinetic Molecular Theory

$$\sigma = \pi d^2$$
$$\rho = \left(\frac{pN_A}{RT}\right)$$
$$z_{12} = \frac{N_2}{V}\sigma\left(\frac{8kT}{\pi\mu}\right)^{1/2}$$
$$\lambda = \frac{1}{\sqrt{2}\rho\sigma}$$
$$Z_{12} = \rho_1\rho_2\sigma\left(\frac{8kT}{\pi M}\right)^{1/2}$$
$$P(v) = 4\pi\left(\frac{M}{2\pi RT}\right)^{3/2} v^2 e^{-Mv^2/2RT}$$
$$\langle v\rangle = \left(\frac{8RT}{\pi M}\right)^{1/2}$$
$$v_{rms} = \left(\frac{3RT}{M}\right)^{1/2}$$
$$v_{mp} = \left(\frac{2RT}{M}\right)^{1/2}$$

Math

Determinants

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

$$\psi(1,2,3,\ldots,n) = \frac{1}{\sqrt{n!}}\begin{vmatrix} u_1(1) & u_2(1) & \cdots & u_n(1) \\ u_1(2) & u_2(2) & \cdots & u_n(2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(n) & u_2(n) & \cdots & u_n(n) \end{vmatrix}$$

Integrals

$$\int_{-\infty}^{+\infty} f(x)\,dx = 0 \text{ for odd } f(x)$$
$$f(-x) = -f(x) \text{ for odd } f(x)$$
$$\int_{-\infty}^{+\infty} f(x)\,dx = 2\int_0^{+\infty} f(x)\,dx \text{ for even } f(x)$$
$$f(-x) = f(x) \text{ for even } f(x)$$
$$\int \sin(ax)\,dx = -\frac{1}{a}\cos(ax)$$
$$\int \cos(ax)\,dx = \frac{1}{a}\sin(ax)$$
$$\int \sin^2(ax)\,dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$
$$\int \cos^2(ax)\,dx = \frac{x}{2} + \frac{\sin(2ax)}{4a}$$
$$\int x\sin^2(ax)\,dx = \frac{x^2}{4} - \frac{\cos(2ax)}{8a^2} - \frac{x\sin(2ax)}{4a}$$
$$\int x\cos^2(ax)\,dx = \frac{x^2}{4} + \frac{\cos(2ax)}{8a^2} + \frac{x\sin(2ax)}{4a}$$
$$\int x^2\sin^2(ax)\,dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) - \frac{x}{4a^2}\cos(2ax)$$
$$\int x^2\cos^2(ax)\,dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) + \frac{x}{4a^2}\cos(2ax)$$
$$\int_0^{\infty} e^{-ax^2}\,dx = \left(\frac{\pi}{4a}\right)^{1/2}$$
$$\int_0^{\infty} x^{2n}e^{-ax^2}\,dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$$
$$\int_0^{\infty} x^{2n+1}e^{-ax^2}\,dx = \frac{n!}{2a^{n+1}}$$
$$\int_0^{\infty} x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$$

Trigonometry

$$\sin(2x) = 2\sin x\cos x$$
$$\cos(2x) = \cos^2 x - \sin^2 x$$
$$\sin^2 x = \frac{1-\cos 2x}{2}$$
$$\cos^2 x = \frac{1+\cos 2x}{2}$$
$$\sin^2 x + \cos^2 x = 1$$
$$\sin x \sin y = \frac{1}{2}\left[\cos(x-y) - \cos(x+y)\right]$$
$$\cos x \cos y = \frac{1}{2}\left[\cos(x-y) + \cos(x+y)\right]$$
$$\sin x \cos y = \frac{1}{2}\left[\sin(x+y) + \sin(x-y)\right]$$

Polar

$$x = r\cos\phi$$
$$y = r\sin\phi$$
$$r = \sqrt{x^2+y^2}$$
$$\phi = \tan^{-1}\frac{y}{x}$$
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)_{r=r_0} = \frac{1}{r_0^2}\frac{\partial^2}{\partial\phi^2}$$

Spherical

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$
$$r = \sqrt{x^2+y^2+z^2}$$
$$\theta = \cos^{-1}\frac{z}{\sqrt{x^2+y^2+z^2}}$$
$$\phi = \tan^{-1}\frac{y}{x}$$
$$dV = dx\,dy\,dz = r^2\,\sin\theta\,dr\,d\theta\,d\phi$$
$$\nabla^2_{r=r_0} = \cdots$$
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)_{r=r_0} = \cdots$$
$$\frac{1}{r_0^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)_{r,\phi} + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)_{r,\theta}\right]$$

