Spherical Bessel function

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Here we discuss the property of the spherical Bessel function which is the wave function of the free particle in the spherical co-ordinates, based on the book written by R.H. Dicke and J.P. Wittke (Introduction to Quantum Mechanics, Addison-Wesley, 1966).

1. Properties of vector operator

Suppose that $\hat{\boldsymbol{V}}$ is a vector and $\hat{\boldsymbol{J}}$ is an angular momentum in the quantum mechanics. As is already discussed before, we have the following commutation relations.

$$[\hat{V}_x, \hat{J}_x] = 0, \qquad [\hat{V}_y, \hat{J}_x] = -i\hbar\hat{V}_z, \qquad [\hat{V}_z, \hat{J}_x] = i\hbar\hat{V}_y,$$

$$[\hat{V}_x, \hat{J}_y] = i\hbar\hat{V}_z, \qquad [\hat{V}_y, \hat{J}_y] = 0, \qquad [\hat{V}_z, \hat{J}_y] = -i\hbar\hat{V}_x,$$

$$[\hat{V}_x, \hat{J}_z] = -i\hbar\hat{V}_y, \qquad [\hat{V}_y, \hat{J}_z] = i\hbar\hat{V}_x, \qquad [\hat{V}_z, \hat{J}_z] = 0.$$

We introduce the operators as

$$\hat{V}_\pm = \hat{V}_x \pm i\hat{V}_y, \qquad \hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y.$$

Using the above relation, we get

$$[\hat{V}_+, \hat{J}_x] = [\hat{V}_x + i\hat{V}_y, \hat{J}_x] = i[\hat{V}_y, \hat{J}_x] = \hbar\hat{V}_z,$$

$$[\hat{V}_-, \hat{J}_x] = [\hat{V}_x - i\hat{V}_y, \hat{J}_x] = -i[\hat{V}_y, \hat{J}_x] = -\hbar\hat{V}_z,$$

$$[\hat{V}_+, \hat{J}_y] = [\hat{V}_x + i\hat{V}_y, \hat{J}_y] = [\hat{V}_x, \hat{J}_y] = i\hbar\hat{V}_z,$$

$$[\hat{V}_-, \hat{J}_y] = [\hat{V}_x - i\hat{V}_y, \hat{J}_y] = [\hat{V}_x, \hat{J}_y] = i\hbar\hat{V}_z,$$

$$[\hat{V}_+, \hat{J}_z] = [\hat{V}_x + i\hat{V}_y, \hat{J}_z] = [\hat{V}_x, \hat{J}_z] + i[\hat{V}_y, \hat{J}_z] = -\hbar\hat{V}_+.$$

$$[\hat{V}_-, \hat{J}_z] = [\hat{V}_x - i\hat{V}_y, \hat{J}_z] = [\hat{V}_x, \hat{J}_z] - i[\hat{V}_y, \hat{J}_z] = \hbar\hat{V}_-.$$

These relations in turn can be shown to lead to

$$[\hat{V}_+, \hat{J}_z] = -\hbar\hat{V}_+, \qquad [\hat{V}_-, \hat{J}_z] = \hbar\hat{V}_-,$$

$$[\hat{V}_+, \hat{J}_+] = 0, \qquad [\hat{V}_-, \hat{J}_-] = 0,$$

$$[\hat{V}_+, \hat{J}_-] = 2\hbar\hat{V}_z, \qquad [\hat{V}_-, \hat{J}_+] = -2\hbar\hat{V}_z.$$

Note that $\hat{\boldsymbol{V}}$ is the vector operator. The momentum vector $\hat{\boldsymbol{p}}$ and position vector $\hat{\boldsymbol{r}}$ are the vector operators.

We also have the commutation relation for the scalar product $\hat{\boldsymbol{V}}_1 \cdot \hat{\boldsymbol{V}}_2$

$$[\hat{\boldsymbol{J}}, \hat{\boldsymbol{V}}_1 \cdot \hat{\boldsymbol{V}}_2] = 0$$

or

$$[\hat{J}_x, \hat{V}_{1x}\hat{V}_{2x} + \hat{V}_{1y}\hat{V}_{2y} + \hat{V}_{1z}\hat{V}_{2z}] = 0,$$

$$[\hat{J}_y, \hat{V}_{1x}\hat{V}_{2x} + \hat{V}_{1y}\hat{V}_{2y} + \hat{V}_{1z}\hat{V}_{2z}] = 0,$$

$$[\hat{J}_z, \hat{V}_{1x}\hat{V}_{2x} + \hat{V}_{1y}\hat{V}_{2y} + \hat{V}_{1z}\hat{V}_{2z}] = 0,$$

