Free Particle in the spherical coordinates
Masatsugu Sei Suzuki
Department of Physics, SUNY Binghamton
(Date: February 23, 2014)

1. Derivation

Free particle wave function ψ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi = E_k\psi ,$$

where μ is the mass of particle,

$$E_k = \frac{\hbar^2 k^2}{2\mu} ,$$

is the energy of the particle, and k is the wave number. This equation can be rewritten as

$$(\nabla^2 + k^2)\psi = 0 .$$

This equation is solved in a formal way as

$$\psi = \varphi_{k\ell m}(r,\theta,\phi) = \langle r\theta\phi | k\ell m\rangle$$

$$\frac{1}{2m}({p_r}^2 + \frac{\boldsymbol{L}^2}{r^2})\varphi_{k\ell m}(r,\theta,\phi) = E_k\varphi_{k\ell m}(r,\theta,\phi)$$

(separation variables), where $\boldsymbol{L}$ is the angular momentum:

$$\varphi_{k\ell m}(r,\theta,\phi) = R_{k\ell}(r)Y_{\ell m}(\theta,\phi) ,$$

with

$$\boldsymbol{L}^2 Y_{\ell m}(\theta,\phi) = \hbar^2\ell(\ell+1)Y_{\ell m}(\theta,\phi) .$$

Since $p_r = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r$, we have

$${p_r}^2 R_{k\ell}(r) = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r(\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r)R_{k\ell}(r) = -\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)],$$

or

$$-\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)]+\frac{1}{r^2}\ell(\ell+1)R_{k\ell}(r)=k^2R_{k\ell}(r),$$

or

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)]+[k^2-\frac{1}{r^2}\ell(\ell+1)]R_{k\ell}(r)=0.$$

((**Note**))

In the limit of $r\to\infty$, we have

$$\frac{\partial^2}{\partial r^2}[rR_{k\ell}(r)]+k^2[rR_{k\ell}(r)]=0$$

Then we get

$$R_{kl}=\frac{e^{\pm ikr}}{r}$$ (outgoing and incoming spherical waves)

Now we put $x=kr$ (dimensionless)

$$\frac{\partial}{\partial r}=\frac{\partial x}{\partial r}\frac{\partial}{\partial x}=k\frac{\partial}{\partial x},\qquad \frac{\partial^2}{\partial r^2}=k\frac{\partial}{\partial x}(k\frac{\partial}{\partial x})=k^2\frac{\partial^2}{\partial x^2}$$

$$[-\frac{k}{x}k^2\frac{\partial^2}{\partial r^2}(\frac{x}{k})+\frac{k^2}{x^2}\ell(\ell+1)]R=k^2R$$

or

$$-\frac{1}{x}\frac{\partial^2}{\partial x^2}(xR)+\frac{1}{x^2}\ell(\ell+1)R=R$$

or

$$-\frac{1}{x}[xR''+2R']+\frac{1}{x^2}\ell(\ell+1)R=R$$

or

$$R''+\frac{2}{x}R'+[1-\frac{\ell(\ell+1)}{x^2}]R=0$$ (Spherical Bessel equation)

where

$$R(x) = R_{kl}(r)$$

Note that the differential equation has of the Sturm-Liouville-type,

$$\frac{d^2}{dx^2}(x^2 R') + [x^2 - \ell(\ell+1)]R = 0 .$$

Suppose that

$$R(x) = \frac{f(x)}{\sqrt{x}},$$

$$\frac{d^2 f}{dx^2} + \frac{1}{x}\frac{df}{dx} + [1 - \frac{(\ell + \frac{1}{2})^2}{x^2}]f = 0 .$$

The solution of this equation is the Bessel functions;

$$f(x) = J_{\ell+1/2}(x), \qquad N_{\ell+1/2}(x) .$$

Then $R(x)$ is expressed by the spherical Bessel functions;

(i) Spherical Bessel function,

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

and

(ii) Spherical Neumann function,

$$n_\ell(x) = \sqrt{\frac{\pi}{2x}} N_{\ell+1/2}(x) .$$

Since the spherical Neumann function $n_\ell(x)$ diverges at x =0, it cannot be chosen as a solution. Finally we get

$$\varphi_{k\ell m}(r,\theta,\phi) = \langle r,\theta,\phi | k,l,m \rangle = \sqrt{\frac{2k^2}{\pi}} j_\ell(kr) Y_{\ell m}(\theta,\phi)$$

with

$$E_k = \frac{\hbar^2 k^2}{2m}$$

and

$$\langle k'l'm'|klm\rangle = \delta(k-k')\delta_{l,l'}\delta_{m,m'}$$

((**Mathematica**))

```
Clear["Global`*"];

eq1 = x^2 D[Rℓ[x], {x, 2}] + 2 x D[Rℓ[x], x] + (x^2 - ℓ (ℓ + 1)) Rℓ[x];

rule1 = {Rℓ → (J[#]/Sqrt[#] &)};

eq11 = eq1 /. rule1 // FullSimplify
```

$$\frac{\left(4x^2 - (1+2\ell)^2\right) J[x] + 4x\,(J'[x] + x J''[x])}{4\sqrt{x}}$$

```
DSolve[eq11 == 0, J[x], x]
```

$$\left\{\left\{J[x] \to \mathrm{BesselJ}\left[\frac{1}{2}(1+2\ell), x\right] C[1] + \mathrm{BesselY}\left[\frac{1}{2}(1+2\ell), x\right] C[2]\right\}\right\}$$

2 Recursion relation

(a) $\ell = 0$

First we consider the case of $\ell = 0$. The differential equation is given by

$$\frac{\partial^2}{\partial x^2}(xR) + xR = 0 .$$

So that the solution of rR are

$$xR = \sin x , \qquad \text{or} \qquad \cos x ,$$

or

$$R = \frac{\cos x}{x} = \frac{e^{ix} + e^{-ix}}{2x} , \qquad \text{or} \qquad \frac{\sin x}{x} = \frac{e^{ix} - e^{-ix}}{2ix}$$

