

## Schrodinger 3D Formulas

xyz Laplacian Operator:  $\nabla^2 F(x, y, z) = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) F(x, y, z)$

xyz Time-Dependent Schrodinger:  $i\hbar \frac{\partial \psi(x, y, z)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) + V(x, y, z) \psi(x, y, z)$

Free-Particle with Momentum  $\vec{p}$ :  $\psi(\vec{x}, t) = A \exp\left(i\left[\vec{k} \cdot \vec{x} - \omega t\right]\right) \quad \vec{k} = \frac{\vec{p}}{\hbar} \quad \omega = \frac{E}{\hbar} = \frac{\vec{p}^2}{2m\hbar} = \frac{\hbar}{2m} \vec{k}^2$

xyz Time-Independent Schrodinger:  $-\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) + V(x, y, z) \psi(x, y, z) = E \psi(x, y, z)$

Rectangular Box:  $V = 0$  for  $0 < x < w_x$  and  $0 < y < w_y$  and  $0 < z < w_z$  and  $V = \infty$  elsewhere

Solutions:  $\psi_{n_x, n_y, n_z} = \sin\left(\frac{n_x \pi x}{w_x}\right) \cdot \sin\left(\frac{n_y \pi y}{w_y}\right) \cdot \sin\left(\frac{n_z \pi z}{w_z}\right) \quad n_x, n_y, n_z = 1, 2, 3, \dots$  in any combination

Energies:  $E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \cdot \left[ \frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} + \frac{n_z^2}{w_z^2} \right] = (0.3759 \text{ eV-nm}^2) \cdot \left[ \frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} + \frac{n_z^2}{w_z^2} \right]$  for electron

xyz Harmonic Oscillator Energies:  $E_{n_x, n_y, n_z} = \frac{\hbar}{\sqrt{m}} \cdot \left[ \left( n_x + \frac{1}{2} \right) \sqrt{k_x} + \left( n_y + \frac{1}{2} \right) \sqrt{k_y} + \left( n_z + \frac{1}{2} \right) \sqrt{k_z} \right]$

if  $k_x = k_y = k_z = k$ :  $E_{n_x, n_y, n_z} = \hbar \sqrt{\frac{k}{m}} \cdot \left[ n_x + n_y + n_z + \frac{3}{2} \right] = \left[ n_x + n_y + n_z + \frac{3}{2} \right] \cdot (0.2761 \sqrt{\text{eV-nm}}) \cdot \sqrt{k}$  for electron

Spherical Gradient:  $\vec{\nabla} F = \hat{r} \frac{\partial F}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial F}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial F}{\partial \phi}$

Spherical Divergence:  $\vec{\nabla} \cdot \vec{G} = \frac{1}{r^2} \frac{\partial}{\partial r} [r^2 G_r] + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} [\sin \theta G_\theta] + \frac{1}{r \sin \theta} \frac{\partial G_\phi}{\partial \phi}$

Spherical Laplacian:  $\nabla^2 F = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial F}{\partial r} \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial F}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 F}{\partial \phi^2}$

Spherical Schrodinger:  $-\frac{\hbar^2}{2M} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial \psi}{\partial r} \right] + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial \psi}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right\} + V(r) \psi = E \psi(r, \theta, \phi)$

Separation:  $\psi = F(r) \cdot G(\theta) \cdot H(\phi)$

$$\frac{2Mr^2}{\hbar^2} [E - V(r)] + \frac{\partial}{\partial r} \left[ r^2 \frac{\partial F}{\partial r} \right] \frac{1}{F} = \lambda = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial G}{\partial \theta} \right] \frac{1}{G} - \frac{1}{\sin^2 \theta} \left[ \frac{\partial^2 H}{\partial \phi^2} \right] \frac{1}{H}$$

$$\lambda \sin^2 \theta + \sin \theta \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial G}{\partial \theta} \right] \frac{1}{G} = \mu = -\left[ \frac{\partial^2 H}{\partial \phi^2} \right] \frac{1}{H}$$

Solutions:  $H_m(\phi) = \exp[i m \phi]$  with integer  $m$  and  $\mu = m^2 \quad G_{lm}(\theta) = P_l^m(\theta)$  Legendre Functions

$m=4$				$105 \sin^4 \theta$
$m=3$			$-15 \sin^3 \theta$	$-105 \sin^3 \theta \cos \theta$
$m=2$		$3 \sin^2 \theta$	$15 \sin^2 \theta \cos \theta$	$\frac{15}{2} \sin^2 \theta (7 \cos^2 \theta - 1)$
$m=1$	$-\sin \theta$	$-3 \sin \theta \cos \theta$	$-\frac{3}{2} \sin \theta (5 \cos^2 \theta - 1)$	$-\frac{5}{2} \sin \theta (7 \cos^3 \theta - 3 \cos \theta)$
$m=0$	1	$\cos \theta$	$\frac{1}{2} (3 \cos^2 \theta - 1)$	$\frac{1}{2} (5 \cos^3 \theta - 3 \cos \theta)$
	$\ell=0$	$\ell=1$	$\ell=2$	$\ell=3$
				$\ell=4$

