FORMULAS ETC

- Particle in box

$$V(x) = 0 \quad \text{for} \quad 0 < x < L, \quad V(x) = \infty \;\; \text{otherwise}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad , \quad n = 1, 2, 3, \ldots$$

- Onedimensional harmonic oscillator

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \tfrac{1}{2}m\omega^2 x^2\right)\psi_n(x) = \hbar\omega(n + \tfrac{1}{2})\psi_n(x); \qquad \langle\, \psi_n, \psi_k \,\rangle = \delta_{nk};$$

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n\, n!}}\, e^{-y^2/2} H_n(y), \qquad y = \frac{x}{\sqrt{\hbar/m\omega}};$$

$$H_0(y) = 1, \quad H_1(y) = 2y, \quad H_2(y) = 4y^2 - 2, \quad H_3(y) = 8y^3 - 12y, \quad \cdots;$$

$$\widehat{\mathcal{P}}\psi_n(x) \equiv \psi_n(-x) = (-1)^n \psi_n(x).$$

- Laplace-operator and angular momentum operators in spherical coordinates

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2};$$

$$\hat{\mathbf{L}}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \qquad \hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi};$$

$$\hat{L}_x = \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\,\cos\phi\frac{\partial}{\partial\phi}\right), \qquad \hat{L}_y = \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\,\sin\phi\frac{\partial}{\partial\phi}\right);$$

$$[\widehat{\mathbf{L}}^2, \widehat{L}_z] = 0, \qquad [\widehat{L}_x, \widehat{L}_y] = i\hbar\widehat{L}_z, \quad \text{osv.}$$

- Spherical harmonics

$$\left\{\begin{array}{c}\hat{\mathbf{L}}^2\\ \hat{L}_z\end{array}\right\} Y_{lm} = \left\{\begin{array}{l}\hbar^2 l(l+1)\\ \hbar m\end{array}\right\} Y_{lm}\,, \quad l = 0, 1, 2, ...; \quad m = 0, \pm1, \pm2, ..., \pm l$$

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) Y^*_{l'm'} Y_{lm} = \delta_{l'l}\delta_{m'm};$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}, \qquad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \equiv Y_{p_z}, \qquad Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi};$$

$$Y_{p_x} = \sqrt{\frac{3}{4\pi}}\frac{x}{r} = \frac{1}{\sqrt{2}}(Y_{1,-1} - Y_{11}), \qquad Y_{p_y} = \sqrt{\frac{3}{4\pi}}\frac{y}{r} = \frac{i}{\sqrt{2}}(Y_{11} + Y_{1,-1});$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1); \qquad Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}; \qquad Y_{2,\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}.$$

$$\widehat{\mathcal{P}}Y_{lm} = (-1)^l Y_{lm}.$$

- Energy eigenfunctions and radial equation, spherically symmetric potential $V(r)$

$$\psi(r,\theta,\phi) = \frac{u(r)}{r}\, Y_{lm}(\theta,\phi);$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V^l_{\text{eff}}(r)\right] u(r) = E\, u(r), \qquad V^l_{\text{eff}}(r) \equiv V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}, \qquad u(0) = 0.$$

- Energy eigenvalues and eigenfunctions, hydrogen atom, $V(r) = -e^2/(4\pi\epsilon_0 r)$

$$E_n = \frac{E_1}{n^2} \equiv \frac{E_1}{(l+1+n_r)^2}, \qquad E_1 = -\tfrac{1}{2}\alpha^2 m_e c^2;$$

$$\psi_{nlm} = R_{nl}(r) Y_{lm}(\theta,\phi);$$

$$R_{10} = \frac{2}{a_0^{3/2}}\, e^{-r/a_0}; \qquad R_{20} = \frac{1}{\sqrt{2}\, a_0^{3/2}}\left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}; \qquad R_{21} = \frac{1}{2\sqrt{6}\, a_0^{3/2}}\,\frac{r}{a_0}\, e^{-r/2a_0}.$$

- Some constants

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 0.529\cdot 10^{-10}\ \text{m} \qquad \text{(Bohr radius)};$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137.0360} \qquad \text{(fine structure constant)};$$

$$\tfrac{1}{2}\alpha^2 m_e c^2 = \frac{\hbar^2}{2m_e a_0^2} \approx 13.6\ \text{eV} \qquad \text{(Rydberg energy)}.$$

$$m_e \simeq 9.11\cdot 10^{-31}\ \text{kg} \qquad \hbar = h/2\pi \simeq 1.05\cdot 10^{-34}\ \text{Js} \qquad e \simeq 1.60\cdot 10^{-19}\ \text{C} \qquad u \simeq 1.66\cdot 10^{-27}\ \text{kg}$$

$$m_p \simeq m_n \simeq 1.67\cdot 10^{-27}\ \text{kg} \qquad k_B \simeq 1.38\cdot 10^{-23}\ \text{J/K} \qquad c \simeq 3.00\cdot 10^8\ \text{m/s} \qquad 1\ \text{Å} = 0.1\ \text{nm}$$

$$1/4\pi\epsilon_0 \simeq 9\cdot 10^9\ \text{Nm}^2/\text{C}^2 \qquad m_e c^2 \simeq 511\ \text{keV} \qquad m_p c^2 \simeq m_n c^2 \simeq 939\ \text{MeV}$$

