PHY294: Review Sheet

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1 The Three-Dimensional Schrödinger Equation.

In general, the Schrödinger Equation can be written as

$$\nabla^2\psi = \frac{2M}{\hbar^2}[U-E]\psi \tag{1}$$

where ∇^2 is the Laplacian, which is a fancy way of writing:

$$\begin{aligned}
\nabla^2\psi &= \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} && \text{(Cartesian)} \\
&= \frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2} && \text{(Cylindrical)} \\
&= \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}
\end{aligned}$$

1.1 Particle in a Box

For a particle in an infinite square well, the allowed energies are

$$E = \frac{\hbar^2\pi^2}{2M}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) \tag{2}$$

Here, n_x, n_y, n_z are known as **quantum numbers**. When the same energy occurs at different quantum numbers, then we call it a **degeneracy.**

1.2 Central Force Problem

2-Dimensions

For the two-dimensional case, our solution is in the form of $\psi(r,\theta) = R(r)\Theta(\theta)$. Solving for $\Theta(\theta)$ gives:

$$\Phi(\phi) = A\sin(m\phi) + B\cos(m\phi),$$

which must satisfy the property $\Phi(\phi) = \Phi(\phi + 2\pi)$, forcing m to be an integer. The radial part $R(r)$ cannot be solved since it depends on the specific potential.

3-Dimensions

The solution is in the form of $\phi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$.

- Solving for $\Phi(\phi)$ gives the same equation as the $\Theta(\theta)$ case in 2-D, leading to the same quantum numbers.
- Solving for $\Theta(\theta)$ gives a parameter $k = l(l+1)$ where $l \geq |m|$ and is an integer.

1.3 Angular Momentum

The magnitude of the angular momentum is quantized and given by

$$L = \sqrt{l(l+1)}\hbar. \tag{3}$$

The angular momentum acts in a certain direction away from the z-axis, and

$$L_z = m\hbar, \tag{4}$$

where m has the usual restrictions. As a result, we can often draw these as vectors on a diagram. For a given l, there are $2l+1$ possible vectors.

1.4 Hydrogen Atom

Consider the simplest (yet useful) potential $U(r) = \dfrac{-ke^2}{r}$, for a hydrogen atom. The $R(r)$ part is given by

$$\frac{d^2}{dr^2}(rR) = \frac{2m_e}{\hbar^2}\left[-\frac{ke^2}{r} + \frac{l(l+1)\hbar^2}{2m_e r^2} - E\right](rR), \tag{5}$$

which only has acceptable solutions if

$$E = -\frac{m_e(ke^2)^2}{2\hbar^2}\frac{1}{n^2} = -\frac{E_R}{n^2}, \tag{6}$$

where n has the restriction $n > l$.

1.5 Hydrogenic Wave Functions

The solution for $R(r)$ is in the form of

$$R(r) = Ae^{-r/(na_B)} \tag{7}$$

where $a_B = \dfrac{h^2}{m_e ke^2}$ is the Bohr radius, and A is some function. The radial probability density is

$$P(r) = 4\pi r^2 |R(r)|^2 \tag{8}$$

1.6 Hydrogen-like Ions

We can extend this discussion to any ion with one electron bounded to a nucleus of charge Ze. Note that Φ, Θ are left unchanged and everything else can be derived by replacing ke^2 with Zke^2 and as a direct consequence, replacing a_B with a_B/Z.