Comment on the paper “Improving Poor Man’s Kramers-Kronig analysis and Kramers-Kronig constrained variational analysis”

Emmanuel Rousseau, Nicolas Izard, Jean-Louis Bantignies, Didier Felbacq

Graphical Abstract

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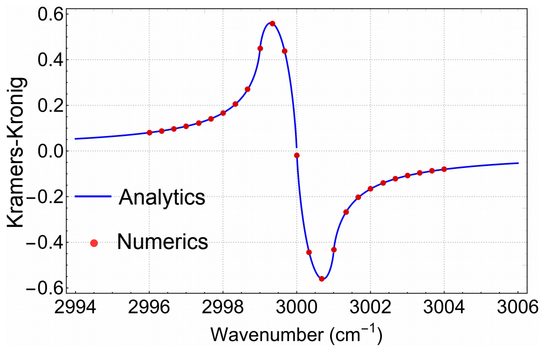

Highlights

Comment on the paper "Improving Poor Man's Kramers-Kronig analysis and Kramers-Kronig constrained variational analysis"

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- A comment on the title paper is reported,
- We clarify some analytical expressions existing in the literature,
- Within the correct formulae we conclude that there is no need for an *ad hoc* improvement on the opposite to the title paper,
- We highlight the symmetry properties of the function to be integrated in order to agree with the usual assumptions made to derive the Kramers-Kronig relations,
- The analytical formula we provide may be used to increase the accuracy of the "Poor Man's Kramers-Kronig analysis" method and the "Kramers-Kronig constrained variational analysis" method.

Comment on the paper "Improving Poor Man's Kramers-Kronig analysis and Kramers-Kronig constrained variational analysis"

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Abstract

The title paper [*Spectrochim. Acta A* **213** (2019): 391-396] reports an improvement of the "Poor Man's Kramers-Kronig analysis" and of the "Kramers-Kronig constrained variational analysis" thanks to an *ad hoc* modification of some analytical formulas existing in the literature. This *ad hoc* modification is not based on mathematical grounds. In this comment we show that no *ad hoc* modification is required but a correction of the analytical formula used by the authors of the title paper [*Spectrochim. Acta A* **213** (2019): 391-396].

Keywords: Kramers-Kronig relations, Poor Man's Kramers-Kronig analysis

1. Introduction

The Kramers-Kronig relations [eq.(1) and eq.(2)] allow to connect the real part and the imaginary part of any holomorphic function [1, p. 28]. As an example, for the dielectric constant $\varepsilon(\sigma) = \varepsilon'(\sigma) + i\varepsilon''(\sigma)$, with real part $\varepsilon'(\sigma)$ and imaginary part $\varepsilon''(\sigma)$, assuming that it converges to 1 for large

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wavenumbers σ, the Kramers-Kronig relations read [2, p. 179]:

$$\varepsilon'(\sigma) - 1 = \frac{2}{\pi}\mathcal{P}\int_0^{+\infty} \frac{\sigma'\varepsilon''(\sigma')}{\sigma'^2 - \sigma^2}\,\mathrm{d}\sigma' \tag{1}$$

$$\varepsilon''(\sigma) = -\frac{2\sigma}{\pi}\mathcal{P}\int_0^{+\infty} \frac{[\varepsilon'(\sigma') - 1]}{\sigma'^2 - \sigma^2}\,\mathrm{d}\sigma' \tag{2}$$

where $\mathcal{P}\int_{\mathbb{R}}$ stands for the Cauchy principal-value integral. They are the eqs.(1) and (2) in the paper to be commented [3].

These relations hold if the analytic continuation of the function to be considered, *i.e.* $[\varepsilon(\sigma) - 1]$ here, is analytic in the upper part of the complex plane and decreases to zero as $|\sigma| \to +\infty$. They also assume the following symmetry properties (see [2, p. 179]):

$$[\varepsilon'(\sigma) - 1] \text{ is even } \Rightarrow [\varepsilon'(-\sigma) - 1] = [\varepsilon'(\sigma) - 1] \tag{3}$$

$$\varepsilon''(\sigma) \text{ is odd } \Rightarrow \varepsilon''(-\sigma) = -\varepsilon''(\sigma) \tag{4}$$

