8.2: Infinite Spherical Potential Well

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

$$V(r)=\begin{cases}0 & \text{for } 0\leq r\leq a\\ \infty & \text{otherwise}\end{cases}. \tag{8.2.1}$$

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 Section [s5.2].) Writing the wavefunction in the standard form

$$\psi(r,\theta,\phi)=R_{n,l}(r)\,Y_{l,m}(\theta,\phi), \tag{8.2.2}$$

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

$$\frac{d^{\,2}R_{n,l}}{dr^{\,2}}+\frac{2}{r}\frac{dR_{n,l}}{dr}+\left[k^{\,2}-\frac{l\,(l+1)}{r^{\,2}}\right]R_{n,l}=0 \tag{8.2.3}$$

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

$$k^{\,2}=\frac{2\,m\,E}{\hbar^{\,2}}. \tag{8.2.4}$$

Defining the scaled radial variable $z=k\,r$, the previous 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.\]

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

$$\begin{aligned}j_l(z)&=z^{\,l}\left(-\frac{1}{z}\frac{d}{dz}\right)^{l}\left(\frac{\sin z}{z}\right),\\ y_l(z)&=-z^{\,l}\left(-\frac{1}{z}\frac{d}{dz}\right)^{l}\left(\frac{\cos z}{z}\right).\end{aligned}$$

Thus, the first few spherical Bessel functions take the form

$$\begin{aligned}j_0(z)&=\frac{\sin z}{z},\\ j_1(z)&=\frac{\sin z}{z^{\,2}}-\frac{\cos z}{z},\\ y_0(z)&=-\frac{\cos z}{z},\\ y_1(z)&=-\frac{\cos z}{z^{\,2}}-\frac{\sin z}{z}.\end{aligned}$$

These functions are also plotted in Figure [sph]. 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

$$k\,a=z_{n,l}, \tag{8.2.5}$$

for $n=1,2,3,\ldots$. Hence, from Equation ([e9.29]), the allowed energy levels are

$$E_{n,l} = z_{n,l}^{\,2}\,\frac{\hbar^{\,2}}{2\,m\,a^{\,2}}. \tag{8.2.6}$$

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

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
[0.5ex] $l=1$	4.493	7.725	10.904	14.066
[0.5ex] $l=2$	5.763	9.095	12.323	15.515
[0.5ex] $l=3$	6.988	10.417	13.698	16.924
[0.5ex] $l=4$	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 Equation ([e9.27]). As is clear from Chapter [sorb], 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, et cetera. 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, et cetera. 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, et cetera. 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 ([e9.39]) 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: that is,

$$\int_0^a j_l(z_{n,l}\,r/a)\,j_l(z_{n',l}\,r/a)\,r^{\,2}\,dr = 0 \tag{8.2.7}$$

when $n\neq n'$. Given that the $Y_{l,m}(\theta,\phi)$ are mutually orthogonal (see Chapter [sorb]), this ensures that wavefunctions ([e9.27]) corresponding to distinct sets of values of the quantum numbers n, l, and m are mutually orthogonal.

Contributors and Attributions

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