ADMR Units:

Algorithm has troubles to compute with very high power of ten therefore, I propose to regroup the constant to make it easier for the memory usage.

First, in the code, velocity is defined with $\hbar = 1$, to instead plug $\hbar$ directly in the movement equation and Chambers formula.

$v = 1 . \nabla_k \mathcal{E}$, in equations v should be $\frac{v}{\hbar}$

a, b, c are expressed in Å, the repated power of ten will be stored in "Angstrom" $= 10^{-10}$

t is expressed in meV, the repated power of ten will be stored in "meVolt" $= 1.605 . 10^{-22}$

τ is expressed in picosecond, the repated power of ten will be stored in "picosecond" $= 10^{-12}$

equivalently Γ is expressed in THz.

This brings to the movement equation:

$$\frac{dk}{dt} = \left(-\frac{e}{\hbar}\right) \vec{v} \times \vec{B}$$

$$\frac{dk'}{dt'} \cdot \frac{\text{Angstrom}^{-1}}{\text{picosecond}} = -\frac{e}{\hbar} \cdot \frac{\text{Angstrom} \cdot \text{meVolt}}{\hbar} \cdot v' \times B$$

$$\frac{dk'}{dt'} = -\frac{e}{\hbar^2} \cdot \text{Angstrom}^2 \cdot \text{meVolt} \cdot \text{picosecond} \, (v' \times B)$$

units_move_eq

The same way the Chambers formula:

$$\sigma_{33} = \frac{e^2}{4\pi^3} \cdot \int d^3k \cdot \left(-\frac{\partial f}{\partial \varepsilon}\right) \cdot v_3(k,0) \int v_3(k,t)\, e^{-\frac{t}{\tau}} \cdot dt$$

$$= \frac{e^2}{4\pi^3} \cdot \frac{\text{Angstrom}^{-3}}{\text{meVolt}} \cdot \int d^3k' \left(-\frac{\partial f}{\partial \varepsilon'}\right) \cdot \frac{\text{Å}^2 \cdot \text{meVolt}^2}{\hbar^2} \cdot v_3' \int v_3' \cdot \text{picosecond} \cdot dt'$$

$$= \frac{e^2}{4\pi^3} \cdot \frac{\text{Angstrom}^{-1}}{\hbar^2} \cdot \text{meVolt} \cdot \text{picosecond} \int d^3k (\dots) v_3' \int v_3' \cdot e^{-\frac{t}{\tau}} \cdot dt'$$

units_chambers

By using these constants for conversion, one can directly enter in the program a, b, c in Å, t in meV and Γ in THz.