Derivation and Solution of the Time Independent Schrödinger Equation of a Particle in an Infinite Cylindrical Potential Energy Well by James Pate Willams, Jr. © May 28-31and June 1, 2024, All Applicable Rights Reserved

We derive the time Independent Schrödinger equation of a particle in an infinite cylindrical potential energy well by first performing the transformation from Cartesian coordinates to polar cylindrical coordinates. For any set of three-dimensional orthogonal coordinates, the following equation for the Laplacian operator holds:

$$\nabla^2 = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial u_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial}{\partial u_1}\right) + \frac{\partial}{\partial u_2}\left(\frac{h_1 h_3}{h_2}\frac{\partial}{\partial u_2}\right) + \frac{\partial}{\partial u_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial}{\partial u_3}\right)\right]$$

$$h_r = \sqrt{g_{rr}}$$

The g is the metric tensor which maybe calculated by the following equation for the line element:

$$ds^2 = g_{rs} x^r x^s$$

In the Cartesian coordinate system, we have the line element:

$$ds^2 = dx^2 + dy^2 + dz^2$$

The transformation to polar cylindrical coordinates uses the following equations:

$$x = r\cos\theta$$

$$y = r\sin\theta$$

$$z' = z$$

$$dx = \cos\theta dr - r\sin\theta\, d\theta$$

$$dy = \sin\theta dr + r\cos\theta\, d\theta$$

$$dz' = dz$$

$$dx^2 = (\cos\theta)^2 dr^2 - 2r\cos\theta\sin\theta dr d\theta + r^2(\sin\theta)^2\, d\theta^2$$

$$dy^2 = (\sin\theta)^2 dr^2 + 2r\cos\theta\sin\theta dr d\theta + r^2(\cos\theta)^2\, d\theta^2$$

$$ds^2 = (\cos\theta)^2 dr^2 + (\sin\theta)^2 dr^2 + r^2(\sin\theta)^2 d\theta^2 + r^2(\cos\theta)^2\, d\theta^2 + dz^2$$
$$= dr^2 + r^2 d\theta^2 + dz^2$$

$$h_r = 1$$

$$h_\theta = r$$

$$h_z = 1$$

$$\nabla^2 = \frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\frac{1}{r}\frac{\partial}{\partial\theta}\right) + r\frac{\partial^2}{\partial z^2}\right]$$

The Schrödinger Equation is shown below:

$$-\frac{h^2}{8\pi^2 m}\nabla^2\psi = E\psi$$

We separate the variables using the functions:

$$\psi(r,\theta,z) = R(r,z)\Theta(\theta)$$

$$\frac{\Theta}{r}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \Theta\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}E + R\Theta + \frac{R}{r^2}\frac{d^2\Theta}{d\theta^2} = 0$$

$$\frac{1}{Rr}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \frac{1}{R}\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}E + \frac{1}{\Theta r^2}\frac{d^2\Theta}{d\theta^2} = 0$$

$$\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \frac{r^2}{R}\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}Er^2 + \frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} = 0$$

$$\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \frac{r^2}{R}\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}Er^2 + \frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} = -\alpha^2 - \beta^2$$

$$\frac{r}{R}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \frac{r^2}{R}\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}Er^2 + \alpha^2 = 0$$

$$\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} + \beta^2 = 0$$

$$\frac{1}{Rr}\frac{\partial}{\partial r}\left(r\frac{\partial R}{dr}\right) + \frac{1}{R}\frac{\partial^2 R}{\partial z^2} + \frac{h^2}{8\pi^2 m}E + \frac{\alpha^2}{r^2} = 0$$

$$R(r,z) = S(r)Z(z)$$

$$\frac{Z}{r}\frac{\partial}{\partial r}\left(r\frac{\partial S}{dr}\right) + S\frac{\partial^2 Z}{\partial z^2} + \frac{h^2}{8\pi^2 m}ESZ + \frac{\alpha^2}{r^2}SZ = 0$$

