

# 1 Extended Tao-Eldrup model

We are given following equations from [2]:

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

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

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

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

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

## 2 Calculating $\tau$ from ETE

### 2.1 Calculating zeros of Bessel functions of the first kind

#### 2.1.1 Approximating

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 decreases precision with bigger values.

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

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

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

For zeros  $j_{v,m}$  where  $v > 0$  I just put it in bounds  $j_{v-1,m-1} < j_{v,m} < j_{v-1,m+1}$  [1, equation 10.21.2] and approximated using Newton's formula until I got what I wanted. I check values for big  $v$  and  $m$  and got correct answer 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

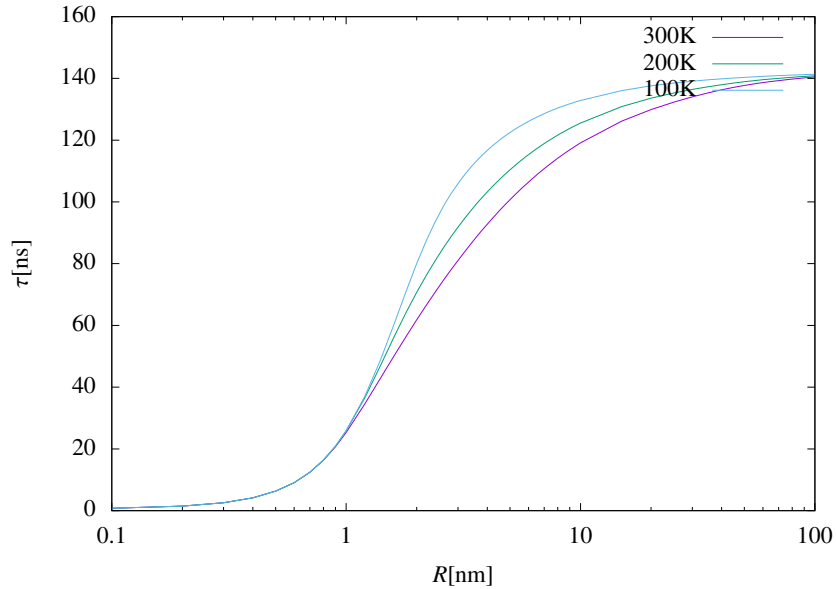


Figure 1: Temperature

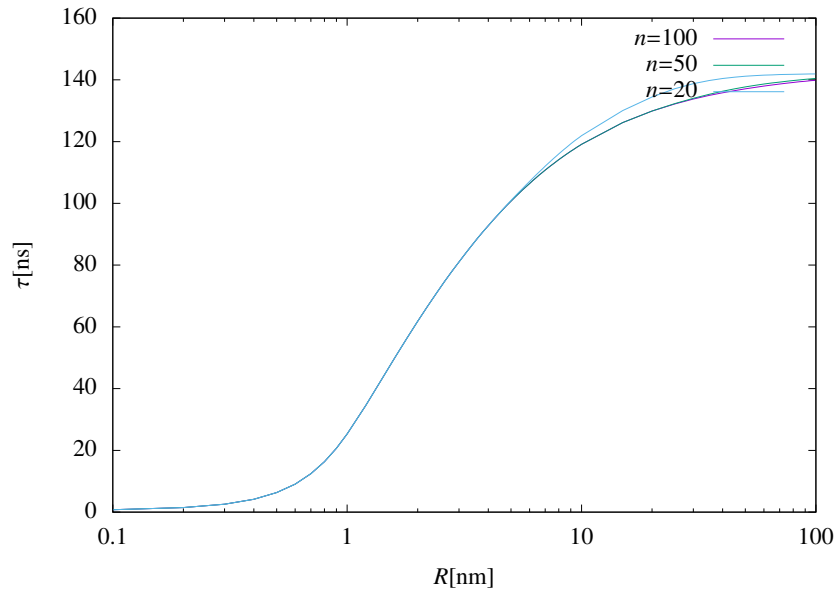


Figure 2: Number of  $n = m$  to sum

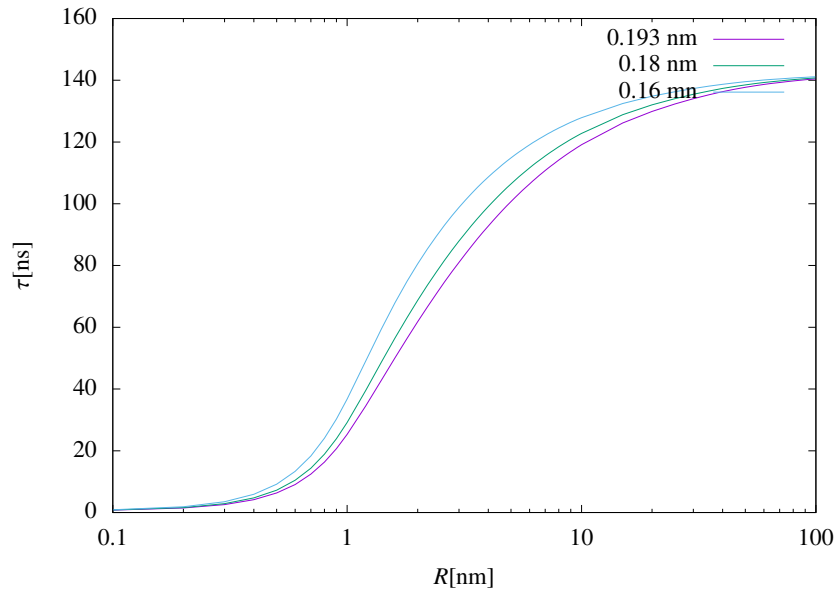


Figure 3:  $\Delta$  parameter

## 4 Calculating $R$ from ETE

### 4.1 Initial guess

I went for approximating  $\tau$  as

$$\tau \approx \frac{140}{1 + x/5^{-3/2}}, \quad (5)$$

which is a CDF of a log-logistic distribution.

It looks quite good but it doesn't matter so much as it will just get corrected. I will check later for comparison against different approximation. I used wxMaxima to calculate inverse of this function which in my case will be

$$R \approx \left( \frac{39480499x}{4993932(140 - x)} \right)^{\frac{2}{3}} \quad (6)$$

## 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.