Finite spherical well

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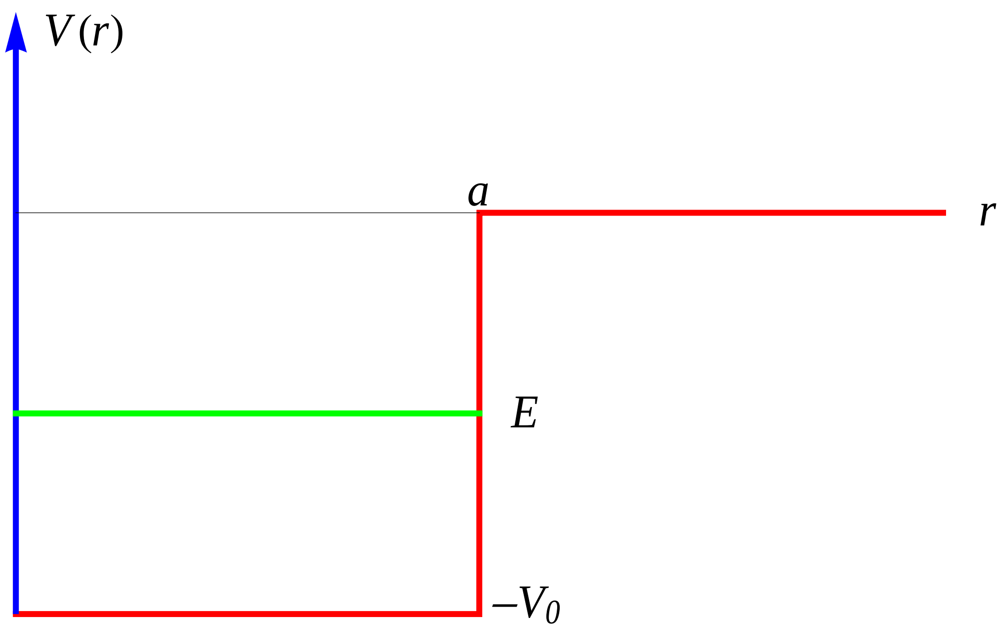
Here we discuss the bound states in a three dimensional square well potential. The potential depends only on the radial co-ordinates.

1. Schrödinger equation for the finite spherical well



The Hamiltonian for the finite spherical well is given by

$$H = \frac{p_r^{\,2}}{2\mu} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r),$$

with the radial momentum

$$p_r = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r.$$

$V(r)$ is the potential energy for the spherical well

$$V(r) = -V_0 \quad \text{for } r<a, \qquad V(r) = 0 \ \text{ for } r>a.$$

Then the Schrodinger equation can be written as

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}[r\psi(r)]+\frac{\hbar^2 l(l+1)}{2\mu r^2}\psi(r)+V(r)\psi(r)=E\psi(r)$$

where

$$E<0$$

and

$$p_r^{\ 2}\psi(r)=\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r(\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r)\psi(r)=-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}[r\psi(r)]$$

(i) For $r<a$,

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}[r\psi(r)]+\frac{\hbar^2 l(l+1)}{2\mu r^2}\psi(r)-V_0\psi(r)=E\psi(r)$$

or

$$-\frac{1}{r}\frac{\partial^2}{\partial r^2}[r\psi(r)]+\frac{l(l+1)}{r^2}\psi(r)-\frac{2\mu}{\hbar^2}(E+V_0)\psi(r)=0$$

We put

$$r\psi(r)=u(r)$$

or

$$\frac{d^2}{dr^2}u(r)-\frac{l(l+1)}{r^2}u(r)+\frac{2\mu}{\hbar^2}(E+V_0)u(r)=0 \qquad \text{(for } r<a\text{).}$$

(ii) $r>a$,

$$\frac{d^2}{dr^2}u(r)-\frac{l(l+1)}{r^2}u(r)+\frac{2\mu}{\hbar^2}Eu(r)=0 \qquad \text{(for } r>a\text{).}$$

2. *l* = 0 case

We consider the case when $l = 0$, for which there is no centrifugal barrier.

