Analytical solution for the absorption coefficient convoluted with the Urbach tail

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We solve analytically the convolution integral between $\alpha(E) \propto \sqrt{E-E_g}$ and the phenomenological Urbach tail $\propto e^{\frac{|E|}{\gamma}}$. Numerical integration with scipy.integrate.quad takes $\sim 10^5$ longer than the analytical solution.

I. THE CONTEXT

Generalized Planck law is a powerful tool to describe luminescence emission from semiconductor under steady-state excitation (photons or electrons)[1–6]. We use the following definition for the absorption coefficient $\alpha_0(\hbar\omega)$ ($\hbar\omega$ is the photon energy) as reported in paper[7] for the absorption coefficient:

$$\alpha_0(\hbar\omega) = \frac{1}{2\gamma}\int_{-\infty}^{\infty} \alpha_{ideal}(\epsilon) \times e^{-\frac{|\hbar\omega-\epsilon|}{\gamma}} d\epsilon \tag{1}$$

$$\alpha_{ideal}(\hbar\omega) = \begin{cases} a_0\sqrt{\frac{\hbar\omega-E_g}{E_0-E_g}} & \hbar\omega \geq E_g \\ 0 & \hbar\omega < E_g \end{cases} \tag{2}$$

II. NUMERICAL IMPLEMENTATION

Numerical integration

A very first attempt has been performed with a basic code based on the scipy.integrate.quad method:

```
from scipy.integrate import quad_vec
def abs_coeff_tail(x, param_abs, param_tail):
        integrand = lambda e : (ideal_abs_function(e, param_abs)
                                  *tail_function(x-e, param_tail))
        _f = quad_vec(integrand, Eg, np.inf)[0]
        return _f
```

It takes in average **12s** to compute the integration for a 1000-long x vector.

Analytical form

The integral in 1 can be rewritten in the following form ($\epsilon' = \epsilon - E_g$):

$$I = C\int_0^{+\infty} \sqrt{\epsilon'} e^{-\frac{|\hbar\omega-\epsilon'-E_g|}{\gamma}} d\epsilon' \xrightarrow[x=\hbar\omega-E_g]{\epsilon'=t^2} C\int_0^{+\infty} t e^{-\frac{\left|x-t^2\right|}{\gamma}} 2t dt \qquad \text{with } x, t \in \mathbb{R} \tag{3}$$

where $C = \frac{a_0}{2\gamma\sqrt{E_0-E_g}}$. At this point we have to split the integral following the $|\ldots|$ definition:

$$e^{-\frac{\left|x-t^2\right|}{\gamma}} = \begin{cases} e^{\frac{x-t^2}{\gamma}} & t^2 \geq x \\ e^{\frac{t^2-x}{\gamma}} & t^2 < x \end{cases}, \tag{4}$$

but we have to be careful to distinguish the $x \geq 0$ and $x < 0$ cases: in the second case $e^{-\frac{\left|x-t^2\right|}{\gamma}} = e^{\frac{x-t^2}{\gamma}}$ since $t^2 \geq x$ is always verified. To summarize we have:

$$\frac{I}{C} = \begin{cases} \overbrace{\int_0^{\sqrt{x}} te^{\frac{t^2-x}{\gamma}} 2tdt}^{I_1^+/C} + \overbrace{\int_{\sqrt{x}}^{+\infty} te^{\frac{x-t^2}{\gamma}} 2tdt}^{I_2^+/C} & x \geq 0 \\ \underbrace{\int_0^{+\infty} te^{\frac{x-t^2}{\gamma}} 2tdt}_{I^-/C} & x < 0\,. \end{cases} \tag{5}$$

Case $x \geq 0$

Integrating by parts both I_1^+ and I_2^+ we arrive to this I^+:

$$I^+ = 2\gamma\sqrt{x} + \gamma e^{\frac{x}{\gamma}} \int_{\sqrt{x}}^{+\infty} e^{-\frac{t^2}{\gamma}} dt - \gamma e^{-\frac{x}{\gamma}} \int_0^{\sqrt{x}} e^{-\frac{t^2}{\gamma}} dt\,. \tag{6}$$

We are lucky since we are now dealing with integrals of the Gaussian function, well known, and well implemented in Scipy[8]. By using the following definitions:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{7}$$