Spherical Harmonics  $Y_\ell^m(\theta, \phi) = P_\ell^m(\theta) \cdot H_m(\phi)$   $\ell = 0, 1, 2, 3, \dots$  and  $|m| \leq \ell$

$m = 4$					$\sin^4 \theta \, e^{4i\phi}$
$m = 3$				$\sin^3 \theta \, e^{3i\phi}$	$\sin^3 \theta \cos \theta \, e^{3i\phi}$
$m = 2$			$\sin^2 \theta \, e^{2i\phi}$	$\sin^2 \theta \cos \theta \, e^{2i\phi}$	$\sin^2 \theta \cdot (7 \cos^2 \theta - 1) e^{2i\phi}$
$m = 1$		$\sin \theta \, e^{i\phi}$	$\sin \theta \cos \theta \, e^{i\phi}$	$\sin \theta \cdot (5 \cos^2 \theta - 1) e^{i\phi}$	$\sin \theta \cdot (7 \cos^3 \theta - 3 \cos \theta) e^{i\phi}$
$m = 0$	1	$\cos \theta$	$3 \cos^2 \theta - 1$	$5 \cos^3 \theta - 3 \cos \theta$	$35 \cos^4 \theta - 30 \cos^2 \theta + 3$
$m = -1$		$\sin \theta \, e^{-i\phi}$	$\sin \theta \cos \theta \, e^{-i\phi}$	$\sin \theta \cdot (5 \cos^2 \theta - 1) e^{-i\phi}$	$\sin \theta \cdot (7 \cos^3 \theta - 3 \cos \theta) e^{-i\phi}$
$m = -2$			$\sin^2 \theta \, e^{-2i\phi}$	$\sin^2 \theta \cos \theta \, e^{-2i\phi}$	$\sin^2 \theta \cdot (7 \cos^2 \theta - 1) e^{-2i\phi}$
$m = -3$				$\sin^3 \theta \, e^{-3i\phi}$	$\sin^3 \theta \cos \theta \, e^{-3i\phi}$
$m = -4$					$\sin^4 \theta \, e^{-4i\phi}$
	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$	$\ell = 4$

Transformation:  $F(r) \rightarrow \frac{U(r)}{r}$  so  $\psi_{k\ell m}(r, \theta, \phi) = \frac{U_{k\ell}(r)}{r} \cdot Y_\ell^m(\theta, \phi)$

Reduced Radial Schrodinger:  $-\frac{\hbar^2}{2M} \frac{\partial^2 U(r)}{\partial r^2} + \left[ V(r) + \frac{\hbar^2 \ell \cdot (\ell + 1)}{2Mr^2} \right] \cdot U(r) = EU(r)$

Boundary Condition:  $U(r) = 0$  at  $r = 0$

Solution  $U_{k\ell}(r)$  and  $E_{k\ell}$  depend on  $k$  and  $\ell$  but don't depend on  $m$

Infinite Spherical Well:  $V(r) = 0$  for  $r < R$  and  $V = \infty$  elsewhere

$\ell = 0$  Solutions:  $\psi_{k00}(r, \theta, \phi) = \frac{U_{k0}(r)}{r}$   $U_{k0}(r) = \sin\left(\frac{k\pi r}{R}\right)$  with  $k = 1, 2, 3, \dots$

$$E_{k0} = k^2 \frac{\hbar^2 \pi^2}{2mR^2} = k^2 \frac{0.3763 \text{ eV-nm}^2}{R^2} \text{ for electron}$$

For  $\frac{1}{r}$  potential ONLY,  $E$  depends on the combination  $n = k + \ell$ , with  $k > 0$

Hydrogen Reduced Radial Equation:  $-\frac{\hbar^2}{2M} \frac{\partial^2 U}{\partial r^2} + \left[ \frac{\hbar^2 \ell \cdot (\ell + 1)}{2Mr^2} - \frac{q_e^2}{4\pi\epsilon_0 r} \right] \cdot U = EU$

Solutions:  $a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e q_e^2} = 52.97 \text{ pm}$   $E_n = -n^2 \cdot \frac{m_e}{2} \cdot \left( \frac{q_e^2}{4\pi\epsilon_0 \hbar} \right)^2 = -n^2 \cdot 13.6 \text{ eV}$   $n = 1, 2, 3, \dots$

$U_{n\ell}(r)$	$\ell = 0, m = 0$	$\ell = 1, m = 0, \pm 1$	$\ell = 2, m = 0, \pm 1, \pm 2$
$\rho = \frac{r}{a_0}$	$n = 3$	$\left[ \rho^3 - 9\rho^2 + \frac{27}{2}\rho \right] \cdot e^{-\frac{\rho}{3}}$	$\left[ \rho^3 - 6\rho^2 \right] \cdot e^{-\frac{\rho}{3}}$ $\rho^3 \cdot e^{-\frac{\rho}{3}}$
	$n = 2$	$\left[ \rho^2 - 2\rho \right] \cdot e^{-\frac{\rho}{2}}$	$\rho^2 \cdot e^{-\frac{\rho}{2}}$
	$n = 1$	$\rho \cdot e^{-\rho}$	