$$\frac{d^2}{dr^2}u(r)=-\frac{2\mu}{\hbar^2}(E+V_0)u(r)=-k_0^{\ 2}u(r) \qquad (r<a)$$

$$\frac{d^2}{dr^2}u(r) = -\frac{2\mu}{\hbar^2}Eu(r) = q^2u(r) \qquad (r>a)$$

where

$$E + V_0 = \frac{\hbar^2 k_0^{\ 2}}{2\mu}, \qquad E = -\frac{\hbar^2 q^2}{2\mu}.$$

This leads to the condition that

$$(k_0 a)^2 + (qa)^2 = \frac{2\mu}{\hbar^2}V_0 a^2 \tag{1}$$

The solution of $u(r)$ is obtained as

$$u(r) = A\sin(k_0 r) \qquad (r<a)$$

$$u(r) = C\exp(-qr) \qquad (r>a)$$

The continuity of $u(r)$ and $u'(r)$ at $r = a$ leads to

$$A\sin(k_0 a) = Ce^{-qa}$$

$$Ak_0\cos(k_0 a) = C(-q)e^{-qa}$$

From these two equations, we have

$$qa = -k_0 a\cot(k_0 a) \tag{2}$$

We assume that

$$qa = y, \qquad k_0 a = x$$

Then we have

$$y = -x\cot(x), \tag{3}$$

$$x^2 + y^2 = \frac{2\mu}{\hbar^2}V_0 a^2 = r_0^{\ 2} \tag{4}$$

Figure shows a plot of Eqs.(3) and (4) in the *x*-*y* plane. There are no bound states for

$$\frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{\pi}{2}\right)^2 .$$

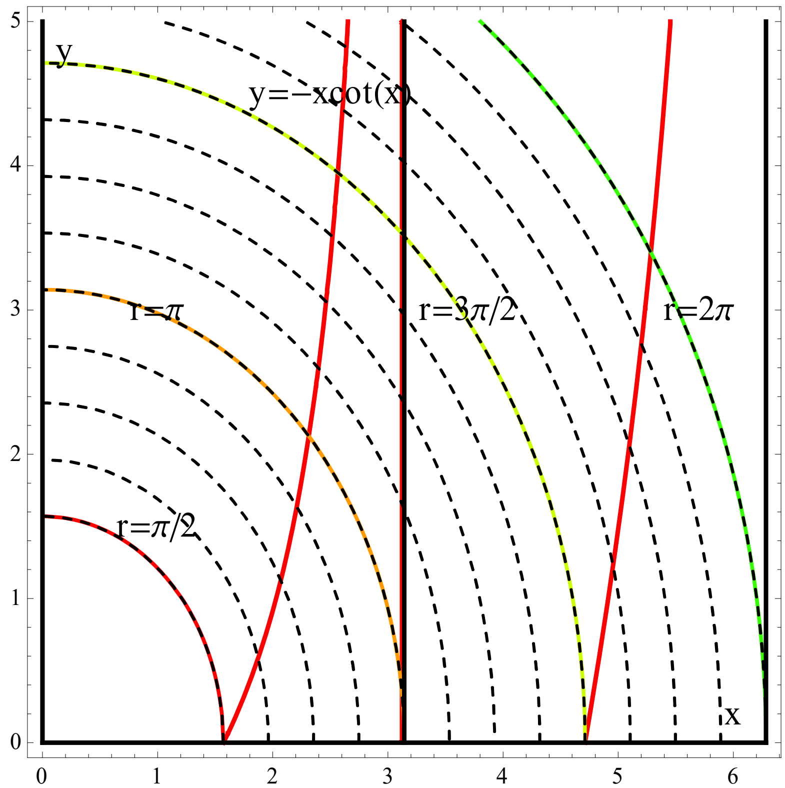


Fig. $l = 0$. A plot of $y = -x\cot(x)$ and $x^2 + y^2 = \frac{2\mu V_0 a^2}{\hbar^2} = r^2$. $x = k_0 a$. $y = qa$. The intersection of two curves leads to the solution (graphically solved). $E = -\frac{\hbar^2 q^2}{2\mu}$. The curve [$y = -x\cot(x)$] crosses the $\boldsymbol{Y}$=0 line at $X = \pi/2, 3\pi/2, 5\pi/2$.