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) \tag{8}$$

$$\mathrm{erfi}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt\,. \tag{9}$$

we can obtain($x = \hbar\omega - E_g$):

$$I^+ = \underbrace{a_0\sqrt{\frac{\hbar\omega - E_g}{E_0 - E_g}}}_{\alpha_{ideal} \text{ in } 2} + \frac{a_0}{4}\frac{\gamma\pi}{E_0 - E_g}\left[e^{\frac{\hbar\omega - E_g}{\gamma}} \mathrm{erfc}\left(\sqrt{\frac{\hbar\omega - E_g}{\gamma}}\right) - e^{\frac{E_g - \hbar\omega}{\gamma}} \mathrm{erfi}\left(\sqrt{\frac{\hbar\omega - E_g}{\gamma}}\right)\right] \tag{10}$$

Case $x < 0$

Following the same procedure as before we obtain for I^-:

$$I^- = \frac{a_0\sqrt{\pi\gamma}}{4\sqrt{E_0 - E_g}} e^{\frac{\hbar\omega - E_g}{\gamma}}\,. \tag{11}$$

Final expression

Putting everything together we finally obtain this analytical expression:

$$I(\hbar\omega) = \begin{cases} I^+ = a_0\sqrt{\frac{\hbar\omega - E_g}{E_0 - E_g}} + \frac{a_0}{4}\frac{\gamma\pi}{E_0 - E_g}\left[e^{\frac{\hbar\omega - E_g}{\gamma}} \mathrm{erfc}\left(\sqrt{\frac{\hbar\omega - E_g}{\gamma}}\right) - e^{\frac{E_g - \hbar\omega}{\gamma}} \mathrm{erfi}\left(\sqrt{\frac{\hbar\omega - E_g}{\gamma}}\right)\right] & \hbar\omega \geq E_g \\ \frac{a_0\sqrt{\pi\gamma}}{4\sqrt{E_0 - E_g}} e^{\frac{\hbar\omega - E_g}{\gamma}} & \hbar\omega < E_g\,, \end{cases} \tag{12}$$

that can easily be implemented in python with the numpy.piecewise function and the Scipy error-functions.

```
def integ(E, g, a0, Eg, E0):
        x = E-Eg
        _c1 = 0.25*a0*np.sqrt(g*np.pi/(E0-Eg))
        _fpos = lambda x : (a0*np.sqrt(x/(E0-Eg))
                        +_c1*(np.exp(x/g)*erfc(np.sqrt(x/g))
                        -np.exp(-x/g)*erfi(np.sqrt(x/g)))
                        )
        _fneg = lambda x : _c1*np.exp(x/g)
          _f = np.piecewise(x, [x>=0, x<0], [_fpos, _fneg])
          return _f
```

III. COMPARISON

Obviously the comparison is perfect, as reported in Figure 1 and we clearly gain in execution time.

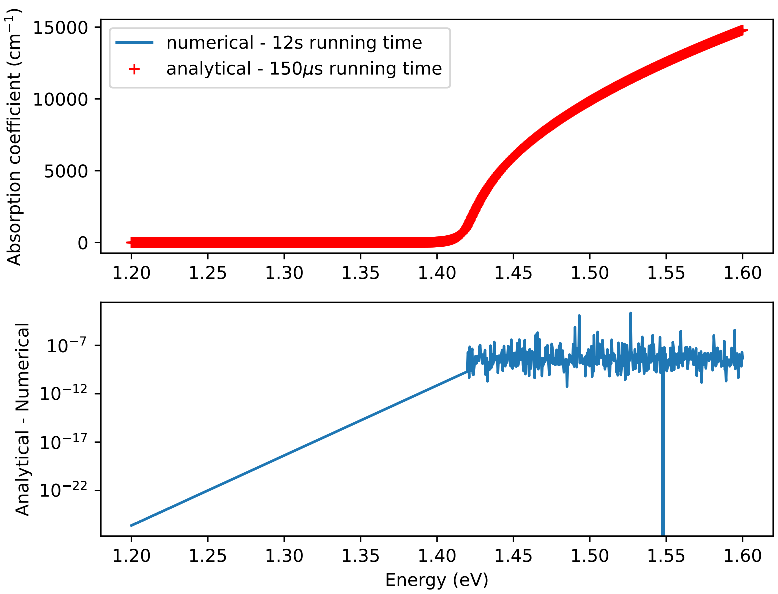

FIG. 1. Comparison between numerical and analytical solutions of 1

.

REFERENCES

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[8]Scipy implementation of erf, erfc and erfi.