If the symmetry conditions do not hold, more general Kramers-Kronig relations can be written but they involve integration range over $\mathbb{R}$ instead over $\mathbb{R}^+$. They read:

$$\varepsilon'(\sigma) - 1 = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\varepsilon''(\sigma')}{\sigma' - \sigma}\,\mathrm{d}\sigma' \tag{1b}$$

$$\varepsilon''(\sigma) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{[\varepsilon'(\sigma') - 1]}{\sigma' - \sigma}\,\mathrm{d}\sigma' \tag{2b}$$

independently on the existence of symmetry conditions or not. Actually the eq.(1) derives from the eq.(1b) with the assumptions that the imaginary part of the dielectric constant $\varepsilon''(\sigma)$ is an odd function of the wavenumbers (see [4, p.789]).

2. The T. Mayerhöfer *et al.* proposal

In the reference[5], T. Mayerhöfer *et al.* proposed a new method to numerically integrate the Kramers-Kronig equations eq.(1) and eq.(2). They named their method the "Poor man's Kramers-Kronig analysis". It consists in interpolating the function to be integrated by a family of functions $b_k(\sigma)$.

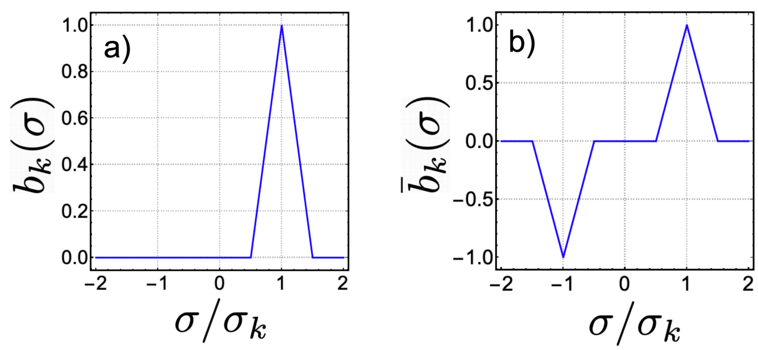

Figure 1: a) Triangular-shape function center on $\sigma = \sigma_k$. b) Odd triangular-shape function center on $\sigma = \sigma_k$.

For example, the interpolation of the imaginary part of the dielectric function reads:

$$\varepsilon''(\sigma) = \sum_{\sigma_k \in \mathcal{S}} \varepsilon''(\sigma_k) b_k(\sigma) \tag{5}$$

where $\mathcal{S} = \{\sigma_k\}_{k=0,..,p-1}$ is the list of the $p \in \mathbb{N}$ discrete wavenumbers and $\varepsilon''(\sigma_k)$ is the value of the imaginary part of the dielectric function at the wavenumber σ_k.

With the help of the eq.(5), the Kramer-Kronig equation (1) can be computed as:

$$\varepsilon'(\sigma) - 1 = \sum_{\sigma_k \in \mathcal{S}} \varepsilon''(\sigma_k) \times \frac{2}{\pi} \mathcal{P} \int_0^{+\infty} \frac{\sigma' b_k(\sigma')}{\sigma'^2 - \sigma^2} \, \mathrm{d}\sigma' \tag{6}$$

$$\varepsilon'(\sigma) - 1 = \sum_{\sigma_k \in \mathcal{S}} \varepsilon''(\sigma_k) a_k(\sigma) \tag{7}$$

where the function $a_k(\sigma)$ is defined by $a_k(\sigma) = \frac{2}{\pi} \mathcal{P} \int_0^{+\infty} \frac{\sigma' b_k(\sigma')}{\sigma'^2 - \sigma^2} \, \mathrm{d}\sigma'$ (see the eq.(5) in [5]).

As a family of interpolating functions $b_k(\sigma)$, T. Mayerhöfer *et al.* choose in the ref. [5] some functions introduced previously by Kuzmenko in the ref.[6] where he described the method denoted "Kramers-Kronig constrained variational analysis". The functions $b_k(\sigma)$ are depicted on the Fig.(1-a).