(b) $\ell \neq 0$

Next we consider the case of $\ell \neq 0$

$$\frac{d}{dx}(x^2 R_\ell') + [x^2 - \ell(\ell+1)]R_\ell = 0$$

where we know the solution $R_\ell = j_l(x)$. When we put

$$R_\ell = x^\ell \chi_\ell(x)$$

we have the differential equation,

$$x\chi_\ell''(x) + 2(1+\ell)\chi_\ell'(x) + x\chi_\ell(x) = 0.$$

If we differentiate this equation with respect to x, we obtain

$$\chi_\ell^{(3)}(x) + \frac{2(1+\ell)}{x}\chi_\ell''(x) + [1 - \frac{2(1+\ell)}{x^2}]\chi_\ell'(x) = 0.$$

By the substitution

$$\chi'_\ell(x) = x\chi_{\ell+1}(x)$$

$$\chi_{\ell+1}''(x) + \frac{2(2+\ell)}{x}\chi_{\ell+1}'(x) + \chi_{\ell+1}(x) = 0$$

which is in fact the equation satisfied by $\chi_{\ell+1}(x)$. Thus the successive function $\chi_{\ell+1}(x)$ is related by

$$\chi_{\ell+1}(x) = \frac{\chi'_\ell(x)}{x}$$

or

$$\frac{R_{\ell+1}}{x^{\ell+1}} = \frac{1}{x}\frac{d}{dx}(\frac{R_\ell}{x^\ell})$$

Since $R_\ell \approx j_\ell(x)$, we have the spherical Bessel function as

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

Similarly we define the spherical Neumann function as

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

((**Mathematica**))

```
Clear["Global`*"]; OP1 := (1/x) D[#, x] &;
J[l_, x_] := (-x)^l Nest[OP1, Sin[x]/x, l]

Table[{l, J[l, x]}, {l, 0, 7}] // Simplify // TableForm
```

0	$\frac{\text{Sin}[x]}{x}$
1	$\frac{-x\,\text{Cos}[x]+\text{Sin}[x]}{x^2}$
2	$-\frac{3\,x\,\text{Cos}[x]+\left(-3+x^2\right)\text{Sin}[x]}{x^3}$
3	$\frac{x\left(-15+x^2\right)\text{Cos}[x]+3\left(5-2\,x^2\right)\text{Sin}[x]}{x^4}$
4	$\frac{5\,x\left(-21+2\,x^2\right)\text{Cos}[x]+\left(105-45\,x^2+x^4\right)\text{Sin}[x]}{x^5}$
5	$\frac{-x\left(945-105\,x^2+x^4\right)\text{Cos}[x]+15\left(63-28\,x^2+x^4\right)\text{Sin}[x]}{x^6}$
6	$-\frac{21\,x\left(495-60\,x^2+x^4\right)\text{Cos}[x]+\left(-10395+4725\,x^2-210\,x^4+x^6\right)\text{Sin}[x]}{x^7}$
7	$\frac{x\left(-135135+17325\,x^2-378\,x^4+x^6\right)\text{Cos}[x]-7\left(-19305+8910\,x^2-450\,x^4+4\,x^6\right)\text{Sin}[x]}{x^8}$

```
OP2 := (1/x) D[#, x] &; H[l_, x_] := -(-x)^l Nest[OP2, Cos[x]/x, l]

Table[{l, H[l, x]}, {l, 0, 7}] // Simplify // TableForm
```

0	$-\frac{\text{Cos}[x]}{x}$
1	$-\frac{\text{Cos}[x]+x\,\text{Sin}[x]}{x^2}$
2	$\frac{\left(-3+x^2\right)\text{Cos}[x]-3\,x\,\text{Sin}[x]}{x^3}$
3	$\frac{3\left(-5+2\,x^2\right)\text{Cos}[x]+x\left(-15+x^2\right)\text{Sin}[x]}{x^4}$
4	$-\frac{\left(105-45\,x^2+x^4\right)\text{Cos}[x]+5\,x\left(21-2\,x^2\right)\text{Sin}[x]}{x^5}$
5	$-\frac{15\left(63-28\,x^2+x^4\right)\text{Cos}[x]+x\left(945-105\,x^2+x^4\right)\text{Sin}[x]}{x^6}$
6	$\frac{\left(-10395+4725\,x^2-210\,x^4+x^6\right)\text{Cos}[x]-21\,x\left(495-60\,x^2+x^4\right)\text{Sin}[x]}{x^7}$
7	$\frac{7\left(-19305+8910\,x^2-450\,x^4+4\,x^6\right)\text{Cos}[x]+x\left(-135135+17325\,x^2-378\,x^4+x^6\right)\text{Sin}[x]}{x^8}$

3. Spherical Hankel functions

We define the spherical Hankel functions as

$$h_n^{(1)}(x) = \sqrt{\frac{\pi}{2x}} H^{(1)}_{n+\frac{1}{2}}(x) = j_n(x) + i n_n(x)$$

$$h_n^{(2)}(x) = \sqrt{\frac{\pi}{2x}} H^{(2)}_{n+\frac{1}{2}}(x) = j_n(x) - i n_n(x)$$

where the spherical Bessel function and spherical Neumann function are given by

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x)$$

$$n_n(x) = \sqrt{\frac{\pi}{2x}} N_{n+\frac{1}{2}}(x) = (-1)^n \sqrt{\frac{\pi}{2x}} J_{-n-\frac{1}{2}}(x)$$

