The Radial Eqn

Our separation of the TISE in spherical coordinates using

$$\psi(r,\theta,\phi) = R(r)\, Y_l^m(\theta,\phi)$$

yielded the same angular solution for all potentials and a radial function with the normalization

$$1 = \int_0^\infty r^2 R^* R \, dr$$

The separated radial equation is

$$\frac{-\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \underbrace{\left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]}_{V_{eff}} R = ER$$

which is reminesant of the equation of orbit from classical mechanics with a effective potential arising from rotation.

As in classical mechanics, consider a change of variables

$$u(r) = r R(r)$$

$$R(r) = \frac{u(r)}{r}$$

$$\frac{dR}{dr} = \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2}$$

$$r^2 \frac{dR}{dr} = r\frac{du}{dr} - u$$

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = \frac{du}{dr} + r\frac{d^2u}{dr^2} - \frac{du}{dr} = r\frac{d^2u}{dr^2}$$

and the radial equation becomes

$$\frac{-\hbar^2}{2mr^2} r \frac{d^2u}{dr^2} + V_{eff} R = E R$$

or

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{eff}\, u = E u$$

Where

$$V_{eff} = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$$

Evidently, things are easier when $l = 0$. This will turn out to be when the angular momentum is zero and classically the particle executes one dimensional motion through the origin.

<u>Ex</u> Particle trapped in a spherical infinite square well with $l = 0$.

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

<u>Radial Eqn</u>

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu$$

Same as the one-dimensional square well.

$$u = \sqrt{\frac{2}{a}} \sin k_n r \qquad k_n = \frac{n\pi}{a}$$

Radial Function

$$R(r) = \frac{u(r)}{r} = \sqrt{\frac{2}{a}} \frac{\sin k_n r}{r}$$

Check finite at $r=0$

$$\lim_{r \to 0} R(r) = \sqrt{\frac{2}{a}} k_n \qquad \text{L'Hopital}$$

Note, there is a subtlety, the $r=a$ boundary condition is the same for the 1-d case but to discard the $\cos k_n x$ solution at $r=0$ requires us to argue the wave function must be finite at the origin.

Check Normalization

$$1 = \int_0^a r^2 R^* R \, dr = \int_0^a u^* u \, dr \quad \checkmark$$

Complete wave function

$$\psi_{n0} = \psi_{n\ell} = \sqrt{\frac{2}{a}}\,\frac{\sin k_n r}{r}\,Y_0^0$$

$$= \left(\frac{1}{4\pi}\right)^{1/2}\sqrt{\frac{2}{a}}\,\frac{\sin k_n r}{r}$$

$$E_{n0} = \frac{\hbar k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

Ex Isotropic Harmonic Oscillator $\ell = 0$

$$V(r) = \tfrac{1}{2} k r^2$$

Radial Eqn

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + \frac{1}{2} k r^2 u = E u$$

$\Rightarrow$ Same eqn as 1-d SHO

Solutions $\qquad \omega = \sqrt{\frac{k}{m}} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, r$

$$u_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}$$

$$u_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{2}\, \xi\, e^{-\xi^2/2}$$

Problem We know the energy spectrum since the potential is separable

$$V = \tfrac{1}{2}kx^2 + \tfrac{1}{2}ky^2 + \tfrac{1}{2}kz^2$$

$$\Rightarrow E_0 = E_{0x} + E_{0y} + E_{0z} = 3\left(\tfrac{1}{2}\hbar\omega\right) = \tfrac{3}{2}\hbar\omega$$

Solution

$$R_0(r) = \frac{u_0}{r} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}/r$$

$$\Rightarrow \infty \quad \text{as} \quad r \to 0$$

Not an allowed solution.

The ground state is then u_1

$$R_1 = \frac{u_1}{r} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{2}\,\frac{\xi}{r}\, e^{-\xi^2/2}$$

$$= \sqrt{\frac{2m\omega}{\hbar}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}$$

Ex Infinite Square Well $\quad l \neq 0$

Radial Eqn

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u = Eu$$

$$\frac{d^2u}{dr^2} = \left(\frac{l(l+1)}{r^2} - k^2\right)u$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Another well investigated differential equation. The solution are spherical Bessel functions, j_l and n_l.

