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.,

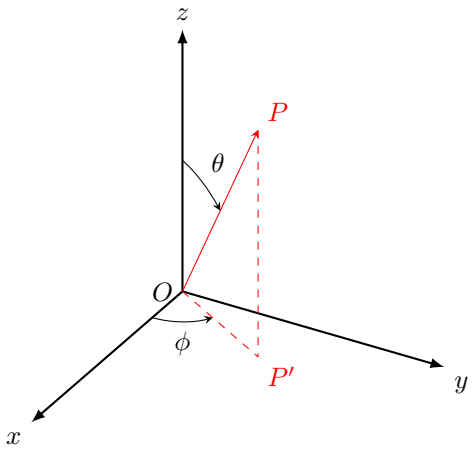
$$Df \;=\; \lambda f.$$

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.



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

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.

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.

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 2.6×10^{-11}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.