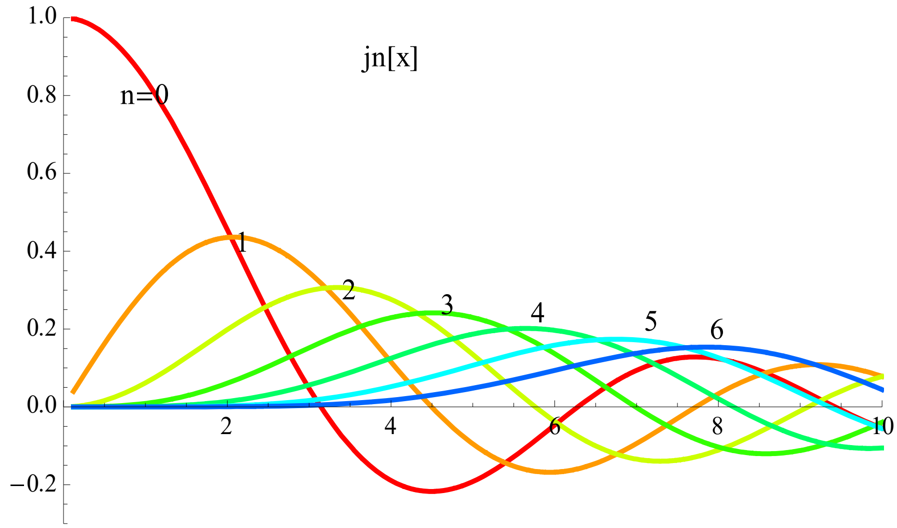


Fig. $j_n(x)$ with n = 0, 1, 2, 3, 4, 5, and 6.

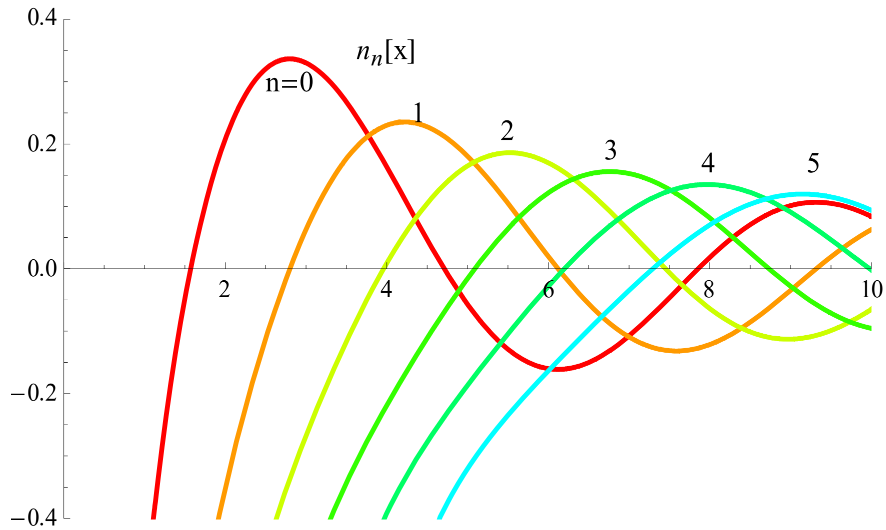


Fig. $n_n(x)$ with n = 0, 1, 2, 3, 4, and 5.

4 Rayleigh formulas

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

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

$$h_\ell^{(1)}(x) = -i(-1)^\ell x^l (\frac{1}{x}\frac{d}{dx})^\ell \frac{e^{ix}}{x}$$

$$h_\ell^{(2)}(x) = i(-1)^\ell x^l (\frac{1}{x}\frac{d}{dx})^\ell \frac{e^{-ix}}{x}$$

5 Asymptotic forms

The asymptotic values of the spherical Bessel functions and spherical Hankel functions may be obtained from the Bessel asymptotic form.

$$j_\ell(x) \approx \frac{1}{x}\sin(x - \frac{l\pi}{2}),$$

$$n_\ell(x) \approx -\frac{1}{x}\cos(x - \frac{l\pi}{2}),$$

$$h_\ell^{(1)}(x) \approx -i\frac{e^{i(x-l\pi/2)}}{x}$$ (outgoing spherical wave)

$$h_\ell^{(2)}(x) \approx i\frac{e^{-i(x-l\pi/2)}}{x}$$ (incoming spherical wave)

6. The behavior near the origin

$$j_l(x) \approx \frac{2^l l!}{(2l+1)!}x^l \qquad \text{for } x \ll 1.$$

$$n_l(x) \approx -\frac{(2l)!}{2^l l!}\frac{1}{x^{l+1}} \qquad \text{for } x \ll 1.$$

7. Energy eigenvalue of particle in an infinite spherical well (spherical quantum dot

We discuss the wave function of a particle in an infinite spherical well in three dimensions. The wave function is given by

$$R(r) = Aj_\ell(kr)$$

with

$$j_\ell(ka) = 0$$

or

$$J_{l+\frac{1}{2}}(x = ka) = 0$$

The energy eigenvalue is dependent on the value of l. Suppose that $x(l, n_r)$ is the n_r-th zero points where $j_l(x)$ becomes zero, where n_r = 1, 2, 3, ... (integer). The energy eigenvalue is

$$E(l,n_r) = \frac{\hbar^2}{2m}\frac{[x(l,n_r)]^2}{a^2}$$

or

$$E_r = \frac{2m}{\hbar^2}a^2 E(l,n_r) = [x(l,n_r)]^2$$

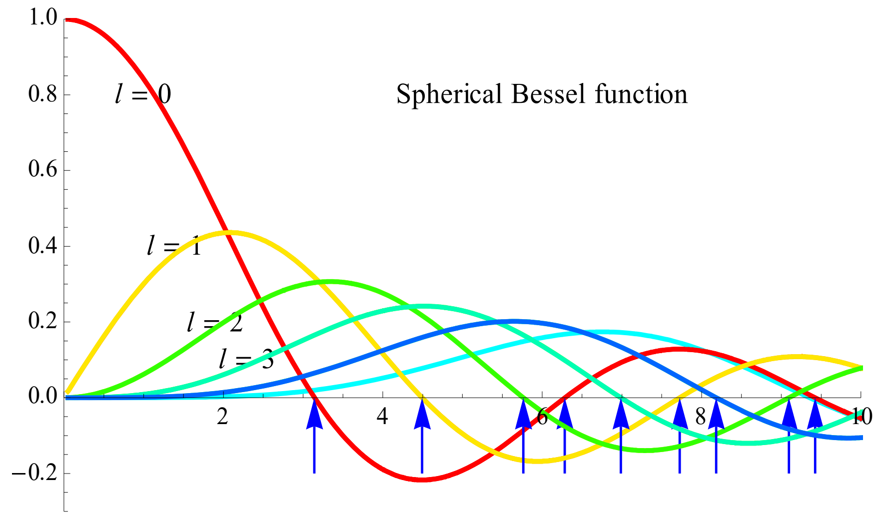


Fig. The plot of $j_\ell(x)$ as a function of x. The values of x when $j_\ell(x) = 0$ are denoted by the blue arrows.