Their analytical formula are:

$$b_k(\sigma) = \begin{cases} \frac{\sigma-\sigma_{k-1}}{\sigma_k-\sigma_{k-1}} & \sigma \in [\sigma_{k-1}, \sigma_k] \\ \frac{\sigma_{k+1}-\sigma}{\sigma_{k+1}-\sigma_k} & \sigma \in]\sigma_k, \sigma_{k+1}] \\ 0 & \text{otherwise} \end{cases} \tag{8}$$
$$0 < \sigma_{k-1} < \sigma_k < \sigma_{k+1}$$

This is the eq.(4) in [3]. These functions are of triangular-shape and centered on the frequency $\sigma_k \in \mathcal{S}$. They get null values outside the range $[\sigma_{k-1}, \sigma_{k+1}]$. Because the functions $b_k(\sigma)$ are piecewise linear, their Hilbert transform can be analytically evaluated. T. Mayerhöfer *et al.* have found [3, 5]:

$$\begin{aligned} a_k^M(\sigma) &= \frac{1}{\pi}\left[\frac{\sigma-\sigma_{k-1}}{\sigma_k-\sigma_{k-1}}\ln\left|\frac{\sigma-\sigma_k}{\sigma-\sigma_{k-1}}\right| - \frac{\sigma_{k+1}-\sigma}{\sigma_{k+1}-\sigma_k}\ln\left|\frac{\sigma-\sigma_k}{\sigma-\sigma_{k+1}}\right|\right] \\ &= -\frac{1}{\pi}\left[\frac{g(\sigma-\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g(\sigma-\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g(\sigma-\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right] \\ \text{with} &\quad g(x) = x\ln|x| \end{aligned} \tag{9}$$

This is the equation (5) in [3] that corresponds partially to a result initially published by A.B. Kuzmenko in [6]. Indeed the equivalent of the function $g(x)$ defined above is in A.B. Kuzmenko's paper[6] $g_K(x, y) = (x + y)\ln|x + y| + (x - y)\ln|x - y|$. T. Mayerhöfer *et al.* retain only the term proportional to $(x - y)\ln|x - y|$ but with a difference in the sign of the prefactor. Indeed it is $-1/\pi$ in the result used by T. Mayerhöfer *et al.* whereas it is $+1/\pi$ in the result reported by A.B. Kuzmenko. We will show below that the prefactor $-1/\pi$ given by T. Mayerhöfer *et al.* is the correct one.

In order to check the accuracy of the "Poor man's Kramers-Kronig analysis" method, T. Mayerhöfer *et al.* computed in the ref. [5] and in the ref. [3], the difference between the eq.(9) and a numerical integration of the Kramers-Kronig equation (1). The numerical integration is based on the Riemann sum approximation [7] of the eq.(1) (see the eq.(2) in [5]). The calculations are done for one single triangular-shape function centered on $\sigma_1 = 3000$ cm^{-1} with $\sigma_0 = 2999$ cm^{-1} and $\sigma_2 = 3001$ cm^{-1}. Denoting by $\Delta(\sigma)$ the difference between the eq.(9) and its numerical calculation, they got in the ref.[5] a maximal discrepancy on the order of $|\Delta(\sigma)| \sim 10^{-2}$ as shown by the Fig.(S1) in the supplementary information of the ref. [5]. In the Fig.(3) of the subsequent publication (ref. [3]) they got a more or less constant disagreement on the order of $|\Delta(\sigma)| \sim 10^{-4}$. These discrepancies lead them to some comments in the two previously mentioned refs.[5, 3]. Indeed, in the ref. [5, p.3167], they wrote: "There is, however, also a drawback, which is that [eqn (8) and (9)] are not fully Kramers-Kronig consistent.". In the ref. [3, p.394] they wrote "[$\Delta(\sigma)$] reflects the deviations from the Kramers-Kronig conformity". T. Mayerhöfer *et al.* concluded that there is a mismatch between the analytical formula and the numerical integration of the eq.(1). They finally assume that the correct result is given by the numerical integration and provide in the ref.[3] an *ad hoc* modification of the analytical equation (9). The *ad hoc* modification leads to an increase of the accuracy, the quantity $\Delta(\sigma)$ being small and center on zero in the range $[2990\ \mathrm{cm}^{-1}, 3010\ \mathrm{cm}^{-1}]$ but with an absolute difference that reachs $|\Delta(\sigma)| \sim 4.10^{-5}$ at maximum. The *ad hoc* modification is the eq.(10) in the ref.[3]. This *ad hoc* modification sounds rather strange since the eq.(9) is *a priori* an exact analytical result. The *ad hoc* modification has no mathematical justifications.

