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Why is Adachi procedure successful to avoid divergences in optical models?

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Abstract

Adachi proposed a procedure to avoid divergences in optical-constant models by slightly shifting photon energies to complex numbers on the real part of the complex dielectric function, ε_1 The imaginary part, ε_2 was ignored in that shift and, despite this, the shifted function would also provide ε_2(in addition to ε_1) in the limit of real energies. The procedure has been successful to model many materials and material groups, even though it has been applied phenomenologically, i.e., it has not been demonstrated. This research presents a demonstration of Adachi procedure. The demonstration is based on that ε_2 is a piecewise function (i.e., it has more than one functionality), which results in a branch cut in the dielectric function at the real photon energies where ε_2 is not null. Adachi procedure is seen to be equivalent to a recent procedure developed to turn optical models into analytic by integrating the dielectric function with a Lorentzian function. Such equivalence is exemplified on models used by Adachi and on popular piecewise optical models: Tauc-Lorentz and Cody-Lorentz-Urbach models.

1. Introduction

Material optical constants are two functions used to evaluate the interaction of the material with the electromagnetic field. Despite their name, optical constants vary over the spectrum and hence they must be measured at each wavelength/photon energy. Often simple optical models can accurately reproduce the optical constants of a material in a certain spectral range. The use of optical models simplifies optical constant determination, since one only needs to determine a few free parameters.

Optical models need to satisfy various requirements if they are to reproduce the optical constants of materials. The optical constants are two real functions varying with wavelength/photon energy, such as ε_1 and ε_2 or n and k, which are combined in a complex function, such as $\varepsilon_1+i\varepsilon_2$. This function being complex is relevant to establish such requirements. They are expressed in what is usually quoted as Titchmarsh theorem [1], although the core of this theorem has been attributed [2] to the combined work of Riesz [3] and of Payley and Wiener [4]. This theorem connects causality in the response of the material to an external electric stimulus with the fact that the two parts of the aforementioned complex dielectric function are Hilbert transforms of each other, in what is known as Kramers-Kronig (KK) relations. The theorem also establishes that the optical constants are the limit on the real axis of an analytic (holomorphic) complex function in the upper complex half plane C^+. The latter property involves extending the spectral variable such as photon energy E, which is a real number, to complex numbers, such as $z=E+ia\in C^+$, with $a>0$.

Even though typically such extension of the optical constants to complex energy numbers is not required to be known, in some cases it is useful. An example of this is a procedure developed by Adachi to model the optical constants of materials, such as for semiconductors with indirect band gap [5], among other models and material groups. This model involves a divergence, which Adachi circumvented by adding in a phenomenological manner a positive imaginary part to photon energy. He supported this in that optical transitions are strongly affected by a damping effect, i.e., a lifetime broadening [5]. Adachi added this energy term only to the real component of the dielectric function ε_1, and not to the imaginary part ε_2. Operating like this, not only the real part of the dielectric function was obtained, but also the imaginary part. Adachi's procedure to add broadening has the benefit of being very simple to apply. However, being developed in a phenomenological manner, it requires mathematical verification and the conditions for this procedure to be applied. Furthermore, in a common situation where an optical-constant model is described by more than one functionality, one wonders if such model can be extended to C^+, or, conversely, how can an analytic function in C^+ have two different functionalities in the limit on the real axis.

Another application of extending photon energies to C^+ is a procedure to turn non-analytic (holomorphic) optical models into analytic [6,7]: it consists in convolving such model with a Lorentzian function, which results in spectral smoothening of the optical constants. Such convolution is equivalent to an energy shift in the imaginary direction amounting the semi-width of a Lorentzian function [8]. Hence a shift of photon energy in the imaginary direction is equivalent to a convolution and to a smoothening, and the larger the shift, the smoother the resulting optical constants.

The present research investigates the basis of Adachi procedure and compares it with the Lorentzian convolution procedure. Section 2 rigorously demonstrates Adachi procedure, which, to the best of our knowledge, had not been reported so far. It also sets the conditions for Adachi procedure to apply. Section 3 demonstrates that Adachi procedure is equivalent to the Lorentzian convolution procedure. Adachi's models have been generalized by various authors [9,10] to extend them from Lorentzian to Gaussian broadening, which can be also implemented through shifting in C^+, which is addressed also in Section 3. Section 4 presents various models that are turned analytic with Adachi's procedure as well as with the Lorentzian convolution procedure to exemplify their equivalence.

2. Fundaments of Adachi's procedure

Adachi developed a procedure to avoid divergences in optical-constant models, which he used to describe various sorts of materials. One example is the group of semiconductors with an indirect gap [5]. Adachi modelled the latter materials through a parabolic band with the following function:

$$\varepsilon_2(E) = \frac{D}{E^2}\left(E - E_g^{id} + E_q\right)^2 \Theta\left(1 - \frac{E}{E_c}\right) \Theta\left(1 - \frac{E_g^{id} - E_q}{E}\right) \quad (1)$$

where Θ stands for Heaviside function, i.e., $\Theta(x) = 1$ for x>0 and $\Theta(x) = 0$ for x<0.

