Solution of the Time Independent Schrödinger Equation of a Particle in a Finite Rectangular Prism Potential Energy Well

For the one-dimensional case see:

[Rectangular potential barrier - Wikipedia]

Suppose the dimensions of the potential energy well are length(L), width(W), and height(H). The length of the well varies between 0 and L. The width of the well is from 0 to W. Finally, the height of the well varies between 0 and H.

The Schrödinger Equation is shown below:

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

The potential energy is *V*, *E* is the total energy, and the Laplacian operator is:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

The potential energy is given by the equations:

$$V = 0 \forall x < 0, y < 0, z < 0$$

$$V = V_0 \forall 0 \leq x \leq L, 0 \leq y \leq W, 0 \leq z \leq H$$

$$V = 0 \forall x > L, y > W, Z > H$$

Our space is divided into three regions. We call the regions left, center, and right. First, we investigate the central region with nonzero potential energy. After minor rearrangements of the equation, we have:

$$\nabla^2\psi_C - \frac{8\pi^2 m}{h^2}V\psi_C + \frac{8\pi^2 m}{h^2}E\psi_C = 0$$

The wave function is separable in Cartesian coordinates:

$$\psi_C(x,y,z) = X_C(x)Y_C(y)Z_C(z) \forall x \in [0,L], y \in [0,W], z \in [0.H]$$

Substituting the separated wave functions and division by the wave function, we obtain:

$$\frac{1}{X_C}\frac{\partial^2 X_C}{\partial x^2} + \frac{1}{Y_C}\frac{\partial^2 Y_C}{\partial y^2} + \frac{1}{Z_C}\frac{\partial^2 Z_C}{\partial z^2} - \frac{8\pi^2 m}{h^2}V_0 + \frac{8\pi^2 m}{h^2}E = 0$$

Introducing the eigenvalues:

$$\frac{1}{X_C}\frac{\partial^2 X_C}{\partial x^2} + \frac{1}{Y_C}\frac{\partial^2 Y_C}{\partial y^2} + \frac{1}{Z_C}\frac{\partial^2 Z_C}{\partial z^2} - \frac{8\pi^2 m}{h^2}V_0 + \frac{8\pi^2 m}{h^2}E = -(\alpha^2 + \beta^2 + \gamma^2)$$

$$\frac{1}{X_C}\frac{\partial^2 X_C}{\partial x^2} - \frac{8\pi^2 m}{h^2}V_0 + \frac{8\pi^2 m}{h^2}E + \alpha^2 = 0$$

$$\frac{1}{Y_C}\frac{\partial^2 Y_C}{\partial y^2} + \beta^2 = 0$$

$$\frac{1}{Z_C}\frac{\partial^2 Z_C}{\partial z^2} + \gamma^2 = 0$$

Multiplying through with the separated wave functions yields:

$$\frac{d^2 X_C}{dx^2} - \frac{8\pi^2 m}{h^2}V_0 X_c + \frac{8\pi^2 m}{h^2}E X_c + \alpha^2 X_c = 0$$

$$\frac{d^2 Y_C}{dy^2} + \beta^2 Y = 0$$

$$\frac{dZ_C}{dz^2} + \gamma^2 Z = 0$$

Rearranging the X wave function:

$$\frac{d^2 X_C}{dx^2} + \left[\frac{8\pi^2 m}{h^2}(E - V_0) + \alpha^2\right] X_C = 0$$

The wave functions are:

$$X_C(x) = A_{Cx}e^{ik_{Cx}x} + B_{Cx}e^{-ik_{Cx}x}$$

$$Y_C(y) = A_{Cy}e^{ik_{Cy}y} + B_{Cy}e^{-ik_{Cy}y}$$

$$Z_C(z) = A_{Cz}e^{ik_{Cz}z} + B_{Cz}e^{-ikC_z z}$$

Where:

$$k_{Cx} = \sqrt{\frac{8\pi^2 m}{h^2}(E - V_0) + \alpha_{Cx}{}^2}$$

The Y wave function is of a similar form to the X wavefunction but with simpler eigenvalues:

$$k_{Cy} = \beta_{Cy}$$

Likewise for the Z equation:

$$k_{Cz} = \gamma_{Cz}$$

To determine the various constants including the eigenvalues we need to solve the equation for zero potential energy namely in the left and right spatial regions.