There is no bound state for $\frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{\pi}{2}\right)^2$.

There is a single bound state for $\left(\frac{\pi}{2}\right)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{3\pi}{2}\right)^2$.

There are two bound states for $\left(\frac{3\pi}{2}\right)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{5\pi}{2}\right)^2$.

3. Solution for *r*<*a* with finite *l*

We solve the differential equation for *r*<*a*

$$\frac{d^2}{dr^2}u(r) - \frac{l(l+1)}{r^2}u(r) + \frac{2\mu}{\hbar^2}(E+V_0)u(r) = 0 \qquad \text{(for } r<a\text{)}.$$

or

$$\frac{d^2}{dr^2}u(r) + [k^2 - \frac{l(l+1)}{r^2}]u(r) = 0$$

where the wave number k is defined as

$$E + V_0 = \frac{\hbar^2}{2\mu}k^2 .$$

Now we introduce a dimensionless variable ρ,

$$\rho = kr$$

Then we have

$$[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + 1]u_{k,l}(\rho) = 0$$

The solution of this differential equation is obtained as

$$u_{k,l}(\rho) = A_1\rho j_l(\rho) + A_2\rho n_l(\rho)$$

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

$$j_l(\rho) = \sqrt{\frac{\pi}{2\rho}}J_{l+\frac{1}{2}}(\rho),$$

$$n_l(\rho) = \sqrt{\frac{\pi}{2\rho}}N_{l+\frac{1}{2}}(\rho).$$

Note that $n_l(\rho)$ becomes infinity in the limit of $\rho \to 0$. So we choose the first term

$$R_{k,l}(r) = A_l j_l(kr).$$

where $rR_{k,l}(r) = u_{k,l}(r)$ and a_l is constant.

((**Mathematica**))

```
Clear["Global`*"];
eq1 = y''[x] + (1 - L (L + 1)/x^2) y[x] == 0;
DSolve[eq1, y[x], x]
```

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

((**Note**))
We note that

$$u(\rho) \propto \sqrt{\rho} J_{l+\frac{1}{2}}(\rho) = \rho \frac{J_{l+\frac{1}{2}}(\rho)}{\sqrt{\rho}} = \sqrt{\frac{2}{\pi}} \rho j_l(\rho)$$

Thus we have

$$R(r) = \frac{u(r)}{r} \propto \frac{u(\rho)}{\rho} = j_l(\rho).$$

3. Solution for $r>a$ with finite l

We solve the differential equation for $r>a$

$$\frac{d^2}{dr^2}u(r) - \frac{l(l+1)}{r^2}u(r) + \frac{2\mu}{\hbar^2}Eu(r) = 0 \qquad \text{(for } r>a\text{).}$$

where

$$E = -\frac{\hbar^2}{2\mu}\kappa^2$$

where κ is the wavenumber.

$$\frac{d^2}{dr^2}u(r) + [(i\kappa)^2 - \frac{l(l+1)}{r^2}]u(r) = 0$$

Now we introduce a dimensionless variable ρ,

$$\rho = ikr$$

Then we get

$$\frac{d^2}{d\rho^2}u_{k,l}(\rho)+[1-\frac{l(l+1)}{\rho^2}]u_{k,l}(\rho)=0$$

The solution of this differential equation is obtained as

$$\begin{aligned} R_{k,l}(r) &= B_1' j_l(i\kappa r)+B_2' n_l(i\kappa r) \\ &= B_1 h_l^{(1)}(i\kappa r)+B_2 h_l^{(2)}(i\kappa r) \end{aligned}$$

where $h_l^{(1)}(x)$ and $h_l^{(2)}(x)$ are the spherical Hankel function of the first and second kind.