Hence ε_2 was nonzero only in $E_g^{id} - E_q < E < E_c$. In the following we will simplify notation with $E_g \equiv E_g^{id} - E_q$. Adachi applied KK dispersion relations to ε_2 to obtain $\varepsilon_1(E)$:

$$\varepsilon_1(E) - 1 = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\varepsilon_2(E')}{E' - E} dE' \quad (2)$$

which resulted in [5]:

$$\varepsilon_1(E) = \frac{2D}{\pi}\left[-\frac{E_g^2}{E^2} ln\left(\frac{E_c}{E_g}\right) + \frac{1}{2}\left(1+\frac{E_g}{E}\right)^2 ln\left(\frac{E+E_c}{E+E_g}\right) + \frac{1}{2}\left(1-\frac{E_g}{E}\right)^2 ln\left(\frac{E-E_c}{E-E_g}\right)\right] \quad (3)$$

ε_1 in Eq. 3 involves a divergence at $E=E_c$; the divergence is due to ε_2's discontinuity at E_c. To avoid it, Adachi introduced a lifetime broadening effect in a phenomenological manner by replacing E with $E+i\Gamma$, where Γ was a real, positive, fitting parameter. But such replacement was not performed in the full $\tilde{\varepsilon}(E) = \varepsilon_1(E) + i\varepsilon_2(E)$ but only in $\varepsilon_1(E)$, so that the full dielectric function was given by $\varepsilon_1(E + i\Gamma)$. Surprisingly, ε_2 was ignored. It has to be taken into account that away from the real axis, in general both ε_1 and ε_2 are not real functions anymore, so that ε_1 would also contribute to $Im\tilde{\varepsilon}$ and ε_2 would also contribute to $Re\tilde{\varepsilon}$. The procedure worked well in this example and it was found that in the $\Gamma \to 0$ limit, $Im[\varepsilon_1(E + i\Gamma)]$ exactly agreed with $\varepsilon_2(E)$ given by Eq. (1). Was this good match just fortuitous? In the case of an optical constant function with more than one functionality over the spectrum, one wonders if Adachi procedure is applicable and, in case it is, which functionality must be selected to extend it to C^+. The present paper provides an answer to these questions.

A similar procedure to avoid divergences was used by the same author to fit the optical constants of several groups of materials [11,12,13,14,15,16,17,18], where functionalities coincident with and also different to the one in Eq. (1) were used. A common feature to all these examples is that the function describing ε_2 was nonzero at some energy range and zero at some other, or more generally, the function was piecewise, i.e., it had more than one functionality over the spectrum. In all these examples, the procedure to avoid divergences was based on adding in a phenomenological manner an extra parameter, Γ, as an imaginary energy.

Apparently, the procedure has not been demonstrated, but it worked with all the materials and models in which it was applied. In the following, a demonstration of the method and the conditions for it to apply are presented.

The dielectric function of any material in nature $\tilde{\varepsilon}(E)$ must satisfy, by virtue of Titchmarsh theorem, that $\tilde{\varepsilon}(E + i\Gamma)$ is analytic in C^+, i.e., for any $\Gamma>0$ and for any real E. There is an important concept for analytic functions: analytic continuation. If a function is analytic in a given subset, it must have a radius of convergence centered at any point within the subset in which the function is analytic. By moving such center point towards the edge of the subset, there may be a new radius of convergence that enables extending further the analytic range, and so on. Since the dielectric function is analytic in the full C^+, one can continue such process to fill C^+. Analytic continuation is unique.

In the process of performing such continuation for an optical-constant function, problems might arise on the real axis R, since $\tilde{\varepsilon}(E)$ is not strictly required to be analytic on R, but only in C^+. Nevertheless, since we will be dealing with specific models with a known functionality, such as Adachi's above example, one will be able to evaluate whether a specific model is or is not analytic in parts of the real axis and in a subset around them.

In the above example of Adachi's model, ε_1 in Eq. (3), interpreted as a function of a complex variable, involves a branch cut in the range $E_g < E < E_c$ originated in the logarithm. Energy points in the branch-cut photon-energy range are not valid to perform analytic continuation, because at a branch cut the function is not analytic in an open subset, since there is a discontinuity when crossing it. Regarding the rest of the real axis, either $0 \leq E < E_g$ or $E > E_c$ (such ranges further extend symmetrically to the negative semi-axis), $\varepsilon_1(E)$ given by Eq. (3) is analytic in these ranges and there are open subsets centered at any such real energies (hence the subsets entering both the upper and the lower complex plane) with no singularity. Hence analytic continuation can be started from such ranges of the real axis towards C^+. In these ranges, ε_2 is null.