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

General quantum mechanics

$$E = h\nu = \frac{hc}{\lambda}$$
$$\lambda = \frac{h}{p}$$
$$\Psi(x,t) = \psi(x)\,e^{-i(E/\hbar)t}$$
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\right]\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\psi(x) = E\psi(x)$$
$$\hat{H}\psi_n(x) = E_n\psi_n(x)$$
$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$
$$\hat{x} = x$$
$$\hat{p_x} = -i\hbar\frac{\partial}{\partial x}$$
$$\int_{-\infty}^{+\infty}\Psi^*(x,t)\,\Psi(x,t)\,dx = 1$$
$$\langle a\rangle = \frac{\int_{-\infty}^{+\infty}\Psi^*(x,t)\,\hat{A}\Psi(x,t)\,dx}{\int_{-\infty}^{+\infty}\Psi^*(x,t)\,\Psi(x,t)\,dx}$$
$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$
$$\left[\hat{A},\hat{B}\right] = -\left[\hat{B},\hat{A}\right]$$
$$\Delta p\Delta x \geq \frac{\hbar}{2}$$
$$E_{variational} = \frac{\int\Phi^*\hat{H}\Phi d\tau}{\int\Phi^*\Phi d\tau} \geq E_0$$

Term symbols

$${}^{2S+1}L_J$$
$$L = \sum_i l_i, M_L = \sum_i l_{z,i}$$
$$S = \sum_i s_i, M_S = \sum_i s_{z,i}$$
$$J = L+S, L+S-1, \ldots, |L-S|$$

${}^{2S+1}\Lambda_\Omega$ for molecules

Particle in a box

$$\psi_{1D}\left(x\right) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right); n = 1, 2, 3 \ldots$$

$$E_n = \frac{h^2 n^2}{8ma^2}$$

$$\psi_{3D}\left(x, y, z\right) = \left(\frac{8}{abc}\right)^{1/2} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

Harmonic oscillator

$$\begin{aligned}
V\left(x\right) &= \frac{1}{2}kx^2 \\
x_{cm} &= \frac{m_1 x_1 + m_2 x_2}{m_1 m_2} \\
\mu &= \frac{m_1 m_2}{m_1 + m_2} \\
\hat{H} &= \left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right] \\
\psi_v\left(x\right) &= A_v H_v\left(\alpha^{1/2} x\right) e^{-\frac{1}{2}\alpha x^2} \\
\psi_0\left(x\right) &= \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} \\
\psi_1\left(x\right) &= \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x e^{-\frac{1}{2}\alpha x^2} \\
\psi_2\left(x\right) &= \left(\frac{\alpha}{4\pi}\right)^{1/4}\left(2\alpha x^2 - 1\right) e^{-\frac{1}{2}\alpha x^2} \\
\alpha &= \sqrt{\frac{k\mu}{\hbar^2}} \\
E_v &= \hbar\sqrt{\frac{k}{\mu}}\left(v + \frac{1}{2}\right) = h\nu\left(v + \frac{1}{2}\right); v = 0, 1, 2, 3, \cdots \\
\nu &= \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} = \tilde{\nu} c
\end{aligned}$$

Anharmonic oscillator

$$V\left(x\right) = D_e\left(e^{-2ax} - 2e^{-ax}\right); a = \sqrt{\frac{k}{2D_e}}$$

$$E_v = h\nu\left(v + \frac{1}{2}\right) - \frac{\left(h\nu\right)^2}{4D_e}\left(v + \frac{1}{2}\right)^2$$

$$G\left(v\right) = \tilde{\nu}\left(v + \frac{1}{2}\right) - \tilde{x}\tilde{\nu}\left(v + \frac{1}{2}\right)^2; \tilde{x} = \frac{hc\tilde{\nu}}{4D_e}$$

Rigid rotor

$$\begin{aligned}
I &= \mu r^2 \\
L &= I\omega \\
KE &= \frac{1}{2}I\omega^2 \\
&= \frac{L^2}{2I}
\end{aligned}$$

