Bohr and Uncertainty

$$\hbar = \frac{h}{2\pi} \qquad \lambda = \frac{\lambda}{2\pi}$$

$$a_0 = \frac{\hbar}{m_e c}\frac{1}{\alpha} = \frac{\hbar^2}{m_e k e^2} \simeq 0.5\mathring{A}$$

$$\alpha = \frac{ke^2}{\hbar c} \simeq \frac{1}{137}$$

$$L = m_e v r = n\hbar n = 1, 2, 3, \ldots$$

$$\begin{aligned} L = m_e v r &= n\hbar \qquad n = 1, 2, 3 \ldots && (1)\\ \frac{v_n}{c} &= Z\alpha\left[\frac{1}{n}\right] && (2)\\ E_n &= -\frac{1}{2}m_e c^2 (Z\alpha)^2\left[\frac{1}{n^2}\right] && (3)\\ &= -\frac{ke^2}{2a_o}Z^2\left[\frac{1}{n^2}\right] && (4)\\ &= -13.6\,\mathrm{eV}\,Z^2\left[\frac{1}{n^2}\right] && (5)\\ r_n &= \frac{a_0}{Z}\left[n^2\right] && (6)\\ &= \frac{\hbar}{m_e c\, Z\alpha}\left[n^2\right] && (7) \end{aligned}$$

$$KE = -\frac{1}{2}PE \qquad \text{for Force} \propto 1/r^2$$

$$\frac{1}{2}m_e c^2\alpha^2 = \frac{ke^2}{2a_0} = 13.6\,\mathrm{eV}$$

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k \qquad (8)$$

$$\Delta x \Delta p \sim \hbar \qquad (9)$$

Quantum Mechanics in 1D

$$P(x)dx = |\psi(x)|^2 dx \qquad (10)$$

$$\int |\psi(x)|^2 = 1 \qquad (11)$$

$$\mathbb{X}\psi(x) = x\psi(x) \qquad (12)$$

$$\mathbb{P}\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi(x) \qquad (13)$$

$$\begin{aligned} \mathbb{H} &= \frac{\mathbb{P}^2}{2M} + U(\mathbb{X}) && (14)\\ &= -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + U(x) && (15) \end{aligned}$$

$$\begin{aligned} \mathbb{H}\psi_n(x) &= E_n\psi_n(x) && (16)\\ \left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + U(x)\right]\psi_n(x) &= E_n\psi_n(x) && (17) \end{aligned}$$

Box wave and energies

$$\begin{aligned} \psi_n(x) &= \sqrt{\frac{2}{L}}\sin(k_n x) \qquad k_n = \frac{n\pi}{L} \qquad n = 1, 2, 3 && (18)\\ &= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) && (19) \end{aligned}$$

$$E_n = \frac{\hbar^2 k_n^2}{2M} = \frac{\hbar^2\pi^2}{2ML^2}n^2 \qquad n = 1, 2, 3 \ldots \qquad (20)$$

Expectations

$$\begin{aligned} \langle x\rangle &= \int dx\,\psi^*(x)\mathbb{X}\psi(x) = \int dx\,x\,|\psi(x)|^2 && (21)\\ \langle x^2\rangle &= \int dx\,\psi^*(x)\mathbb{X}^2\psi(x) = \int dx\,x^2\,|\psi(x)|^2 && (22)\\ \langle(\Delta x)^2\rangle &= \int dx(x - \langle x\rangle)^2\,|\psi(x)|^2 && (23)\\ &= \langle x^2\rangle - \langle x\rangle^2 && (24)\\ \Delta x &\equiv \sqrt{\langle(\Delta x)^2\rangle} && (25) \end{aligned}$$

$$\langle p\rangle = \langle\mathbb{P}\rangle = \int dx\,\psi^*(x)\mathbb{P}\psi(x) = \int dx\psi^*(x) - i\hbar\frac{\partial}{\partial x}\psi(x) \qquad (26)$$

$$\langle p^2\rangle = \langle\mathbb{P}^2\rangle = \int dx\,\psi^*(x)\mathbb{P}\psi(x) = \int dx\psi^*(x) - \hbar^2\frac{\partial^2}{\partial x^2}\psi(x) \qquad (27)$$

$$(\Delta p)^2 = \langle\mathbb{P}^2\rangle - \langle\mathbb{P}\rangle^2 \qquad (28)$$

$$\langle KE\rangle = \left\langle\frac{\mathbb{P}^2}{2M}\right\rangle = \int dx\,\psi^*(x)\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2}\right]\psi(x) \qquad (29)$$