$$X_L(x) = A_{Lx}e^{ik_{Lx}x} + B_{Lx}e^{-ik_{Lx}x} \forall x < 0$$

$$Y_L(y) = A_{Ly}e^{ik_{Ly}y} + B_{Ly}e^{-ik_{Ly}y} \forall y < 0$$

$$Z_L(z) = A_{Lz}e^{ik_{Lz}z} + B_{Lz}e^{-ik_{Lz}z} \forall z < 0$$

Using the well-known Euler's identity:

$$e^{ix} = \cos x + i \sin x$$

$$\begin{aligned} X_L(x) &= C_{Lx} \cos k_{Lx}x + i\, C_{Lx} \sin k_{Lx}x + D_{Lx} \cos k_{Lx}x - iD_{Lx} \sin k_{Lx}x \\ &= (C_{Lx} + D_{Lx}) \cos k_{Lx}x + i\, (C_{Lx} - D_{Lx}) \sin k_{Lx}x \end{aligned}$$

$$\begin{aligned} Y_L(x) &= E_{Ly} \cos k_{Ly}y + i\, E_{Ly} \sin k_{Ly}y + F_{Ly} \cos k_{Ly}y - iF_{Ly} \sin k_{Ly}y \\ &= (E_{Ly} + F_{Ly}) \cos k_{Ly}y + i\, (E_{Ly} - F_{Ly}) \sin k_{Ly}y \end{aligned}$$

$$\begin{aligned} Z_L(x) &= G_{Lz} \cos k_{Lz}z + i\, H_{Lz} \sin k_{Lz}z + G_{Lz} \cos k_{Lz}z - iH_{Lz} \sin k_{Lz}z \\ &= (G_{Lz} + H_{Lz}) \cos k_{Lz}z + i\, (G_{Lz} - H_{Lz}) \sin k_{Lz}z \end{aligned}$$

$$\frac{dX_L}{dx} = -k_{Lx}(C_{Lx} + D_{Lx}) \sin k_{Lx}x + ik_{Lx}(C_{Lx} - D_{Lx}) \cos k_{Lx}x$$

$$\frac{dY_L}{dy} = -k_{Ly}(E_{Ly} + F_{Ly}) \sin k_{Lx}y + ik_{Ly}(C_{Ly} - D_{Ly}) \cos k_{Ly}y$$

$$\frac{dX_L}{dz} = -k_{Lz}(G_{Lz} + H_{Lz}) \sin k_{Lz}z + ik_{Lz}(C_{Lz} - D_{Lz}) \cos k_{Lz}z$$

I resort to using the real and imaginary parts since I have a real number function for solving an underdetermined system of equations.

Where the wave numbers (k-values) are:

$$k_{Lx} = \sqrt{\frac{8\pi^2 m}{h^2} E + {\alpha_{Lx}}^2}$$

$$k_{Ly} = \beta_{Ly}$$

$$k_{Lz} = \gamma_{Lz}$$

$$X_C(x) = A_{Cx}e^{ik_{Cx}x} + B_{Cx}e^{-ik_{Cx}x}\forall 0 \leq \ x \leq L$$

$$Y_C(y) = A_{Cy}e^{ik_{Ry}y} + B_{Cy}e^{-ik_{Ry}y}\forall 0 \leq y \leq W$$

$$Z_C(z) = A_{Cz}e^{ik_{Cz}z} + B_{Cz}e^{-ik_{Cz}z}\forall 0 \leq z \leq H$$

$$\begin{aligned} X_C(x) &= C_{Cx}\cos k_{Cx}x + i\,C_{Cx}\sin k_{Cx}x + D_{Cx}\cos k_{Cx}x - iD_{Cx}\sin k_{Lx}x \\ &= (C_{Cx} + D_{Cx})\cos k_{Cx}x + i\,(C_{Cx} - D_{Cx})\sin k_{Cx}x \end{aligned}$$

$$\begin{aligned} Y_C(x) &= E_{Cy}\cos k_{Cy}y + i\,E_{Cy}\sin k_{Cy}y + F_{Cy}\cos k_{Cy}y - iF_{Cy}\sin k_{Cy}y \\ &= (E_{Cy} + F_{Cy})\cos k_{Cy}y + i\,(E_{Cy} - F_{Cy})\sin k_{Cy}y \end{aligned}$$

$$\begin{aligned} Z_C(x) &= G_{Cz}\cos k_{Cz}z + i\,H_{Cz}\sin k_{Cz}z + G_{Cz}\cos k_{Cz}z - iH_{Cz}\sin k_{Cz}z = \\ &= (G_{Cz} + H_{Cz})\cos k_{Cz}z + i\,(G_{Cz} - H_{Cz})\sin k_{Cz}z \end{aligned}$$

$$\frac{dX_C}{dx} = -k_{Cx}(C_{Cx} + D_{Cx})\sin k_{Cx}x + ik_{Cx}(C_{Cx} - D_{Cx})\cos k_{Cx}x$$

$$\frac{dY_C}{dy} = -k_{Cy}(E_{Cy} + F_{Cy})\sin k_{Cx}y + ik_{Cy}(E_{Cy} - F_{Cy})\cos k_{Cy}y$$

$$\frac{dZ_C}{dz} = -k_{Cz}(G_{Cz} + H_{Cz})\sin k_{Cz}z + ik_{Cz}(G_{Cz} - H_{Cz})\cos k_{Cz}z$$

$$k_{Rx} = \sqrt{\frac{8\pi^2 m}{h^2}E + \alpha_{Rx}{}^2}$$

$$k_{Ry} = \beta_{Ry}$$

$$k_{Rz} = \gamma_{Rz}$$

$$X_R(x) = A_{Rx}e^{ik_{Rx}x} + B_{Rx}e^{-ik_{Rx}x}\forall x > L$$

$$Y_R(y) = A_{Ry}e^{ik_{Ry}y} + B_{Ry}e^{-ik_{Ry}y}\forall y > W$$

$$Z_R(z) = A_{Rz}e^{ik_{Rz}z} + B_{Rz}e^{-ik_{Rz}z}\forall z > H$$

$$\begin{aligned} X_R(x) &= C_{Rx}\cos k_{Rx}x + i\,C_{Rx}\sin k_{Rx}x + D_{Rx}\cos k_{Rx}x - iD_{Rx}\sin k_{Lx}x \\ &= (C_{Rx} + D_{Rx})\cos k_{Rx}x + i\,(C_{Rx} - D_{Rx})\sin k_{Rx}x \end{aligned}$$

$$\begin{aligned} Y_R(x) &= E_{Ry}\cos k_{Ry}y + i\,E_{Ry}\sin k_{Ry}y + F_{Ry}\cos k_{Ry}y - iF_{Ry}\sin k_{Ry}y \\ &= (E_{Ry} + F_{Ry})\cos k_{Ry}y + i\,(E_{Ry} - F_{Ry})\sin k_{Ry}y \end{aligned}$$

$$\begin{aligned} Z_R(x) &= G_{Rz}\cos k_{Rz}z + i\,H_{Rz}\sin k_{Rz}z + G_{Rz}\cos k_{Rz}z - iH_{Rz}\sin k_{Rz}z = \\ &= (G_{Rz} + H_{Rz})\cos k_{Rz}z + i\,(G_{Rz} - H_{Rz})\sin k_{Rz}z \end{aligned}$$

$$\frac{dX_R}{dx} = -k_{Rx}(C_{Rx} + D_{Rx}) \sin k_{Rx}x + ik_{Rx}(C_{Rx} - D_{Rx}) \cos k_{Rx}x$$

$$\frac{dY_R}{dy} = -k_{Ry}(E_{Ry} + F_{Ry}) \sin k_{Rx}y + ik_{Ry}(E_{Ry} - F_{Ry}) \cos k_{Ry}y$$

$$\frac{dZ_R}{dz} = -k_{Rz}(G_{Rz} + H_{Rz}) \sin k_{Rz}z + ik_{Rz}(G_{Rz} - H_{Rz}) \cos k_{Rz}z$$

$$k_{Rx} = \sqrt{\frac{8\pi^2 m}{h^2}E + {\alpha_{Rx}}^2}$$

$$k_{Ry} = \beta_{Ry}$$

$$k_{Rz} = \gamma_{Rz}$$

The wave functions and their derivatives must be continuous everywhere and satisfy the boundary conditions:

$$X_L(0) = X_C(0)$$

$$Y_L(0) = Y_C(0)$$

$$Z_L(0) = Z_C(0)$$

$$\frac{dX_L}{dx} = \frac{dX_C}{dx} at\ x = 0$$

$$\frac{dY_L}{dy} = \frac{dY_C}{dy} at\ y = 0$$

$$\frac{dZ_L}{dz} = \frac{dZ_C}{dz} at\ z = 0$$

$$X_R(L) = X_C(L)$$

$$Y_R(W) = Y_C(W)$$

$$Z_R(H) = Z_C(H)$$

$$\frac{dX_R}{dx} = \frac{dX_C}{dx} at\ x = L$$

$$\frac{dY_R}{dy} = \frac{dY_C}{dy} at\ y = W$$

$$\frac{dZ_R}{dz} = \frac{dZ_C}{dz} at\ z = H$$

Now we fill in the boundary conditions:

$$C_{Lx} + D_{Lx} - C_{Cx} - D_{Cx} = 0 \; for \; x = 0$$

$$E_{Ly} + F_{Ly} - E_{Cy} - F_{Cy} = 0 \; for \; y = 0$$

$$G_{LZ} + H_{LZ} - G_{Cz} - H_{Cz} = 0 \; for \; z = 0$$

$$(C_{Rx} + D_{Rx}) \cos k_{Rx}L + i\,(C_{Rx} - D_{Rx}) \sin k_{Rx}L$$
$$= (C_{Cx} + D_{Cx}) \cos k_{Cx}L + i\,(C_{Cx} - D_{Cx}) \sin k_{Cx}L$$

$$\left(E_{Ry} + F_{Ry}\right) \cos k_{Ry}W + i\left(E_{Ry} - F_{Ry}\right) \sin k_{Ry}W =$$
$$= \left(E_{Cy} + F_{Cy}\right) \cos k_{Cy}W + i\left(E_{Cy} - F_{Cy}\right) \sin k_{Cy}W$$

$$(G_{Rz} + H_{Rz}) \cos k_{Rz}H + i\,(G_{Rz} - H_{Rz}) \sin k_{Rz}H$$
$$= (G_{Cz} + H_{Cz}) \cos k_{Cz}H + i\,(G_{Cz} - H_{Cz}) \sin k_{Cz}H$$

$$-k_{Rx}(C_{Rx} + D_{Rx}) \sin k_{Rx}L + ik_{Rx}(C_{Rx} - D_{Rx}) \cos k_{Rx}L$$
$$= -k_{Cx}(C_{Cx} + D_{Cx}) \sin k_{Cx}L + ik_{Cx}(C_{Cx} - D_{Cx}) \cos k_{Cx}L$$

$$-k_{Ry}\left(E_{Ry} + F_{Ry}\right) \sin k_{Ry}W + ik_{Ry}\left(E_{Ry} - F_{Ry}\right) \cos k_{Ry}W$$
$$= -k_{Cy}\left(C_{Cy} + D_{Cy}\right) \sin k_{Cy}W + ik_{Cy}\left(C_{Cy} - D_{Cy}\right) \cos k_{Cy}W$$

$$-k_{Rz}(G_{Rz} + H_{Rz}) \sin k_{Rz}H + ik_{Rz}(G_{Rz} - H_{Rz}) \cos k_{Rz}H = -\,k_{Cz}(G_{Cz} + H_{Cz}) \sin k_{Cz}H$$
$$+ ik_{Cz}(G_{Cz} - H_{Cz}) \cos k_{Cz}H$$

Rewriting the equations and then equating the real and imaginary components, we have two sets of equations, one set for the real parts and one set for the imaginary parts. The real part yields:

$$C_{Lx} + D_{Lx} - C_{Cx} - D_{Cx} = 0$$

$$E_{Ly} + F_{Ly} - E_{Cy} - F_{Cy} = 0$$

$$G_{LZ} + H_{LZ} - G_{Cz} - H_{Cz} = 0$$

$$(C_{Rx} + D_{Rx}) \cos k_{Rx} L - (C_{Cx} + D_{Cx}) \cos k_{Cx} L = 0$$

$$\left(E_{Ry} + F_{Ry}\right) \cos k_{Ry} W - \left(E_{Cy} + F_{Cy}\right) \cos k_{Cy} W = 0$$

$$(G_{Rz} + H_{Rz}) \cos k_{Rz} H - (G_{Cz} + H_{Cz}) \cos k_{Cz} H = 00$$

$$-k_{Rx}(C_{Rx} + D_{Rx}) \sin k_{Rx} L + k_{Cx}(C_{Cx} + D_{Cx}) \sin k_{Cx} L = 0$$

$$-k_{Ry}\left(E_{Ry} + F_{Ry}\right) \sin k_{Ry} W + k_{Cy}\left(E_{Cy} + F_{Cy}\right) \sin k_{Cy} W = 0$$

$$-k_{Rz}(G_{Rz} + H_{Rz}) \sin k_{Rz} H + k_{Cz}(G_{Cz} + H_{Cz}) \sin k_{Cz} H = 0$$

This gives us 18 unknowns in 9 equations. The set of unknown variables is:

$$C_{Lx}, D_{Lx}, E_{Ly}, F_{Ly}, G_{LZ}, H_{LZ}, C_{Cx}, D_{Cx}, E_{Cy}, F_{Cy}, G_{CZ}, H_{CZ}, C_{Rx}, D_{Rx}, E_{Ry}, F_{Ry}, G_{Rz}, H_{Rz}$$

This is an underdetermined system of linear equations. I wonder if it is possible to combine the real and imaginary parts into a single matrix would give us an 18 by 18 matrix.

We use functions from the "A Numerical Library in C for Scientists and Engineers" © H. T. Lau, PhD to compute a solution to the set of equations. I have eight Dynamic Link Libraries that implement the NUMAL C library. I use Chapter 1, Chapter 3, and the Utility DLLs. First, we give the matrix for the real parts with 18 rows and 9 columns, named M:

1	1	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0	0	0
0	0	1	1	0	0	0	0	-1	-1	0	0	0	0	0	0	0	0
0	0	0	0	1	1	0	0	0	0	-1	-1	0	0	0	0	0	0

$$M[7,4] = -\cos k_{Cx} L$$

$$M[8,4] = -\cos k_{Cx} L$$

$$M[13,4] = \cos k_{Rx} L$$

$$M[14,4] = \cos k_{Rx} L$$

$$M[9,5] = -\cos k_{Cy} W$$

$$M[10,5] = -\cos k_{Cy} W$$

$$M[15,5] = \cos k_{Ry} W$$

$$M[16][5] = \cos k_{Ry}W$$

$$M[11,6] = -k_{Cx}\cos k_{Cx}L$$

$$M[12,6\ ] = -k_{Cx}\cos k_{Cx}L$$

$$M[16,6] = k_{Rx}\cos k_{Rx}L$$

$$M[16.6] = k_{Rx}\cos k_{Rx}L$$

$$M[1,7] = k_{Cx}\sin k_{Cx}L$$

$$M[2,7] = k_{Cx}\sin k_{Cx}L$$

$$M[13,7] = -k_{Rx}\sin k_{Rx}L$$

$$M[14,7] = -k_{Rx}\sin k_{Rx}L$$

$$M[9,8] = k_{Cy}\sin k_{Cy}W$$

$$M[10,8] = k_{Cy}\sin k_{Cy}W$$

$$M[15,8] = -k_{Ry}\sin k_{Cy}W$$

$$M[16,8] = -k_{Ry}\sin k_{Ry}W$$

$$M[11,9] = k_{Cz}\sin k_{Cz}H$$

$$M[12, 9] = k_{Cz}\sin k_{Cz}H$$

$$M[17,9] = -k_{Rz}\sin k_{Cz}H$$

$$M[18,9] = -k_{Rz}\sin k_{Rz}H$$

The imaginary parts equations are illustrated below:

$$(C_{Rx} - D_{Rx})\sin k_{Rx}L - (C_{Cx} - D_{Cx})\sin k_{Cx}L = 0$$

$$\left(E_{Ry} - F_{Ry}\right)\sin k_{Ry}W - \left(E_{Cy} - F_{Cy}\right)\sin k_{Cy}W = 0$$

$$(G_{Rz} - H_{Rz})\sin k_{Rz}H - (G_{Cz} - H_{Cz})\sin k_{Cz}H = 0$$

$$k_{Rx}(C_{Rx} - D_{Rx})\cos k_{Rx}L - k_{Cx}(C_{Cx} - D_{Cx})\cos k_{Cx}L = 0$$

$$k_{Ry}\left(E_{Ry} - F_{Ry}\right)\cos k_{Ry}W - k_{Cy}\left(E_{Cy} - F_{Cy}\right)\cos k_{Cy}W = 0$$

$$k_{Rz}(G_{Rz} - H_{Rz})\cos k_{Rz}H - k_{Cz}(G_{Cz} - H_{Cz})\cos k_{Cz}H = 0$$

Again, we have 18 unknowns and 6 six equations in this case. Our matrix has 6 rows and 18 columns. The transpose is an 18 by 6 matrix.

$$M[7,1] = -\sin k_{Cx} L$$

$$M[8,1] = \sin k_{Cx} L$$

$$M[13,1] = \sin k_{Rx} L$$

$$M[14,1] = -\sin k_{Rx} L$$

$$M[9,2] = -\sin k_{Cy} W$$

$$M[10,2] = \sin k_{Cy} W$$

$$M[15,2] = \sin k_{Ry} W$$

$$M[16,2] = -\sin k_{Ry} W$$

$$M[11,3] = -\sin k_{Cz} H$$

$$M[12,3] = \sin k_{Cz} H$$

$$M[17,3] = \sin k_{Rz} H$$

$$M[18,3] = -\sin k_{Rz} H$$

$$M[7,4] = -k_{Cx} \cos k_{Cx} L$$

$$M[8,4] = k_{Cx} \cos k_{Cx} L$$

$$M[13,4] = k_{Rx} \cos k_{Rx} L$$

$$M[14.4] = -k_{Rx} \cos k_{Rx} L$$

$$M[9,5] = -k_{Cy} \cos k_{Cy} W$$

$$M[10,5] = k_{Cy} \cos k_{Cy} W$$

$$M[15,5] = k_{Ry} \cos k_{Ry} W$$

$$M[16,5] = -k_{Ry} \cos k_{Ry} W$$

$$M[11,6] = -k_{Cz} \cos k_{Cz} H$$

$$M[12,6] = k_{Cz} \cos k_{Cz} H$$

$$M[17,6] = k_{Rz} \cos k_{Rz} H$$

$$M[18,6] = -k_{Rz} \cos k_{Rz} H$$

The particle’s probability distribution is given by:

$$\iiint \psi^*(x,y,z)\psi(x,y,z)dxdydz$$

$$X_L^*(x)X_L(x) = (C_{Lx} + D_{Lx})^2(\cos k_{Lx}x)^2 + (C_{Lx} - D_{Lx})^2(\sin k_{Lx}x)^2$$

$$Y_L^*(y)Y_L(y) = \left(E_{Ly} + F_{Ly}\right)^2\left(\cos k_{Ly}y\right)^2 + \left(E_{Ly} - F_{Ly}\right)^2\left(\sin k_{Ly}y\right)^2$$

$$Z_L^*(z)Z_L(z) = (G_{Lz} + H_{Lz})^2(\cos k_{Lz}z)^2 + (G_{Lz} - H_{Lz})^2(\sin k_{Lz}z)^2$$

$$X_c^*(x)X_c(x) = (C_{Cx} + D_{Cx})^2(\cos k_{Cx}x)^2 + (C_{Cx} - D_{Cx})^2(\sin k_{Cx}x)^2$$

$$Y_c^*(y)Y_c(y) = \left(E_{Cy} + F_{Cy}\right)^2\left(\cos k_{Cy}y\right)^2 + \left(E_{Cy} - F_{Cy}\right)^2\left(\sin k_{Cy}y\right)^2$$

$$Z_C^*(z)Z_C(z) = (G_{Cz} + H_{Cz})^2(\cos k_{Cz}z)^2 + (G_{Cz} - H_{Cz})^2(\sin k_{Cz}z)^2$$

$$X_R^*(x)X_R(x) = (C_{Rx} + D_{Rx})^2(\cos k_{Rx}x)^2 + (C_{Rx} - D_{Rx})^2(\sin k_{Rx}x)^2$$

$$Y_R^*(y)Y_R(y) = \left(E_{Ry} + F_{Ry}\right)^2\left(\cos k_{Ry}y\right)^2 + \left(E_{Ry} - F_{Ry}\right)^2\left(\sin k_{Ry}y\right)^2$$

$$Z_R^*(z)Z_R(z) = (G_{Rz} + H_{Rz})^2(\cos k_{Rz}z)^2 + (G_{Rz} - H_{Rz})^2(\sin k_{Rz}z)^2$$

Input file:

```
2
25
50
75
1
1
1
1
1
1
1
1
1
0.50
0.25
```

The output file:

```
neutron
mass in kg  =  1.674927e-27
L in meters =  2.500000e+01
W in meters =  5.000000e+01
H in meters =  7.500000e+01
E in MeV    =  9.395641e+02
V in MeV    =  4.697820e+02

Number of singular values not found :   0
Norm : 2.309533e+00
```

```
Maximal neglected subdiagonal element : 2.702730e-13
Number of iterations :  13
Rank :   9

-4.754111e+03
-4.754111e+03
 7.737880e-02
 7.737868e-02
-4.754101e+03
-4.754101e+03
-4.754361e+03
-4.754361e+03
-1.726213e-01
-1.726213e-01
-4.754351e+03
-4.754351e+03
-4.754080e+03
-4.754080e+03
 9.524253e-02
 9.524253e-02
-4.753706e+03
-4.753706e+03

Number of singular values not found :  0
Norm : 1.123517e+00
Maximal neglected subdiagonal element : 0.000000e+00
Number of iterations :   2
Rank :   6

 1.090898e+00
 1.062536e+00
 1.000000e+00
 3.188956e-01
 6.961330e-01
 2.273501e-01
-1.717595e-01
 1.717595e-01
-2.043760e-01
 2.043760e-01
-2.095603e-01
 2.095603e-01
 1.718111e-01
-1.718111e-01
-1.406285e-01
-2.043760e-01
 2.095603e-01
-2.095603e-01
```

```
Probability lt outside  =  5.000000e-01
Probability inside      =  4.540083e-08
Probability rt outside  =  5.000000e-01
```