This can be proved as follows.
((**Proof**))

$$\begin{aligned}
[\hat{J}_x, \hat{V}_{1x}\hat{V}_{2x} + \hat{V}_{1y}\hat{V}_{2y} + \hat{V}_{1z}\hat{V}_{2z}] &= [\hat{J}_x, \hat{V}_{1x}]\hat{V}_{2x} + \hat{V}_{1x}[\hat{J}_x, \hat{V}_{2x}] + [\hat{J}_x, \hat{V}_{1y}]\hat{V}_{2y} + \hat{V}_{1y}[\hat{J}_x, \hat{V}_{2y}] \\
&\quad + [\hat{J}_x, \hat{V}_{1z}]\hat{V}_{2z} + \hat{V}_{1z}[\hat{J}_x, \hat{V}_{2z}] \\
&= -[\hat{V}_{1x}, \hat{J}_x]\hat{V}_{2x} - \hat{V}_{1x}[\hat{V}_{2x}, \hat{J}_x] - [\hat{V}_{1y}, \hat{J}_x]\hat{V}_{2y} - \hat{V}_{1y}[\hat{V}_{2y}, \hat{J}_x] \\
&\quad - [\hat{V}_{1z}, \hat{J}_x]\hat{V}_{2z} - \hat{V}_{1z}[\hat{V}_{2z}, \hat{J}_x] \\
&= i\hbar\hat{V}_{1z}\hat{V}_{2y} + i\hbar\hat{V}_{1y}\hat{V}_{2z} - i\hbar\hat{V}_{1y}\hat{V}_{2z} - i\hbar\hat{V}_{1z}\hat{V}_{2y} \\
&= 0
\end{aligned}$$

2. Eigenket $|\lambda, j, m\rangle$

From the above formula, we can derive the following relations,

$$[\hat{\boldsymbol{J}}, \hat{\boldsymbol{V}}^2] = 0,$$

$$[\hat{J}_z, \hat{V}_+] = \hbar\hat{V}_+,$$

$$[\hat{\boldsymbol{J}}^2, \hat{V}_+] = 2\hbar(\hat{V}_+\hat{J}_z - \hat{V}_z\hat{J}_+) + 2\hbar^2\hat{V}_+.$$

We assume that

$$\hat{H}|\lambda, j, m\rangle = E_\lambda|\lambda, j, m\rangle ,$$

$$\hat{\boldsymbol{L}}^2|\lambda, j, m\rangle = \hbar^2 j(j+1)|\lambda, j, m\rangle ,$$

$$\hat{L}_z|\lambda, j, m\rangle = \hbar m|\lambda, j, m\rangle .$$

where $|\lambda, j, m\rangle$ is the simultaneous eigenket of the Hamiltonian $\hat{H}$, the angular momentum ($\hat{\boldsymbol{L}}^2$, $\hat{L}_z$).

We now show that

$$\hat{V}_+|\lambda, j, m = j\rangle \approx |\lambda, j+, m = j+1\rangle$$

((**Proof**))
In order to verify this, we use the relation

$$[\hat{\boldsymbol{J}}^2, \hat{V}_+]|\lambda, j, m = j\rangle = 2\hbar(\hat{V}_+\hat{J}_z - \hat{V}_z\hat{J}_+)|\lambda, j, m = j\rangle + 2\hbar^2\hat{V}_+|\lambda, j, m = j\rangle ,$$

or

$$\hat{\boldsymbol{J}}^2\hat{V}_+|\lambda, j, j\rangle - \hbar^2 j(j+1)\hat{V}_+|\lambda, j, j\rangle = 2\hbar^2 j\hat{V}_+|\lambda, j, j\rangle - \hat{V}_z\hat{J}_+|\lambda, j, j\rangle + 2\hbar^2\hat{V}_+|\lambda, j, j\rangle ,$$

or

$$\hat{\boldsymbol{J}}^2\hat{V}_+|\lambda, j, j\rangle - \hbar^2 j(j+1)\hat{V}_+|\lambda, j, j\rangle = 2\hbar^2 j\hat{V}_+|\lambda, j, j\rangle + 2\hbar^2\hat{V}_+|\lambda, j, j\rangle ,$$

since $\hat{J}_+|\lambda, j, j\rangle = 0$. Then we get

$$\hat{\boldsymbol{J}}^2\hat{V}_+|\lambda, j, j\rangle =^2 (j+1)(j+2)\hat{V}_+|\lambda, j, j\rangle .$$