$$h_l^{(1)}(x)=\sqrt{\frac{\pi}{2x}}H_{l+\frac{1}{2}}^{(1)}(x)=j_l(x)+in_l(x)$$

$$h_l^{(2)}(x)=\sqrt{\frac{\pi}{2x}}H_{l+\frac{1}{2}}^{(2)}(x)=j_l(x)-in_l(x)$$

The asymptotic forms of $h_n^{(1)}(x)$ and $h_n^{(2)}(x)$ are given by

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

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

in the limit of large *x*. Then we get

$$h_\ell^{(1)}(i\kappa r)\approx -i\frac{e^{i(i\kappa r-l\pi/2)}}{i\kappa r}=-\frac{e^{(-\kappa r-il\pi/2)}}{\kappa r}$$

$$h_\ell^{(2)}(i\kappa r)\approx i\frac{e^{-i(i\kappa r-l\pi/2)}}{i\kappa r}=\frac{e^{(\kappa r+il\pi/2)}}{\kappa r}$$

which means that $h_\ell^{(2)}(i\kappa r)$ becomes diverging for large *r*, while $h_\ell^{(1)}(i\kappa r)$ becomes zero for large *r*. So we choose $h_\ell^{(1)}(i\kappa r)$ as the solution of $R_{k,l}(r)$ for *r*>*a*,

$$R_{k,l}(r)=B_l h_l^{(1)}(i\kappa r).$$

where B_1 is constant.

4. Bound states with finite *l*

Using the boundary condition at $r = a$, we determine the energy eigenvalues. We note that the wave function and its derivative should be continuous at $r = a$.

$$A_l j_l(ka) = B_l h_l^{(1)}(i\kappa a),$$

$$A_l k j_l'(ka) = B_l i\kappa h_l^{(1)}{}'(i\kappa a)$$

or

$$ka\frac{1}{j_l(x)}\frac{\partial j_l(x)}{\partial x}|_{x=ka} = i\kappa a\frac{1}{h_l^{(1)}(x)}\frac{\partial h_l^{(1)}(x)}{\partial x}|_{x=i\kappa a} \qquad (1)$$

where

$$\xi = ka, \qquad \eta = \kappa a$$

((Note))
The following equations for the condition of the continuity of the wave function and its derivative with respect to r at $r = a$ are equivalent.

$$(i\kappa a)\frac{1}{h_l^{(1)}(x)}\frac{\partial h_l^{(1)}(x)}{\partial x}|_{x=i\kappa a} = \frac{x}{h_l^{(1)}(x)}\frac{\partial h_l^{(1)}(x)}{\partial x}|_{x=i\kappa a}$$
$$= \frac{iy}{h_l^{(1)}(iy)}\frac{\partial h_l^{(1)}(iy)}{\partial (iy)}|_{y=\kappa a}$$
$$= \frac{y}{h_l^{(1)}(iy)}\frac{\partial h_l^{(1)}(iy)}{\partial y}|_{y=\kappa a}$$

From the conditions of

$$E = -\frac{\hbar^2}{2\mu}\kappa^2, \quad \text{and} \qquad E + V_0 = \frac{\hbar^2}{2\mu}k^2,$$

we have

$$(ka)^2 + (\kappa a)^2 = \frac{2\mu V_0}{\hbar^2}a^2 = r_0{}^2,$$

or

$$\xi^2 + \eta^2 = \frac{2\mu V_0}{\hbar^2} a^2 = r_0^{\ 2}. \qquad (2)$$

We solve the problem using the graphs. These graphs can be drawn in the (ξ, η) plane by using the Mathematica (ContourPlot), where the radius r0 is changed as a parameter.

