Next Up Previous
Next: Hydrogen Atom **Up:** Central Potentials **Previous:** Derivation of Radial Equation

Infinite Spherical Potential Well

Consider a particle of mass m and energy $E > 0$ moving in the following simple central potential:

$$V(r) = \begin{cases} 0 & \text{for } 0 \leq r \leq a \\ \infty & \text{otherwise} \end{cases}. \tag{647}$$

Clearly, the wavefunction ψ is only non-zero in the region $0 \leq r \leq a$. Within this region, it is subject to the physical boundary conditions that it be well behaved (*i.e.*, square-integrable) at $r = 0$, and that it be zero at $r = a$ (see Sect. 5.2). Writing the wavefunction in the standard form

$$\psi(r, \theta, \phi) = R_{n,l}(r)\, Y_{l,m}(\theta, \phi), \tag{648}$$

we deduce (see previous section) that the radial function $R_{n,l}(r)$ satisfies

$$\frac{d^2 R_{n,l}}{dr^2} + \frac{2}{r}\frac{dR_{n,l}}{dr} + \left(k^2 - \frac{l\,(l+1)}{r^2}\right) R_{n,l} = 0 \tag{649}$$

in the region $0 \leq r \leq a$, where

$$k^2 = \frac{2\,m\,E}{\hbar^2}. \tag{650}$$

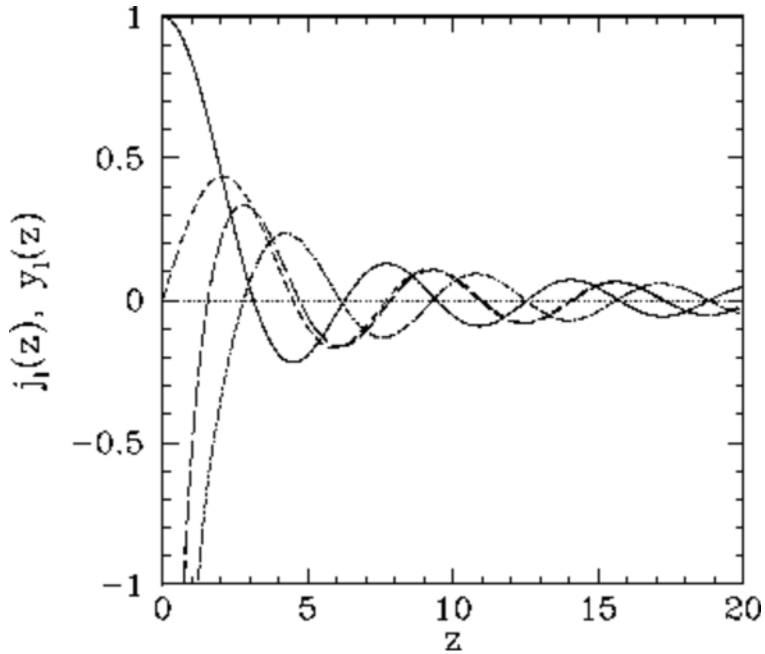

Figure 20: *The first few spherical Bessel functions. The solid, short-dashed, long-dashed, and dot-dashed curves show $j_0(z)$, $j_1(z)$, $y_0(z)$, and $y_1(z)$, respectively.*

Defining the scaled radial variable $z = k\,r$, the above differential equation can be transformed into the standard form

$$\frac{d^2 R_{n,l}}{dz^2} + \frac{2}{z}\frac{dR_{n,l}}{dz} + \left[1 - \frac{l\,(l+1)}{z^2}\right] R_{n,l} = 0. \tag{651}$$

The two independent solutions to this well-known second-order differential equation are called *spherical Bessel functions*, and can be written

$$j_l(z) \quad = \quad z^l \left(-\frac{1}{z}\frac{d}{dz}\right)^l \left(\frac{\sin z}{z}\right), \tag{652}$$

$$y_l(z) = -z^l\left(-\frac{1}{z}\frac{d}{dz}\right)^l\left(\frac{\cos z}{z}\right). \tag{653}$$

Thus, the first few spherical Bessel functions take the form

$$j_0(z) = \frac{\sin z}{z}, \tag{654}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}, \tag{655}$$

$$y_0(z) = -\frac{\cos z}{z}, \tag{656}$$

$$y_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}. \tag{657}$$

These functions are also plotted in Fig. 20. It can be seen that the spherical Bessel functions are oscillatory in nature, passing through zero many times. However, the $y_l(z)$ functions are badly behaved (*i.e.*, they are not square-integrable) at $z = 0$, whereas the $j_l(z)$ functions are well behaved everywhere. It follows from our boundary condition at $r = 0$ that the $y_l(z)$ are unphysical, and that the radial wavefunction $R_{n,l}(r)$ is thus proportional to $j_l(k\,r)$ only. In order to satisfy the boundary condition at $r = a$ [*i.e.*, $R_{n,l}(a) = 0$], the value of k must be chosen such that $z = k\,a$ corresponds to one of the zeros of $j_l(z)$. Let us denote the nth zero of $j_l(z)$ as $z_{n,l}$. It follows that

$$k\,a = z_{n,l}, \tag{658}$$

for $n = 1, 2, 3, \ldots$. Hence, from (650), the allowed energy levels are

$$E_{n,l} = z_{n,l}^2 \frac{\hbar^2}{2m\,a^2}. \tag{659}$$

The first few values of $z_{n,l}$ are listed in Table 1. It can be seen that $z_{n,l}$ is an increasing function of both n and l.

Table 1: *The first few zeros of the spherical Bessel function* $j_l(z)$.

	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	3.142	6.283	9.425	12.566
$l=1$	4.493	7.725	10.904	14.066
$l=2$	5.763	9.095	12.323	15.515
$l=3$	6.988	10.417	13.698	16.924
$l=4$	8.183	11.705	15.040	18.301

We are now in a position to interpret the three quantum numbers-- n, l, and m--which determine the form of the wavefunction specified in Eq. (648). As is clear from Sect. 8, the azimuthal quantum number m determines the number of nodes in the wavefunction as the azimuthal angle ϕ varies between 0 and 2π. Thus, $m=0$ corresponds to no nodes, $m=1$ to a single node, $m=2$ to two nodes, *etc*.

Likewise, the polar quantum number l determines the number of nodes in the wavefunction as the polar angle θ varies between 0 and π. Again, $l=0$ corresponds to no nodes, $l=1$ to a single node, *etc*. Finally, the radial quantum number n determines the number of nodes in the wavefunction as the radial variable r varies between 0 and a (not counting any nodes at $r=0$ or $r=a$). Thus, $n=1$ corresponds to no nodes, $n=2$ to a single node, $n=3$ to two nodes, *etc*. Note that, for the case of an infinite potential well, the only restrictions on the values that the various quantum numbers can take are that n must be a positive integer, l must be a non-negative integer, and m must be an integer lying between $-l$ and l. Note, further, that the allowed energy levels (659) only depend on the values of the quantum numbers n and l. Finally, it is easily demonstrated that the spherical Bessel functions are mutually orthogonal: *i.e.*,

$$\int_0^a j_l(z_{n,l}\,r/a)\,j_l(z_{n',l}\,r/a)\,r^2\,dr = 0 \tag{660}$$

when $n \neq n'$. Given that the $Y_{l,m}(\theta,\phi)$ are mutually orthogonal (see Sect. 8), this ensures that wavefunctions (648) corresponding to distinct sets of values of the quantum numbers n, l, and m are mutually orthogonal.

Next Up Previous

Next: Hydrogen Atom **Up:** Central Potentials **Previous:** Derivation of Radial Equation

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