Appendix B - Mathematical Formulae

DO NOT READ THIS APPENDIX

This appendix is included for completeness and for those of you who are curious to see the relevant mathematical formulae and equations, even if you do not understand the notation. It is *not* necessary to read this.

Waves

The disturbance $\Psi(x,t)$ of a monochromatic wave with wavelength λ moving in the positive x-direction, with amplitude A:

$$\Psi(x,t) \;=\; A\sin\left(\frac{2\pi}{\lambda}(x-ct)+\phi\right), \tag{B.1}$$

where c is the wave speed and ϕ is the initial phase at $x=t=0$.

The frequency of the wave is:

$$f \;=\; \frac{c}{\lambda} \tag{B.2}$$

Interference

The intensity of monochromatic radiation, $I(x)$ with wavelength λ from two narrow slits separated by a distance a at a distance x from the centre of a screen placed at a distance D from the slits ($x \ll D$):

$$I(x) \;=\; I(0)\cos^2\left(\frac{2\pi xa}{\lambda D}\right) \tag{B.3}$$

The intensity of monochromatic radiation, $I(x)$ with wavelength λ from a narrow object (such as a pin) of width a at a distance x from the centre of a screen placed at a distance D from the object:

$$I(x) \;=\; I(0)\frac{\lambda^2 D^2}{4\pi^2 x^2 a^2}\sin^2\left(\frac{2\pi xa}{\lambda D}\right) \tag{B.4}$$

Wavepackets

The disturbance $\Psi(x,t)$ due to a wavepacket moving along the positive x-axis may be described by

$$\Psi(x,t) \;=\; f\,(x-ct)\,. \tag{B.5}$$

$f(x)$ can be any continuous function of x but for a localized wavepacket it would be a function with local support and a single maximum at the peak of the wavefunction.

This may be written in terms of a superposition of disturbances due to harmonic wave with wavelength λ by

$$\Psi(x,t) \;=\; \int_0^\infty \left[A^{(e)}(\lambda)\cos\left(\frac{2\pi}{\lambda}(x-ct)\right) + A^{(o)}(\lambda)\sin\left(\frac{2\pi}{\lambda}(x-ct)\right)\right] d\lambda, \qquad \text{(B.6)}$$

where

$$A^{(e)}(\lambda) \;=\; \frac{4}{\lambda^2}\int_0^\infty f^{(e)}(y)\cos\left(\frac{2\pi y}{\lambda}\right) dy$$

and

$$A^{(o)}(\lambda) \;=\; \frac{4}{\lambda^2}\int_0^\infty f^{(o)}(y)\sin\left(\frac{2\pi y}{\lambda}\right) dy.$$

The even and odd parts of the function $f(y)$ are defined by

$$f^{(e)}(y) \;=\; \frac{1}{2}\left(f(y)+f(-y)\right)$$

$$f^{(o)}(y) \;=\; \frac{1}{2}\left(f(y)-f(-y)\right)$$

Classical Particle Physics

The kinetic energy, T, of a particle of mass m with a velocity v (much smaller than the speed of light):

$$T \;=\; \frac{1}{2}mv^2 \qquad \text{(B.7)}$$

The (vector) momentum $\mathbf{p}$ of a particle of mass m with a velocity $\mathbf{v}$:

$$\mathbf{p} \;=\; m\mathbf{v} \qquad \text{(B.8)}$$

Rutherford Scattering

An α-particle with electric charge $4e$ and kinetic energy E scattering off a nucleus with electric charge Ze with impact parameter b scatters through an angle θ where

$$b \;=\; \frac{Ze^2}{2\pi\epsilon_0 E}\cot\left(\frac{\theta}{2}\right). \qquad \text{(B.9)}$$

This leads to a differential scattering cross-section (per unit solid-angle)

$$\frac{d\sigma}{d\Omega} \;=\; \frac{Z^2e^4}{16\pi^2\epsilon_0^2E^2\sin^4(\theta/2)} \qquad \text{(B.10)}$$

Blackbody Radiation

The energy radiated, $R(\lambda, T)\,d\lambda$, per unit time per unit area in a wavelength interval between λ and $\lambda + d\lambda$ at temperature T, from a blackbody :

Rayleigh-Jeans' Formula:

$$R(\lambda, T) \;=\; \frac{2\pi c}{\lambda^4} k_B T \tag{B.11}$$

Planck's Radiation Law:

$$R(\lambda, T) \;=\; \frac{2\pi h c^2}{\lambda^5} \frac{1}{(e^{hc/\lambda k_B T} - 1)} \tag{B.12}$$