In this comment, we show that no *ad hoc* modification is needed but actually a correction of the analytical formula eq.(9) to get a fully "Kramers-Kronig conformity" between the analytical result and the numerical evaluation of the equation (1). From the mathematical side, this is reassuring because the function $f_k(\sigma) = a_k(\sigma) + ib_k(\sigma)$ being analytic in the complex plane, its real and imaginary parts have to satisfied the Kramers-Kronig relations eqs.(1b-2b) in the general case or eqs.(1-2) if $a_k(\sigma)$ and $b_k(\sigma)$ have some specific symmetries.

3. Main results

The equation (1) and consequently its numerical integration assume that the function to be integrated $\varepsilon''(\sigma)$ is an odd function of the wavenumber (see [2, eq.(6.32)]). But the interpolating functions considered by T. Mayerhöfer *et al.* are neither odd or even. In order to get an agreement between an analytical result and the numerical integration of the eq.(1) a family of odd interpolating-functions has to be considered. The basis functions we considered are then:

$$\bar{b}_k(\sigma) = \begin{cases} b_k(\sigma) \text{ for } \sigma > 0 \\ \\ -b_k(|\sigma|) \text{ for } \sigma < 0 \end{cases} \tag{10}$$

where the function $b_k(\sigma)$ has been previously defined by the eq.(8) and $|\sigma|$ stands for the modulus of σ. The function $\bar{b}_k(\sigma)$ is depicted on the Fig.(1-b). The Hilbert transform of the functions $\bar{b}_k(\sigma)$ is:

$$\begin{aligned}
a_k^R(\sigma) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\bar{b}_k(\sigma')}{\sigma'-\sigma}\,\mathrm{d}\sigma' \\
&= \frac{1}{\pi}\mathcal{P}\int_{0}^{+\infty} \frac{\bar{b}_k(\sigma')}{\sigma'-\sigma}\,\mathrm{d}\sigma' + \frac{1}{\pi}\mathcal{P}\int_{0}^{+\infty} \frac{\bar{b}_k(-\sigma')}{\sigma'+\sigma}\,\mathrm{d}\sigma' \\
&= \frac{1}{\pi}\mathcal{P}\int_{0}^{+\infty} \frac{b_k(\sigma')}{\sigma'-\sigma}\,\mathrm{d}\sigma' - \frac{1}{\pi}\mathcal{P}\int_{0}^{+\infty} \frac{b_k(\sigma')}{\sigma'+\sigma}\,\mathrm{d}\sigma'
\end{aligned}$$

We have found more convenient to start from the eq.(1b) rather than from the eq.(1). The result of the analytical calculations is:

$$a_k^R(\sigma) = a_k^M(\sigma) + c_k(\sigma) \tag{11}$$

with

$$c_k(\sigma) = -\frac{1}{\pi}\left[\frac{\sigma+\sigma_{k-1}}{\sigma_k-\sigma_{k-1}}\ln\left(\frac{\sigma+\sigma_k}{\sigma+\sigma_{k-1}}\right) + \frac{\sigma_{k+1}+\sigma}{\sigma_{k+1}-\sigma_k}\ln\left(\frac{\sigma+\sigma_k}{\sigma+\sigma_{k+1}}\right)\right] \tag{12}$$

$$c_k(\sigma) = \frac{1}{\pi}\left[\frac{g(\sigma+\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g(\sigma+\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g(\sigma+\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right]$$

$a_k^M(\sigma)$ is given by the eq.(9). As compared to the result studied by T. Mayerhöfer *et al.*, our solution includes an extra term $c_k(\sigma)$ due to the contribution of the function $\bar{b}_k(\sigma)$ at negative wavenumbers whereas the term $a_k^M(\sigma)$ comes from the contribution of the positive-wavenumbers range.