2D

$$\begin{aligned}
\hat{H} &= -\frac{\hbar^2}{2\mu r_0^2}\frac{\partial^2}{\partial\phi^2} \\
\Phi_{m_l}\left(\phi\right) &= \frac{1}{\sqrt{2\pi}} e^{i m_l \phi} \\
m_l &= 0, \pm 1, \pm 2, \cdots \\
E_{m_l} &= \frac{\hbar^2 m_l^2}{2I} \\
\hat{L}_z \Phi_{m_l}\left(\phi\right) &= m_l \hbar \Phi_{m_l}\left(\phi\right)
\end{aligned}$$

3D

$$\begin{aligned}
\hat{H} &= -\frac{\hbar^2}{2\mu r_0^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)_{r,\phi} + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)_{r,\theta}\right] \\
Y\left(\theta, \phi\right) &= Y_l^{m_l}\left(\theta, \phi\right) = \Theta_l^{m_l}\left(\theta\right)\Phi_{m_l}\left(\phi\right) \\
E_l &= \frac{\hbar^2}{2I} l\left(l + 1\right) \\
l &= 0, 1, 2, 3, \ldots \\
m_l &= -l, -\left(l - 1\right), \ldots, 0, \ldots, \left(l - 1\right), l \\
E_J &= hc\tilde{B}J\left(J + 1\right) \\
\tilde{B} &= \frac{h}{8\pi^2 c\mu r_0^2} \\
\hat{L}_z Y_l^{m_l}\left(\theta, \phi\right) &= m_l \hbar Y_l^{m_l}\left(\theta, \phi\right) \\
\hat{L}^2 Y_l^{m_l}\left(\theta, \phi\right) &= \hbar^2 l\left(l + 1\right) Y_l^{m_l}\left(\theta, \phi\right) \\
\hat{L}_{\substack{x\\y\\z}} &= -i\hbar\left(\substack{y\\z\\x}\frac{\partial}{\partial\substack{z\\x\\y}} - \substack{z\\x\\y}\frac{\partial}{\partial\substack{y\\z\\x}}\right) \\
\left[\hat{L}_{\substack{x\\y\\z}}, \hat{L}_{\substack{y\\z\\x}}\right] &= i\hbar\hat{L}_{\substack{z\\x\\y}}
\end{aligned}$$

Spherical Harmonics

Complex

$$Y_l^{m_l}(\theta,\phi) = \cdots$$

$$Y_0^0(\theta,\phi) = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$

$$Y_1^{\pm1}(\theta,\phi) = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$$

$$Y_2^0(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{1/2}\left(3\cos^2\theta - 1\right)$$

$$Y_2^{\pm1}(\theta,\phi) = \mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$$

$$Y_2^{\pm2}(\theta,\phi) = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm 2i\phi}$$

Real

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

$$p_x = \frac{-1}{\sqrt{2}}\left(Y_1^1 - Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$$

$$p_y = \frac{-1}{\sqrt{2}i}\left(Y_1^1 + Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi$$

$$d_{z^2} = Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

$$d_{xz} = \frac{-1}{\sqrt{2}}\left(Y_2^1 - Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\phi$$

$$d_{yz} = \frac{-1}{\sqrt{2}i}\left(Y_2^1 + Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\phi$$

$$d_{xy} = \frac{1}{\sqrt{2}i}\left(Y_2^2 - Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\phi$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left(Y_2^2 + Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\phi$$

Hydrogen atom

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2 n^2} = -\frac{e^2}{8\pi\varepsilon_0 a_0 n^2}$$

$$a_0 = \frac{\varepsilon_0 h^2}{\pi m_e e^2}$$

$$n = 1, 2, 3, \cdots$$

$$l = 0, 1, 2, \cdots, n-1$$

$$m_l = 0, \pm1, \pm2, \cdots, \pm l$$

Radial functions

$$R_{nl}(r) = \cdots$$

$$R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

$$R_{20}(r) = \frac{1}{\sqrt{8}}\left(\frac{1}{a_0}\right)^{3/2}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}$$

$$R_{21}(r) = \frac{1}{\sqrt{24}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}$$

$$R_{30}(r) = \frac{2}{81\sqrt{3}}\left(\frac{1}{a_0}\right)^{3/2}\left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$$

$$R_{31}(r) = \frac{4}{81\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right)e^{-r/3a_0}$$

$$R_{32}(r) = \frac{4}{81\sqrt{30}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r^2}{a_0^2}e^{-r/3a_0}$$

$$P_{nl}(r)\,dr = R_{nl}^2(r)\,r^2 dr$$

Full wavefunctions

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)\,Y_l^{m_l}(\theta,\phi)$$
$$= R_{nl}(r)\,Y_{s,p,d,f,\ldots x,y,z}(\theta,\phi)$$