- Some formulas

$$\sin a = (e^{ia} - e^{-ia})/2i\ , \qquad \cos a = (e^{ia} + e^{-ia})/2;$$

$$\tan y = \frac{1}{\cot y} = \tan(y + n\pi), \quad n = 0, \pm 1, \cdots;$$

$$\sinh y = \tfrac{1}{2}(e^y - e^{-y}); \qquad \cosh y = \tfrac{1}{2}(e^y + e^{-y}); \qquad \tanh y = \frac{1}{\coth y} = \frac{\sinh y}{\cosh y};$$

$$\cosh^2 y - \sinh^2 y = 1; \qquad \frac{d}{dy}\sinh y = \cosh y; \qquad \frac{d}{dy}\cosh y = \sinh y.$$

$$|y| \ll 1 \Rightarrow \exp(y) \simeq 1 + y$$

$$|z_1 + z_2|^2 = |z_1|^2 + |z_2|^2 + 2\text{Re}(z_1^* z_2)$$

- A couple of integrals:

$$\int_0^\pi \sin Nx \sin^2 x dx = 4/(4N - N^3) \;\; ; \;\; N = 1, 3, 5 \ldots$$

$$\int_{-\infty}^{\infty} x^2 \exp(-x^2) dx = \sqrt{\pi}/2$$

- de Broglie:

$$\lambda = h/p \;\; , \;\; \nu = E/h$$

- Average translational energy pr particle in ideal gas (in 3 dimensions): $3k_B T/2$
- Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}\Psi$$

- Time independent Schrödinger equation:

$$\widehat{H}\psi = E\psi$$

- Momentum operator:

$$\widehat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \;\; , \;\; \widehat{\boldsymbol{p}} = \frac{\hbar}{i}\nabla \;\; , \;\; f(p) \to f(\widehat{p})$$

- Kinetic energy:

$$K = \frac{p^2}{2m}$$

- Angular momentum:

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$$

- Rotational energy:

$$K_{\text{rot}} = \frac{1}{2} I \omega^2 \quad , \quad \boldsymbol{L} = I\boldsymbol{\omega}$$

- Heisenberg's uncertainty relation:

$$\Delta x \Delta p \geq \hbar/2$$

$$\Delta A \Delta B \geq \frac{1}{2}\left| \langle i[\widehat{A}, \widehat{B}] \rangle \right|$$

- Commutator:

$$[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$$

- Stationary state:

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

- Expectation values:

$$\begin{aligned} \langle x \rangle &= \int \Psi^* x \Psi dx \\ \langle p \rangle &= \int \Psi^* \frac{\hbar}{i}\frac{\partial}{\partial x} \Psi dx \\ \langle F \rangle &= \int \Psi^* \widehat{F} \Psi d\tau \end{aligned}$$

- Wave packet:

$$\Psi(x,t) = \sum_j c_j \psi_j(x) e^{-iE_j t/\hbar}$$

$$c_j = \int \psi_j^*(x) \Psi(x,0) dx$$

- Boundary conditions:
  $\psi(x)$ continuous everywhere, $d\psi/dx$ discontinuous at ∞ jump in $V(x)$

- Probability current:

$$j = \text{Re}\left[\Psi^* \left(\frac{\hbar}{mi}\frac{\partial}{\partial x}\right)\Psi\right]$$

- Uncertainty (standard deviation):

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \;\;,\;\; \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

- Ehrenfest's theorem:

$$\frac{d}{dt}\langle \boldsymbol{r} \rangle = \frac{\langle \boldsymbol{p} \rangle}{m} \;\;,\;\; \frac{d}{dt}\langle \boldsymbol{p} \rangle = -\langle \nabla V \rangle$$

- Relativistic energy (K is kinetic energy):

$$E^2 = p^2c^2 + m^2c^4 \;\;;\;\; E = K + mc^2$$

- Relativistic momentum:

$$p = \frac{mv}{\sqrt{1 - v^2/c^2}}$$

- Prefixes:
  f $= 10^{-15}$, p $= 10^{-12}$, n $= 10^{-9}$, $\mu = 10^{-6}$, m $= 10^{-3}$, k $= 10^{3}$, M $= 10^{6}$, G $= 10^{9}$, T $= 10^{12}$

- Spherical coordinates: $z = r\cos\theta$, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$

- A couple of potentially useful numerical values:
  $\hbar^2/2m_e = 0.0378$ eV nm^2
  $hc = 1237$ eV nm

- Selection rules for radiative transitions: $\Delta l = \pm 1$, $\Delta m = 0$ or ± 1