EXACT SOLUTIONS to the SCHRODINGER EQUATION **Chemistry BC3253x**

Free particle of mass m moving in one-dimension x: $V(x) = 0$

$\psi(x) = A \sin(kx + \delta)$ (not normalized)

$k^2 = 2mE$, no quantization of energy

Particle in a one-dimensional box: mass m, $V(x) = 0$ when $0 < x < L$, $V(x) = \infty$ otherwise

$E_n = n^2 h^2/8mL^2$ $n = 1, 2, 3...\infty$

$\psi_n(x) = (2/L)^{1/2} \sin(n\pi x/L)$

Simple Harmonic Oscillator: particle of mass m with harmonic force constant k

$V(x) = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2$ where $\omega^2 = k/m$ Reduced variable $\xi = x/(\hbar/m\omega)^{1/2}$

$E_v = (v + \frac{1}{2}) \hbar\omega$ $v = 0, 1, 2, 3...\infty$

$\psi_v(\xi) = N_v H_v(\xi) e^{-\xi^2/2}$ $N_v = (2^v v! \pi^{1/2})^{-1/2}$

Hermite Polynomials $H_v(\xi)$

v	0	1	2	3
$H_v(\xi)$	1	2x	$4x^2 - 2$	$8x^3 - 12x$

Particle on a Ring: Particle mass m, ring of radius r, no torques: $V(\varphi) = 0$

$E_M = \hbar^2 M^2 /2I$ where $I = mr^2$ $M = 0 \pm1, \pm2, \pm3... \pm\infty$

$\Phi_M(\varphi) = (2\pi)^{-1/2} \exp(iM\varphi)$

Rigid rotor: particle on mass m moving on a sphere of radius r: $V(\theta, \varphi) = 0$

$E_J = (\hbar^2/2\mu r^2) J(J+1) = BJ(J+1)$ $J = 0,1,2\ldots\infty$; $M= 0 \pm1, \pm2, \pm3.. \pm J$

$\psi_{J,M}(\theta,\varphi) = Y_{J,M}(\theta,\varphi) = \Theta_{J,M}(\theta)\, \Phi_M(\varphi)$ $Y_{J,M}(\theta, \varphi)$ called Spherical Harmonics

$\Theta_{J,M}(\theta) = N_{J,M}\, P_{J,M}(\cos\theta)$ $\Phi_M(\varphi) = (2\pi)^{-1/2} \exp(i M\varphi)$

Associated Legendre Polynomials $P_{J,M}(\cos\theta)$

J	0	1	1	2	2	2
M	0	0	±1	0	±1	±2
P	1	$\cos\theta$	$\sin\theta$	$\frac{1}{2}(3\cos^2\theta - 1)$	$\sin\theta\cos\theta$	$\sin^2\theta$
N	$\sqrt{(1/2)}$	$\sqrt{(3/2)}$	$\sqrt{(3/4)}$	$\sqrt{(5/8)}$	$\sqrt{(15/4)}$	$\sqrt{(15/16)}$

Hydrogenlike atom (nucleus with charge Z, one electron with mass m_e)

$E_n = -m_e (Ze^2/4\pi\varepsilon_0)^2 / 2\hbar^2 n^2 = -Z^2 R_\infty /n^2$ (identical to Bohr result)

three quantum numbers (n, ℓ, m) where $n= 1, 2, 3...\infty$; $0 \le \ell < n$; $|m| \le \ell$

$\psi_{n,\ell,m}(r, \theta,\varphi) = R_{n,\ell}(r)\, Y_{\ell,m}(\theta, \varphi)$ Y same as above, with $(J,M) \rightarrow (\ell, m)$

n	ℓ	**Normalized Radial Functions $R_{n,\ell}$**
1	0	$2 (Z/a_0)^{3/2} \exp(-Zr/a_0)$
2	0	$(1/2\sqrt{2}) (Z/a_0)^{3/2} (2 - Zr/a_0) \exp(-Zr/2a_0)$
2	1	$(1/2\sqrt{6}) (Z/a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0)$
3	0	$(2/81\sqrt{3}) (Z/a_0)^{3/2} [27 - 18(Zr/a_0) + 2(Zr/a_0)^2] \exp(-Zr/3a_0)$
3	1	$(4/81\sqrt{6}) (Z/a_0)^{3/2} [6(Zr/a_0) - Zr/a_0)^2] \exp(-Zr/3a_0)$
3	2	$(4/81\sqrt{30}) (Z/a_0)^{3/2} (Zr/a_0)^2 \exp(-Zr/3a_0)$