

Equations

$$E_n = -\frac{me^4}{8\epsilon_0^2 \hbar^2 n^2}$$

$$l = mvr$$

$$\Delta E = h\nu = \hbar\omega$$

$$2\pi r = n\lambda$$

$$\hat{H}\phi_n(x) = E_n\phi_n(x)$$

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

$$\langle a \rangle = \int_{-\infty}^{\infty} \Psi^*(\tau) \hat{A} \Psi(\tau) d\tau$$

$$\hat{H}\Psi(x, t) = i\hbar \frac{\partial \Psi(x, t)}{\partial t}$$

$$\int g^* \hat{A} f dx = \int f \hat{A}^* g^* dx$$

$$c_n = \int \phi_n^*(x) \psi(x) dx$$

$$\sigma = \frac{2\pi^5 k^4}{15h^3 c^2}$$

$$l_x = yp_z - zp_y$$

$$\lambda = h/p$$

$$\hat{P}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x)$$

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\sigma_a^2 = \langle a^2 \rangle - \langle a \rangle^2$$

$$\Psi_n(x, t) = \psi_n(x) e^{-iE_n t/\hbar}$$

$$\psi(x) = \sum_n c_n \phi_n(x)$$

$$p_n = |c_n|^2$$

Harmonic oscillator:

$$E_n = (n + \frac{1}{2})\hbar\omega$$

$$\Psi_0(x) = (\alpha/\pi)^{1/4} e^{-\alpha x^2/2}$$

$$\alpha = \sqrt{k\mu}/\hbar$$

$$\omega = \sqrt{k/\mu}$$

$$\Psi_1(x) = (\alpha/4\pi)^{1/4} 2\sqrt{\alpha} x e^{-\alpha x^2/2}$$

Rigid rotor:

$$E_l = \hbar^2 l(l+1)/2I$$

$$I = \mu r^2$$

$$\Delta E = \hbar^2(l+1)/I$$

$$\hat{H} = \hat{L}^2/2I$$

Spherical harmonics:

$$\hat{L}^2 Y_l^m = \hbar^2 l(l+1) Y_l^m$$

$$\hat{L}_z Y_l^m = \hbar m Y_l^m$$

$$Y_0^0(\theta, \phi) = 1/\sqrt{4\pi}$$

$$Y_1^1(\theta, \phi) = \sqrt{3/8\pi} \sin\theta e^{i\phi}$$

$$l = 0, 1, 2, \dots \quad -l \leq m \leq l$$

$$Y_l^m(\theta, \phi) = N_{lm} P_l^{|m|}(\cos\theta) e^{im\phi}$$

$$Y_1^0(\theta, \phi) = \sqrt{3/4\pi} \cos\theta$$

$$Y_1^{-1}(\theta, \phi) = \sqrt{3/8\pi} \sin\theta e^{-i\phi}$$

Spin of electron:

$$\hat{S}^2 \alpha = \hbar^2 \frac{1}{2} (\frac{1}{2} + 1) \alpha$$

$$\hat{S}_z \alpha = \frac{\hbar}{2} \alpha$$

$$\hat{S}^2 \beta = \hbar^2 \frac{1}{2} (\frac{1}{2} + 1) \beta$$

$$\hat{S}_z \beta = -\frac{\hbar}{2} \beta$$

Some useful integrals:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\pi/a}$$

$$\int_{-\infty}^{\infty} x^4 e^{-ax^2} dx = (3/4) \sqrt{\pi/a^5}$$

$$\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = a/2$$

$$\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \left(\frac{a}{2\pi n}\right)^3 \left(\frac{4\pi^3 n^3}{3} - 2n\pi\right)$$

$$\int x \sin(ax) dx = \frac{\sin(ax)}{a^2} - \frac{x \cos(ax)}{a}$$

$$\int x^2 \sin(ax) dx = \frac{2x}{a^2} \sin(ax) + \left(\frac{2}{a^3} - \frac{x^2}{a}\right) \cos(ax)$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = (1/2) \sqrt{\pi/a^3}$$

$$\int_{-\infty}^{\infty} x^6 e^{-ax^2} dx = (15/8) \sqrt{\pi/a^7}$$

$$\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx = a^2/4$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du$$

Wave functions for H-like atoms:

$$\Psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$$

$$\Psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \cos\theta$$

$$\sigma = Zr/a_0$$

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (2 - \sigma) e^{-\sigma/2}$$

$$\Psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2} \sin\theta \cos\phi$$

First order perturbation correction:

$$\Delta E_n = \int \psi_n^{(0)*} \hat{H}^{(1)} \psi_n^{(0)} d\tau$$

Variational principle:

$$E_\phi = \frac{\int \phi^* \hat{H} \phi d\tau}{\int \phi^* \phi d\tau}$$

$$E_\phi \geq E_0$$