Photoelectric Effect

Energy, E of a photon (quantum) of electromagnetic radiation with frequency f

$$E \;=\; h\,f \tag{B.13}$$

The stopping potential, V_0, for photoelectrons emitted from a metal with work function ϕ_0, illuminated with radiation of frequency f;

$$e\,V_0 \;=\; h\,f \,-\, \phi_0 \tag{B.14}$$

Compton Scattering

A photon of wavelength λ which scatters off a target of mass m through a scattering angle θ emerges with wavelength λ':

$$\lambda' \;=\; \lambda + \frac{h}{m\,c}\,(1 - \cos\theta) \tag{B.15}$$

Bragg Scattering

The intensity of scattered of X-rays with wavelength λ from a crystal lattice whose lattice planes are separated by d has a maximum at angles of incidence θ between the incident radiation and the lattice planes whenever:

$$2d\sin\theta \;=\; n\,\lambda \quad \text{(integer } n\text{)} \tag{B.16}$$

Matter (de Broglie) Waves

A particle with momentum p has a wavelength, λ:

$$\lambda \;=\; \frac{h}{p} \tag{B.17}$$

Heisenberg Uncertainty Relation

The uncertainty, Δp, in momentum and the uncertainty, Δx, in position obey the inequality

$$\Delta x \, \Delta p \ > \ \frac{1}{2}\hbar \tag{B.18}$$

Schrödingers Equation

One Dimension

Wavefunction $\Psi(x,t)$ for a particle of mass m moving in one dimension in a force field whose potential is $V(x)$:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} \ = \ -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \tag{B.19}$$

Example 1: A particle of mass m confined to a square well with walls at $x = 0$ and $x = L$:

$$\begin{aligned} V(x) &= 0 \quad \leq x \ < L \\ &= \infty \quad x \ < 0, \text{ or } x \ > L \end{aligned}$$

Solutions:

$$\Psi_n(x,t) \ = \ \sqrt{\frac{2}{L}} e^{-iE_n t/\hbar} \sin\left(\frac{n\pi x}{L}\right) \tag{B.20}$$

where the energy levels E_n are given by

$$E_n \ = \ \frac{n^2 h^2}{8mL^2} \tag{B.21}$$

Example 2: A particle of mass m performing harmonic motion with frequency f:

$$V(x) \ = \ 2\pi^2 m f^2 x^2$$

Solutions:

$$\Psi_n(x,t) \ = \ e^{-iE_n t/\hbar}\left(\frac{4\pi m f}{h}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n\, n!}} H_n\left(2\pi\sqrt{\frac{mf}{h}}x\right) \tag{B.22}$$

where the energy levels E_n are given by

$$E_n \ = \ \left(n + \frac{1}{2}\right) h\, f \tag{B.23}$$

and $H_n(y)$ are Hermite polynomials of the argument y.

Three dimensions

Wavefunction $\Psi(\mathbf{r},t)$ for a particle of mass m moving in one dimension in a force field whose potential is $V(\mathbf{r})$:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t), \tag{B.24}$$

where the Laplacian operator, ∇^2, is given in cartesian coordinates by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

and in spherical polar coordinates (r,θ,ϕ) by

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Example: The Hydrogen atom. An electron of mass m_e and electric charge $-e$ moving in the electric field of a proton whose electric charge $+e$.

$$V(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0 r} = \alpha^2 m_e c^2\left(\frac{a_0}{r}\right),$$

where the dimensionless constant α known as the “fine-structure constant” is defined by

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c},$$

(c being the speed of light in vacuo), and the Bohr radius a_0 is given by

$$a_0 = \frac{\hbar}{\alpha m_e c}$$

The spherically symmetric (i.e. angular independent) solutions are:

$$\Psi_n(\mathbf{r},t) = \frac{2}{n}\left(\frac{1}{na_0}\right)^{\frac{3}{2}} e^{-iE_n t/\hbar}e^{-r/(na_0)}L^1_{(n-1)}\left(\frac{2r}{na_0}\right) \tag{B.25}$$

where $L^i_n(y)$ are associated Laguerre polynomials of the argument y.

The energy levels E_n are given by

$$E_n = \frac{\alpha^2 m_e c^2}{2n^2} \tag{B.26}$$

The wavelength, λ_{mn}, of electromagnetic radiation emitted or absorbed when a hydrogen atom makes a transition between energy level E_n and E_m is given by

$$\frac{1}{\lambda_{mn}} = \frac{1}{hc}|E_n - E_m| = R_H\left|\frac{1}{n^2} - \frac{1}{m^2}\right| \tag{B.27}$$

Inserting eq.(B.26) into eq.(B.27) gives the expression for the Rydberg constant R_H

$$R_H = \frac{\alpha^2 m_e c}{2h}.$$

Spin

The spin-wavefunction, Ψ_+ for a spin-$\frac{1}{2}$ particle whose component of spin measured in the direction with polar angle θ and azimuthal angle ϕ is $+\frac{1}{2}\hbar$ is given by:

$$\Psi_+ \;=\; \cos\left(\frac{\theta}{2}\right)\Psi_\uparrow + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\Psi_\downarrow \tag{B.28}$$

where $\Psi_\uparrow$ and $\Psi_\downarrow$ are the spin wavefunctions corresponding to spin component $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ (respectively) in the z-direction.

The spin-wavefunction, Ψ_- corresponding to a component $-\frac{1}{2}\hbar$ in the (θ, ϕ) direction is given by:

$$\Psi_- \;=\; \sin\left(\frac{\theta}{2}\right)e^{-i\phi}\Psi_\uparrow - \cos\left(\frac{\theta}{2}\right)\Psi_\downarrow \tag{B.29}$$