Time dependence

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) = +i\hbar\frac{\partial}{\partial t}\psi(x,t) \qquad (30)$$

$$\psi(x,t) = e^{-iE_n t}\hbar\psi_n(x) \qquad (31)$$

$$\Delta E\Delta t \sim \hbar \qquad (32)$$

Finite box

$$\psi(x) \sim e^{-\frac{x}{\delta}} \qquad (33)$$

where the penetration depth is δ

$$\delta = \sqrt{\frac{\hbar^2}{2M(V-E)}} \tag{34}$$

Spring:

$$\omega_o = \sqrt{\frac{k}{M}} \qquad k = M\omega_o^2 \tag{35}$$

$$E_n = \hbar\omega_o\left(n+\frac{1}{2}\right) \qquad n = 0,1,2,3\ldots \tag{36}$$

$$L = \sqrt{\frac{\hbar}{M\omega_o}} \tag{37}$$

$$\frac{\hbar^2}{2ML^2} = \frac{1}{2}m\omega_o^2 L^2 \tag{38}$$

In the harmonic oscillator figure

$$y = \frac{x}{L} \qquad \text{with} \qquad L = \sqrt{\frac{\hbar}{M\omega_o}} \qquad \alpha = \frac{1}{L^2} \tag{39}$$

3D Box

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n_x}{L}x\right)\times\sqrt{\frac{2}{L}}\sin\left(\frac{\pi n_y}{L}y\right) \tag{40}$$

$$\times\sqrt{\frac{2}{L}}\sin\left(\frac{\pi n_y}{L}z\right) \tag{41}$$

$$n_x, n_y, n_z = 1,2,3,\ldots \tag{42}$$

The Energies are

$$E_{n_x,n_y,n_z} = KE_x + KE_y + KE_z \tag{43}$$

$$= \frac{\hbar^2 k_x^2}{2M} + \frac{\hbar^2 k_y^2}{2M} + \frac{\hbar^2 k_z^2}{2M} \tag{44}$$

with

$$k_x = \frac{\pi n_x}{L} \qquad k_y = \frac{\pi n_y}{L} \qquad k_z = \frac{\pi n_z}{L} \tag{45}$$

Sperhical Problems

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi) \tag{46}$$

$$n = 1,2,3,4\ldots \tag{47}$$

$$\ell = 0,1,\ldots n-1 \tag{48}$$

or

$$\ell = s,p,d,f,g\ldots \tag{49}$$

$$m = -\ell\ldots\ell \tag{50}$$

$$\mathbb{L}^2 Y_{\ell m} = \ell(\ell+1)\hbar^2\, Y_{\ell m} \tag{51}$$

$$\mathbb{L}_z Y_{\ell m} = m\hbar\, Y_{\ell m} \tag{52}$$

$$\mathbb{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos(\theta)}{\sin(\theta)}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right) \tag{53}$$

$$\mathbb{L}_z = -i\hbar\frac{\partial}{\partial\phi} \tag{54}$$

Hydrogen

$$V(r) = -\frac{k_C e^2}{r} \tag{55}$$

$$E_{n\ell} = -\frac{\hbar^2}{2ma_0^2}\frac{Z^2}{n^2} = -\frac{k_C e^2}{2a_0}\frac{Z^2}{n^2} \qquad n = 1,2,3,4\ldots \tag{56}$$

Radial Schrödinger. We define

$$u_{n\ell}(r) \equiv rR_{n\ell}(r) \tag{57}$$

which satisfies

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right]u_{nl} = E_{nl}u_{nl} \tag{58}$$

classically

$$KE = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} \tag{59}$$

Probabilities

$$P(x,y,z)\,dV = |\psi(x,y,z)|^2\; dV \tag{60}$$

$$P(r)\,dr = |rR(r)|^2\,dr = |u_{n\ell}(r)|^2\,dr \tag{61}$$

$$\int_0^\infty P(r)dr = \int_0^\infty |u_{n\ell}(r)|^2 = 1 \tag{62}$$

$$\bar{r} = \langle r\rangle = \int_0^\infty r|u_{n\ell}(r)|^2 \tag{63}$$

$$\langle V(r)\rangle = \int_0^\infty -\frac{k_C e^2}{r}\,|u_{n\ell}(r)|^2 \tag{64}$$

$$(\Delta r)^2 = \left\langle r^2\right\rangle - \langle r\rangle^2 \tag{65}$$

$$\langle KE\rangle = \int_0^\infty u_{n\ell}(r)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}\right]u_{n\ell}(r) \tag{66}$$

$$\langle \text{Radial KE} \rangle = \int_0^\infty u_{n\ell}(r) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \right] u_{n\ell}(r) \tag{67}$$