In order to check that our analytical solution eq.(11) is consistent with the eq.(1), we numerically integrate the eq.(1) with the built-in function for integration of the software Mathematica® (denoted $NI(\sigma)$). In order to get a precise numerical result, we specify the option "Principal Value" in the Mathematica® function. The solution we propose eq.(11) and the numerical calculation $NI(\sigma)$ are compared on the Fig.(2-a) as respectively the plain black-line and the red dots. They perfectly fit. Indeed as shown by the Fig.(2-b) the absolute difference $|\bar{\Delta}(\sigma)| = |a_k^R(\sigma) - NI(\sigma)|$ is less than 5×10^{-13} *i.e* on the order of magnitude of the numerical rounding.

The correction we make to the analytical formula provided by T. Mayerhöfer *et al.*, *i.e.* the term $c_k(\sigma)$, decreases linearly in the range $[2990, 3010]$

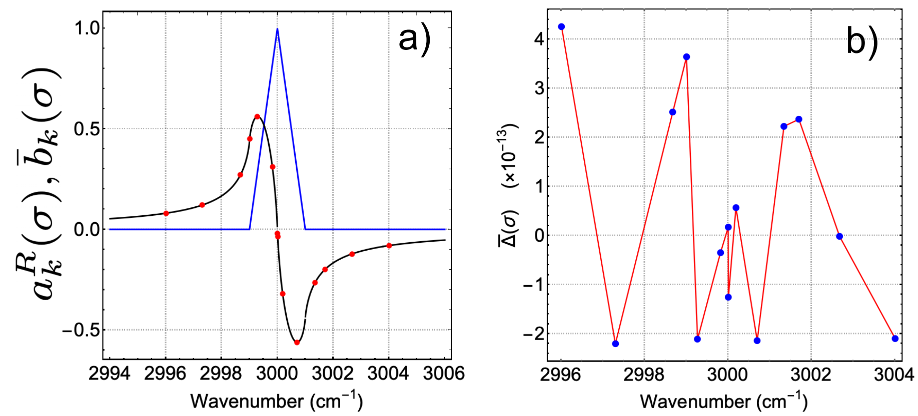

Figure 2: Comparison between the analytical formula $a_k^R(\sigma)$ and the numerical integration $NI(\sigma)$. a) Blue curve: $\bar{b}_k(\sigma)$ given by the eq.(10) with parameters $\sigma_0 = 2999\text{cm}^{-1}$,$\sigma_1 = 3000\text{cm}^{-1}$ and $\sigma_2 = 3001\text{cm}^{-1}$; Black curve: $\bar{a}_k(\sigma)$ given the eq.(11) ; Red dots: $NI(\sigma)$, *i.e.* the numerical integration of the eq.(1) with the software Mathematica®. b) Difference between the numerical calculation $NI(\sigma)$ and the analytical expression $a_k^R(\sigma)$.

varying from $c_k(2990) \simeq 5.314 \times 10^{-5}$ to $c_k(3010) \simeq 5.296 \times 10^{-5}$. These values are small but larger by several orders of magnitude than the numerical precision on the order of $\sim 5 \times 10^{-13}$. This numerical accuracy is reached thanks to the option "Principal Value" of the Mathematica® built-in function for integration. This option was needed in order to check the adequacy between the analytical result and the numerical integration of the eq.(1). Indeed as already said the function $c_k(\sigma)$ takes values on the order of $\sim 5.10^{-5}$ in the range $[2990, 3010]\text{cm}^{-1}$. An accuracy better than 10^{-5} is then required to get a conclusion. On the opposite, according to their Fig.(3) in ref.[3] T. Mayerhöfer *et al.* got an absolute difference on the order of $\sim 4.10^{-5}$ between their numerical calculations and their analytical formula augmented by the *ad hoc* correction. This value of $\sim 4.10^{-5}$ reflects the fact that the analytical formula (9) given by T. Mayerhöfer *et al.* missed the contribution of the negative-frequencies part that is taken into account when the eq.(1) is integrated numerically. Restoring the negative-frequency contribution to the Kramer-Kronig relations leads to a "Kramers-Kronig consistency" between the imaginary part $b_k(\sigma)$ and the real part $a_k(\sigma)$ of the analytic function $f_k(\sigma) = a_k(\sigma) + ib_k(\sigma)$.