5. A finite spherical well with *l* = 1

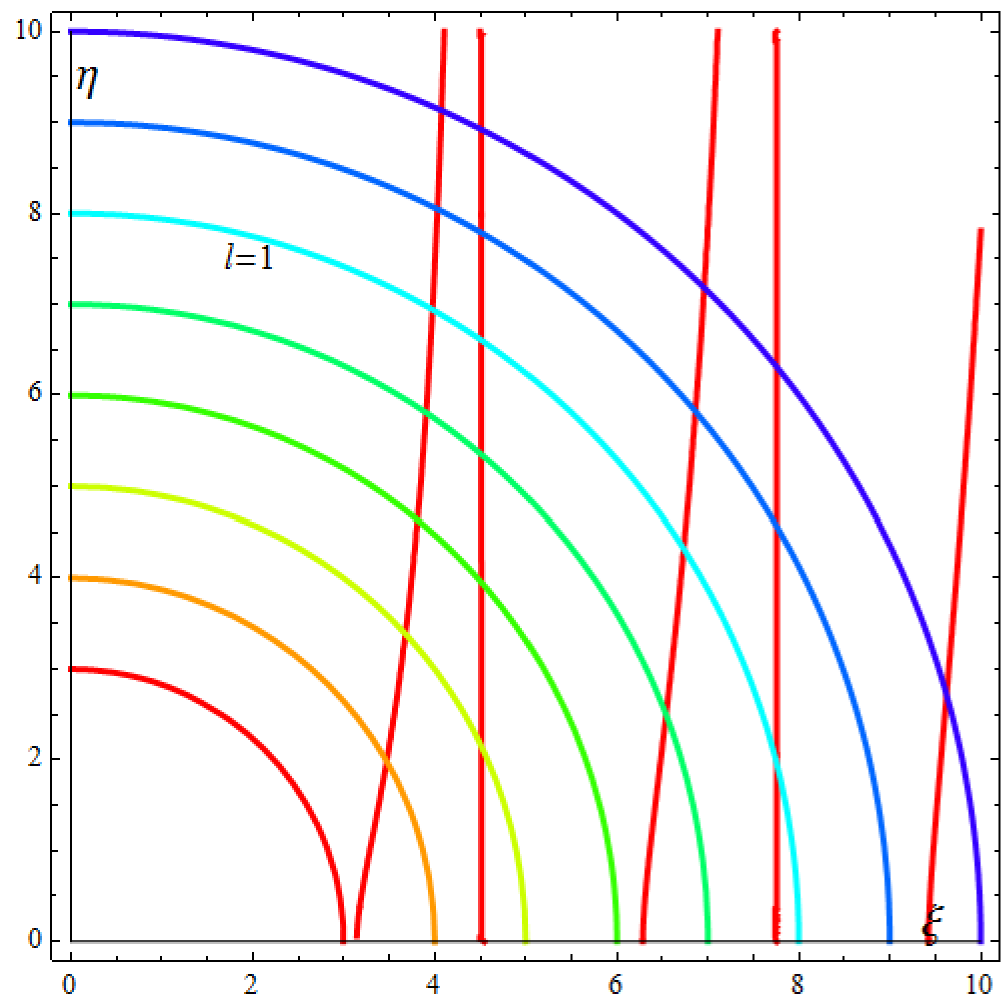


Fig. $l = 1$. Curve -1 denoted by Eq.(1), which cross the $\eta = 0$ line at $\xi = \pi$, 2π, and 3π. The curve-2 denoted by Eq.(2) (circle with radius r_0), where r_0 is changed as a parameter.

There is no bound state for $\frac{2\mu V_0 a^2}{\hbar^2} < \pi^2$

There is a single bound state for $(\pi)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < (2\pi)^2$.

There are two bound states for $(2\pi)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < (3\pi)^2$.

There are three bound states for $(3\pi)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < (4\pi)^2$.

((**Schiff**))

For l = 1, Eq.(1) can be expressed as

$$\frac{\cot\xi}{\xi} - \frac{1}{\xi^2} = \frac{1}{\eta} + \frac{1}{\eta^2}$$

or

$$\eta^2 \xi \cos\xi = [\xi^2 (1+\eta) + \eta^2] \sin\xi \qquad (1')$$

together with

$$\xi^2 + \eta^2 = \frac{2\mu V_0}{\hbar^2} a^2 = r_0^{\ 2} \qquad (2)$$

where

$$\xi = ka, \qquad \eta = \kappa a$$

These two equations can be solved graphically by using the ContourPlot of the Mathematica. See the detail the APPENDIX.