$$\frac{Z}{r}\frac{\partial}{\partial r}\left(r\frac{\partial S}{\partial r}\right) + S\frac{\partial^2 Z}{\partial z^2} + \frac{h^2}{8\pi^2 m}ESZ + \frac{\alpha^2}{r^2}SZ = 0$$

$$\frac{1}{Sr}\frac{d}{dr}\left(r\frac{dS}{dr}\right)+\frac{h^2}{8\pi^2 m}E+\frac{\alpha^2}{r^2}+\gamma^2=0$$

$$\frac{1}{Z}\frac{d^2Z}{dz^2}+\delta^2=0$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dS}{dr}\right)+\frac{h^2}{8\pi^2 m}ES+\frac{\alpha^2}{r^2}S+\gamma^2S=0$$

$$r\frac{d}{dr}\left(r\frac{dS}{dr}\right)+\frac{h^2}{8\pi^2 m}Er^2S+\alpha^2S+\gamma^2r^2S=0$$

$$\frac{d^2\Theta}{d\theta^2}+\beta^2=0$$

$$\frac{d^2Z}{dz^2}+\delta^2Z=0$$

$$r\frac{d}{dr}\left(r\frac{dS}{dr}\right)+\left\{\left[\frac{h^2}{8\pi^2 m}E+\gamma^2\right]r^2+\alpha^2\right\}S=0$$

$$r^2\frac{d^2S}{dr^2}+r\frac{dS}{dr}+\left\{\left[\frac{h^2}{8\pi^2 m}E+\gamma^2\right]r^2+\alpha^2\right\}S=0$$

$$\Theta(\theta)=Ae^{i\beta z}+Be^{-i\beta z}$$

$$Z(z)=Ce^{i\delta z}+De^{-i\delta z}$$

The dimensions of the infinite cylindrical potential energy well are:

$$0\le r\le R, 0\le\theta\le 2\pi, 0\le z\le H$$

The boundary values are:

$$S(0,0)=0, S(0,R)=0$$

$$\frac{dS}{dr}=0\ for\ r=0$$

$$\frac{dS}{dr}=0\ for\ r=R$$

$$Z(0)=C+D$$

$$Z(R)=Ce^{i\delta R}+De^{-i\delta R}$$

$$\frac{dZ}{dr}=i\delta(C-D), for\ r=0$$

$$\frac{dZ}{dr} = i\delta\left(Ce^{i\delta R} + De^{-i\delta R}\right), for\ r = R$$

$$\Theta(0) = A + B$$

$$\Theta(2\pi) = Ae^{2\pi i\beta} + Be^{-2\pi i\beta z}$$

$$\frac{d\Theta}{d\theta} = i\delta(A - B), for\ \theta = 0$$

$$\frac{d\Theta}{d\theta} = i\delta\left(Ce^{2\pi i\delta} + De^{-2\pi i\delta}\right), for\ \theta = 2\pi$$

We solve the *S* equation using the finite difference method:

$$k = \frac{R}{N}$$

$$r_n = nk\forall n \in \{0,1,\dots,N\}$$

$$\frac{dS}{dr} \approx \frac{S_{n+1} - S_{n-1}}{2k}$$

$$\frac{d^2S}{dr^2} = \frac{S_{n+1} - 2S_n + S_{n-1}}{k^2}$$

$$r^2\frac{d^2S}{dr^2} + r\frac{dS}{dr} + \left\{\left[\frac{h^2}{8\pi^2 m}E + \gamma^2\right]r^2 + \alpha^2\right\}S \approx r^2\frac{S_{n+1} - 2S_n + S_{n-1}}{k^2} + r\frac{S_{n+1} - S_{n-1}}{2k} + \left\{\left[\frac{h^2}{8\pi^2 m}E + \gamma^2\right]r^2 + \alpha^2\right\}S_n = 0$$