We also use the relation

$$[\hat{J}_z, \hat{V}_+] = \hbar\hat{V}_+ .$$

Then we have

$$[\hat{J}_z, \hat{V}_+]|\lambda, j, j\rangle = (\hat{J}_z\hat{V}_+ - \hat{V}_+\hat{J}_z)|\lambda, j, j\rangle = \hbar\hat{V}_+|j, j\rangle ,$$

or

$$\hat{J}_z \hat{V}_+ \left|\lambda, j, j\right\rangle = \hbar(j+1)\hat{V}_+ \left|\lambda, j, j\right\rangle .$$

These indicate that

$$\hat{V}_+ \left|\lambda, j, j\right\rangle \approx \left|\lambda, j+1, j+1\right\rangle.$$

As a trivial example of the usefulness of vectors, we assume that

$$\hat{V}_+ = \hat{p}_+ .$$

Then we have

$$\hat{p}_+ \left|\lambda, l, l\right\rangle \approx \left|\lambda, l+1, l+1\right\rangle$$

Here we use the notation for the wave function

$$\psi_{\lambda lm}(\boldsymbol{r}) = \left\langle \boldsymbol{r} \middle| \lambda, l, m \right\rangle$$

Then we get the relations

$$p_+ \psi_{\lambda 00}(\boldsymbol{r}) \approx \psi_{\lambda 11}(\boldsymbol{r}) ,$$

$$p_+{}^2 \psi_{\lambda 00}(\boldsymbol{r}) \approx \psi_{\lambda 22}(\boldsymbol{r}) ,$$

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$$p_+{}^l \psi_{\lambda 00}(\boldsymbol{r}) \approx \psi_{\lambda ll}(\boldsymbol{r}) ,$$

Since

$$\psi_{\lambda lm}(\boldsymbol{r}) \approx L_-{}^{l-m} \psi_{\lambda ll}(\boldsymbol{r})$$

we get

$$L_-{}^{l-m} p_+{}^l \psi_{\lambda 00}(\boldsymbol{r}) \approx L_-{}^{l-m} \psi_{\lambda ll}(\boldsymbol{r}) \approx \psi_{\lambda lm}(\boldsymbol{r}) .$$

3. Spherical Bessel function as wave function of free particle

We use the relation

$$\left\langle \boldsymbol{r} \middle| \hat{p}_+ \middle| \psi \right\rangle = -i\hbar\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi(\boldsymbol{r}) = -i\hbar(x+iy)\frac{1}{r}\frac{\partial}{\partial r}\psi(\boldsymbol{r})$$

or

$$p_+\psi(\boldsymbol{r}) = -i\hbar(x+iy)\frac{1}{r}\frac{d}{dr}\psi(\boldsymbol{r})$$

We repeat this process,

$$\begin{aligned} p_+{}^2\psi(\boldsymbol{r}) &= -i\hbar p_+(x+iy)\frac{1}{r}\frac{\partial}{\partial r}\psi(\boldsymbol{r}) \\ &= -i\hbar(x+iy)p_+\frac{1}{r}\frac{\partial}{\partial r}\psi(\boldsymbol{r}) \\ &= (-i\hbar)^2(x+iy)^2\left(\frac{1}{r}\frac{d}{dr}\right)^2\psi(\boldsymbol{r}) \end{aligned}$$

Similarly we have

$$p_+{}^l\psi(\boldsymbol{r}) = (-i\hbar)^l(x+iy)^l\left(\frac{1}{r}\frac{d}{dr}\right)^l\psi(\boldsymbol{r}).$$

Here we note that

$$[p_+, x+iy] = 0,$$

or

$$[\hat{p}_+, \hat{x}+i\hat{y}] = 0. \qquad \text{(commutation relation)}$$

This relation can be checked using Mathematica.

