Notes for Lectures on Quantum Mechanics *

Particle in a Rigid Spherical Box

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The potential for a rigid spherical box can be written as

$$V(r) = \begin{cases} 0, & 0 < r < a \\ \infty, & r > a \end{cases}. \tag{1}$$

The problem is separable in spherical polar coordinates and form of the full wave function is

$$\psi(r, \theta, \phi) = R(r) Y_{\ell m}(\theta, \phi). \tag{2}$$

We need to consider solutions of the radial equation only. No solution can be found for $E < 0$, therefore we consider $E > 0$. For $r > a$ the potential is infinite and hence the radial wave function must be zero, Next we consider $r < a$, where the potential is zero. The radial equation assumes the form

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{dR(r)}{dr} + \frac{\ell(\ell+1)\hbar^2}{2mr^2}R(r) - ER(r) = 0. \tag{3}$$

The most general solution of this equation is given in terms of spherical Bessel functions j_ℓ, n_ℓ and we write it as

$$R_{E\ell(r)} = Aj_\ell(kr) + Bn_\ell(kr), \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{4}$$

Recall that near $r = 0$, $n_\ell(r) \sim r^{-\ell-1}$ and blows up as $r \to 0$. Therefore we must set $B = 0$ if the solution is to remain finite at $r = 0$. Thus we get

$$R_\ell(r) = \begin{cases} Aj_\ell(kr), & 0 < r < a \\ 0 & r > a \end{cases}. \tag{5}$$

Next we must demand that the radial wave function $R(r)$ must be continuous at $r = a$. Remember that there is no corresponding requirement on the derivative for this case of infinite jump in the potential at $r = a$ The continuity requirement of $R_{E\ell}(r)$ becomes

$$j_\ell(ka) = 0. \tag{6}$$

The solutions of the above equation determine allowed values of k and hence allowed bound state energies.

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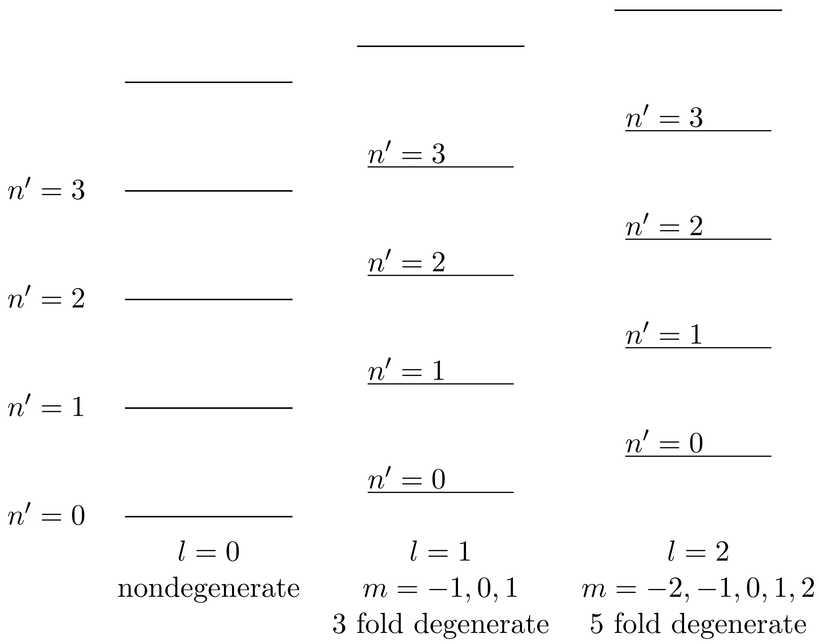
Energy levels and degeneracy

To get all the solutions, one proceeds as follows. First set $\ell = 0$ and locate the roots of $j_0(ka) = 0$. We call the roots as $\rho_{0n}, n = 0, 1, 2, \ldots$ and the corresponding energies are given by $E = \dfrac{\hbar^2 \rho_{0n}^2}{2ma^2}$.. Here n denotes the number of nodes of the radial wave function for $\ell = 0$.

Next, we set $\ell = 1$ and find the roots of $j_1(kr) = 0$, calling these roots as $\rho_{1n}, n = 0, 1, 2, \ldots$ the $\ell = 1$ energy levels are given by $E = \frac{\hbar^2 \rho_{1n}^2}{2ma^2}$. This process is to be repeated for all values of angular momentum ℓ and the number of bound states for each ℓ turns out to be infinite. The states of definite energy depend on quantum numbers $n\ell m$ and the energy does not depend on magnetic quantum number m. Therefore for a given azimuthal quantum number ℓ we have $(2\ell+1)$ wave functions $N_{n\ell} R_{n\ell}(r/\rho_{n\ell}) Y_{\ell m}(\theta, \phi), (m = -\ell, -\ell+1, \cdots, \ell)$ and the energy levels $E_{n\ell}$ are $(2\ell + 1)$ fold degenerate. The energy increases with ℓ and also with increasing n. Thus schematic energy level diagram would appear as follows.


$n' = 3$
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$n' = 0$
$l = 0$
nondegenerate
$l = 1$
$m = -1, 0, 1$
3 fold degenerate
$l = 2$
$m = -2, -1, 0, 1, 2$
5 fold degenerate