$$\alpha^2 S_0 = 0 \to \alpha = 0$$

$$\frac{dS_1}{dr} \approx 0 for\ r = 0 \to S_2 = S_1$$

$$\frac{dS}{dr} \approx 0 for\ r = R, \frac{S_n - S_{n-2}}{2k} = 0$$

$$\varepsilon = \frac{h^2}{8\pi^2 m}E + \gamma^2$$

The nonrelativistic kinetic energy = total energy is calculated by the equation:

$$E = T = \frac{m}{2}(\beta c)^2$$

$$0 < \beta < 1$$

$$R^2\frac{S_N - 2S_{N-1} + S_{N-2}}{k^2} + R\frac{S_N - S_{N-2}}{2k}\varepsilon R^2 S_{N-1} = 0$$

$$r_n^2\frac{S_{n+1} - 2S_n + S_{n-1}}{k^2} + r_n\frac{S_{n+1} - S_{n-1}}{2k} + \varepsilon r_n^2 S_n = 0$$

We arrive at the recurrence equation as follows:

$$S_{n+1} - 2S_n + S_{n-1} + \frac{k}{2r_n}(S_{n+1} - S_{n-1}) + k^2\varepsilon S_n = 0$$

$$S_{n+1} = 2S_n - \frac{k}{2r_n}(S_{n+1} - S_{n-1}) - k^2\varepsilon S_n$$

$$\left(1 + \frac{k}{2r_n}\right)S_{n+1} = 2S_n + \frac{k}{2r_n}S_{n-1} - k^2\varepsilon S_n$$

$$S_{n+1} = \frac{2S_n + \frac{k}{2r_n}S_{n-1} - k^2\varepsilon S_n}{1 + \frac{k}{2r_n}}$$

$$S_0 = S_1 = 1$$

For instance, the case *n* = 1 and *n* = N yields the recurrences:

$$S_2 = \frac{2S_1 + \frac{k}{2r_2}S_0 - k^2\varepsilon S_0}{1 + \frac{k}{2r_1}}$$

$$S_N = \frac{2S_{N-1} + \frac{k}{2r_{N-1}}S_{N-2} - k^2\varepsilon S_{N-1}}{1 + \frac{k}{2r_{N-1}}}$$

```
neutron
mass in kg  =  1.674927e-27
R in meters =  1.000000e+01
beta        =  2.500000e-01
T in Joules =  4.704218e-12
T in MeV    =  2.936138e+01
gamma       =  4.000000e+00
N           = 32
S[ 0] =  1.000000e+00
S[ 1] =  1.000000e+00
S[ 2] =  5.500000e-01    density =  2.148438e-01
S[ 3] =  3.491071e-01    density =  3.068324e-01
S[ 4] =  1.968750e-01    density =  3.076172e-01
S[ 5] =  1.100396e-01    density =  2.686513e-01
```

```
S[ 6] =  5.958329e-02    density =  2.094725e-01
S[ 7] =  3.166581e-02    density =  1.515259e-01
S[ 8] =  1.654376e-02    density =  1.033985e-01
S[ 9] =  8.523577e-03    density =  6.742282e-02
S[10] =  4.339288e-03    density =  4.237586e-02
S[11] =  2.186488e-03    density =  2.583643e-02
S[12] =  1.091897e-03    density =  1.535480e-02
S[13] =  5.409930e-04    density =  8.928498e-03
S[14] =  2.661745e-04    density =  5.094747e-03
S[15] =  1.301462e-04    density =  2.859659e-03
S[16] =  6.327945e-05    density =  1.581986e-03
S[17] =  3.061223e-05    density =  8.639585e-04
S[18] =  1.474114e-05    density =  4.664188e-04
S[19] =  7.068812e-06    density =  2.492032e-04
S[20] =  3.376716e-06    density =  1.319030e-04
S[21] =  1.607348e-06    density =  6.922270e-05
S[22] =  7.626259e-07    density =  3.604599e-05
S[23] =  3.607488e-07    density =  1.863634e-05
S[24] =  1.701704e-07    density =  9.572086e-06
S[25] =  8.006327e-08    density =  4.886674e-06
S[26] =  3.757754e-08    density =  2.480705e-06
S[27] =  1.759696e-08    density =  1.252752e-06
S[28] =  8.222860e-09    density =  6.295627e-07
S[29] =  3.834780e-09    density =  3.149463e-07
S[30] =  1.785014e-09    density =  1.568860e-07
S[31] =  8.294171e-10    density =  7.783885e-08
S[32] =  3.847491e-10    density =  3.847491e-08
```