Finally, even if T. Mayerhöfer *et al.* had ruled out[1] this possibility, we think that the solution we propose here was already included in the ref. [8, eqs. (8) and (12)]. The main goal of this comment was to clarify the assertion made by Mayerhöfer *et al.* in [3] that an *ad hoc* modification of the existing formula was needed to reach a good accuracy between the analytical expression and a numerical integration of the equation (1). Our comment shows that this assertion is unfounded. To clearly explain why we think no *ad hoc* modification is needed, we have found worth to derive in this comment the set of eq.(9) and eq.(11). This derivation highlights the importance of the symmetry of the function to be integrated in order to satisfy the assumptions made while deriving the Kramers-Kronig relations (1). Finally, our result also disagrees with A. B. Kuzmenko's solution [6] by some sign difference and finally clarifies some existing formulae available in the literature. In order for the reader to appreciate the difference between our result and the equations available in the literature,the table (1) summarized in a uniform notational way the result provided by A.B. Kuzmenko[6] and the two results derived by T. Mayerhöfer *et al.*. The differences and similarities can be appreciated.

The analysis detailed in the previous paragraph shows that the contribution of the negative-frequencies part [*i.e.* the term $c_k(\sigma)$, eq.(12)] is on the order of 5×10^{-5} in the range [2990 cm^{-1}, 3010 cm^{-1}]. As a consequence, considering a scale similar to the Fig.2-a) there would be no significant differences between our result and the equation used by T. Mayerhöfer *et al.* without and with the *ad hoc* correction. Nevertheless Kramer-Kronig analysis often require the integration of the Kramer-Kronig equations over a wide range of frequencies. Indeed, rigorously speaking the Kramers-Kronig equations have to be integrated over $\mathbb{R}$. The low-frequency part of a spectrum can contribute to the final result and it could be interesting to compare the behavior of the formulae existing in the literature at low frequency. This is done here for a central frequency of $\sigma_k = 20$ cm^{-1}. We can also investigate situation where the experimental frequency-increment is larger than 1cm^{-1}, the only case considered in [3]. As a consequence we test our equation and the equations available in the literature (summarized in the table 1) with the parameters $\sigma_k = 20$ cm^{-1}, $\sigma_{k-1} = 10$ cm^{-1}, $\sigma_{k+1} = 30$ cm^{-1}. Such a compar-

[1] They wrote in[3] "An alternative explanation could be that the derivation of Eq. (5) contains an error, but since B-spline analysis shares the same mathematical base [14] we rule out this explanation."

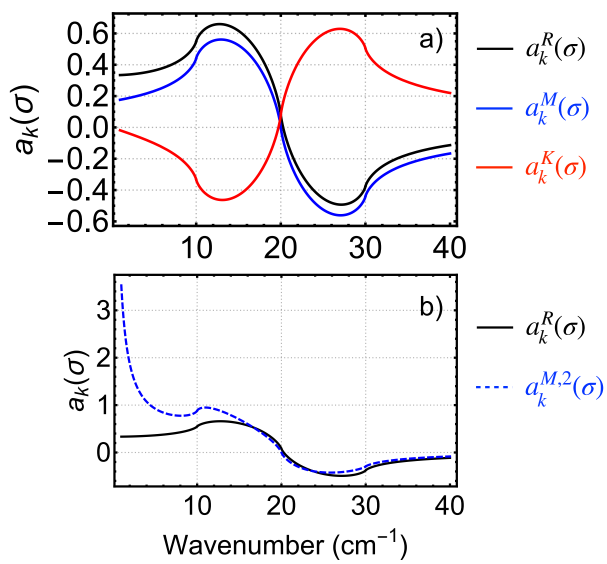

Figure 3: Comparison between the different equations available in the literature as summarized in the table 1. The calculations are performed with $\sigma_{k-1} = 10$ cm^{-1}, $\sigma_k = 20$ cm^{-1}, $\sigma_{k+1} = 30$ cm^{-1}. a) black line: this work, equation $a_k^R(\sigma)$, blue line: $a_k^M(\sigma)$, solution proposed in [3], red line: $a_k^K(\sigma)$, solution proposed in [6]. b) black line: this work, equation $a_k^R(\sigma)$, dashed blue line: $a_k^{M,2}(\sigma)$, solution with an *ad hoc* modification proposed in [3].