The energy levels of the infinite spherical well is shown for each l (= 0, 1, 2, 3, 4,...)

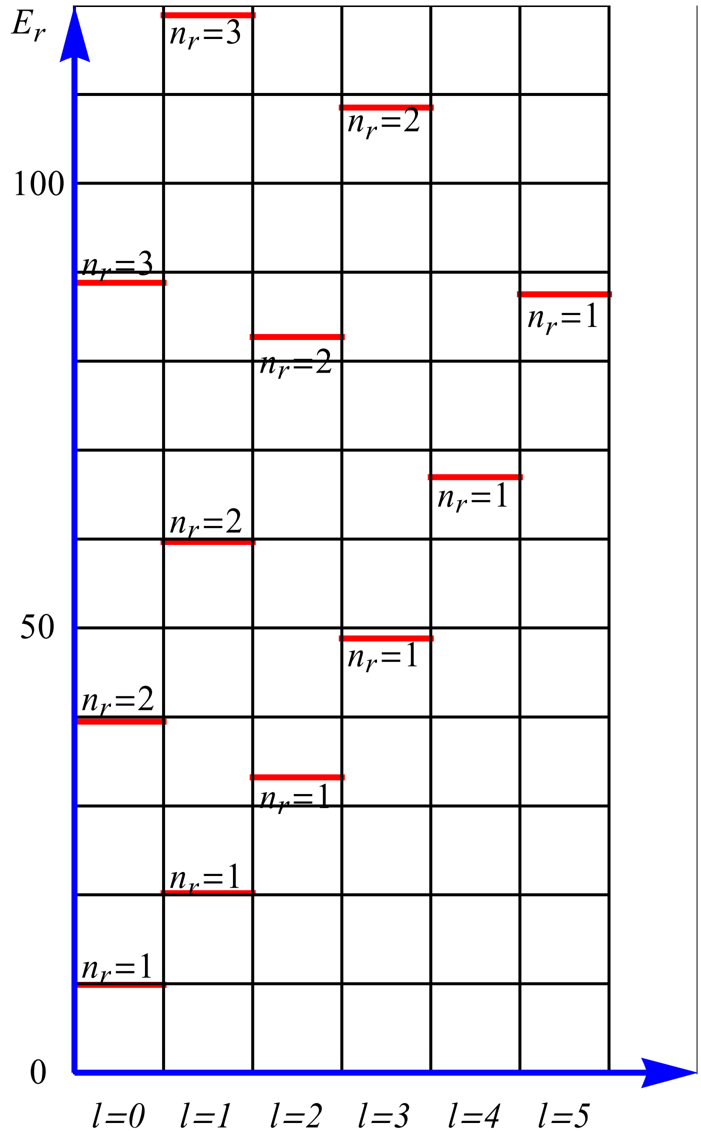
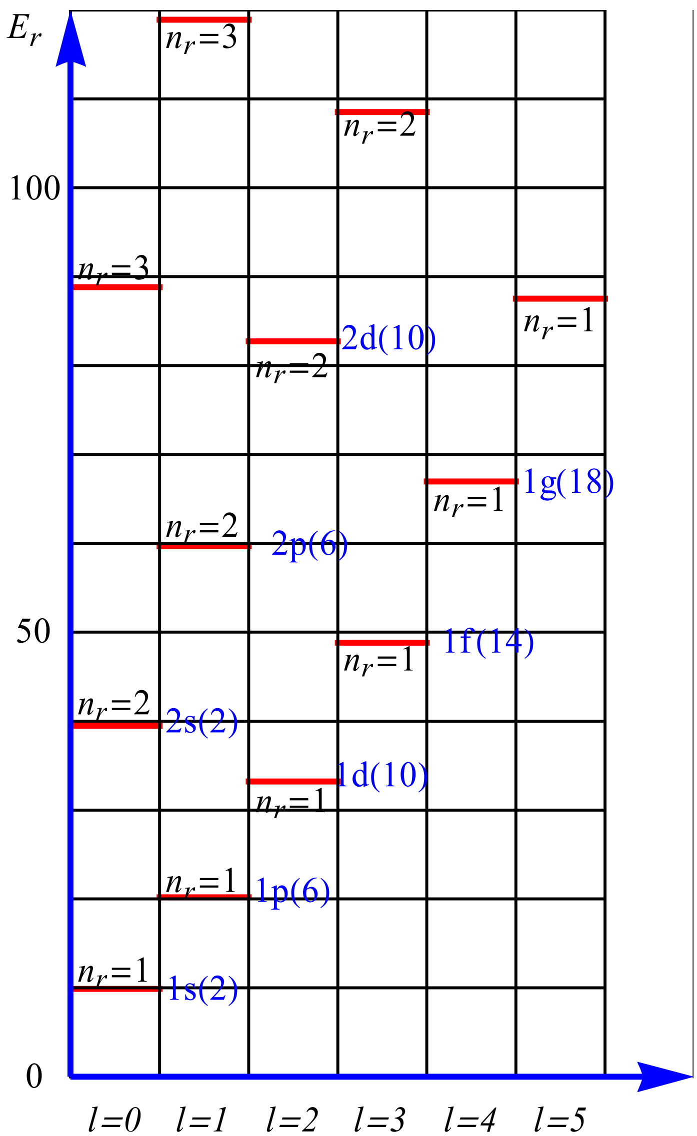


Fig. The energy levels of the infinite spherical well. $E_r = E(l, n_r)\dfrac{2m}{\hbar^2}a^2 = [x(l, n_r)]^2$.

