Casida-realtime equivalence

We want to find the relationship between the exponential damping used in the real-time calculations and the Lorentzian function used in the python script. Both of these functions, are used to to give a certain broadening to the calculated excitations. We will try to find the relationship between τ and Γ.

$$damp(t) = e^{(-\frac{t}{\tau})} \quad \& \quad L(x) = \frac{1}{\pi}\frac{\frac{1}{2}\Gamma}{(x-x_0)^2 + (\frac{1}{2}\Gamma)^2}$$

The fourier transform of the exponential function $e^{-2\pi k_0|x|}$ would be:

$$F_x[e^{-2\pi k_0|x|}](k) = \int_{-\infty}^{\infty} e^{-2\pi k_0|x|}e^{-2\pi ikx}dx$$

Partitioning the integral in the two parts of the module and then, using the Euler's formula $e^{i\theta} = \cos(\theta) - i\sin(\theta)$, we got:

$$\begin{aligned}F_x[e^{-2\pi k_0|x|}](k) &= \int_{-\infty}^{\infty} e^{-2\pi k_0|x|}e^{-2\pi ikx}dx \\ &= \int_{-\infty}^{0} e^{2\pi k_0 x}e^{-2\pi ikx}dx + \int_{0}^{\infty} e^{-2\pi k_0 x}e^{-2\pi ikx}dx \\ &= \int_{-\infty}^{0} [\cos(2\pi kx) - i\sin(2\pi kx)]e^{2\pi k_0 x}dx \\ &\quad + \int_{0}^{\infty} [\cos(2\pi kx) - i\sin(2\pi kx)]e^{2\pi k_0 x}dx\end{aligned}$$

Now, we propose a variable change using $u = -x$ (so $du = -dx$). Using the new variable and the properties of trigonometric functions:

$$
\begin{aligned}
F_x[e^{-2\pi k_0|x|}](k) =& \int_{\infty}^{0} [\cos(2\pi ku) + i\sin(2\pi ku)]e^{-2\pi k_0 u}(-du) \\
&+ \int_{0}^{-\infty} [\cos(2\pi ku) + i\sin(2\pi ku)]e^{2\pi k_0 x}(-du) \\
\text{inverting limits:} & \\
=& \int_{0}^{\infty} [\cos(2\pi ku) + i\sin(2\pi ku)]e^{-2\pi k_0 u}du \\
&+ \int_{-\infty}^{0} [\cos(2\pi ku) + i\sin(2\pi ku)]e^{2\pi k_0 x}du \\
\text{by simetry:} & \\
=& \int_{0}^{\infty} [\cos(2\pi ku) + i\sin(2\pi ku)]e^{-2\pi k_0 u}du \\
&+ \int_{0}^{\infty} [\cos(2\pi ku) - i\sin(2\pi ku)]e^{-2\pi k_0 x}du \\
\text{simplyfying:} & \\
F_x[e^{-2\pi k_0|x|}](k) =& 2\int_{0}^{\infty} \cos(2\pi ku)e^{-2\pi k_0 u}du
\end{aligned}
$$

The integral argument of the right side of the equation represents an exponential damped cosene function and can be resolved by double integration by parts (use always the exponential as dv). So we finally got:

$$
F_x[e^{-2\pi k_0|x|}](k) = \frac{1}{\pi}\frac{k_0}{k^2 + k_0^2}
$$

which is the Lorentzian function. This last equation represents our relationship between the damping parameter τ of the real time calculation (k_0 inside the exponential) and the damping from the Lorentian spectrum Γ from Casida (related to the wide parameter k_0 in the Lorentzian function).