Solution of the equation:

Using a Galerkin method function, femlagsym, found in Chapter 5 of the tome *A Numerical Library in C for Scientists and Engineers* © 1994 by H. T. Lau, PhD. We recast a previous equation in the form required by the femlagsym, namely the new equation is:

$$-\frac{d}{dr}\left(r\frac{dS}{dr}\right)-\frac{h^2}{8\pi^2 m}ErS-\frac{\alpha^2}{r}S-\gamma^2 rS=rhs$$

Simplifying using the definition of epsilon above and setting alpha in the previous equation to zero we have:

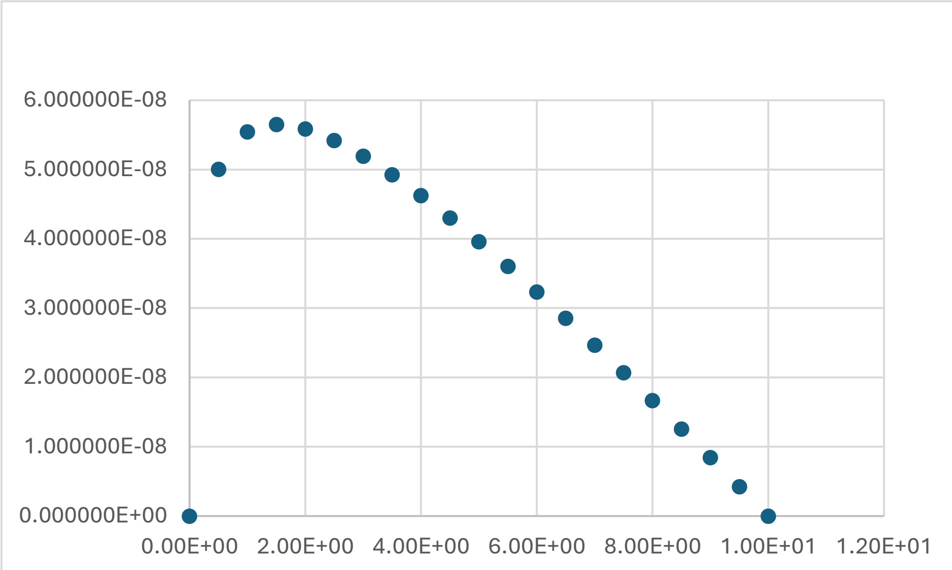
$$-\frac{d}{dr}\left(r\frac{dS}{dr}\right)-\varepsilon rS=0,0\le r\le R,S(0)=0,\frac{dS}{dr}=0\ at\ r=0,S(R)=0,\frac{dS}{dr}=0\ at\ r=R$$

Using Lau’s function we must have non-zero *S(0)* and *S(R)*. Also, the right-hand side (rhs) of the preceding equation must not vanish. Below are some runs of my program that uses Lau’s femlagsym function:

```
Enter a particle specifier (1 - 3):
2
Enter the cylinder's radius:
10
Enter the velocity as a fraction of c (0.05 - 0.60)
0.25
Enter the quantum number gamma:
0
Enter the right-hand side:
1.0e-8

Particle is a(n) neutron
Rest mass in kilograms    =  1.674927e-27
Velocity in meters/second =  7.494811e+07
Kinetic energy in Joules  =  4.704218e-12
Kinetic energy in MeV     =  2.936138e+01

       r             S(r)
 0.000000e+00    0.000000e+00
 5.000000e-01    5.003545e-08
 1.000000e+00    5.543897e-08
 1.500000e+00    5.652486e-08
 2.000000e+00    5.584287e-08
 2.500000e+00    5.419218e-08
 3.000000e+00    5.192877e-08
 3.500000e+00    4.924252e-08
 4.000000e+00    4.624678e-08
 4.500000e+00    4.301466e-08
 5.000000e+00    3.959609e-08
 5.500000e+00    3.602667e-08
 6.000000e+00    3.233268e-08
 6.500000e+00    2.853409e-08
 7.000000e+00    2.464643e-08
 7.500000e+00    2.068199e-08
 8.000000e+00    1.665069e-08
 8.500000e+00    1.256064e-08
 9.000000e+00    8.418574e-09
 9.500000e+00    4.230105e-09
 1.000000e+01    0.000000e+00
```