Spherical Bessel Functions

$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \frac{\sin x}{x}$$

Spherical Neumann Functions

$$n_\ell(x) = -(-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \frac{\cos x}{x}$$

General Solution

$$u(r) = A r j_\ell(kr) + B r n_\ell(kr)$$

Neumann functions $\rightarrow \infty$ as $x \rightarrow 0$, so $B = 0$

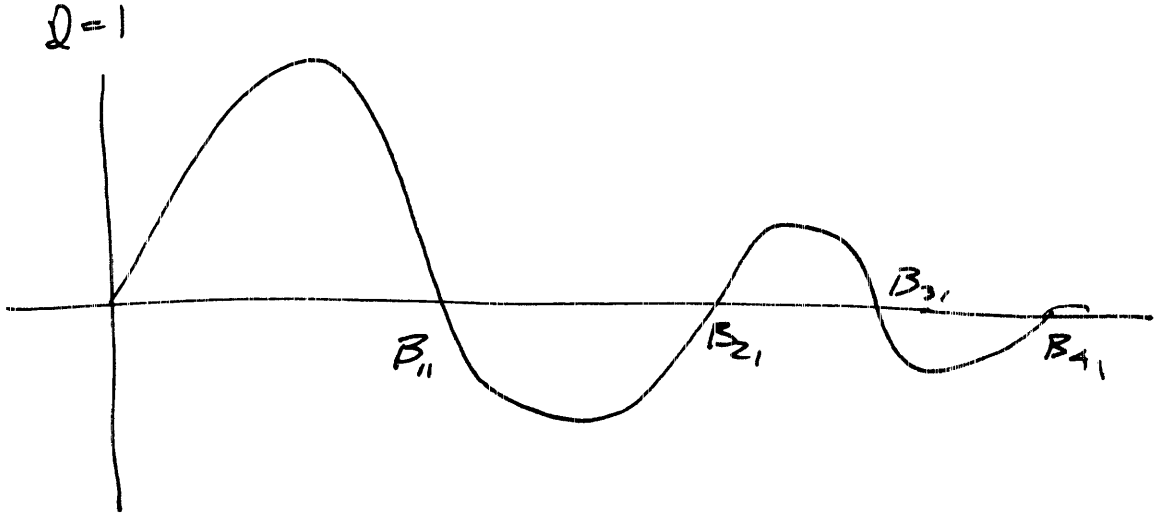
$$R(r) = \frac{u}{r} = A j_\ell(kr)$$

Apply BC

$$R(a) = 0 = A j_\ell(ka)$$

The Bessel functions oscillate like sines, but the zeros are not constantly spaced.

Let $\beta_{n\ell}$ be the nth zero of $j_\ell(x)$



So $\quad k_{n\ell}\, a = \beta_{n\ell} \qquad k_{n\ell} = \dfrac{\beta_{n\ell}}{a}$

$$E_{n\ell} = \frac{\hbar^2 k_{n\ell}^2}{2m} = \frac{\hbar^2 \beta_{n\ell}^2}{2ma^2}$$

ℓ from spherical harmonic

nth energy state

So how do we find zeros of Spherical Bessel functions?

The spherical Bessel functions are defined in terms of the normal Bessel functions $J_\ell(z)$

$$j_\ell(z) \sqrt{\frac{\pi}{2z}} \, J_{\ell+1/2}(z)$$

$\Rightarrow$ If $J_{\ell+1/2}(z) = 0$, $j_\ell(z) = 0$.

$\Rightarrow$ For $\ell = 1$, $J_{3/2}(z) = 0$ at

$$z_1 = B_{11} = 4.49 \qquad z_1 = 7.725 = B_{21}$$

The Maple code which evaluates these zeros follows on the next page.

$$K_{11} = \frac{B_{11}}{a} \qquad K_{21} = \frac{B_{21}}{a}$$

Wave function $(\ell = 1)$ $m=1$

$$\psi_{11} = A \, j_1(K_{11} r) \, Y_1^1$$

$$= -A \, j_1(K_{11} r) \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \, e^{i\phi}$$

> $BesselJZero(1, 1)$;

$$BesselJZero(1, 1) \tag{1}$$

> $evalf(\%)$;

$$BesselJZero(1, 1) \tag{2}$$

> $evalf\left(\mathrm{BesselJZeros}\left(\frac{3}{2}, 1\right)\right)$;

$$4.493409458 \tag{3}$$

> $evalf\left(\mathrm{BesselJZeros}\left(\frac{3}{2}, 0\right)\right)$;

$$0. \tag{4}$$

> $evalf\left(\mathrm{BesselJZeros}\left(\frac{3}{2}, 2\right)\right)$;

$$7.725251837 \tag{5}$$

>

The energy of this state is

$$E_{11} = \frac{\hbar^2 k_{11}^2}{2m} = \frac{\hbar^2}{2ma^2}\beta_{11}^2 = \frac{\hbar^2}{2ma^2}(4.49)^2$$

n l

One could also look up the zeros in

Abramowitz + Stegun

UNITED STATES DEPARTMENT OF COMMERCE • Luther H. Hodges, *Secretary*
NATIONAL BUREAU OF STANDARDS • A. V. Astin, *Director*