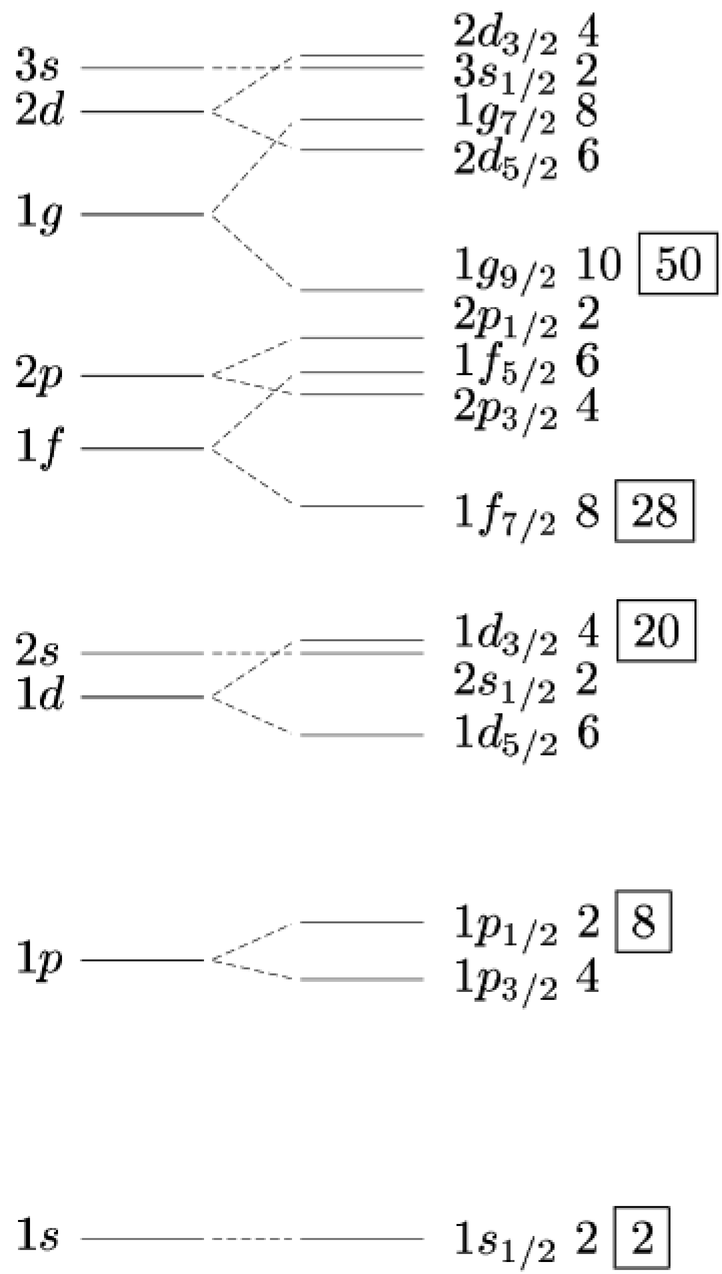


8. Nuclear shell model: Magic number for nucleus

We consider one particle on the spherical shell. It is just like a quantum box for the one dimension. The particle is free inside the spherical shell. Outside the shell, the potential energy is infinite. We consider either proton or neutron. As the first approximation, there is no repulsive Coulomb interaction. These particles are both spn-1/2 particles. These particles obey the Pauli's exclusion principle. First we determine the energy eigenvalues for the one-particle system. This problem is just like the quantum box for the one dimension. According to the Paili's exclusion principle, there are two states in the ground state with the spin-up state and spin-down state. When the two states are occupied, the first excited state will be occupied next.

In nuclear physics and nuclear chemistry, the **nuclear shell model** is a model of the atomic nucleus which uses the Pauli exclusion principle to describe the structure of the nucleus in terms of energy levels. The first shell model was proposed by Dmitry Ivanenko (together with E. Gapon) in 1932. The model was developed in 1949 following independent work by several physicists, most notably Eugene Paul Wigner, Maria Goeppert-Mayer and J. Hans D. Jensen, who shared the 1963 Nobel Prize in Physics for their contributions.

The shell model is partly analogous to the atomic shell model which describes the arrangement of electrons in an atom, in that a filled shell results in greater stability. When adding nucleons (protons or neutrons) to a nucleus, there are certain points where the binding energy of the next nucleon is significantly less than the last one. This observation, that there are certain magic numbers of nucleons: 2, 8, 20, 28, 50, 82, 126 which are more tightly bound than the next higher number, is the origin of the shell model. (http://en.wikipedia.org/wiki/Nuclear_shell_model).



((**Our model**))

We now try to make a nucleus by filling the energy levels with protons and neutrons. Protons and neutrons are both spin 1/2 particles (fermions). According to the Pauli's exclusion principle, there are more than two particles in each energy level. Suppose that we fill the levels with just protons. The first level is a (1s) level where 2 protons can occupy. The second level is a (1p) level where 6 protons can occupy. The third level is a (1d) level where 10 protons can occupy. In such a way, we see that the energy levels will be completely filled when the number of protons is

$(1s)^2$	2
$(1p)^6$	2+6=8
$(1d)^{10}$	2+6+10=18
$(2s)^2$	2+6+10+2=20
$(1f)^{14}$	2+6+10+2+14=34
$(2p)^6$	2+6+10+2+14+6=40
$(1g)^{18}$	2+6+10+2+14+6+18=58
$(2d)^{10}$	2+6+10+2+14+6+18+10=68

with a similar sequence of neutrons. Note that real nuclei exhibits the magic numbers such that

2, 8, 20, 28, 50, 82, and 126.