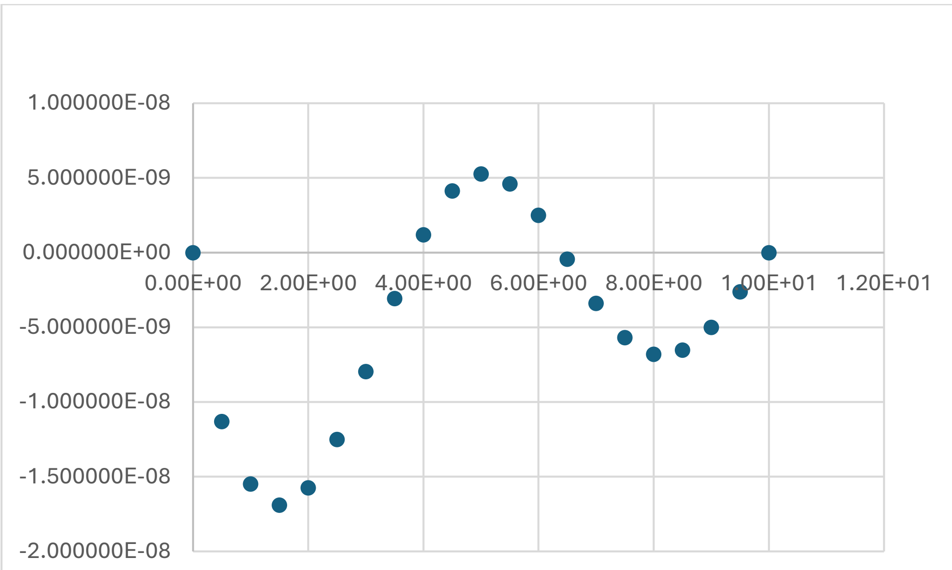



```
Enter a particle specifier (1 - 3):
2
Enter the cylinder's radius:
10
Enter the velocity as a fraction of c (0.05 - 0.60)
0.25
Enter the quantum number gamma:
1
Enter the right-hand side:
1.0e-8

Particle is a(n) neutron
Rest mass in kilograms      =  1.674927e-27
Velocity in meters/second =  7.494811e+07
Kinetic energy in Joules   =  4.704218e-12
Kinetic energy in MeV       =  2.936138e+01

       r              S(r)
 0.000000e+00     0.000000e+00
 5.000000e-01    -1.130861e-08
 1.000000e+00    -1.549232e-08
 1.500000e+00    -1.689591e-08
 2.000000e+00    -1.574405e-08
 2.500000e+00    -1.250852e-08
 3.000000e+00    -7.968882e-09
 3.500000e+00    -3.082726e-09
 4.000000e+00     1.200362e-09
 4.500000e+00     4.123892e-09
 5.000000e+00     5.265212e-09
```

```
 5.500000e+00     4.601915e-09
 6.000000e+00     2.491607e-09
 6.500000e+00    -4.278074e-10
 7.000000e+00    -3.392921e-09
 7.500000e+00    -5.688982e-09
 8.000000e+00    -6.804553e-09
 8.500000e+00    -6.533428e-09
 9.000000e+00    -5.003445e-09
 9.500000e+00    -2.628825e-09
 1.000000e+01     0.000000e+00
```



