1 Extended Tao-Eldrup model

We are given following equations from [2]:

$$P_{nm} = \frac{\int\limits_{Z_{nm}\frac{R}{R+\Delta}}^{Z_{nm}} J_m(r)^2 r dr}{\int\limits_0^{Z_{nm}} J_m(r)^2 r dr} \tag{1}$$

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

$$\tau = \frac{\sum\limits_n \sum\limits_m g_m \exp\left(-\frac{E_{nm}}{kT}\right)}{\sum\limits_n \sum\limits_m g_m \lambda_{nm} \exp\left(-\frac{E_{nm}}{kT}\right)} \tag{3}$$

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

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 ($g_0 = 1$, $g_{m>0} = 2$).

2 Calculating τ from ETE

2.1 Calculating zeroes of Bessel functions of the first kind

2.1.1 Approxmiating

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

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

we can use approximation techniques for finding zeroes that use derivatives. I'm thinking mainly about Newton's or Halley's methodes.

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 innitialy 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.

2.1.2 Initial guess

This wasn't easy because you can't use finite equation for it because it decreses precision with bigger values.

For zeros of $J_0(x)$ I used approximation given by McMahon's asymptotic expansion [1, equation 10.21.19]

$$j_{\nu,m} \sim a - \frac{\mu - 1}{8a} - \frac{4(\mu-1)(7\mu-31)}{3(8a)^3} - \frac{32(\mu-1)(83\mu^2 - 982\mu + 3779)}{15(8a)^5} - \dots \tag{4}$$

where $j_{\nu,m}$ is the m-th zero of the Bessel function $J_\nu(x)$, $\mu = 4\nu^2$ and $a = (m + \frac{1}{2}\nu - \frac{1}{4})\pi$.

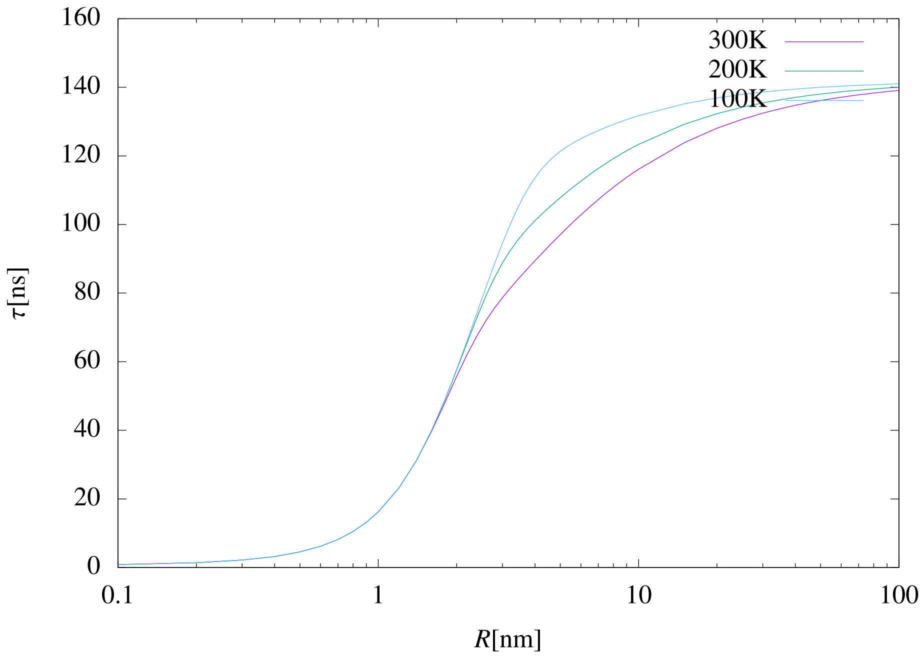
For zeros $j_{\nu,m}$ where $\nu > 0$ I just put it in bounds $j_{\nu-1,m-1} < j_{\nu,m} < j_{\nu-1,m+1}$ [1, equation 10.21.2] and approximated using Newton's formula until I got what I wanted. I check values for big ν and m and got correct anserw so it is assumed that my code is working.

