CH1101 : Elements of Chemistry

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1. An *eigenfunction* of a given operator D is any (non-zero) function f which, when operated upon by D, gets multiplied by some scalar λ called its *eigenvalue*, i.e.,

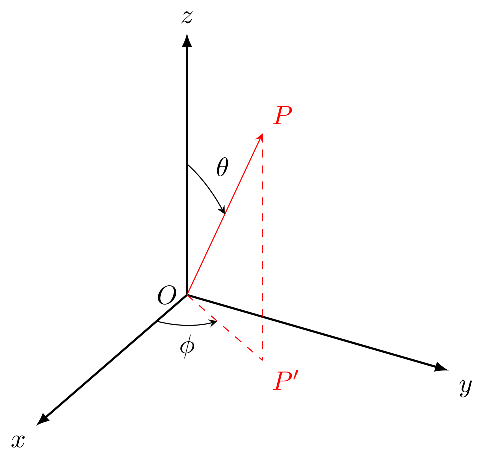
$$Df = \lambda f.$$

For example, consider the differentiation operator $D_x = \frac{\mathrm{d}}{\mathrm{d}x}$. Note that

$$D_x \exp(kx) = k \cdot \exp(kx).$$

Thus, $\exp(kx)$ is an eigenfunction of the operator D_x, with an eigenvalue of k.

2. Below is the point $P(x, y, z)$ in a spherical polar coordinate system.



$$r = \sqrt{x^2 + y^2 + z^2}$$
$$\theta = \arccos\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right)$$
$$\phi = \arctan\left(\frac{y}{x}\right)$$

We must have $r \geq 0$, $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$.

3. The *wavefunction* ψ of a particle is a mathematical entity (a complex valued function) which contains all of the dynamical information about the system. In this way, it can be considered as the central carrier of information in quantum mechanics.

4. (a) **Wave:** Particles were not known to be able to pass through seemingly solid metal foil.
   (b) **Particle:** All known particles were known to travel at speeds less than that of light – the speed of an electron is consistent with this.
   (c) **Wave:** Shadows are commonly cast by waves such as light.
   (d) **Particle:** Charged particles in motion were known to interact with electrical fields, while waves do not do so.

5. The first transition involves the absorption of a 95 nm photon, which corresponds to a frequency of $\approx 3.2 \times 10^{15}$ Hz, i.e., near ultraviolet light.

   The second transition involves the emission of a photon of 1282 nm, which corresponds to a frequency of $\approx 2.3 \times 10^{14}$ Hz, i.e., near infrared light.

   We shall use $E = -13.6\text{ eV}/n^2$ and $\Delta E = hc/\lambda$. For the first transition, we calculate $|\Delta E| = 13.6\text{ eV} \cdot (1 - (1/n_1^2)) = hc/(95\text{ nm})$, thus, $n_1 = 5$. Similarly, for the second transition, we calculate $|\Delta E| = 13.6\text{ eV} \cdot ((1/n_2^2) - (1/n_1^2)) = hc/(1282\text{ nm})$, thus, $n_2 = 3$.

6. We will use $\lambda = h/p$, $p = mv$. An O_2 molecule weighs 32 amu $\approx 5.3 \times 10^{-26}$ kg. Thus, its momentum is 2.5×10^{-23} kg m/s, and its de Broglie wavelength is $2.6 \times 10^{-11}\text{m} = 26$ pm. Clearly, this is a small fraction (10.7 %) of the molecular length of O_2.

7. (a) We have $l \in \{0, 1, 2, \ldots, (n-1)\}$, i.e., $n = 7$ possible values for l.
   (b) A 6d subshell corresponds to $n = 6$, $l = 2$. Thus, we have $m \in \{0, \pm 1, \ldots, \pm l\}$, i.e., $2l + 1 = 5$ possible values for m.
   (c) A 3p subshell corresponds to $n = 3$, $l = 1$. Thus we have $2l + 1 = 3$ possible values for m.
   (d) For $n = 4$, we have exactly 4 subshells, i.e, 4s, 4p, 4d and 4f.

8. (a) 6p consists of a linear combination of the ψ_{61-1}, ψ_{610} and ψ_{611} wavefunctions, such that it has no imaginary component.
   (b) 3d consists of a linear combination of the ψ_{32-2}, ψ_{32-1}, ψ_{320}, ψ_{321} and ψ_{322} wavefunctions.