The difference between the observed magnetic numbers and those in the simple model arises there is a strong inverted spin-orbit coupling that shifts the energy levels.

((**Maria Goeppert-Mayer, nuclear shell model**))

Maria Goeppert-Mayer (June 28, 1906 – February 20, 1972) was a German-born American theoretical physicist, and Nobel laureate in Physics for proposing the nuclear shell model of the atomic nucleus. She is the second female laureate in physics, after Marie Curie.

Goeppert-Mayer's model explained why certain numbers of nucleons in an atomic nucleus result in particularly stable configurations. These numbers are called *magic numbers*. She postulated that the nucleus is a series of closed shells, and pairs of neutrons and protons tend to couple together in what is called spin orbit coupling.

http://en.wikipedia.org/wiki/Maria_Goeppert-Mayer

((Note))
Magneic number:

- 2
- 8=2+6
- 20=2+6+12
- 28=2+6+12+8
- 50=2+6+12+8+22
- 82=2+6+12+8+22+32
- 126=2+6+12+8+22+32+44
- 184=2+6+12+8+22+32+44+58

N: the number of neutron
Z: the number of proton.
These are fermion with spin 1/2, obeying the Pauli exclusion principle.

Either *N* or *Z* equal to the magic number
Both *N* and *Z* are equal to the magic number (double magic number)\

${}_{2}^{4}He: N = 2, Z = 2$ (double magic number)

${}_{8}^{16}O: N = 8, Z = 8$ (double magic number)

${}_{20}^{40}Ca: N = 20, Z = 20$ (double magic number)

${}_{50}^{119}Sn: N = 69, Z = 50$ (magic number)

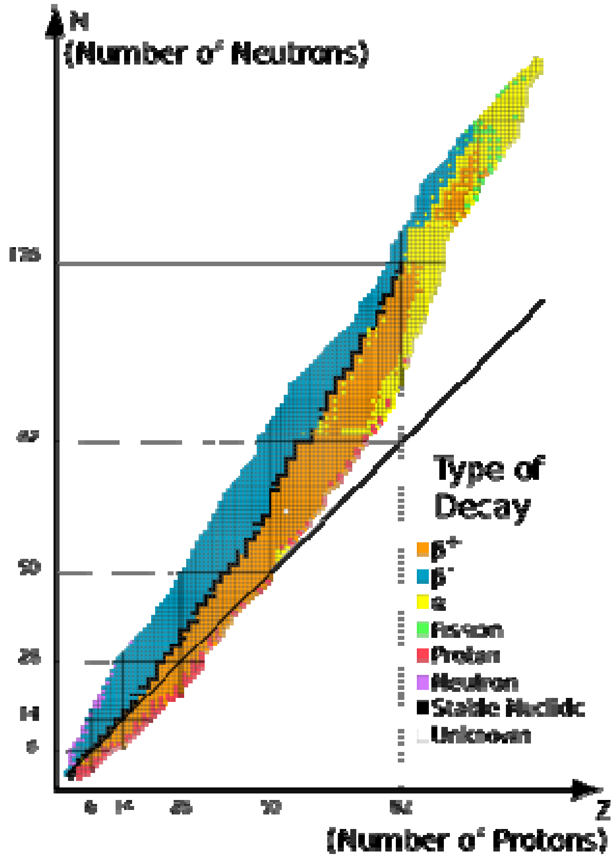


Fig. Graph of isotope stability
http://en.wikipedia.org/wiki/Magic_number_%28physics%29

((**Mathematica-1**))
The roots [zero point, $x(l, n_r)$] of the spherical Bessel function for $l = 0, 1, 2, 3, 4$.

$$J_{l+\frac{1}{2}}(x) = 0\text{; } k = 1 \text{ (first zero), } k = 2 \text{ (second zero), } k = 3 \text{ (third zero),...}$$

$l = 0$

```
Clear["Global`*"];
Table[{k, N[BesselJZero[1 / 2, k]]}, {k, 1, 9}] //
 TableForm
```

1	3.14159
2	6.28319
3	9.42478
4	12.5664
5	15.708
6	18.8496
7	21.9911
8	25.1327
9	28.2743

$l = 1$

```
Table[{k, N[BesselJZero[3 / 2, k]]}, {k, 1, 9}] //
 TableForm
```

1	4.49341
2	7.72525
3	10.9041
4	14.0662
5	17.2208
6	20.3713
7	23.5195
8	26.6661
9	29.8116

$l = 2$

```
Table[{k, N[BesselJZero[5 / 2, k]]}, {k, 1, 9}] //
 TableForm
```

1	5.76346
2	9.09501
3	12.3229
4	15.5146
5	18.689
6	21.8539
7	25.0128
8	28.1678
9	31.3201

$l = 3$

```
Table[{k, N[BesselJZero[7 / 2, k]]}, {k, 1, 9}] //
 TableForm
```

1	6.98793
2	10.4171
3	13.698
4	16.9236
5	20.1218
6	23.3042
7	26.4768
8	29.6426
9	32.8037

$l = 4$

```
Table[{k, N[BesselJZero[9 / 2, k]]}, {k, 1, 9}] //
 TableForm
```

1	8.18256
2	11.7049
3	15.0397
4	18.3013
5	21.5254
6	24.7276
7	27.9156
8	31.0939
9	34.2654

7 Plane wave expression

The wave function ψ can be described by

$$\psi(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm} Y_l^m(\theta,\phi) j_l(kr)$$

We consider the plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$, which is one of the solution of the Schrödinger equation.