Figure 1 displays the process of analytic continuation for the above example with a branch cut between E_g and E_c. If one starts at any real energy in the small energy range ($x_1<E_g$) or large energy range ($x_2>E_c$) and one continues through C^+ following any continuous curve, such as γ_1 for x_1 or γ_2 for x_2, one can fill up all C^+ assuming that the model function is analytic and has no poles in C^+, which are required conditions for any function describing the optical constants of any material; the example of Eqs. (1) and (3) satisfies these requirements. The only range that we precisely know not to be able to continue analytically to is $[E_g, E_c]$ branch cut (and the negative-energy symmetric range). In analogy, there is no analytic continuation starting from any energy on the branch cut, since there is no open subset where the function is analytic. The possibility to continue the function from outside the branch cut but not from the branch cut is key to the present demonstration. Yet, the limit of the analytic function on the real axis at the branch-cut range, even though not analytic any more at the branch cut, it must still provide both ε_1 and ε_2 in the limit, by virtue of Titchmarsh's theorem.

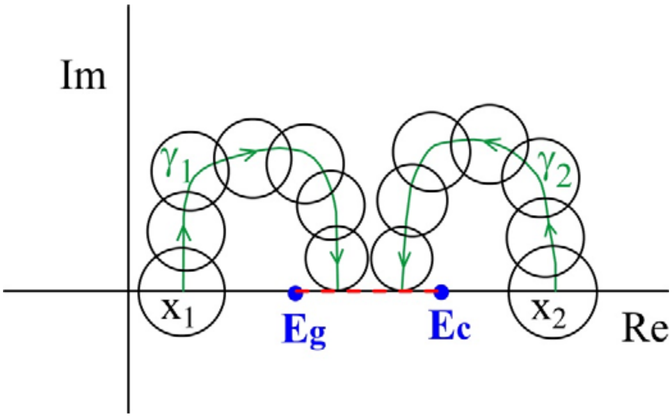

Fig. 1. Analytic continuation of a function starting on the real axis at x_1 or x_2, where the function is analytic in an open subset, following curves γ_1 and γ_2. E_g and E_c are the limits of the branch cut (dashed line). γ_1 and γ_2 can approach the branch cut but cannot cross it, just reach it in the limit.

Analytic continuation of the dielectric function in the allowed range is performed in the following way:

$$\tilde{\varepsilon}(E+i\Gamma)=\sum_{k=0}^{\infty}\frac{d^k\tilde{\varepsilon}(E)}{dE^k}\frac{(i\Gamma)^k}{k!}=\sum_{k=0}^{\infty}\frac{d^k\varepsilon_1(E)}{dE^k}\frac{(i\Gamma)^k}{k!}+i\sum_{k=0}^{\infty}\frac{d^k\varepsilon_2(E)}{dE^k}\frac{(i\Gamma)^k}{k!}=\varepsilon_1(E+i\Gamma) \quad (4)$$

Such expansion assumes that the dielectric function is analytic at the real energy E and in an open subset. Summations correspond to Taylor series expansion around E. However, the expansion of ε_2 in the allowed range is null since ε_2 and all its derivatives are null in the $[0,E_g)$ and (E_c,∞) ranges according to Eq. (1), which gets to the desired result: the full dielectric function at the shifted energy E+iΓ equals ε_1 at that same energy. This means that an imaginary energy shift of ε_1 results in a shift of the full dielectric function $\tilde{\varepsilon}$ to C^+. This shift turns it analytic and, according to [8], it results in optical-constant smoothening, which regularizes possible divergences. This explains Adachi's procedure.

As said above, the expansion of Eq. (4) cannot be made from any photon energy in the $[E_g,E_c]$ range (the branch cut, including its edges), because the dielectric function is not analytic in an open subset. If continuation were possible also from the branch cut, where ε_2 is not null, its expansion would not be null anymore and its contribution would be added to the expansion of ε_1, whereas the expansion of ε_1 would keep functionally the same as in Eq. (3), since ε_1 has a single functionality. Therefore, a hypothetical analytic continuation from the [E_g,E_c] range would not be coincident with the one from outside this range, and hence the analytic continuation would not be unique, but it must be. This helps interpret why analytic continuation cannot be made from [E_g,E_c] range.

