19.4: The Rigid Rotor

The rigid rotor is a simple model of a rotating stick in three dimensions (or, if you prefer, of a molecule). We consider the stick to consist of two point-masses at a fixed distance. We then reduce the model to a one-dimensional system by considering the rigid rotor to have one mass fixed at the origin, which is orbited by the reduced mass μ, at a distance r. The cartesian coordinates, x, y, z, are then replaced by three spherical polar coordinates: the co-latitude (zenith) angle θ, the longitudinal (azimuth) angle ϕ, and the distance r. The TISEq of the system in spherical coordinates is:

$$-\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r)=E_\ell\psi(r), \tag{19.4.1}$$

where $I=\mu r^2$ is the moment of inertia. After a little effort, the eigenfunctions can be shown to be the spherical harmonics $Y_\ell^{m_\ell}(\theta,\phi)$.[1] The eigenvalues are simply:

$$E_\ell=\frac{\hbar^2}{2I}\ell(\ell+1), \tag{19.4.2}$$

where $\ell=0,1,2,\ldots$ is the *azimuthal quantum number*, and $m_\ell=-\ell,-\ell+1,\ldots,\ell-1,\ell$ is the *magnetic quantum number*. Each energy level E_ℓ is $(2\ell+1)$-fold degenerate in m_ℓ. Notice that the energy does not depend on the second index m_ℓ, and the functions with fixed $m_\ell=-\ell,-\ell+1,\ldots,\ell-1,\ell$ have the same energy. Since this problem was, in fact, a one-dimensional problem, it results in just one quantum number ℓ, similarly to the previous two cases. The index m_ℓ that appears in the spherical harmonics will assume some importance in future chapters.

1. For a description of the spherical harmonics see here