When

$\psi(\boldsymbol{r}) = f(r)$ (independent of θ and ϕ, an arbitrary function of r)

We get

$$\begin{aligned} p_+{}^l f(r) &= (-i\hbar)^l(x+iy)^l\left(\frac{1}{r}\frac{d}{dr}\right)^l f(r) \\ &= Y_l^l r^l\left(\frac{1}{r}\frac{d}{dr}\right)^l f(r) \end{aligned}$$

where

$$Y_l^l \approx e^{il\phi}(\sin\theta)^l = \left(\frac{x+iy}{r}\right)^l = \frac{(x+iy)^l}{r^l}.$$

Since

$$p_+{}^l \psi_{\lambda 00}(\boldsymbol{r}) \approx \psi_{\lambda ll}(\boldsymbol{r}),$$

with

$$\psi_{\lambda 00} = \frac{\sin(kr)}{kr},$$

we obtain

$$\begin{aligned} p_+{}^l \psi_{\lambda 00} &= (-i\hbar)^l (x+iy)^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \psi_{\lambda 00} \\ &= Y_l^l r^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \psi_{\lambda 00} \\ &\approx \psi_{\lambda ll} = Y_l^l R_\lambda(r) \end{aligned}$$

Then

$$R_\lambda(r) \approx \left(\frac{r}{k}\right)^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \psi_{\lambda 00},$$

or

$$j_l(kr) \approx (-1)^l \left(\frac{r}{k}\right)^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{\sin(kr)}{kr}.$$

Where

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}.$$

4. Summary

This radial function is a spherical Bessel function. Combining these radial functions with the spherical harmonic gives as the wave function for a free particle.

$$\psi_{\lambda lm}(\boldsymbol{r}) \approx R_\lambda(r) Y_l^m(\theta,\phi).$$

Eigenvalue problem for free particle:

$$H\psi_{\lambda lm}(\boldsymbol{r}) = E_k\psi_{\lambda lm}(\boldsymbol{r}) = \frac{\hbar^2 k^2}{2\mu}\psi_{\lambda lm}(\boldsymbol{r}),$$

$$\boldsymbol{L}^2\psi_{\lambda lm}(\boldsymbol{r}) = \hbar^2 l(l+1)\psi_{\lambda lm}(\boldsymbol{r}),$$

$$L_z\psi_{\lambda lm}(\mathbf{r}) = m\hbar\psi_{\lambda lm}(\mathbf{r}),$$

where

$$H = \frac{1}{2\mu}p_r{}^2 + \frac{\hbar^2 l(l+1)}{2\mu r^2} = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hbar^2 l(l+1)}{2\mu r^2}.$$

Schrodinger equation:

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi_{\lambda lm}) + \frac{\hbar^2 l(l+1)}{2\mu r^2}\psi_{\lambda lm} = \frac{\hbar^2 k^2}{2\mu}\psi_{\lambda lm}(\boldsymbol{r}).$$

When l = 0 (thus m = 0),

$$\frac{\partial^2}{\partial r^2}[r\psi_{\lambda 00}(\boldsymbol{r})] + k^2[r\psi_{\lambda 00}(\boldsymbol{r})] = 0,$$

or

$$\psi_{\lambda 00}(\mathbf{r}) = \frac{\sin(kr)}{kr}.$$

Instead of considering the radial differential equation for states other than l = 0, one can find a way of generating all the other wave functions from the state of l = 0. The momentum operator is a vector operator. We introduce the operator

$$p_+ = p_x + ip_y$$

p_+ commutes with the Hamiltonian.

$$f(r) = \frac{\sin(kr)}{kr}$$

$$\begin{aligned} p_+ f(r) &= (p_x + ip_y) f(r) \\ &= \frac{\hbar}{i}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) f(r) \\ &= \frac{\hbar}{i}(x+iy)\frac{1}{r}\frac{\partial}{\partial r} f(r) \end{aligned}$$

$$\begin{aligned} p_+{}^2 f(r) &= \frac{\hbar}{i} p_+ (x+iy)\frac{1}{r}\frac{\partial}{\partial r} f(r) \\ &= \left(\frac{\hbar}{i}\right)(x+iy) p_+ [\frac{1}{r}\frac{\partial}{\partial r} f(r)] \\ &= \left(\frac{\hbar}{i}\right)^2 (x+iy)^2 \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^2 f(r) \end{aligned}$$