The above example involves the existence of a branch cut (and a second symmetric branch cut at negative energies). Let us see that such a branch cut arises in that ε_2 is piecewise and it is null in a spectral range, regardless of the specific function used for ε_2. Let $\varepsilon_2(E)$ be a piecewise function (of real energy E) that is null outside (a,b), with $b>a\geq 0$. $\varepsilon_2(E)$ must be odd, so it must satisfy $\varepsilon_2(E)=-\varepsilon_2(-E)$ in the $(-b,-a)$ range. $\varepsilon_1(E)$ is obtained with KK dispersion relation (Hilbert transform) [Eq. (2)]:

$$\varepsilon_1(E)-1=\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')}{E'-E}dE'+\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')}{E'+E}dE' \tag{5}$$

The second integral of Eq. (5) arises in the contribution of ε_2 symmetric term at negative energies in the $(-b,-a)$ range. A procedure to calculate the Hilbert transform of Eq. (5) consists in subtracting out the singularity due to the denominator cancellation at $E'=E$ or at $E'=-E$ [19]:

$$\varepsilon_1(E)-1=\frac{1}{\pi}\varepsilon_2(E)\int_a^b\frac{1}{E'-E}dE'+\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')-\varepsilon_2(E)}{E'-E}dE'-\frac{1}{\pi}\varepsilon_2(E)\int_a^b\frac{1}{E'+E}dE'+\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')+\varepsilon_2(E)}{E'+E}dE' \tag{6}$$

which results in:

$$\varepsilon_1(E)-1=\frac{1}{\pi}\varepsilon_2(E)\left[ln\left|\frac{b-E}{a-E}\right|+ln\left|\frac{a+E}{b+E}\right|\right]+\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')-\varepsilon_2(E)}{E'-E}dE'+\frac{1}{\pi}\int_a^b\frac{\varepsilon_2(E')+\varepsilon_2(E)}{E'+E}dE' \tag{7}$$

The intrinsic singularity of the Hilbert transform has turned into removable in the integrals of Eq. (7), whereas the singularity has been transferred to the logarithm terms.

The above integral resulting in the logarithm terms was performed for real energies. If one shifts the integration axis slightly upwards or downwards in the complex plane, the logarithms involve a complex argument and hence the logarithm undergoes a discontinuity when crossing the negative real semi-axis, i.e., for energies satisfying $a<E<b$ or $-b<E<-a$. Such discontinuity is proportional to 2πi and it is due to the branch cut of the logarithm function such as when using the logarithm principal value. Hence each logarithm gives rise to a branch cut, which extends to the (a,b) range and to its symmetrical range, i.e., to the range where the original $\varepsilon_2(E)$ function was not identically zero. This explains why the piecewise function results in a branch cut. The branch cut results in a discontinuity of the imaginary part of the dielectric function when crossing the real axis at (a,b) and $(-b,-a)$ ranges.

The logarithms in Eq. (7) turn null for all real energies only when $b\to\infty$ and $a\to 0$, i.e., when the original $\varepsilon_2(E)$ function stops being piecewise. In other words, by extending the range where $\varepsilon_2(E)$ is nonzero, the term involving the branch cut decays until it turns 0 when $\varepsilon_2(E)$ is defined with a single functionality in the full spectrum. The obtained branch cut is then intrinsic to the use of a piecewise function. Additionally, there might be extra branch cuts, poles or branch points originated in the specific functionality of ε_2 and hence of ε_1. Here we only refer to the specific branch cut originated in that ε_2 is piecewise, and any extra branch cut or singularity originated in the specific functionality of $\varepsilon_2(E)$ does not undermine the fundamental reasoning.

Adachi's procedure can be also extended to more general piecewise functions, regardless of being or not null in some spectral range. Let us assume that ε_2 is defined with one functionality $\varepsilon_{2,1}$ in the (a_0, a_1) energy range, with functionality $\varepsilon_{2,2}$ in the (a_1, a_2) energy range,…, and so on to the m-th functionality; each $\varepsilon_{2,k}$ term is assumed to be null outside its definition range. We represent this as:

$$\varepsilon_2(E) = \sum_{k=1}^{m} \varepsilon_{2,k}(E) \tag{8}$$

Let $\tilde{\varepsilon}$ be the optical-constant model with such $\varepsilon_2(E)$. Each k-range defined with a specific $\varepsilon_{2,k}$ function can be treated separately to provide $\tilde{\varepsilon}_k$ to finally add all separate ranges together: $\sum_k \tilde{\varepsilon}_k$. According to the above demonstration for a function that was null outside its definition range, each $\tilde{\varepsilon}_k$ satisfies:

$$\tilde{\varepsilon}_k(E + i\Gamma) = \varepsilon_{1,k}(E + i\Gamma) \tag{9}$$

where $\tilde{\varepsilon}_k(E + \mathrm{i}\Gamma)$ represents the new dielectric function for the k-th functionality obtained after introducing Adachi's damping coefficient Γ. Hence the full dielectric function, which involves all individual functionalities of the piecewise function, is given by:

$$\tilde{\varepsilon}(E + i\Gamma) = \sum_k \tilde{\varepsilon}_k(E + i\Gamma) = \sum_k \varepsilon_{1,k}(E + i\Gamma) = \varepsilon_1(E + i\Gamma) \qquad (10)$$

Hence Adachi procedure works for any piecewise function, regardless of being or not null at any range. Regarding branch cuts of the total dielectric function, there will be a branch cut for each of the above m terms, which will extend to the aggregated (a_0, a_m) range for the total dielectric function. If we now extend the aggregated spectral range to the full spectrum (as it was done above for a function with a single non-identically null functionality), i.e., we do a_0=0 and a_m=∞, this is not enough to turn null the term that involves the aggregated branch cut: it would be also required that all functionalities of ε_2 be the same, so that, again, the term with the branch cut turns null only when the function stops being piecewise.