((a part of Mathematica))

```
Clear["Global`*"]; L = 1;
f1[x_] := Sin[x]/x^2 - Cos[x]/x;
f2[x_] := ⅈ (1/x + 1/x^2) Exp[-x];

eq1 = x/f1[x] D[f1[x], x] /. x → X // Simplify;
eq2 = x/f2[x] D[f2[x], x] /. x → Y // Simplify;
h1 = eq1 - eq2 // Simplify;

h1
```

$$\frac{X\,Y^2\,\mathrm{Cos}[X] - \left(Y^2 + X^2\,(1+Y)\right)\,\mathrm{Sin}[X]}{(1+Y)\,(X\,\mathrm{Cos}[X] - \mathrm{Sin}[X])}$$

6. A finite spherical well with *l* = 2

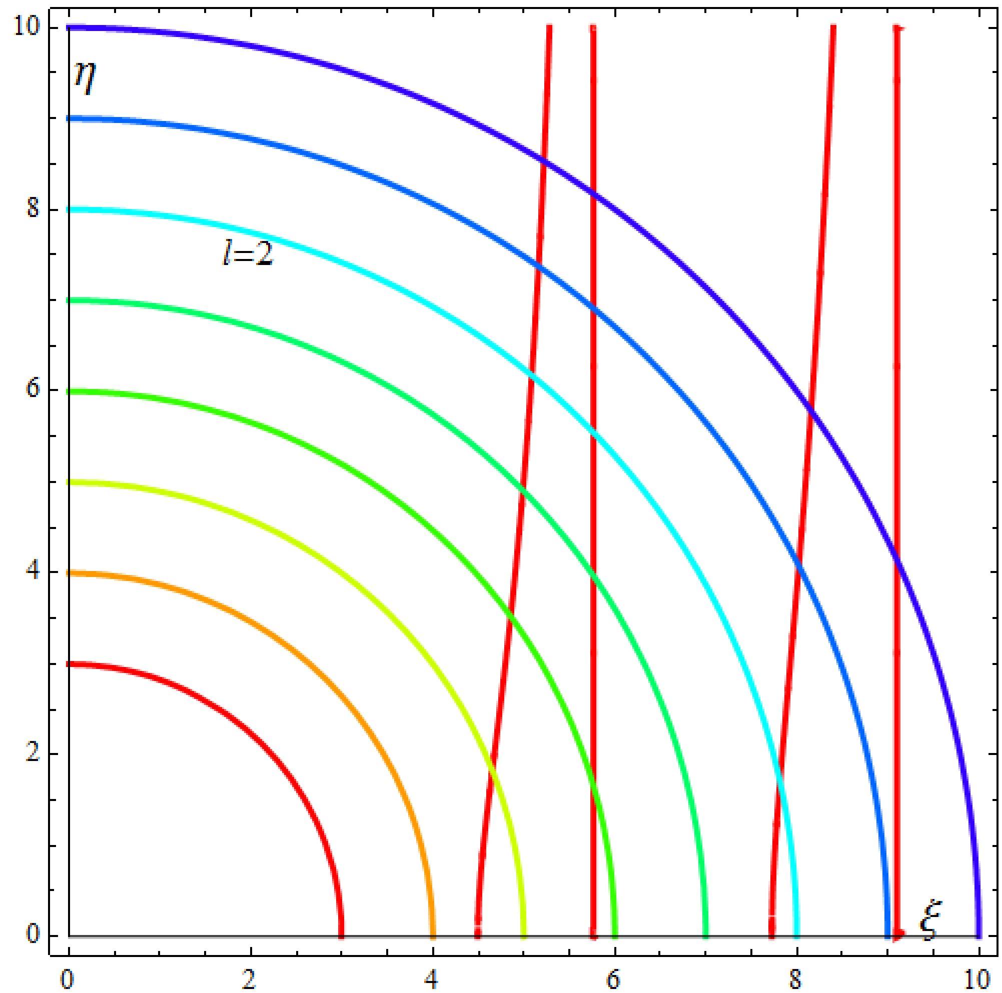


Fig. l = 2. Curve -1 denoted by Eq.(1), which cross the $\eta = 0$ line at $\xi = 3\pi/2$, $5\pi/2$, and $7\pi/2$ The curve-2 denoted by Eq.(2) (circle with radius r_0), where r_0 is changed as a parameter.