Table 1: Equations for the quantity $a_k(\sigma)$ that can be found in some references in the literature. The notations have been unified for a greater clarity.

Reference	equation
eq.(13) in [6]	$a_k^K(\sigma) = +\frac{1}{\pi}\left[\frac{g_K(\sigma,\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g_K(\sigma,\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g_K(\sigma,\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right]$ with $g_K(x,y) = (x-y)\ln\lvert x-y\rvert + (x+y)\ln\lvert x+y\rvert$
eq.(5) in [3]	$a_k^M(\sigma) = -\frac{1}{\pi}\left[\frac{g_M(\sigma,\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g_M(\sigma,\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g_M(\sigma,\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right]$ with $g_M(x,y) = (x-y)\ln\lvert x-y\rvert$
eq.(10) in [3]	$a_k^{M,2}(\sigma) = -\frac{1}{\pi}\left(\frac{\sigma_k}{\sigma}\right)\left[\frac{g_M(\sigma,\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g_M(\sigma,\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g_M(\sigma,\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right]$ with $g_M(x,y) = (x-y)\ln\lvert x-y\rvert$
This work and ref.[8]	$a_k^R(\sigma) = -\frac{1}{\pi}\left[\frac{g_R(\sigma,\sigma_{k-1})}{\sigma_k-\sigma_{k-1}} - \frac{(\sigma_{k+1}-\sigma_{k-1})g_R(\sigma,\sigma_k)}{(\sigma_k-\sigma_{k-1})(\sigma_{k+1}-\sigma_k)} + \frac{g_R(\sigma,\sigma_{k+1})}{\sigma_{k+1}-\sigma_k}\right]$ with $g_R(x,y) = (x-y)\ln\lvert x-y\rvert - (x+y)\ln\lvert x+y\rvert$

ison is shown in the Fig.3. Our result $a_k^R(\sigma)$ is plotted as the black curve in Fig.3-a). Again it differs from a numerical integration of the eq.(1) only by the numerical accuracy on the order of 10^{-13} cm^{-1}. The blue curve in the Fig.3-a) is the eq.(5) in [3] [see formula $a_k^M(\sigma)$ in the table 1]. This result differs by an amount close to 0.1 cm^{-1} [*i.e* $\sim 18\%$] as compared to the exact analytical result. In this frequency range, the difference between the solution proposed by T. Mayerhöfer *et al.* and the exact solution is clearly visible. The red curve in the Fig.3-a) is the solution $a_k^K(\sigma)$ proposed by Kuzmenko as his equation (13) in [6]. Because of the incorrect sign for the contribution of the positive-frequency his solution is mirrored with respect to the exact solution $a_k^R(\sigma)$. Finally, we can also compare our solution with the *ad hoc* modification proposed by T. Mayerhöfer *et al.* in the paper [3] that is the subject of this comment. This is done in the Fig. 3-b) where the black curve is our exact analytical solution and the blue dashed curve is the equation $a_k^{M,2}(\sigma)$ proposed by T. Mayerhöfer *et al.* [see the table (1) for the formula]. A very clear difference is shown. Indeed, the *ad hoc* solution proposed by T. Mayerhöfer *et al.* diverges at low frequency because of the prefactor $\frac{\sigma_k}{\sigma}$. This divergence can significantly decrease the accuracy of the *ad hoc* modification proposed by T. Mayerhöfer *et al.* in [3].

4. Conclusion

As noted by T. Mayerhöfer *et al.* there is a problem of consistency between the analytical formula they used eq.(9) and the Kramers-Kronig equation (1). This assertion sounds rather weird since the considered functions are analytics in the upper part of the complex plane. The remedy to this inconsistency is not an *ad hoc* modification of the analytical formula on the contrary to the proposition of the title paper[3]. Indeed, the consistency can be reached if the considered functions fulfill all the assumptions that lead to the Kramers-Kronig equations (1). Notably the functions must be odd. Considering odd and triangular-shape functions, we recovered an analytical formula [8] that is consistent with the numerical evaluation of the Kramers-Kronig equation (1). This analytical formula eq.(11) can be used to improve the accuracy of the "Kramers-Kronig constrained variational analysis"[6] and the accuracy of the "Poor Man's Kramers-Kronig analysis"[5].

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