A discontinuity of ε_2 at the connection energy between two adjacent definition ranges originates a divergence at ε_1, which is solved with Adachi's imaginary energy shift, such as at E_c of Eq. (1). But even if the connection energy between two adjacent functionalities results in no discontinuity of the dielectric function, the two different functionalities assure a divergence starting at a certain derivation order. The discontinuity at such derivation order and above is solved with Adachi procedure too, such as at E_g of Eq. (1), where the dielectric function is discontinuous starting at the second derivative.

An analogous procedure to the one invented by Adachi could be applied when $\varepsilon_1(E)$ were the piecewise function that is non-null in one range and zero elsewhere, and one would want to solve the corresponding divergences of $\varepsilon_2(E)$. All reasoning would be the same as above. In such case, $\varepsilon_2(E)$ would be obtained from $\varepsilon_1(E)$ through the inverse Hilbert transform (the ε_1-to-ε_2 KK relation), and its continuation in C^+ would be performed as:

$$\tilde{\varepsilon}(E + i\Gamma) = \varepsilon_1(E + i\Gamma) + i\varepsilon_2(E + i\Gamma) = i\varepsilon_2(E + i\Gamma) \qquad (11)$$

because the continuation would be performed starting from a spectral range where ε_1 and all its derivatives were null. With the same reasoning, a branch cut is expected at the nonzero range of $\varepsilon_1(E)$, and the real part of the complex dielectric function is expected to be discontinuous at the branch cut. An analogous extension of $\varepsilon_1(E)$ to a piecewise function with various functionalities is also straightforward.

Let us see the conditions for Adachi procedure to apply. According to Titchmarsh theorem, any pair of square-integrable Hilbert transforms on the real axis may be extended as an analytic function in C^+ from which the Hilbert transformed functions are the limit of that extended function onto the real axis. But to apply Adachi procedure we need that analytic continuation can be performed from some real energy in which the function is analytic in an open subset. If ε_2 is a piecewise function with various functionalities, we need that each contribution to ε_2 can be continued analytically from some real energy in the null-range of each contribution. In order to select an optical model to describe a material, one would try to use an as-smooth and as-simple a function as possible, so that the analyticity condition might be typically satisfied at some real energy.

Such analytic continuation from a given real energy needs to satisfy Titchmarsh theorem conditions. The theorem requires that the function be analytic in C^+, so that one has to check that Adachi's continuation has no poles, branch cuts or branch points in C^+. Finally, it requires that the continued function in C^+ be square integrable along any line in C^+ that is parallel to the real axis.

Summarizing, the conditions for Adachi procedure to be applicable are the following: 1) there is some real energy range where ε_1, obtained as ε_2 Hilbert transform, is analytic in an open subset of energies (hence somewhat penetrating the complex plane), 2) ε_1 extended to C^+ is analytic and has no poles or singularities there, and 3) ε_1 extended to C^+ is square integrable along any line in C^+ that is parallel to the real axis. For a piecewise dielectric function with various non-null functionalities, it is sufficient that each individual contributions to the piecewise function satisfies conditions 1) to 3).

3. Adachi procedure compared with the Lorentzian integration procedure

A procedure was developed to turn non-analytic optical-constant models into analytic by integrating the full dielectric function (or the complex refractive index) with a Lorentzian function [7]:

$$\int_{-\infty}^{\infty}[\tilde{\varepsilon}(E')-1]\frac{a/\pi}{a^2+(E'-E)^2}dE'=\tilde{\varepsilon}_A(E)-1 \tag{12a}$$

Such integration avoids singularities or discontinuities of the optical function $\tilde{\varepsilon}$ and the result is an analytic function $\tilde{\varepsilon}_A(E)$, even if the original function $\tilde{\varepsilon}$ was not analytic. Integration is governed by parameter a>0; the smaller a, the closer the modified model $\tilde{\varepsilon}_A$ to the original model $\tilde{\varepsilon}$, but analyticity may be lost again when a=0, which recovers the original model (the Lorentzian function turns a Dirac delta). Integration can be also performed starting only with ε_1

$$-\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_1(E')-1}{E'-E-ia}dE' = \tilde{\varepsilon}_A(E) - 1 \tag{12b}$$

or starting only with ε_2:

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\varepsilon_2(E')}{E'-E-ia}dE' = \tilde{\varepsilon}_A(E) - 1 \tag{12c}$$

A recent research [8] has shown that optical constants can be extended for photon energies in C$^+$ through convolution of the optical constants with a Lorentzian weight function:

$$\int_{-\infty}^{\infty}[\tilde{\varepsilon}(E') - 1]\frac{a/\pi}{a^2+(E'-E)^2}dE' = \tilde{\varepsilon}(E + ia) - 1 \tag{13}$$

Hence integration of $\tilde{\varepsilon}(E)$ with a Lorentzian weight function provides $\tilde{\varepsilon}(E + ia)$, i.e., the dielectric function at the energy shifted to C$^+$ by ia. Such integration is mathematically a convolution and in practice it results in progressive optical-constant smoothening as one gets farther away from the real axis. If we compare Eq. (12a) with Eq. (13) it is seen that the analyticized function is coincident with the function shifted to C$^+$. The above is valid for dielectrics or semiconductors that have no poles. Conductors with a Drude-like pole at E=0 require an extra term in Eq. (13).

Here comes the question: if shifting the optical constants to C$^+$ results in optical-constant regularization by turning it analytic, hence avoiding poles or other singularities on the real axis, is the above convolution coincident with Adachi procedure? The answer is yes. Let us see why.

Let $\tilde{\varepsilon}$ be an optical-constant model with ε_2 (a parallel reasoning can be made starting with ε_1) defined through a piecewise function with a single, non-identically null functionality in a given range (a,b), the function being null outside that range, except for the aforementioned symmetric term. If we integrate it with a Lorentzian function, we get an analytic dielectric function [7] that equals the dielectric function shifted in C$^+$ [8]. From any such energy in C$^+$

one can continue analytically to any other energy in C^+. One can even reach the real axis in the limit, according to Tichmarsh theorem. On the real axis ε_1 must be the Hilbert transform of ε_2 by virtue of Titchmarsh theorem. On the real axis away from [*a*,*b*], $\varepsilon_2(E)$=0 and the full dielectric function is coincident with ε_1. Hence the Lorentzian integration procedure is consistent with Adachi procedure.

Let us now start with Adachi procedure and see how it converges with the Lorentzian integration procedure. Let ε_2 be null outside [*a*,*b*]. Let ε_1 be the Hilbert transform of ε_2. In fact, to apply Titchmarsh theorem it must be satisfied that ε_1 (ε_2) be the direct (inverse) Hilbert transform of ε_2 (ε_1) and that ε_1+iε_2 be a square integrable function over the spectrum of real energies. Let us start analytic continuation of ε_1 at an energy on the real axis away from [*a*,*b*] where it is satisfied that ε_1 is analytic in an open subset; the latter is not any requirement from Titchmarsh theorem, but it is an extra requirement that is added here. Let us continue ε_1 to C^+ through Adachi procedure. Adachi extends the specific function of the optical model, which originally is a real function, to C^+ by just replacing the real variable with a complex one. Most standard functions enable such extension, although one would have to check if the specific function makes sense in C^+ and if it is analytic and lacks poles, branch cuts and branch points in C^+, and if it is square integrable on any horizontal line parallel to the real axis, as it was specified in the previous section. Obviously, Adachi function extended to C^+ must also converge on the real axis to the original value of ε_1, since otherwise such continuation would be nonsense. Now let us see that Adachi continuation equals the above continuation with the Lorentzian integration procedure. In [8] it was proved that the continuation of the dielectric function from the real axis to C^+ with an analytic function satisfying the conditions of Titchmarsh theorem is unique; hence the present two procedures of analytic continuation must converge on the same function. Even though it may seem that Adachi continuation was not performed from the full $\tilde{\varepsilon}$ but from only ε_1, in the real energy range from which ε_1 was continued, it is satisfied that $\tilde{\varepsilon} = \varepsilon_1$, so that in fact the full function was used. Additionally, parameter Γ of Adachi procedure and parameter *a* of the Lorentzian integration procedure represent the same parameter and have the same value.

In principle, it cannot be discarded that Adachi's continuation of a given function might result in a non-fully analytic function in C^+, or in a function that is not square integrable. In that case Adachi procedure would not provide a function satisfying the requirements of a causal optical model and it would not be coincident with the Lorentzian integration procedure.

The above demonstration was limited to a piecewise function with a single non-null functionality; the case of a piecewise function with any number of functionalities is again straightforward following the reasoning in Section 2. Summarizing, Adachi procedure, assuming the function satisfies the above requirements, is equivalent to integrating the dielectric function with a Lorentzian function.