In general,

$$\begin{aligned} p_+{}^l f(r) &= \left(\frac{\hbar}{i}\right)^l (x+iy)^l \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l f(r) \\ &= \left(\frac{\hbar}{i}\right)^l r^l e^{il\phi} \sin^l\theta \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l f(r) \\ &\approx \left(\frac{\hbar}{i}\right)^l Y_l^l(\theta,\phi) r^l \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l f(r) \approx \psi_{\lambda ll} = Y_l^l(\theta,\phi) g_l(r) \end{aligned}$$

or

$$g_l(r) = r^l \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l f(r) = r^l \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l \frac{\sin(kr)}{kr}$$

or

$$j_l(kr) = (-1)^l \left(\frac{r}{k}\right)^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{\sin(kr)}{kr}$$

((Note))

The definition of the spherical Bessel function:

$$j_l(x) = (-1)^l x^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin(x)}{x}.$$

$$j_0(x) = \frac{\sin x}{x},$$

$$j_1(x) = \frac{\sin x - x\cos x}{x^2}.$$

5. Mathematica for the Spherical Bessel function.

Here we compare two functions,

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

and a standard function provided by Mathematica: SphericalBesselJ[*L*, *x*]

((**Mathematica**))

```
P1 := (1/x) D[#, x] &;
J[L_, x_] := (-1)^L x^L Nest[P1, Sin[x]/x, L];

J[0, x] // Simplify
Sin[x]/x

J[1, x] // Simplify
(-x Cos[x] + Sin[x])/x^2

J[2, x] // Simplify
-(3 x Cos[x] + (-3 + x^2) Sin[x])/x^3
```

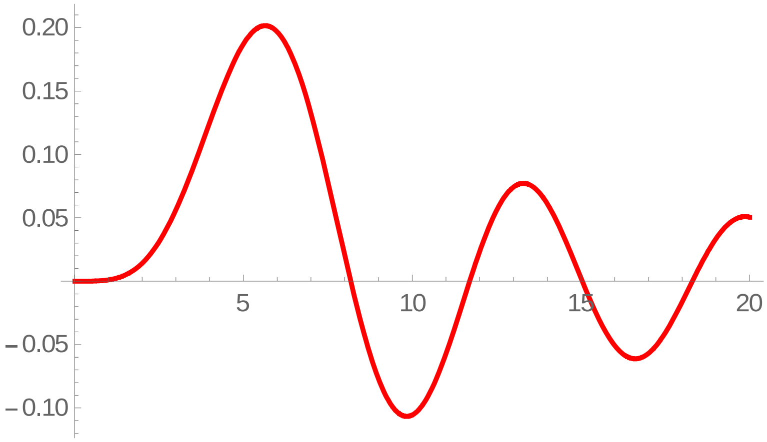
```
J[3, x] // Simplify
```

$$\frac{x\left(-15+x^2\right)\mathrm{Cos}[x]+3\left(5-2x^2\right)\mathrm{Sin}[x]}{x^4}$$

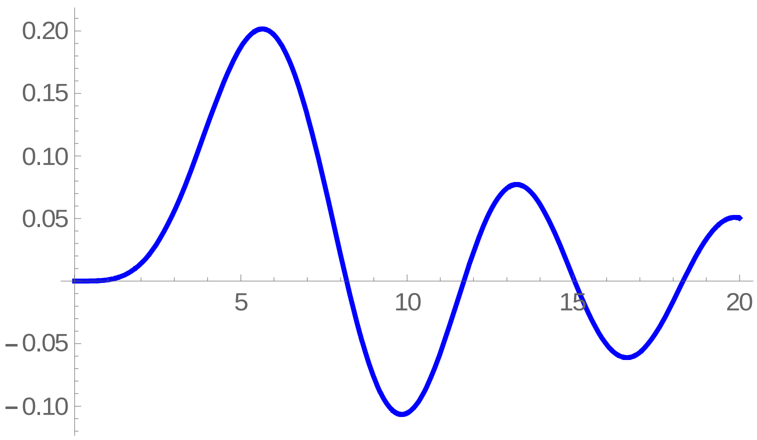
```
J[4, x] // Simplify
```

$$\frac{1}{x^5}\left(5x\left(-21+2x^2\right)\mathrm{Cos}[x]+\left(105-45x^2+x^4\right)\mathrm{Sin}[x]\right)$$

```
Plot[Evaluate[J[4, x]], {x, 0.01, 20},
 PlotStyle → {Red, Thick}]
```




```
f2 = Plot[SphericalBesselJ[4, x],
  {x, 0, 20}, PlotStyle → {Blue, Thick}]
```



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