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

Energies: $E_{nx,ny,nz} = \frac{\hbar^2\pi^2}{2m}\cdot\left[\frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} + \frac{n_z^2}{w_z^2}\right] = \left(0.3763\text{ eV-nm}^2\right)\cdot\left[\frac{n_x^2}{w_x^2} + \frac{n_y^2}{w_y^2} + \frac{n_z^2}{w_z^2}\right]$ for electron

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

if $k_x = k_y = k_z = k$: $E_{nx,ny,nz} = \hbar\sqrt{\frac{k}{m}}\cdot\left[n_x + n_y + n_z + \frac{3}{2}\right] = \left[n_x + n_y + n_z + \frac{3}{2}\right]\cdot\left(0.2761\sqrt{\text{eV}}\text{-nm}\right)\cdot\sqrt{k}$ 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: $\vec{\nabla}\cdot\vec{G} = \frac{1}{r^2}\frac{\partial\left[r^2 G_r\right]}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial\left[\sin\theta\, G_\theta\right]}{\partial\theta} + \frac{1}{r\sin\theta}\frac{\partial G_\phi}{\partial\phi}$

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

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

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

Solutions: $H_m(\phi) = \exp\left[im\phi\right]$ with integer m and $\mu = m^2$ $\quad G_{\ell m}(\theta) = P_\ell^m(\theta)$ Legendre Functions

$m=4$					$105\sin^4\theta$
$m=3$				$-15\sin^3\theta$	$-105\sin^3\theta\cos\theta$
$m=2$			$3\sin^2\theta$	$15\sin^2\theta\cos\theta$	$\frac{15}{2}\sin^2\theta\left(7\cos^2\theta - 1\right)$
$m=1$		$-\sin\theta$	$-3\sin\theta\cos\theta$	$-\frac{3}{2}\sin\theta\left(5\cos^2\theta - 1\right)$	$-\frac{5}{2}\sin\theta\left(7\cos^3\theta - 3\cos\theta\right)$
$m=0$	1	$\cos\theta$	$\frac{1}{2}\left(3\cos^2\theta - 1\right)$	$\frac{1}{2}\left(5\cos^3\theta - 3\cos\theta\right)$	$\frac{1}{8}\left(35\cos^4\theta - 30\cos^2\theta + 3\right)$
	$\ell=0$	$\ell=1$	$\ell=2$	$\ell=3$	$\ell=4$

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

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

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

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

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

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

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

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

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

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

Hydrogen Reduced Radial Equation: $-\dfrac{\hbar^2}{2M}\dfrac{\partial^2 U}{\partial r^2}+\left[\dfrac{\hbar^2\ell\cdot(\ell+1)}{2Mr^2}-\dfrac{q_e^2}{4\pi\varepsilon_0 r}\right]\cdot U=EU$

Solutions: $a_0=\dfrac{4\pi\varepsilon_0\hbar^2}{m_e q_e^2}=52.97\text{ pm}$ $\quad E_n=-n^2\cdot\dfrac{m_e}{2}\cdot\left(\dfrac{q_e^2}{4\pi\varepsilon_0\hbar}\right)^2=-n^2\cdot 13.6\text{ eV}$ $\quad n=1,2,3,...$

$\rho=\dfrac{r}{a_0}$

$U_{n\ell}(\rho)$	$\ell=0,\ m=0$	$\ell=1,\ m=0,\pm1$	$\ell=2,\ m=0,\pm1,\pm2$
$n=3$	$\left[\rho^3-9\rho^2+\frac{27}{2}\rho\right]\cdot e^{\frac{-\rho}{3}}$	$\left[\rho^3-6\rho^2\right]\cdot e^{\frac{-\rho}{3}}$	$\rho^3\cdot e^{\frac{-\rho}{3}}$
$n=2$	$\left[\rho^2-2\rho\right]\cdot e^{\frac{-\rho}{2}}$	$\rho^2\cdot e^{\frac{-\rho}{2}}$	
$n=1$	$\rho\cdot e^{-\rho}$		