The Lorentzian integration procedure provides us with a second interpretation of the origin of the branch cut. Let us start with $\varepsilon_2(E)$ which is non-identically null in a certain range and null outside it. The dielectric function can be anlyticized either with the full dielectric function using Eq. (12a) or with only $\varepsilon_2(E)$ using Eq. (12c). If the latter integral were replaced with a summation over discrete $1/(E_i'-E-\mathrm{i}a)$ functions, one would get a pole at each $E= E_i'-\mathrm{i}a$ energy. Such pole is located in the lower half plane C^- as long as a is positive. By going back from the summation to the integral in the non-null range of $\varepsilon_2(E)$, the discrete poles turn into a full segment of infinitesimal singularities between the extreme energies, which results in the branch cut.

The above has demonstrated that Adachi procedure is equivalent to the Lorentzian integration procedure for a dielectric function with one part defined as a piecewise function. For a dielectric function that is not piecewise but defined with a single functionality, the two procedures must be still equivalent. The only difference here is that, if no part of $\tilde{\varepsilon}$ is piecewise, what must be shifted to C^+ is then the full dielectric function: $\varepsilon_1(E+i\Gamma)+i\varepsilon_2(E+i\Gamma)$.

Adachi's broadening with a constant damping parameter is equivalent to a Lorentzian broadening. Kim et al. [9] tried to generalize such broadening to include Gaussian broadening; even though this resulted in integration that could not be done analytically in closed form, they found a simplification of the problem by turning the damping parameter Γ into a Gaussian function of energy, which was also used in [10] and [20]. Such generalization can still be solved by a shift of the dielectric function to C^+. In this case the shift is not constant over the spectrum, but it depends on photon energy in the same way as the damping parameter does.

4. Examples of Adachi procedure and comparison with Lorentzian integration

Three different functions used by Adachi to model several materials and material groups are addressed in this research. Each of these functions was turned analytic both with Adachi procedure and with the Lorentzian integration procedure in order to illustrate that the two procedures are coincident. In the examples, it was taken $\Gamma = a$ and two values were used for all functions: 0.01 and 0.2 eV.

The first Adachi function F1 is the one given by Eqs. (1) and (3). Adachi used this function to model the indirect bandgap contribution in semiconductors (Eqs. 5 and 7 in [5]), specifically in III-V semiconductors (Eq. 24 in [12]), in $Al_xGa_{1-x}As$ alloys (Eq. 17 in [14]), in $In_{1-x}Ga_xAs_yP_{1-y}$ alloys (Eq. 27 in [15]), and in Si and Ge (Eq. 19 in [17]). Figure 2 compares the two procedures applied on F1. Adachi procedure was calculated with Eq. (3), where E was replaced with $E+i\Gamma$. ε_1 divergence at E_c is solved with either procedure, and the larger Γ, the smoother both ε_1 and ε_2. The divergence of the second derivative at E_g is also removed.

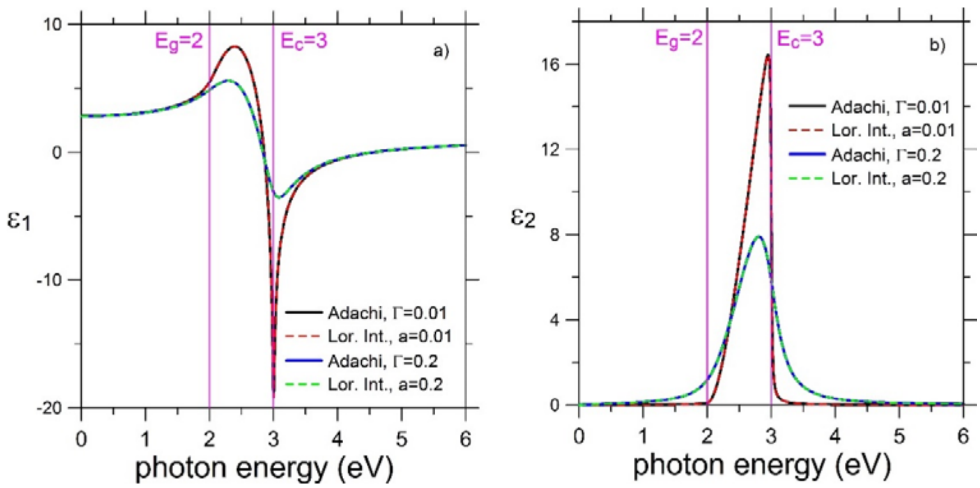

Fig. 2. F1 dielectric function [a) ε_1, b) ε_2] once analyticized both with Adachi and with the Lorentzian integration procedure. Two shift parameters were used: $\Gamma = a = 0.01$ eV and 0.2 eV.

Figure 3 presents a 3-dimensional plot of F1. To help the eye, the non-null ranges of the original ε_2, with real energy in (2,3) and (-3,-2) ranges (hence

E_g=2 eV and E_c=3 eV), are plotted with a different color. The line *ImE*=+*a* is highlighted in red. The branch cuts are at the intersection of the black line at *ImE*=0 with the non-null ranges of ε_2.

