Notes for Lectures on Quantum Mechanics *

Spherically Symmetric Square Well

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The potential for a spherical well can be written as

$$V(r) = \begin{cases} -V_0, & 0 < r < a, \qquad V_0 > 0, \\ 0, & r > a \end{cases}. \tag{1}$$

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 $E < -V_0$, therefore we consider $E > -V_0$. We shall consider two cases of

(a) $-V_0 < E < 0$. This case corresponds to bound states,

(b) $E > 0$. In this case the there is no bound state. This case is of interest for scattering from the potential.

Bound states

The bound states correspond to $-V_0 < E < 0$. The radial equation in regions $r < a$ and $r > a$ assumes the forms

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{dR(r)}{dr} + \Big(q^2 - \frac{\ell(\ell+1)}{r^2}\Big)R(r) = 0, \qquad r > a, \tag{3}$$

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{dR(r)}{dr} + \Big(-\alpha^2 + \frac{\ell(\ell+1)}{r^2}\Big)R(r) = 0, \qquad 0 < r < a. \tag{4}$$

where

$$q^2 = \frac{2m(E+V_0)}{\hbar^2}, \quad \alpha^2 = \frac{2m|E|}{\hbar^2}. \tag{5}$$

The most general solution of this equation is given in terms of spherical Bessel functions j_ℓ, n_ℓ and is given by

$$R(r) = \begin{cases} A j_\ell(qr) + B n_\ell(qr), & 0 < r < a \\ C h^{(1)}(\alpha r) + D h^{(2)}(\alpha r) & r > a \end{cases}. \tag{6}$$

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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 $r = 0$. Also as $r \to \infty$ the Hankel function $h^{(2)}(\alpha r)$ increases exponentially, hence we must set $D = 0$. Thus we get

$$R_\ell(r) = \begin{cases} Aj_\ell(qr), & 0 < r < a \\ Ch_\ell^{(1)}(\alpha r) & r > a \end{cases}. \tag{7}$$

Next we must demand that the radial wave function $R(r)$ and its derivative must be continuous at $r = 0$. These continuity requirements become give the following restrictions of the coefficients A, C.

$$Aj_\ell(qa) = Ch_\ell^{(1)}(\alpha a). \tag{8}$$

$$A\frac{dj_\ell(qr)}{dr}\Big|_{r=a} = C\frac{dh_\ell^{(1)}(\alpha r)}{dr}\Big|_{r=a}. \tag{9}$$

Noting that A, C cannot be zero and eliminating A and C we get condition on the bound state energy to be

$$\frac{1}{j_\ell(qr)}\frac{dj_\ell(qr)}{dr}\Big|_{r=a} = \frac{1}{h_\ell(qr)}\frac{dh_\ell^{(1)}(\alpha r)}{dr}\Big|_{r=a}.. \tag{10}$$

The above equation can be solved numerically to obtain allowed values energies. In this case of square well only a finite number of states exist for a given ℓ below a maximum value. In general there will be no bound state for ℓ greater that a certain values. The states of definite energy depend on quantum number $n\ell$ 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 $N_{n\ell}R_{n\ell}(\rho)Y_{\ell m}(\theta, \phi)$ and the energy levels $E_{n\ell}$ are $(2\ell + 1)$ fold degenerate. The energy increases with ℓ and also with increasing n. Thus energy level diagram would appear as follows.

Continuous energy solutions

The energy levels for $E > 0$ are continuous. We shall write the corresponding solutions which are important for discussion of scattering from a square well. When $E > 0$ we define

$$q^2 = \frac{2m(E + V_0)}{\hbar^2}, \quad k^2 = \frac{2mE}{\hbar^2}. \tag{11}$$

A most general form of the solution of the radial equation is given by

$$R_\ell(r) = \begin{cases} Aj_\ell(qr) + Bn_\ell(qr), & r < a \\ Cj_\ell(kr) + Bn_\ell(kr), & r > a \end{cases}. \tag{12}$$

In order that the radial wave function be finite at $r = 0$, we must set $B = 0$. This gives

$$R_\ell(r) = \begin{cases} Aj_\ell(qr), & r < a \\ Cj_\ell(kr) + Bn_\ell(kr), & r > a \end{cases}. \tag{13}$$

Next we demand continuity of the radial wave function and its derivative at $r = a$ and get

$$
\begin{aligned}
A j_\ell(qa) &= C j_\ell(ka) + B n_\ell(ka) \qquad (14)\\
A \frac{d}{dr} j_\ell(qr)\Big|_{r=a} &= C \frac{d}{dr} j_\ell(kr)\Big|_{r=a} + B \frac{d}{dr} n_\ell(kr)\Big|_{r=a} \qquad (15)
\end{aligned}
$$

These two equations constrain the three constants A, B, C and determine their ratios, the overall normalization constant remains, as expected, undetermined. For a given energy E there is solution for each $\ell = 0, 1, 2, ...$ and $m = -\ell, ..., \ell$ giving rise to infinite degeneracy for $E > 0$. These continuous energy solutions will be required for physical applications to scattering problems.