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm} Y_l^m(\theta,\phi) j_l(kr)$$

We choose the direction of $\boldsymbol{k}$ along the z direction.

$$\boldsymbol{k} = (0,0,k), \qquad \boldsymbol{k}\cdot\boldsymbol{r} = kr\cos\theta$$

We note that $e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta}$ is independent of ϕ. $Y_l^m(\theta,\phi)$ is independent of ϕ only for m = 0.

$$Y_l^{m=0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

Then we get

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} c_l P_l(\cos\theta) j_l(kr)$$

where

$$c_l = i^l (2l+1)$$

((**Proof**))

$$\int_0^\pi e^{ikr\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \sum_{s=0}^\infty c_s j_s(kr) \int_0^\pi P_s(\cos\theta) P_l(\cos\theta)\sin\theta d\theta,$$

or

$$\int_0^\pi e^{ikr\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \sum_{s=0}^\infty c_s j_s(kr) \frac{1}{2s+1}\delta_{l,s} = \frac{2}{2l+1} c_l j_l(kr).$$

Differentiate l times with respect to $x = kr$.

$$\frac{d^l}{dx^l}\int_0^\pi e^{ix\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \frac{2}{2l+1} c_l \frac{d^l}{dx^l} j_l(x),$$

or

$$\int_0^\pi (i\cos\theta)^l e^{ix\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \frac{2}{2l+1} c_l \frac{d^l}{dx^l} j_l(x),$$

Note that

$$j_l(x) \approx \frac{2^l l!}{(2l+1)!} x^l, \qquad \text{for } x \ll 1$$

$$\frac{d^l j_l(x)}{dx^l} = \frac{2^l (l!)^2}{(2l+1)!}.$$

When $x = 0$,

$$\frac{2}{2l+1} c_l \frac{2^l (l!)^2}{(2l+1)!} = i^l \int_0^\pi \cos^l\theta P_l(\cos\theta)\sin\theta d\theta = i^l \int_0^\pi \varsigma^l P_l(\varsigma) d\varsigma = i^l \frac{2^{l+1}(l!)^2}{(2l+1)!},$$

or

$$c_l = i^l (2l+1),$$

or

$$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$$ (Rayleigh's expansion)

This formula is especially useful in scattering theory. For kr>>1, we get

$$\begin{aligned}
e^{i\boldsymbol{k}\cdot\boldsymbol{r}} &\approx \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) j_l(kr) \\
&\approx \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) \frac{\sin(kr - \frac{l\pi}{2})}{kr} \\
&= \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) \frac{\cos[kr - \frac{(l+1)\pi}{2}]}{kr} \\
&= \frac{1}{2ikr} \sum_{l=0}^{\infty} \{e^{\frac{il\pi}{2}} (2l+1) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) [e^{i(kr - \frac{(l+1)\pi}{2})} + e^{-i(kr - \frac{(l+1)\pi}{2})}] \\
&= \frac{e^{ikr}}{2ikr} \sum_{l=0}^{\infty} (2l+1) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) - \frac{e^{-ikr}}{2ikr} \sum_{l=0}^{\infty} (2l+1)(-1)^l P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) \\
&= \frac{2\pi e^{ikr}}{ikr} \delta(\hat{\boldsymbol{k}}, \hat{\boldsymbol{r}}) - \frac{2\pi e^{-ikr}}{ikr} \delta(\hat{\boldsymbol{k}}, -\hat{\boldsymbol{r}})
\end{aligned}$$

where

$$\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}} = \frac{\boldsymbol{k}\cdot\boldsymbol{r}}{kr} = \cos\theta$$

and

$$\langle \boldsymbol{n} | \boldsymbol{n}' \rangle = \delta(\boldsymbol{n} - \boldsymbol{n}') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\boldsymbol{n}\cdot\boldsymbol{n}'),$$

8 Bessel-Fourier transform

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$$

$$\int_0^{\pi} e^{ikr\cos\theta} P_l(\cos\theta) \sin\theta d\theta = \sum_{s=0}^{\infty} i^s (2s+1) j_s(kr) \int_0^{\pi} P_s(\theta) P_l(\cos\theta) \sin\theta d\theta$$

$$\int_0^{\pi} e^{ikr\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \sum_{s=0}^{\infty} i^s (2s+1) j_s(kr) \frac{2}{2s+1}\delta_{s,l} = 2i^l j_l(kr)$$

or

$$j_l(kr) = \frac{1}{2i^l}\int_0^{\pi} e^{ikr\cos\theta} P_l(\cos\theta)\sin\theta d\theta = \frac{1}{2i^l}\int_{-1}^{1} e^{ikrx} P_l(x) dx$$

This means that (apart from constant factor) the spherical Bessel function $j_l(kr)$ is the Fourier transform of the Legendre polynomial $P_l(x)$.

9 Green's function for the spherical Bessel function

We consider the Green's function given by

$$(\nabla^2 + k^2) G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'),$$

The solution of the Green's function is given by

$$G(\mathbf{r}, \mathbf{r}') = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi |\mathbf{r} - \mathbf{r}'|}$$

with the boundary condition

$$G(\mathbf{r}, \mathbf{r}') \to 0 \quad \text{for } r \to 0 \text{ and for } r \to \infty.$$

where $\boldsymbol{r}$ is the variable and $\boldsymbol{r}'$ is fixed.

Within each region (region I ($0<r<r'$) and region II ($r'<r$), we have the simpler equation

$$(\nabla^2 + k^2) G(\mathbf{r}, \mathbf{r}') = 0.$$

The solution of the Green's function is given by the form

$$G(\mathbf{r}, \mathbf{r}') = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}(r, r', \theta', \phi') Y_l^m(\theta, \phi).$$

Then the differential equation of the Green's function is given by

$$\sum_{l',m'} [\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'}) + (k^2 - \frac{l'(l'+1)}{r^2}) A_{l'm'}] Y_{l'}^{m'}(\theta, \phi) = -\frac{\delta(r - r')}{r^2}\delta(\phi - \phi')\delta(\mu - \mu').$$