Handbook of Mathematical Functions

With

Formulas, Graphs, and Mathematical Tables

Edited by
Milton Abramowitz and Irene A. Stegun

National Bureau of Standards
Applied Mathematics Series • 55

Issued June 1964

Ninth Printing, November 1970, with corrections

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 - Price $9.00

ZEROS OF BESSEL FUNCTIONS OF HALF-INTEGER ORDER

Table 10.6

$J_\nu(j_{\nu,s})=0 \qquad Y_\nu(y_{\nu,s})=0$

ν	s	$j_{\nu,s}$	$J'_\nu(j_{\nu,s})$	$y_{\nu,s}$	$Y'_\nu(y_{\nu,s})$
1/2	1	3.141593	−0.45015 82	1.570796	−0.63661 98
	2	6.283185	+0.31830 99	4.712389	+0.36755 26
	3	9.424778	−0.25989 89	7.853982	−0.28470 50
	4	12.566370	+0.22507 91	10.995574	+0.24061 97
	5	15.707963	−0.20131 68	14.137167	−0.21220 66
	6	18.849556	+0.18377 63	17.278760	+0.19194 81
	7	21.991149	−0.17014 38	20.420352	−0.17656 66
	8			23.561945	+0.16437 45
3/2	1	4.493409	−0.36741 35	2.798386	+0.44914 84
	2	7.725252	+0.28469 20	6.121250	−0.31827 37
	3	10.904122	−0.24061 69	9.317866	+0.25989 33
	4	14.066194	+0.21220 57	12.486454	−0.22507 76
	5	17.220755	−0.19194 77	15.644128	+0.20131 63
	6	20.371303	+0.17656 64	18.796404	−0.18377 61
	7	23.519452	−0.16437 44	21.945613	+0.17014 37
5/2	1	5.763459	−0.31710 58	3.959528	−0.36184 68
	2	9.095011	+0.25973 30	7.451610	+0.28430 75
	3	12.322941	−0.22503 59	10.715647	−0.24053 93
	4	15.514603	+0.20130 14	13.921686	+0.21218 15
	5	18.689036	−0.18376 96	17.103359	−0.19193 81
	6	21.853874	+0.17014 05	20.272369	+0.17656 19
	7			23.433926	−0.16437 21
7/2	1	6.987932	−0.28223 71	5.088498	+0.30882 36
	2	10.417119	+0.24019 23	8.733710	−0.25896 77
	3	13.698023	−0.21208 02	12.067544	+0.22485 68
	4	16.923621	+0.19189 90	15.315390	−0.20124 01
	5	20.121806	−0.17654 40	18.525210	+0.18374 36
	6	23.304247	+0.16436 28	21.714547	−0.17012 77
	7			24.891503	+0.15914 62
9/2	1	8.182561	−0.25620 49	6.197831	−0.27236 25
	2	11.704907	+0.22432 53	9.982466	+0.23908 76
	3	15.039665	−0.20107 12	13.385287	−0.21179 27
	4	18.301256	+0.18367 44	16.676625	+0.19179 35
	5	21.525418	−0.17009 46	19.916796	−0.17649 69
	6	24.727566	+0.15912 86	23.128642	+0.16433 89
11/2	1	9.355812	−0.23580 60	7.293692	+0.24538 14
	2	12.966530	+0.21109 29	11.206497	−0.22293 49
	3	16.354710	−0.19155 58	14.676387	+0.20067 86
	4	19.653152	+0.17639 49	18.011609	−0.18352 21
	5	22.904551	−0.16428 83	21.283249	+0.17002 38
	6			24.518929	−0.15909 15
13/2	1	10.512835	−0.21926 48	8.379626	−0.22441 70
	2	14.207392	+0.19983 04	12.411301	+0.20946 65
	3	17.647975	−0.18321 82	15.945983	−0.19106 59
	4	20.983463	+0.16988 82	19.324820	+0.17619 60
	5	24.262768	−0.15902 21	22.628417	−0.16419 26
15/2	1	11.657032	−0.2[illegible] 46	[illegible]	[illegible]
	2	15.431288	+0.19058 8[illegible]	13.[illegible]	[illegible] 11
	3	18.922999	−0.17582 99	17.[illegible]	[illegible] 01
	4	22.295348	+0.16402 38	20.61[illegible]12	−0.16[illegible] 44
	5			23.9[illegible]	+0.1[illegible] 14
17/2	1	12.790782	−0.19382 82	10.529969	+0.19361 38
	2	16.641003	+0.18155 15	14.[illegible]	+0.18[illegible] 97
	3	20.182471	−0.16922 10	18.434[illegible]	−0.17[illegible] 27
	4	23.591275	+0.15870 04	21.898[illegible]	+0.16[illegible] 75
19/2	1	13.915823	−0.18376 11	11.[illegible]	+0.18186 42
	2	17.838643	+0.17398 86	15.[illegible]	−0.17344 10
	3	21.428487	−0.16326 17	19.[illegible]	+0.16347 33
	4	24.873214	+0.15383 84	23.16[illegible]	−0.15337 45
21/2	1	15.033469	−0.17496 82	12.659840	−0.17179 22
	2	19.025854	+0.16722 59	17.099480	+0.17176 97
	3	22.662721	−0.15785 09	20.870973	−0.16247 13
	4			24.4[illegible]6749	+0.15347 56
23/2	1	16.144743	−0.16723 39	13.719013	+0.16394 06
	2	20.203943	+0.16113 25	18.2[illegible]	−0.16491 86
	3	23.886531	−0.15290 87	22.073[illegible]	+0.15739 50
25/2	1	17.250455	−0.16028 44	14.775[illegible]	−0.15534 97
	2	21.373972	+0.15560 47	19.389462	+0.15876 20
	3			23.267630	−0.15201 34
27/2	1	18.351261	−0.15406 83	15.828[illegible]	+0.14852 56
	2	22.536817	+0.15056 00	20.[illegible]	−0.15316 36
	3			24.45[illegible]	+0.14742 15
29/2	1	19.447703	−0.14844 69	16.879170	−0.14242 04
	2	23.693208	+0.14593 21	21.654309	+0.14806 91
31/2	1	20.540230	−0.14333 12	17.927842	+0.13691 88
	2	24.843763	+0.14166 70	22.[illegible]78902	−0.14340 05
33/2	1	21.629221	−0.13865 11	18.974[illegible]	−0.13192 99
	2			23.898931	+0.13910 20
35/2	1	22.715002	−0.13434 93	20.019515	+0.12738 05
37/2	1	23.797849	−0.13037 81	21.062860	−0.12321 13
39/2	1	24.878005	−0.12669 81	22.104735	+0.11937 34

