Formulas and Numerical Constants

<u>De Broglie relations:</u> De Broglie postulated the following relations between (E, p) and (λ, f)

$$E = hf, \qquad (E = \hbar\omega)$$
 (1)

$$p = h/\lambda, \qquad (p = \hbar k)$$
 (2)

where $\hbar = h/(2\pi)$. The most important dispersion relations are

$$E = pc \quad (light), \tag{3}$$

$$E = \frac{p^2}{2m} \quad \text{(nonrelativistic matter)}. \tag{4}$$

<u>Bohr's model:</u> Bohr's model of hydrogen like atoms is based on the quantization condition $L = mvr = n\hbar$. The allowed energies and radii are

$$r_n = \frac{n^2 a_0}{Z}, \qquad a_0 = \frac{\hbar^2}{m_e k e^2},$$
 (5)

$$E_n = -\frac{Z^2 E_0}{n^2}, \qquad E_0 = \frac{m_e k^2 e^4}{2\hbar^2},$$
 (6)

where $k = 1/(4\pi\epsilon_0)$ is the Coulomb constant, e is the charge, and m_e is the mass of the electron. Z is the charge of the nucleus (in units of e). The constant a_0 is called the Bohr radius. The quantity

$$\alpha = \frac{ke^2}{\hbar c} \simeq \frac{1}{137} \tag{7}$$

is called the fine structure constant.

Schrödinger equation: The time-dependent and time-independent Schrödinger equations are

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x,t),$$
 (8)

$$E\psi(x) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x). \tag{9}$$

The wave function is related to the probability

$$P(x,t) dx = \psi^*(x,t)\psi(x,t) dx. \tag{10}$$

More generally, expectation values are given by

$$\langle f \rangle = \int dx \, f(x) \psi^*(x, t) \psi(x, t).$$
 (11)

3d Schrödinger equation: Solutions of the Schrödinger equation for a potential with rotational symmetry have the form

$$\psi(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi), \tag{12}$$

where Y_{lm} are the spherical harmonics, (l,m) label $L^2 = \hbar^2 l(l+1)$ and $L_z = \hbar m \ (m \leq l)$, and $R_{nl}(r)$ is the radial wave function (labeled by the quantum number n). The ground state wave function of the hydrogen atom is

$$R_{10}(r) = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}, \quad Y_{00}(\theta, \phi) = \frac{1}{\sqrt{4\pi}},$$
 (13)

where a_0 is the Bohr radius defined above.

<u>Selection rules:</u> Dipole transitions involving the emission or absorption of a photon are allowed if

$$\Delta m_l = \pm 1, 0 \quad \text{and} \quad \Delta l = \pm 1.$$
 (14)

<u>Vibrational and rotational energies:</u> The energy levels of a one-dimensional harmonic oscillator are

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right),\tag{15}$$

where $\omega = \sqrt{k/m}$ and k is the spring constant. The energy levels of a rigid rotor are

$$E_l = \frac{\hbar^2}{2I}l(l+1),\tag{16}$$

where I is the moment of inertia.

Fermi gas: The Fermi energy is

$$E_F = \frac{h^2}{8m} \left(\frac{3N}{\pi V}\right)^{2/3} \,, \tag{17}$$

The average energy is $E_{av} = (3/5)E_F$, the Fermi temperature is $T_F = E_F/k_B$, and the Fermi velocity is $v_F = \sqrt{2E_F/m}$. The Fermi-Dirac distribution is

$$f(E) = \frac{1}{\exp((E - E_F)/(k_B T)) + 1}.$$
 (18)

Conductivity: The resistivity is

$$\rho = \frac{m_e v_{av}}{e^2 n_e \lambda} \,, \tag{19}$$

where n_e is the density of electrons and v_{av} is the average velocity. The mean free path is $\lambda = 1/(n_I \sigma)$, where n_I is the density of scatterers and σ is the cross section.

Numerical Constants:

$$k = 1/(4\pi\epsilon_0) = 8.987 \cdot 10^9 \,\text{N} \cdot \text{m}^2 \cdot \text{C}^{-2}$$

$$k_B = 1.381 \times 10^{-23} \,\text{J/K} = 8.617 \times 10^{-5} \,\text{eV/K}$$

$$N_A = 6.022 \times 10^{23}$$

$$h = 6.626 \times 10^{-34} \,\text{J} \cdot \text{s}$$

$$c = 2.998 \times 10^8 \,\text{m/sec}$$

$$hc = 1240 \,\text{eV} \cdot \text{nm}$$

$$\hbar c = 197.33 \,\text{MeV} \cdot \text{fm}$$

$$E_0 = 0.5 \, m_e c^2 \alpha^2 = 13.6 \,\text{eV}$$

$$e = 1.602 \times 10^{-19} \,\text{C}$$

$$1 \,\text{cal} = 4.186 \,\text{J}$$

$$1 \,\text{eV} = 1.602 \times 10^{-19} \,\text{J}$$

$$1 \,u = 1.661 \times 10^{-27} \,\text{kg} = 931.49 \,\text{MeV/}c^2$$

$$m_e c^2 = 512 \,\text{keV}$$

$$m_e = 9.109 \times 10^{-31} \,\text{kg}$$

$$m_p c^2 = 935 \,\text{MeV}$$