Note that

$$\delta_{l,l'}\delta_{m,m'} = \int d\Omega \langle l',m'|\mathbf{n}\rangle\langle \mathbf{n}|l,m\rangle = \iint \sin\theta d\theta d\phi Y_{l'}^{m'^*}(\theta,\phi)Y_l^m(\theta,\phi)$$

where

$$d\Omega = \sin\theta d\theta d\phi .$$

Then

$$\sum_{l',m'}\int d\Omega Y_l^{m^*}(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'.}) + (k^2 - \frac{l'(l'+1)}{r^2})A_{l'm'}]$$
$$= -\int d\Omega Y_l^{m^*}(\theta,\phi)\frac{\delta(r-r')}{r^2}\delta(\phi-\phi')\delta(\mu-\mu')$$

or

$$\sum_{l',m'}[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{l'm'}) + (k^2 - \frac{l'(l'+1)}{r^2})A_{l'm'}]\delta_{l,l'}\delta_{m,m'}$$
$$= -\int d\Omega Y_l^{m^*}(\theta,\phi)\frac{\delta(r-r')}{r^2}\delta(\phi-\phi')\delta(\mu-\mu')$$

or

$$\begin{aligned}\frac{1}{r}\frac{\partial^2}{\partial r^2}(rA_{lm}) + [k^2 - \frac{l(l+1)}{r^2}]A_{lm} &= -\frac{\delta(r-r')}{r^2}\int d\Omega Y_l^{m^*}(\theta,\phi)\delta(\phi-\phi')\delta(\mu-\mu') \\ &= -\frac{\delta(r-r')}{r^2}Y_l^{m^*}(\theta',\phi')\int d\mu d\phi\delta(\phi-\phi')\delta(\mu-\mu') \\ &= -\frac{\delta(r-r')}{r^2}Y_l^{m^*}(\theta',\phi')\end{aligned}$$

Since $Y_l^{m^*}(\theta',\phi')$ is constant, we put

$$G_l(r,r') = \frac{A_{lm}(r,r',\theta',\phi')}{Y_l^{m^*}(\theta',\phi')} .$$

Then we get

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}(rG_l) + [k^2 - \frac{l(l+1)}{r^2}]G_l = -\frac{\delta(r-r')}{r^2} ,$$

The possible solutions of G_l are $j_l(kr)$, $n_l(kr)$, $h_l^{(1)}(kr)$, $h_l^{(1)}(kr)$, or a linear combination of these functions.

$$G_{lI} = Aj_l(kr), \qquad \text{for } r<r' \text{ (region I)}$$

$$G_{lII} = Bh_l^{(1)}(kr), \qquad \text{for } r>r' \text{ (region II)}$$

where A and B are constant. Note that If we use the positive sign for $G(\mathbf{r}, \mathbf{r}')$, we need to choose $h_l^{(1)}(kr)$;

$$h_\ell^{(1)}(kr) \approx -i\frac{e^{i(kr-l\pi/2)}}{kr} \approx \frac{e^{ikr}}{r}. \qquad \text{(outgoing spherical wave)}$$

(i) The continuity of G_l at $r = r'$

$$Aj_l(kr') = Bh_l^{(1)}(kr'),$$

or

$$\frac{A}{h_l^{(1)}(kr')} = \frac{B}{j_l(kr')} = C.$$

(ii) The discontinuity of dG_l/dr at $r = r'$.

$$\int_{r'-\varepsilon}^{r'+\varepsilon} \{\frac{d^2}{dr^2}(rG_l) + [k^2 r - \frac{l(l+1)}{r}]G_l\}dr = -\int_{r'-\varepsilon}^{r'+\varepsilon} \frac{\delta(r-r')}{r}dr,$$

or

$$[\frac{d}{dr}(rG_l)]_{r'-\varepsilon}^{r'+\varepsilon} = -\frac{1}{r'},$$

or

$$(G_l + r\frac{dG_l}{dr})|_{r'-\varepsilon}^{r'+\varepsilon} = -\frac{1}{r'},$$

$$\frac{dG_l^{II}(k,r,r')}{dr}|_{r'+\varepsilon} - \frac{dG_l^{I}(k,r,r')}{dr}|_{r'-\varepsilon} = -\frac{1}{r'^2},$$

or

$$kC[j_l(kr')h_l^{(1)}{}'(kr') - j_l'(kr')h_l^{(1)}(kr')] = -\frac{1}{r'^2}.$$

We need to calculate the Wronskian

$$W = \begin{vmatrix} j_l(kr') & n_l(kr') \\ j_l'(kr') & n_l'(kr') \end{vmatrix} = \frac{i}{k^2 r'^2}.$$

((Note)) We can calculate W by using Mathematica.

```
Wronskian[{SphericalBesselJ[l, x],
  SphericalHankelH1[l, x]}, x]
```

$$\frac{i}{x^2}$$

Thus we get

$$C = ik.$$

In general, we have

$$G(\mathbf{r},\mathbf{r}') = ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi').$$

This means that

$r_< = r$
$r_> = r'$ in the region I ($r<r'$)

$r_> = r$
$r_< = r'$ in the region II ($r'<r$)

We also get

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = 4\pi ik\sum_{l=0}^{\infty}\sum_{m=-l}^{l} j_l(kr_<)h_l^{(1)}(kr_>)Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi').$$

APPENDIX
Mathematica

Bessel functions

BesselJ[n,z] for $J_n(z)$
BesselI[n,z] for $I_n(z)$
BesselK[n,z] for $K_n(z)$
BesselY[n,z] for $N_n(z)$ (or $Y_n(z)$)

Hankel functions

HankelH1[n,z] for $H_n^{(1)}(z)$
HankelH2[n,z] for $H_n^{(2)}(z)$

Spherical Bessel functions

SphericalBesselJ[n,z] for $j_n(z)$
SphericalBesselI[n,z] for $i_n(z)$
SphericalBesselK[n.z] for $k_n(z)$
SphericalBesselY[n,z] for $n_n(z)$

Spherical Hankel functions

SphericalHankelH1 [n,z] for $h_n^{(1)}(z)$
SphericalKankelH2[n,z] for $h_n^{(2)}(z)$

REFERENCES

G.B. Arfken and H.J. Weber, *Mathematical Methods for Physicists*, 6-th edition (Elsevier, 2005)