So, from the left-side of the last equation we got the equivalence for real-time:

$$
\begin{aligned}
-2\pi k_0 &= -\frac{1}{\tau} \\
k_0 &= \frac{1}{2\pi\tau}
\end{aligned}
$$

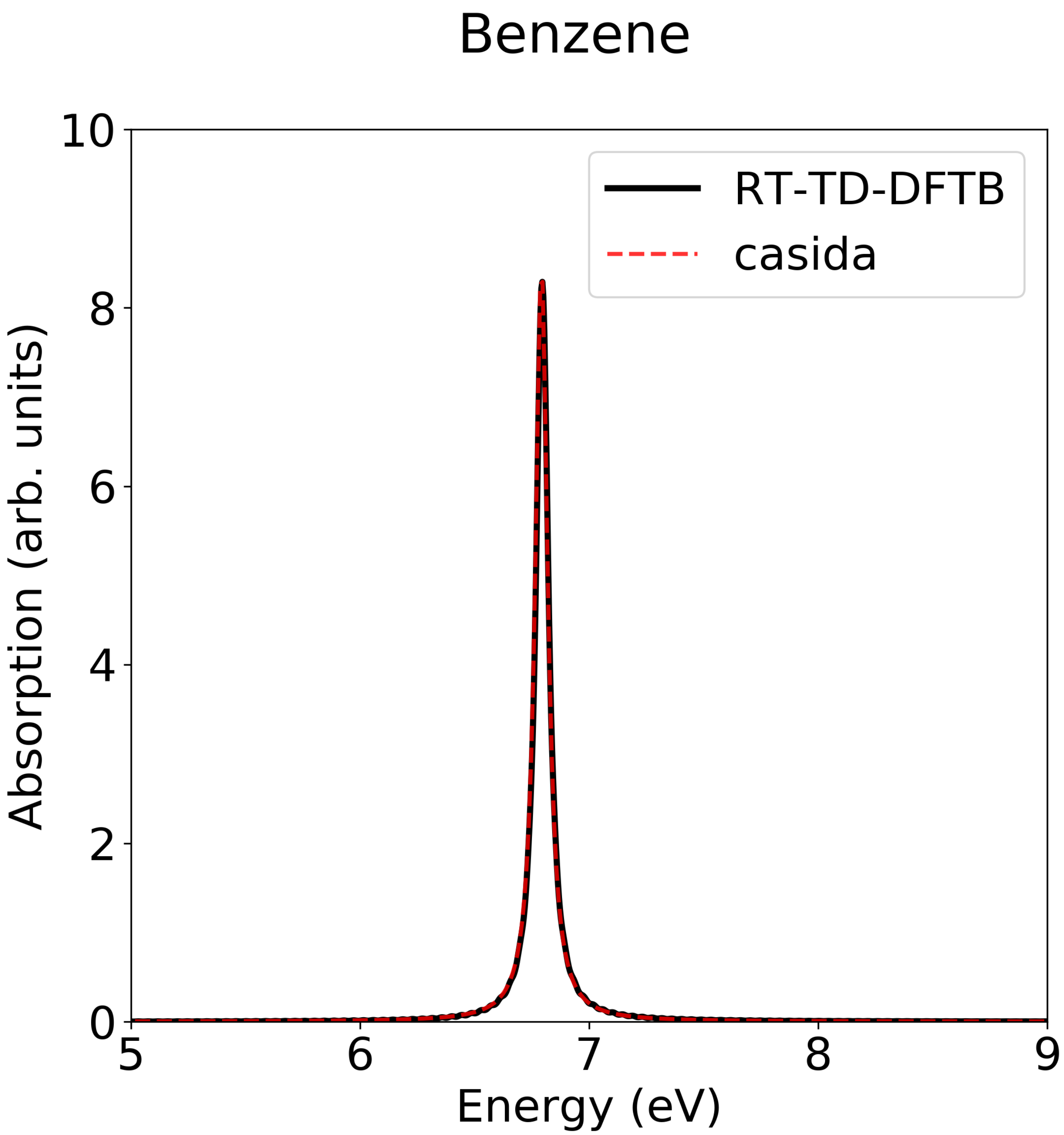
From the right-side we got the equivalence for the Lorentzian function (Casida):

$$k_0 = \frac{1}{2}\Gamma$$
$$2k_0 = \Gamma$$

replacing

$$\frac{1}{\pi\tau} = \Gamma$$

So, in order to have the same curve shape, the Γ parameter for the Lorentzian function need to be related with the τ from real time as shown in the las equation.
As the τ in the FT for the real time spectrum is defined in fs and the Γ unit is eV, a **factor of** $h10^{15}$**.**



Bibliography:

Fourier Transform–Exponential Function – from Wolfram MathWorld
Euler's formula