Values to greater accuracy and over a wider range are given in [10.31].

From National Bureau of Standards, Tables of spherical Bessel functions, vols. I, II. Columbia Univ. Press, New York, N.Y., 1947 (with permission).

Extracting Spherical Bessel Eqn from TISE

Divide by k^2 Let $\rho = kr$

$$\frac{d^2u}{d\rho^2} = \left(\frac{l(l+1)}{\rho^2} - 1 \right) u$$

Maple's Solution Appears on the next page

If $u = \rho R' = rR = krR' \Rightarrow R' = \frac{R}{k}$

$$\frac{du}{d\rho} = R + \rho \frac{dR}{d\rho}$$

$$\frac{d^2u}{d\rho^2} = \frac{dR}{d\rho} + \frac{dR}{d\rho} + \rho \frac{d^2R}{d\rho^2}$$

So the equation becomes

$$\rho \frac{d^2R'}{d\rho^2} + 2\frac{dR'}{d\rho} = \left(\frac{l(l+1)}{\rho^2} - 1 \right) \rho R'$$

$$\rho^2 \frac{d^2R'}{d\rho^2} + 2\rho \frac{dR'}{d\rho} + \left(\rho^2 - l(l+1) \right) R' = 0$$

spherical Bessel equation $\Rightarrow$ Solution A+S two pages following.

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10. Bessel Functions of Fractional Order

Mathematical Properties

10.1. Spherical Bessel Functions

Definitions

Differential Equation

10.1.1

$$z^2w''+2zw'+[z^2-n(n+1)]w=0 \qquad (n=0, \pm 1, \pm 2, \ldots)$$

Particular solutions are the *Spherical Bessel functions of the first kind*

$$j_n(z)=\sqrt{\tfrac{1}{2}\pi/z}\,J_{n+\frac{1}{2}}(z),$$

the *Spherical Bessel functions of the second kind*

$$y_n(z)=\sqrt{\tfrac{1}{2}\pi/z}\,Y_{n+\frac{1}{2}}(z),$$

and the *Spherical Bessel functions of the third kind*

$$h_n^{(1)}(z)=j_n(z)+iy_n(z)=\sqrt{\tfrac{1}{2}\pi/z}\,H_{n+\frac{1}{2}}^{(1)}(z),$$

$$h_n^{(2)}(z)=j_n(z)-iy_n(z)=\sqrt{\tfrac{1}{2}\pi/z}\,H_{n+\frac{1}{2}}^{(2)}(z).$$