2.2 Numerical integration

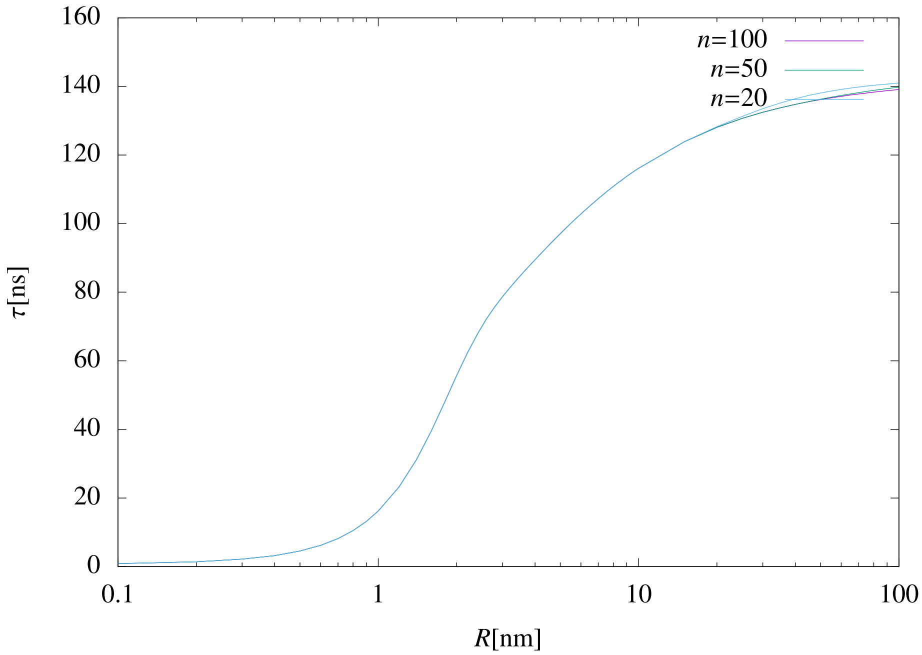
Next mission is to calculate 1 by using numerical integration algorithms. Use of simple midpoint rule is inefficient so there's need to use Gauss' quadrature. I arbitrarily chose 10 points given in [1, table 3.5.2]

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

3.1 Temperature



3.2 Resolution

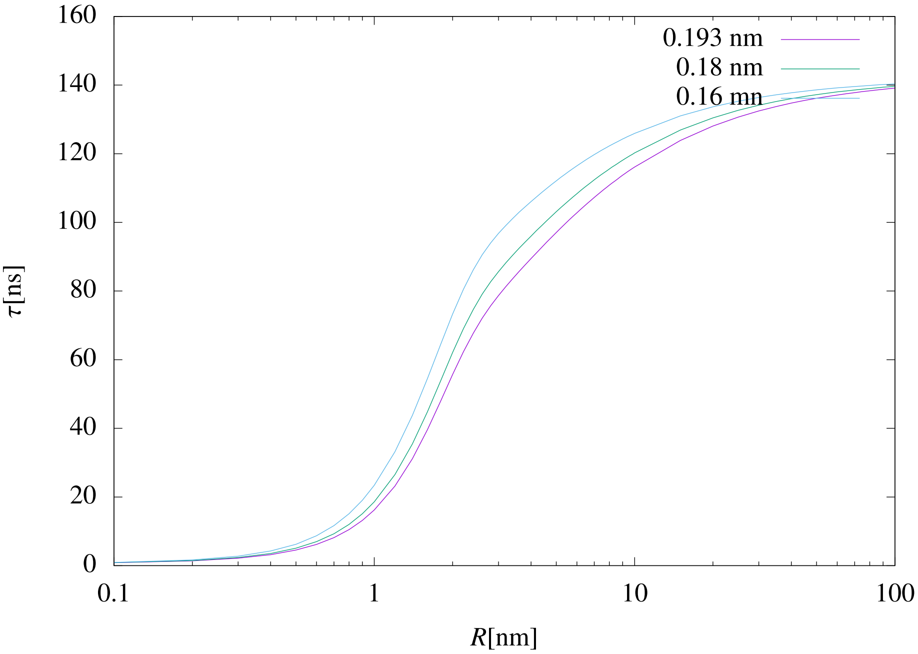


3.3 Δ

References

[1] *NIST Digital Library of Mathematical Functions*. http://dlmf.nist.gov/, Release 1.1.3 of 2021-09-15. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller, B. V. Saunders, H. S. Cohl, and M. A. McClain, eds. URL: `http://dlmf.nist.gov/`.

[2] R. Zaleski. Principles of positron porosimetry. *Nukleonika*, 60(4):795–800, 2015. `doi:10.1515/nuka-2015-0143`.



0.193 nm
0.18 nm
0.16 mn
τ[ns]
R[nm]
160
140
120
100
80
60
40
20
0
0.1
1
10
100