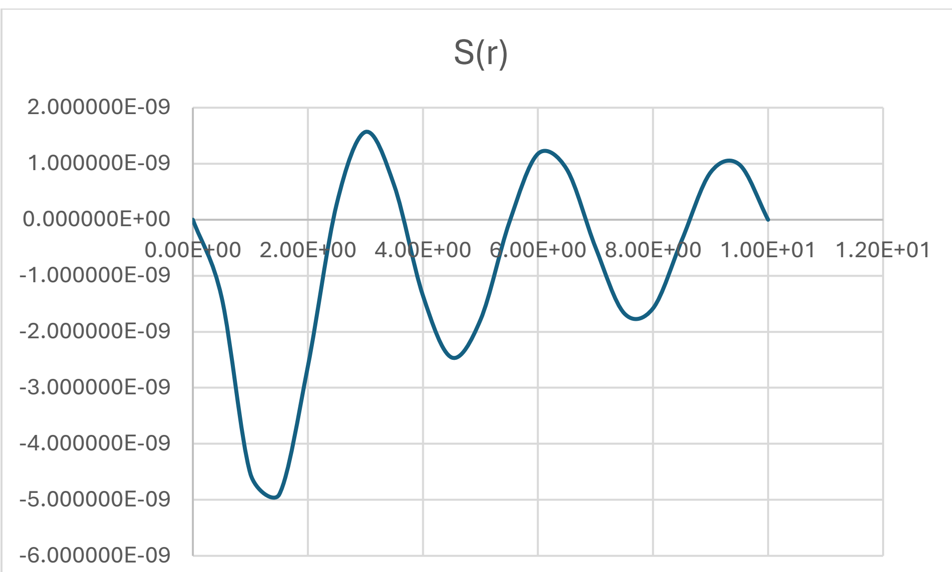

```
Enter a particle specifier (1 - 3):
2
Enter the cylinder's radius:
10
Enter the velocity as a fraction of c (0.05 - 0.60)
0.25
Enter the quantum number gamma:
2
Enter the right-hand side:
1.0e-8

Particle is a(n) neutron
Rest mass in kilograms     =  1.674927e-27
Velocity in meters/second =  7.494811e+07
Kinetic energy in Joules   =  4.704218e-12
Kinetic energy in MeV      =  2.936138e+01

       r               S(r)
 0.000000e+00     0.000000e+00
```

```
 5.000000e-01   -1.387299e-09
 1.000000e+00   -4.535852e-09
 1.500000e+00   -4.906512e-09
 2.000000e+00   -2.612249e-09
 2.500000e+00    2.796105e-10
 3.000000e+00    1.567112e-09
 3.500000e+00    6.127807e-10
 4.000000e+00   -1.355453e-09
 4.500000e+00   -2.459533e-09
 5.000000e+00   -1.787808e-09
 5.500000e+00   -5.207268e-11
 6.000000e+00    1.178082e-09
 6.500000e+00    9.011929e-10
 7.000000e+00   -4.942424e-10
 7.500000e+00   -1.671757e-09
 8.000000e+00   -1.582110e-09
 8.500000e+00   -3.657489e-10
 9.000000e+00    8.449813e-10
 9.500000e+00    9.855633e-10
 1.000000e+01    0.000000e+00
```

A graph of the immediately above data is illustrated below:

