Thursday 2nd June 2011

# Quantum Physics: Numbers and Formulae

Please bear in mind that learning physics is NOT about rote memorisation. It will do you no harm to learn the contents of this handout, but it will not guarantee that you pass the exam, or even help all that much. Much more important is to appreciate the interconnected group of ideas and experiments that led to the equations, understand their physical meanings and relationships, know how to work through the main derivations, and practise plenty of problems.

## Units and sizes

| | |
|---|---|
| 1 nm | $10^{-9}$ m |
| 1 Å | $10^{-10}$ m |
| 1 eV | $1.6 \times 10^{-19}$ J |
| Distance between air molecules | few nm |
| Distance between atoms in molecules/solids | few Å |
| Radius of atom | $\sim$ 1Å |
| Radius of nucleus | $\sim$ few $\times 10^{-15}$m |
| Typical thermal energy | $\sim k_B T$ $\quad$ ($\frac{1}{2} k_B T$ per degree of freedom) |
| Chemical bond energy | $\sim$ few eV |
| Atomic ionisation energy | $\sim$ few eV |
| Work function | $\sim$ few eV |

## Equations from other courses

### Ideal gas law

$$PV = Nk_BT$$

### Newtonian mechanics

$$E = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x) \qquad\qquad F = -\frac{dV}{dx}$$

### Relativistic energy and momentum

$$\begin{aligned} E &= m\gamma c^2 \\ p &= m\gamma v \\ E^2 &= p^2c^2 + m^2c^4 \quad (E^2 = p^2c^2 \text{ if } m = 0) \end{aligned}$$

**Waves**

Travelling wave moving right:

$$\psi(x,t) = a\cos(kx - \omega t + \phi) = \text{Re}\left(Ae^{i(kx-\omega t)}\right) \quad (A = ae^{i\phi})$$

Travelling wave moving left:

$$\psi(x,t) = a\cos(-kx - \omega t + \phi) = \text{Re}\left(Ae^{i(-kx-\omega t)}\right) \quad (A = ae^{i\phi})$$

Wave vector and angular frequency:

$$k = \frac{2\pi}{\lambda} \qquad \omega = 2\pi\nu$$

Intensity:

$$I(x) = \text{square of max displacement at } x$$

Intensity of travelling wave:

$$I(x) = a^2 = |A|^2 \quad \text{(independent of } x\text{)}$$

Phase and group velocities:

$$v_p = \frac{\omega}{k} \qquad v_g = \frac{d\omega}{dk}$$

## Equations from this course

**Dispersion relations**

$$\text{light:} \quad \omega = ck$$
$$\text{non-relativistic massive particle:} \quad \omega = \frac{\hbar k^2}{2m}$$

**Photoelectric effect**

$$eV_0 = h\nu - W$$
$$\frac{1}{2}mv_{\text{max}}^2 = eV_0$$

**Planck and de Broglie equations**

$$E = h\nu = \hbar\omega$$
$$p = \frac{h}{\lambda} = \hbar k$$

(Note: these apply to *all* particles — massive and massless, relativistic and non-relativistic.)

**For photons only**

$$E = pc = \frac{hc}{\lambda} = \hbar ck$$

**For non-relativistic massive particles only**

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m}$$

**Probability densities**

If $f(x)$ is a probability density function (pdf), then

$$\begin{aligned} f(x) &\geq 0 \\ \int_{-\infty}^{\infty} f(x)\,dx &= 1 \\ f(x)\,dx &= \begin{cases}\text{probability that } x \text{ lies in the range } x \\ \text{to } x + dx.\end{cases} \end{aligned}$$

Expected values of $x$ and $x^2$:

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} x f(x)\,dx \\ \langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 f(x)\,dx \end{aligned}$$

The root-mean-square (rms) uncertainty $\Delta x$ (also known as the standard deviation of $f(x)$) is defined by:

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

**Probabilities in QM**

If $\psi(x) = \int A(k) e^{ikx}\,dk$ is a QM wave function (or rather a snapshot of the QM wave function $\psi(x,t)$ at some fixed time $t$), then

$$\begin{aligned} |\psi(x)|^2 dx &\propto \begin{cases}\text{probability that a measurement of the particle's position yields a} \\ \text{result in the range } x \text{ to } x + dx.\end{cases} \\ |A(k)|^2 dk &\propto \begin{cases}\text{probability that a measurement of the particle's momentum yields} \\ \text{a result in the range } \hbar k \text{ to } \hbar(k + dk).\end{cases} \end{aligned}$$

If $\psi(x)$ is *normalised*,

$$\int |\psi(x)|^2 dx = 1 \,,$$

then $|\psi(x)|^2$ is a pdf.

**Bandwidth theorem**

For any function $\psi(x) = \int A(k)e^{ikx}dk$,

$$\Delta x\, \Delta k \;\; \geq \;\; \frac{1}{2}\,,$$

where $\Delta x$ is the rms width of $|\psi(x)|^2$ and $\Delta k$ is the rms width of $|A(k)|^2$.

For any function $\psi(t) = \int A(\omega)e^{i\omega t}d\omega$,

$$\Delta t\, \Delta \omega \;\; \geq \;\; \frac{1}{2}\,,$$

where $\Delta t$ is the rms width of $|\psi(t)|^2$ and $\Delta\omega$ is the rms width of $|A(\omega)|^2$.

**Uncertainty principle**

$$\Delta x\, \Delta p \;\; \geq \;\; \frac{\hbar}{2} \qquad\qquad \Delta t\, \Delta E \;\; \geq \;\; \frac{\hbar}{2}$$

**Time-dependent Schrödinger equation**

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

**Time-independent Schrödinger equation**

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_n(x)}{dx^2} + V(x)\phi_n(x) \;\; = \;\; E_n\phi_n(x)$$

**Simple harmonic oscillator**

The energy levels of a quantum mechanical simple harmonic oscillator with spring constant $s$ and mass $m$ are

$$E_n \;\; = \;\; \left(n + \frac{1}{2}\right)\hbar\omega_{\rm cl}\,, \qquad\qquad n = 0, 1, 2, 3, \ldots\;,$$

where $\omega_{\rm cl} = \sqrt{s/m}$ is the angular frequency of a *classical* simple harmonic oscillator with spring constant $s$ and mass $m$. The zero-point energy of the QM oscillator is $E_0 = \frac{1}{2}\hbar\omega_{\rm cl}$.