Hunds Rule

$$O : \underbrace{[\uparrow\downarrow]}_{1s^2} \; \underbrace{[\uparrow\downarrow]}_{2s^2} \; \underbrace{[\; \overbrace{\uparrow\uparrow\uparrow}^{m=-1,0,1} \quad \downarrow]}_{2p^4}$$

Two particles in Box, +/- is boson/fermion

$$\Psi(r_2, r_1) = \pm\Psi(r_1, r_2) \tag{68}$$

$$\Psi_{ab}(r_1, r_2) \propto \psi_a(r_1)\psi_b(r_2) \pm \psi_a(r_2)\psi_b(r_1) \tag{69}$$

$$E_{\text{tot}} = E_a + E_b \tag{70}$$

Statistical Mechanics

$$P(E) \propto e^{-\frac{E}{k_B T}} \tag{71}$$

$$P(v) \underbrace{d^3\mathbf{v}}_{dv_x dv_y dv_z} = \left(\frac{M}{2\pi k_B T} \right)^{3/2} e^{-\frac{Mv^2}{2k_B T}} \, d^3\mathbf{v} \tag{72}$$

$$P(v)\, dv = \left(\frac{M}{2\pi k_B T} \right)^{3/2} e^{-\frac{Mv^2}{2k_B T}} \, 4\pi v^2 \, dv \tag{73}$$

Quantum gas

$$\lambda_{\text{thermal}} \sim \frac{\hbar}{\sqrt{m\, k_B T}} \tag{74}$$

particle spacing

$$d \sim \left(\frac{V}{N} \right)^{1/3} \tag{75}$$

For classical gas

$$\lambda_{\text{thermal}} \ll d \tag{76}$$

Mode Counting

$$g(k)\, dk = 2\frac{dk}{\Delta k} = 2\,\frac{L\, dk}{\pi} \qquad \text{1D} \tag{77}$$

$$g(\mathbf{k})\, d^2\mathbf{k} = 2\frac{d^2k}{(\Delta k)^2} = 2\,\frac{A\, d^2k}{\pi^2} \qquad 2D \tag{78}$$

$$g(\mathbf{k})\, d^3\mathbf{k} = 2\frac{d^3k}{(\Delta k)^3} = 2\,\frac{V\, d^3k}{\pi^3} \qquad 3D \tag{79}$$

$$g(k)\, dk = 2\,\frac{L}{\pi}\, dk \qquad \text{1D} \tag{80}$$

$$g(k)\, dk = 2\,\frac{A}{\pi^2}\,\frac{2\pi k}{4} dk \qquad 2D \tag{81}$$

$$g(k)\, dk = 2\,\frac{V}{\pi^3}\,\frac{4\pi k^2}{8} dk \qquad 3D \tag{82}$$

Fermi Gas

$$E_F = \frac{\hbar^2 k_F^2}{2M} \qquad \text{all dimensions} \tag{83}$$

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3} \qquad \text{3D} \tag{84}$$

or

$$N = 2\, V \frac{\frac{4}{3}\pi k_F^3}{8\pi^3} \qquad \text{3D} \tag{85}$$

Black Body Radiation

$$N(\omega)\, d\omega = \frac{V}{\pi^2 c^3}\, \frac{\omega^2 d\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1} \tag{86}$$

$$\hbar\omega_{\text{mp}} = 1.6\, k_B T \tag{87}$$

$$\lambda \sim \frac{\hbar c}{k_B T} \tag{88}$$

$$\frac{N}{V} = 0.244 \left(\frac{\hbar c}{k_B T} \right)^3 \tag{89}$$

$$u_E \equiv \frac{E}{V} = (k_B T) \left(\frac{k_B T}{\hbar c} \right)^3 \frac{\pi^2}{15} \tag{90}$$

$$e = u_E\, \frac{c}{4} \tag{91}$$

$$e = \sigma T^4 \qquad \sigma = \frac{\pi^2}{60}\, \frac{c k_B^4}{(\hbar c)^3} = 5.67 \times 10^{-8}\, \frac{W}{m^2 K^4} \tag{92}$$