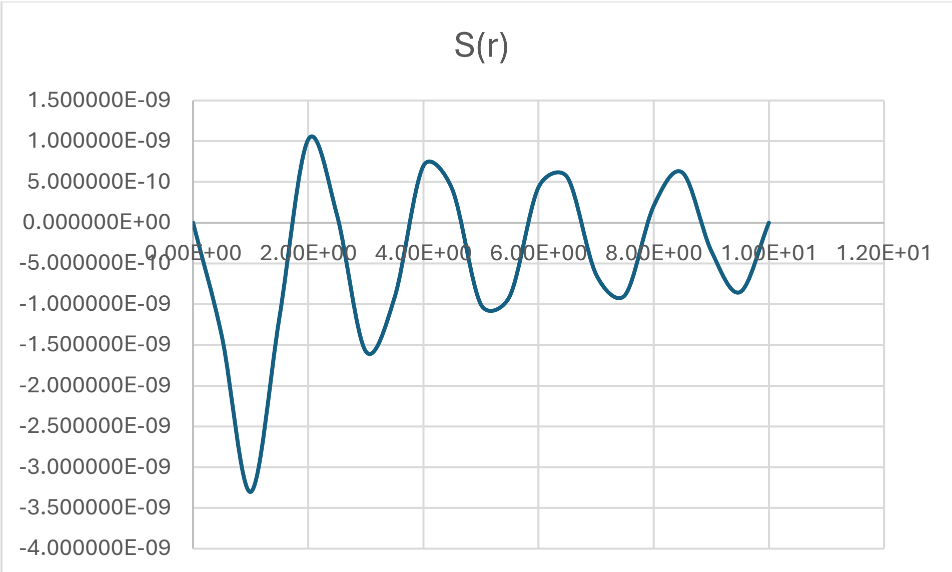



```
Enter a particle specifier (1 - 3):
2
Enter the cylinder's radius:
10
Enter the velocity as a fraction of c (0.05 - 0.60)
0.25
Enter the quantum number gamma:
```

```
3
Enter the right-hand side:
1.0e-8

Particle is a(n) neutron
Rest mass in kilograms    =  1.674927e-27
Velocity in meters/second =  7.494811e+07
Kinetic energy in Joules  =  4.704218e-12
Kinetic energy in MeV     =  2.936138e+01

      r              S(r)
 0.000000e+00    0.000000e+00
 5.000000e-01   -1.395648e-09
 1.000000e+00   -3.304094e-09
 1.500000e+00   -1.160366e-09
 2.000000e+00    1.021705e-09
 2.500000e+00    9.280386e-11
 3.000000e+00   -1.579327e-09
 3.500000e+00   -9.167849e-10
 4.000000e+00    6.972301e-10
 4.500000e+00    4.127783e-10
 5.000000e+00   -1.004782e-09
 5.500000e+00   -9.013081e-10
 6.000000e+00    4.368105e-10
 6.500000e+00    5.571964e-10
 7.000000e+00   -6.352666e-10
 7.500000e+00   -8.900980e-10
 8.000000e+00    2.063484e-10
 8.500000e+00    6.138226e-10
 9.000000e+00   -3.466826e-10
 9.500000e+00   -8.515446e-10
 1.000000e+01    0.000000e+00
```




```
Enter a particle specifier (1 - 3):
2
Enter the cylinder's radius:
10
Enter the velocity as a fraction of c (0.05 - 0.60)
0.25
Enter the quantum number gamma:
4
Enter the right-hand side:
1.0e-8

Particle is a(n) neutron
Rest mass in kilograms     =  1.674927e-27
Velocity in meters/second =  7.494811e+07
Kinetic energy in Joules   =  4.704218e-12
Kinetic energy in MeV      =  2.936138e+01

       r             S(r)
 0.000000e+00    0.000000e+00
 5.000000e-01    6.646304e-10
 1.000000e+00   -3.663503e-09
 1.500000e+00    7.350352e-10
 2.000000e+00    1.032564e-09
 2.500000e+00   -2.142161e-09
 3.000000e+00    1.459520e-10
 3.500000e+00    1.151152e-09
 4.000000e+00   -1.499519e-09
 4.500000e+00   -2.532961e-10
 5.000000e+00    1.168356e-09
 5.500000e+00   -1.037587e-09
```

```
 6.000000e+00   -5.468316e-10
 6.500000e+00    1.108798e-09
 7.000000e+00   -6.466970e-10
 7.500000e+00   -7.560878e-10
 8.000000e+00    9.863005e-10
 8.500000e+00   -3.016943e-10
 9.000000e+00   -8.881176e-10
 9.500000e+00    8.139855e-10
 1.000000e+01    0.000000e+00
```