The pairs $j_n(z)$, $y_n(z)$ and $h_n^{(1)}(z)$, $h_n^{(2)}(z)$ are linearly independent solutions for every n. For general properties see the remarks after **9.1.1.**

Ascending Series (See 9.1.2, 9.1.10)

10.1.2

$$j_n(z)=\frac{z^n}{1\cdot 3\cdot 5\ldots(2n+1)}\left\{1-\frac{\frac{1}{2}z^2}{1!(2n+3)}+\frac{(\frac{1}{2}z^2)^2}{2!(2n+3)(2n+5)}-\ldots\right\}$$

10.1.3

$$y_n(z)=-\frac{1\cdot 3\cdot 5\ldots(2n-1)}{z^{n+1}}\left\{1-\frac{\frac{1}{2}z^2}{1!(1-2n)}+\frac{(\frac{1}{2}z^2)^2}{2!(1-2n)(3-2n)}-\ldots\right\} \qquad (n=0, 1, 2, \ldots)$$

Limiting Values as $z\to 0$

10.1.4 $$z^{-n}j_n(z)\to\frac{1}{1\cdot 3\cdot 5\ldots(2n+1)}$$

Wronskians

10.1.6 $$W\{j_n(z), y_n(z)\}=z^{-2}$$

10.1.7

$$W\{h_n^{(1)}(z), h_n^{(2)}(z)\}=-2iz^{-2} \qquad (n=0,$$

Representations by Elementary Func

10.1.8

$$j_n(z)=z^{-1}[P(n+\tfrac{1}{2}, z)\sin(z-\tfrac{1}{2}n\pi)$$
$$+Q(n+\tfrac{1}{2}, z)\ \mathrm{co}$$

10.1.9

$$y_n(z)=(-1)^{n+1}z^{-1}[P(n+\tfrac{1}{2}, z)\cos(z+\tfrac{1}{2}n$$
$$-Q(n+\tfrac{1}{2}, z)\ \mathrm{si}$$

$$P(n+\tfrac{1}{2}, z)=1-\frac{(n+2)!}{2!\,\Gamma(n-1)}(2z)^{-2}$$
$$+\frac{(n+4)!}{4!\,\Gamma(n-3)}($$
$$=\sum_0^{[\frac{1}{2}n]}(-1)^k(n+\tfrac{1}{2}, 2k)(2z)^{-2k}$$

$$Q(n+\tfrac{1}{2}, z)=\frac{(n+1)!}{1!\,\Gamma(n)}(2z)^{-1}-\frac{(n+3)!}{3!\,\Gamma(n-2)}($$
$$+\frac{(n+5)!}{5!\,\Gamma(n-4)}($$
$$=\sum_0^{[\frac{1}{2}(n-1)]}(-1)^k(n+\tfrac{1}{2}, 2k+1)(2$$

$$(n=$$

$$(n+\tfrac{1}{2}, k)=\frac{(n+k)!}{k!\,\Gamma(n-k+1)}$$

n \ k	1	2	3	4
1	2			
2	6	12		
3	12	60	120	

```
> ode:= diff(u(x), x, x) -(l*(l+1)/x^2)*u(x)+u(x)=0;
```

$$ode := \frac{d^2}{dx^2}\,u(x) - \frac{l\,(l+1)\,u(x)}{x^2} + u(x) = 0 \qquad (1)$$

```
> dsolve(ode);
```

$$u(x) = \_C1\,\sqrt{x}\,\mathrm{BesselJ}\left(l+\frac{1}{2}, x\right) + \_C2\,\sqrt{x}\,\mathrm{BesselY}\left(l+\frac{1}{2}, x\right) \qquad (2)$$

```
> assume(l :: integer);
> dsolve(ode);
```

$$u(x) = \_C1\,\sqrt{x}\,\mathrm{BesselJ}\left(l\sim+\frac{1}{2}, x\right) + \_C2\,\sqrt{x}\,\mathrm{BesselY}\left(l\sim+\frac{1}{2}, x\right) \qquad (3)$$

```
>
```

solve j_1(x)=0

Input interpretation

$$\text{solve} \quad j_1(x) = 0$$

$j_n(x)$ is the spherical Bessel function of the first kind

Results

$x \approx -14.0661939128315\ldots$

$x \approx \pm 10.9041216594289\ldots$

$x \approx \pm 7.72525183693771\ldots$

$x \approx \pm 4.49340945790906\ldots$

$x = 0$

Root plot: