

1 Calculating τ from ETE

1.1 Calculating zeroes of Bessel functions of the first kind

1.1.1 Initial thoughts

Values of Bessel functions of the first kind are kindly provided by the Go's mathematics package. Because Bessel functions' derivatives can be defined by

$$\frac{d}{dx}J_n(x) = J_{n-1}(x) - \frac{n}{x}J_n(x)$$

or by

$$\frac{d}{dx}J_n(x) = \frac{1}{2}(J_{n-1}(x) - J_{n+1}(x))$$

(which might be better because we don't perform needless division by floating-point numbers), we can use approximation techniques for finding zeroes that use derivatives. I'm thinking mainly about Newton's or Halley's methods.

Recursive sequence in Newton's method is defined in our case by

$$x_{n+1} = x_n - \frac{J_v(x_n)}{J'_v(x_n)} = x_n - \frac{J_v(x_n)}{J_{v-1}(x) - \frac{v}{x_n}J_v(x)} = x_n - \frac{2J_v(x)}{J_{v-1}(x) + J_{v+1}(x)}$$

The last equation might be actually worse than I initially thought because we would need to calculate Bessel function 3 times compared to 2 times in the second to last equation.

Halley's method can be defined by

$$x_{n+1} = x_n - \frac{2J_v(x_n)J'_v(x_n)}{2(J'_v(x_n))^2 - J_v(x_n)J''_v(x_n)}$$

which looks not as easy by I will check how fast it converges compared to Newton's method. Optimal function that calculates derivatives might be easily constructed.

1.1.2 Code and comparisons

2 A study of the extended Tao-Eldrup model's parameters

We are given following equations from [1]:

$$P_{nm} = \frac{\int_{\frac{R}{R+\Delta}}^{Z_{nm}} J_m(r)^2 r dr}{\int_0^{Z_{nm}} J_m(r)^2 r dr} \quad (1)$$

$$\lambda_{nm} = \lambda_p P_{nm} + \lambda_i (1 - P_{nm}) \quad (2)$$

$$\tau = \frac{\sum_n \sum_m g_m \exp\left(-\frac{E_{nm}}{kT}\right)}{\sum_n \sum_m g_m \lambda_{nm} \exp\left(-\frac{E_{nm}}{kT}\right)} \quad (3)$$

$$E_{nm} = \frac{\hbar^2}{4m_e} \frac{Z_{nm}^2}{(R + \Delta)^2}$$

where Z_{nm} is the n -th node of the Bessel function of the first kind $J_m(r)$ and g_m is the statistical weight of the m -th state ($g_0 = 1$, $g_{m>0} = 2$).

References

- [1] R. Zaleski. Principles of positron porosimetry. *Nukleonika*, 60(4):795–800, 2015.
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