Blog Entry © Saturday, November 30, 2024, by James Pate Williams, Jr. Partial Solution of the Schrödinger Equation for Hydrogen in Parabolic Coordinates

References:

Parabolic coordinates - Wikipedia

Orthogonal coordinates - Wikipedia

In my blog entry yesterday, Friday, November 29, 2024, I computed the Christoffel symbols of the second kind in parabolic coordinates. We can use the metric tensor, g, to compute the scale factors, h:

$$h_\sigma = \sqrt{g_{\sigma\sigma}} = \sqrt{\sigma^2 + \tau^2} = h_\tau, h_\varphi = \sigma\tau$$

The parabolic coordinates are:

$$x = \sigma\tau\cos\varphi$$

$$y = \sigma\tau\sin\varphi$$

$$z = \frac{1}{2}(\tau^2 - \sigma^2)$$

$$r = \sqrt{x^2 + y^2 + z^2} = \sqrt{\sigma^2\tau^2 + \frac{1}{4}(\tau^4 - 2\sigma^2\tau^2 + \sigma^4)} = \sqrt{\frac{4\sigma^2\tau^2}{4} + \frac{1}{4}(\tau^4 - 2\sigma^2\tau^2 + \sigma^4)}$$
$$= \frac{1}{2}\sqrt{\tau^4 + 2\sigma^2\tau^2 + \sigma^4} = \frac{1}{2}\sqrt{(\sigma^2 + \tau^2)^2} = \frac{\sigma^2 + \tau^2}{2}$$

The Laplacian operator is:

$$\nabla^2 = \frac{1}{h_\sigma h_\tau h_\varphi}\left[\frac{\partial}{\partial\sigma}\left(\frac{h_\tau h_\varphi}{h_\sigma}\frac{\partial}{\partial\sigma}\right) + \frac{\partial}{\partial\tau}\left(\frac{h_\sigma h_\varphi}{h_\tau}\frac{\partial}{\partial\tau}\right) + \frac{\partial}{\partial\varphi}\left(\frac{h_\sigma h_\tau}{h_\varphi}\frac{\partial}{\partial\varphi}\right)\right]$$
$$= \frac{1}{(\sigma^2 + \tau^2)\sigma\tau}\left[\frac{\partial}{\partial\sigma}\left(\sigma\tau\frac{\partial}{\partial\sigma}\right) + \frac{\partial}{\partial\tau}\left(\sigma\tau\frac{\partial}{\partial\tau}\right) + \frac{\partial}{\partial\varphi}\left(\frac{\sigma^2 + \tau^2}{\sigma\tau}\frac{\partial}{\partial\varphi}\right)\right]$$
$$= \frac{1}{\sigma^2 + \tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial}{\partial\sigma}\right) + \frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial}{\partial\tau}\right)\right] + \frac{1}{\sigma^2\tau^2}\frac{\partial^2}{\partial\varphi^2}$$

The Schrödinger equation in parabolic coordinates is:

$$-\frac{h^2}{8\pi^2\mu}\frac{1}{\sigma^2 + \tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\psi}{\partial\sigma}\right) + \frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\psi}{\partial\tau}\right)\right] + \frac{1}{\sigma^2\tau^2}\frac{\partial^2\psi}{\partial\varphi^2} - \frac{2Ze^2\psi}{\sigma^2 + \tau^2} = E\psi$$

After a multiplication and using atomic units:

$$-\frac{1}{2}\frac{\sigma^2\tau^2}{\sigma^2+\tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\psi}{\partial\tau}\right)\right]-\frac{2Z\sigma^2\tau^2\psi}{\sigma^2+\tau^2}+\frac{\partial^2\psi}{\partial\varphi^2}-\sigma^2\tau^2E\psi=0$$

Now Suppose the wavefunction is as follows:

$$\psi(\sigma,\tau,\varphi)=\Psi(\sigma,\tau)\Phi(\varphi)$$

$$-\frac{1}{2}\frac{\sigma^2\tau^2}{\sigma^2+\tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\Psi}{\partial\tau}\right)\right]-\frac{2Z\sigma^2\tau^2\Psi}{\sigma^2+\tau^2}-\sigma^2\tau^2E\Psi=-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=m^2$$

$$\frac{d^2\Phi}{d\varphi^2}+m^2\Phi=0$$

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}e^{im\varphi}\forall m=0,\pm1,\pm2,\ldots$$

$$-\frac{1}{2}\frac{\sigma^2\tau^2}{\sigma^2+\tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\Psi}{\partial\tau}\right)\right]-\frac{2Z\sigma^2\tau^2\Psi}{\sigma^2+\tau^2}-\sigma^2\tau^2E\Psi-m^2=0$$

$$\frac{\sigma^2\tau^2}{\sigma^2+\tau^2}\left[\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\Psi}{\partial\tau}\right)\right]+\frac{4Z\sigma^2\tau^2\Psi}{\sigma^2+\tau^2}+2\sigma^2\tau^2E\Psi+2m^2=0$$

$$\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\Psi}{\partial\tau}\right)+4Z\Psi+2(\sigma^2+\tau^2)\mathrm{E}\Psi+\frac{2m^2(\sigma^2+\tau^2)}{\sigma^2\tau^2}=0$$

Let m = 0:

$$\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Psi}{\partial\sigma}\right)+\frac{1}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\Psi}{\partial\tau}\right)+4Z\Psi+2(\sigma^2+\tau^2)\mathrm{E}\Psi=0$$

Now suppose:

$$\Psi(\sigma,\tau)=\Xi(\sigma)\mathrm{T}(\tau)$$

$$\frac{T}{\sigma}\frac{\partial}{\partial\sigma}\left(\sigma\frac{\partial\Xi}{\partial\sigma}\right)+\frac{\Xi}{\tau}\frac{\partial}{\partial\tau}\left(\tau\frac{\partial\mathrm{T}}{\partial\tau}\right)+4Z\Xi T+2\sigma^2E\Xi\mathrm{T}+2\tau^2E\Xi\mathrm{T}=0$$

$$\frac{1}{\sigma\Xi}\frac{d}{d\sigma}\left(\sigma\frac{d\Xi}{d\sigma}\right)+4Z+2\sigma^2E=-n^2$$

$$\frac{1}{\tau\mathrm{T}}\frac{d}{d\tau}\left(\tau\frac{d\mathrm{T}}{d\tau}\right)+2\tau^2E=-n^2$$

$$\frac{1}{\sigma}\frac{d}{d\sigma}\left(\sigma\frac{d\Xi}{d\sigma}\right)+4Z\Xi+2\sigma^2E\Xi+n^2\Xi=0$$

$$\frac{1}{\tau}\frac{d}{d\tau}\left(\tau\frac{d\mathrm{T}}{d\tau}\right)+2\tau^2E\mathrm{T}+n^2\mathrm{T}=0$$

$$\frac{d}{d\sigma}\left(\sigma\frac{d\Xi}{d\sigma}\right)+4Z\sigma\Xi+2\sigma^3E\Xi+n^2\sigma\Xi=0$$

$$\frac{d}{d\tau}\left(\tau\frac{d\mathrm{T}}{d\tau}\right)+2\tau^3E\mathrm{T}+n^2\tau\mathrm{T}=0$$

Now we setup the equations for solution using the femlagsym function found in ***A Numerical Library in C for Scientists and Engineers*** © 1995 by H. T. Lau, PhD. The function uses Galerkin's Method.

$$-\frac{d}{d\sigma}\left(\sigma\frac{d\Xi}{d\sigma}\right)-4Z\sigma\Xi-2\sigma^3E\Xi-n^2\sigma\Xi=0$$

The functions in my C/C++ implementation of the previous equation for Lau's function femlagsym are:

$$p(\sigma)=\ \sigma,r(\sigma)=-4Z\sigma-2\sigma^3E-n^2\sigma,f(\sigma)=0=0$$

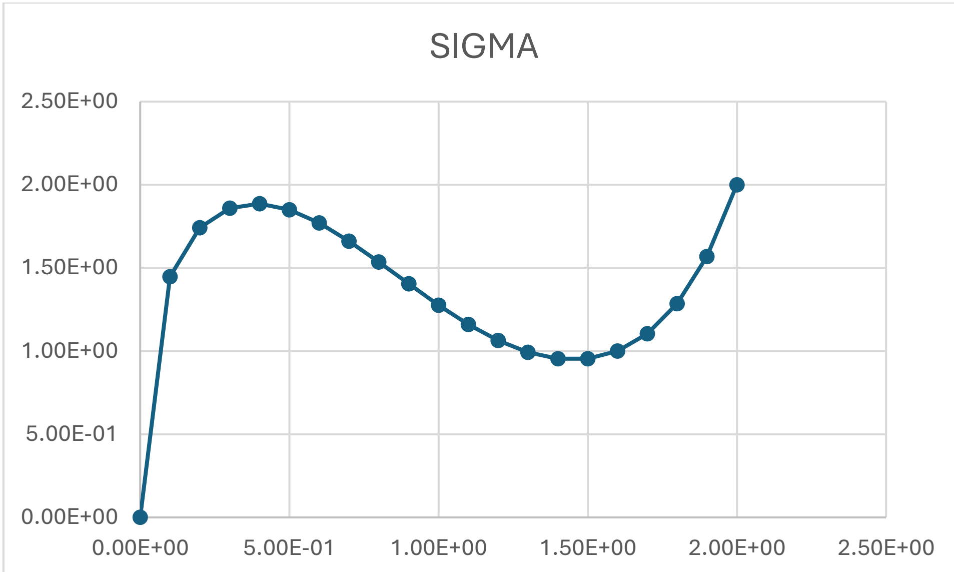
$$-\frac{d}{d\tau}\left(\tau\frac{d\mathrm{T}}{d\tau}\right)-2\tau^3E\mathrm{T}-n^2\tau\mathrm{T}=0$$

$$p(\tau)=\tau,r(\tau)=-2\tau^3E-n^2\tau,f(\tau)=0$$

Let E = -2, Z = 1, a = 0, b = 2, and n = 0:

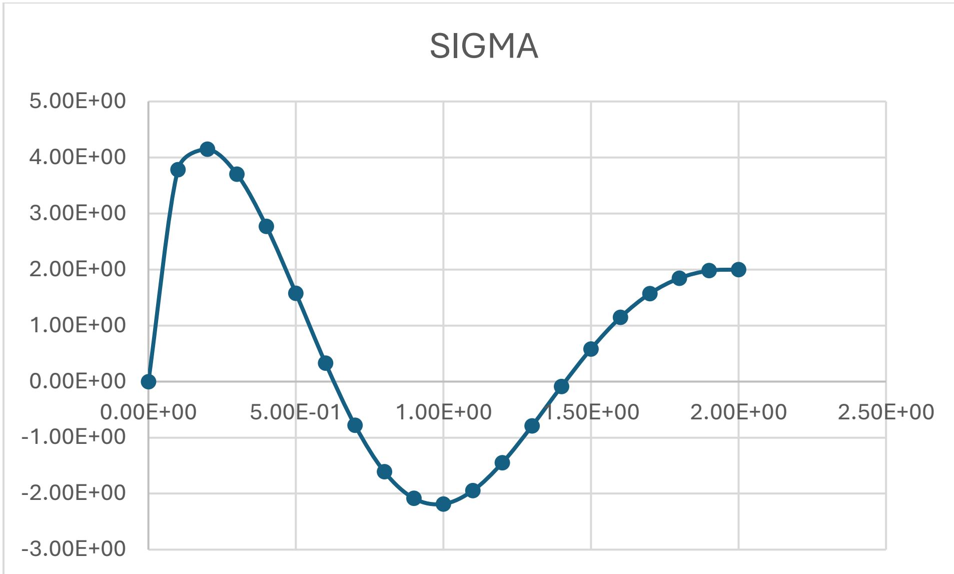
sigma	SIGMA
0.00E+00	0.00E+00
1.00E-01	1.45E+00
2.00E-01	1.74E+00
3.00E-01	1.86E+00
4.00E-01	1.89E+00
5.00E-01	1.85E+00
6.00E-01	1.77E+00
7.00E-01	1.66E+00
8.00E-01	1.54E+00
9.00E-01	1.40E+00
1.00E+00	1.28E+00
1.10E+00	1.16E+00
1.20E+00	1.06E+00
1.30E+00	9.93E-01
1.40E+00	9.54E-01
1.50E+00	9.54E-01
1.60E+00	1.00E+00
1.70E+00	1.10E+00
1.80E+00	1.28E+00
1.90E+00	1.57E+00

2.00E+00	2.00E+00



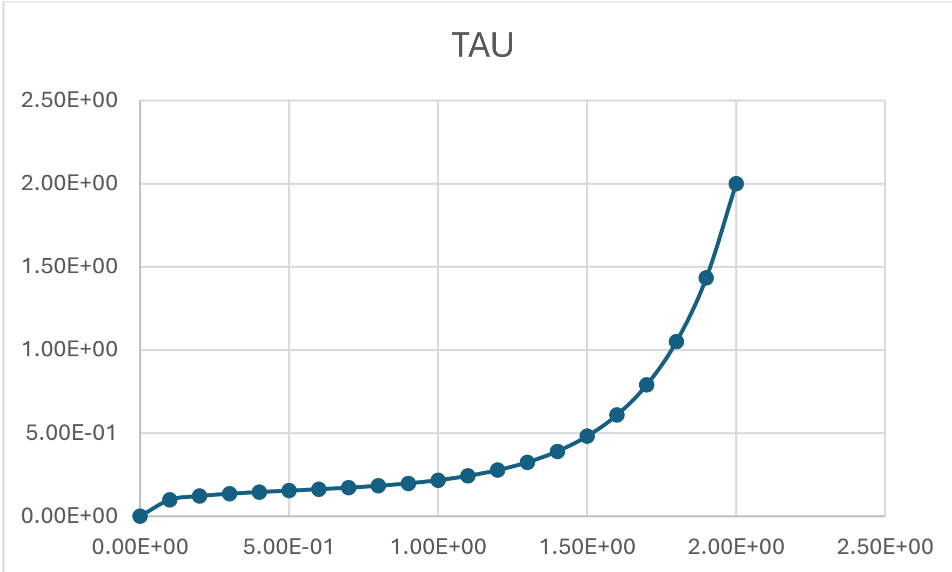
Now suppose E = -2, Z = 1, a = 0, b = 2, and n = 4.

sigma	SIGMA
0.00E+00	0.00E+00
1.00E-01	3.78E+00
2.00E-01	4.15E+00
3.00E-01	3.70E+00
4.00E-01	2.77E+00
5.00E-01	1.58E+00
6.00E-01	3.32E-01
7.00E-01	-7.77E-01
8.00E-01	-1.61E+00
9.00E-01	-2.09E+00
1.00E+00	-2.18E+00
1.10E+00	-1.94E+00
1.20E+00	-1.45E+00
1.30E+00	-7.93E-01
1.40E+00	-8.67E-02
1.50E+00	5.82E-01
1.60E+00	1.15E+00
1.70E+00	1.57E+00
1.80E+00	1.85E+00
1.90E+00	1.98E+00
2.00E+00	2.00E+00



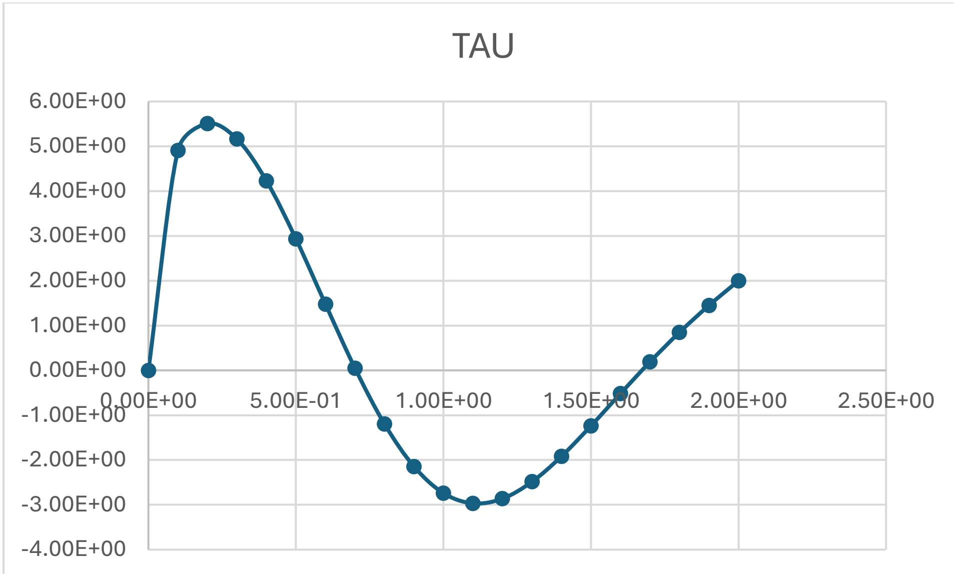
Let E = -2, Z = 1, a = 0, b = 2, and n = 0:

Tau	TAU
0.00E+00	0.00E+00
1.00E-01	9.91E-02
2.00E-01	1.22E-01
3.00E-01	1.36E-01
4.00E-01	1.46E-01
5.00E-01	1.54E-01
6.00E-01	1.63E-01
7.00E-01	1.72E-01
8.00E-01	1.84E-01
9.00E-01	1.98E-01
1.00E+00	2.17E-01
1.10E+00	2.43E-01
1.20E+00	2.78E-01
1.30E+00	3.25E-01
1.40E+00	3.90E-01
1.50E+00	4.81E-01
1.60E+00	6.09E-01
1.70E+00	7.90E-01
1.80E+00	1.05E+00
1.90E+00	1.43E+00
2.00E+00	2.00E+00



Now suppose E = -2, Z = 1, a = 0, b = 2, and n = 4.

Tau	TAU
0.00E+00	0.00E+00
1.00E-01	4.91E+00
2.00E-01	5.51E+00
3.00E-01	5.16E+00
4.00E-01	4.23E+00
5.00E-01	2.93E+00
6.00E-01	1.48E+00
7.00E-01	5.05E-02
8.00E-01	-1.19E+00
9.00E-01	-2.14E+00
1.00E+00	-2.74E+00
1.10E+00	-2.97E+00
1.20E+00	-2.86E+00
1.30E+00	-2.49E+00
1.40E+00	-1.92E+00
1.50E+00	-1.24E+00
1.60E+00	-5.17E-01
1.70E+00	1.90E-01
1.80E+00	8.50E-01
1.90E+00	1.45E+00
2.00E+00	2.00E+00


TAU
6.00E+00
5.00E+00
4.00E+00
3.00E+00
2.00E+00
1.00E+00
0.00E+00
-1.00E+00
-2.00E+00
-3.00E+00
-4.00E+00
0.00E+00
5.00E-01
1.00E+00
1.50E+00
2.00E+00
2.50E+00