There is no bound state for $\frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{3\pi}{2}\right)^2$.

There is a single bound state for $\left(\frac{3\pi}{2}\right)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{5\pi}{2}\right)^2$.

There are two bound states for $\left(\frac{5\pi}{2}\right)^2 < \frac{2\mu V_0 a^2}{\hbar^2} < \left(\frac{7\pi}{2}\right)^2$.

7. Conclusion

The minimum value of $V_0 a^2$ for the p-wave binding (l = 1) is larger than that for the s-wave binding (l = 0), and so on.

$$\frac{2\mu V_0 a^2}{\hbar^2} \geq \left(\frac{\pi}{2}\right)^2 \qquad (l = 0)$$

$$\frac{2\mu V_0 a^2}{\hbar^2} \geq (\pi)^2 \qquad (l = 1)$$

$$\frac{2\mu V_0 a^2}{\hbar^2} \geq \left(\frac{3\pi}{2}\right)^2 \qquad (l = 2).$$

Physically, the meaning of this is as follows. In the case of $l = 2$ and $l = 1$, there exists a centrifugal barrier and, therefore, a particle requires stronger attraction for the binding.

REFERENCES

A. Das, Lectures on Quantum Mechanics, 2nd edition (World Scientific Publishing, 2012)

L.I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc, New York, 1955).

F.S. Levin, An Introduction to Quantum Theory (Cambridge University Press, 2002).

APPENDIX-I

(a) Spherical Hankel function of the first kind.

$$h_0^{(1)}(x) = -ie^{ix}\frac{1}{x},$$

$$h_1^{(1)}(x) = -e^{ix}\left(\frac{x+i}{x^2}\right),$$

$$h_2^{(1)}(x) = ie^{ix}\left(\frac{x^2+3ix-3}{x^3}\right),$$

$$h_3^{(1)}(x) = e^{ix}\left(\frac{x^3+6ix^2-15x-15i}{x^4}\right).$$

(b) Spherical Bessel function

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

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

$$j_2(x) = \frac{(3-x^2)\sin x - 3x\cos x}{x^3},$$

$$j_3(x) = \frac{3(5-2x^2)\sin x + x(-15+x^2)\cos x}{x^4}.$$

Rayleigh formula:

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

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

APPENDIX II

Finite spherical well with $l = 1$

Mathematica program

```
Clear["Global`*"]; L = 1;
f1[x_] := SphericalBesselJ[L, x];
f2[x_] := SphericalHankelH1[L, x];

eq1 = x/f1[x] D[f1[x], x] /. x → X // Simplify;
eq2 = x/f2[x] D[f2[x], x] /. x → ⅈ Y // Simplify;
h1 = eq1 - eq2;

g1 = ContourPlot[Evaluate[h1 == 0], {X, 0, 10},
    {Y, 0, 10}, ContourStyle → {Red, Thick},
    PlotPoints → 40] // Simplify;

g2 = ContourPlot[
   Evaluate[Table[X^2 + Y^2 == a^2, {a, 3, 10, 1}]],
   {X, 0, 10}, {Y, 0, 10},
   ContourStyle → Table[{Hue[0.1 i], Thick},
     {i, 0, 10}]];
```

```
g3 =
 Graphics[{Black, Thin,
   Line[{{0, 0}, {10, 0}}],
   Line[{{0, 0}, {0, 10}}],
   Text[Style["ξ", Black, 15], {9.5, 0.2}],
   Text[Style["η", Black, 15], {0.2, 9.5}],
   Text[Style["l=" <> ToString[L], Black,
     12], {2, 7.5}]}];
Show[g1, g2, g3]
```