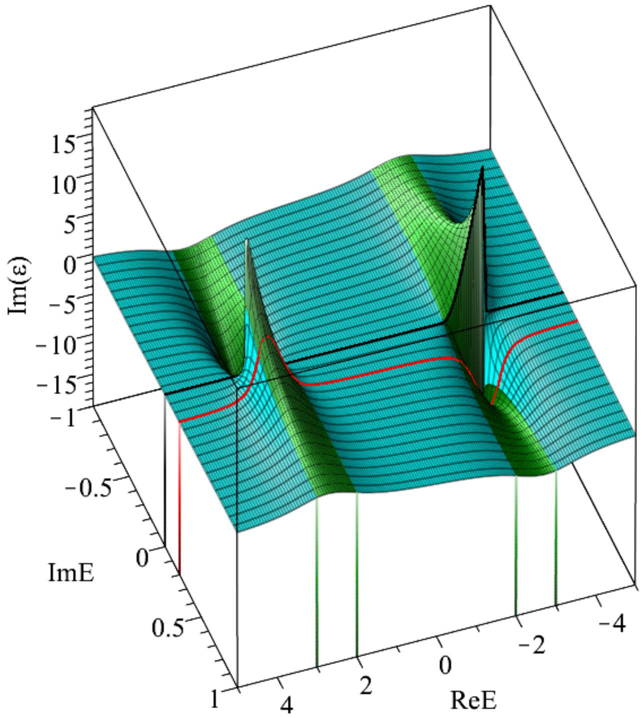

Fig. 3. $Im[\tilde{\varepsilon}(ReE + iImE)]$ vs. ReE (the real part of energy) and vs. ImE (the imaginary part of energy) for Adachi F1 function with the same parameters of the function plotted in Fig. 2. Calculations were performed with Γ=*a*=0 eV. The non-null range of ε_2 on the real axis (from 2 to 3 eV and from -3 to -2 eV) is plotted with a different color. *ImE*=0 eV, which contains the branch cut, is plotted as a black line. The branch cut is the intersection of this black line with the non-null ranges of ε_2. The cross section *ImE*=0.2 eV, which is shown in blue color in Fig. 2b), is plotted here as a red line.

The second Adachi function F2 that was addressed is the following:

$$\varepsilon_2(E) = \frac{\pi B E_1^2}{E^2}\Theta(E - E_1) \tag{14}$$

$$\varepsilon_1(E) - 1 = -\frac{B E_1^2}{E^2}\ln\left(1 - \frac{E^2}{E_1^2}\right) \tag{15}$$

Hence ε_2 is non-null for E>E_1. It was used to model 2-dimensional M_0 minima of E_1 and $E_1+\Delta_1$ transitions in III-V semiconductors (Eqs. 16 and 17 in [12]), in Si and Ge (Eqs. 11 and 12 in [13]), in $Al_xGa_{1-x}As$ alloys (Eqs. 10 and 11 in [14]), in $In_{1-x}Ga_xAs_yP_{1-y}$ alloys (Eqs. 17 and 18 in [15]), and in α-Sn (Eqs. 6 and 8 in [16]). This function has a divergence at E_1. This divergence was removed with the two procedures and again the two procedures provided the same function. Adachi procedure was applied on Eq. (15), The resulting functions are not displayed for shortness.

The third Adachi function F3 is defined as follows:

$$\varepsilon_2(E) = \frac{A}{E^2}(E - E_0)^{1/2}\Theta(E - E_0) \tag{16}$$

$$\varepsilon_1(E) = \frac{AE_0^{1/2}}{E^2}\left[2 - \left(1 + \frac{E}{E_0}\right)^{1/2} - \left(1 - \frac{E}{E_0}\right)^{1/2}\Theta(E_0 - E)\right] \tag{17}$$

It was used in 3-dimensional M_0 critical points of E_0 and $E_0+\Delta_0$ transitions in III-V semiconductors (Eqs. 3 and 5 in [12]), in Si and Ge (Eqs. 2 and 3 in [13]), in $In_{1-x}Ga_xAs_yP_{1-y}$ alloys (Eqs. 5 and 6 in [15]), and in semiconductors in general (Eqs. 16 and 17 in [5]). In fact, Adachi did not apply his procedure on this function since neither Eq. (16) nor Eq. (17) involves any divergence. However, the first derivative of both ε_1 and ε_2 diverge at E_0, so that F3 is not analytic at this energy. In practice, this divergence at the derivative may not be found in real materials, so that it is worth avoiding it. The divergence at the derivative was also removed with Adachi procedure using Eq. (17) and with the Lorentzian integration procedure too. The two procedures were successfully applied to avoid such divergence. Hence either procedure is valid to solve a lack of analyticity not only for a discontinuity at the dielectric function but at any of its derivatives. The resulting functions are not displayed for shortness.

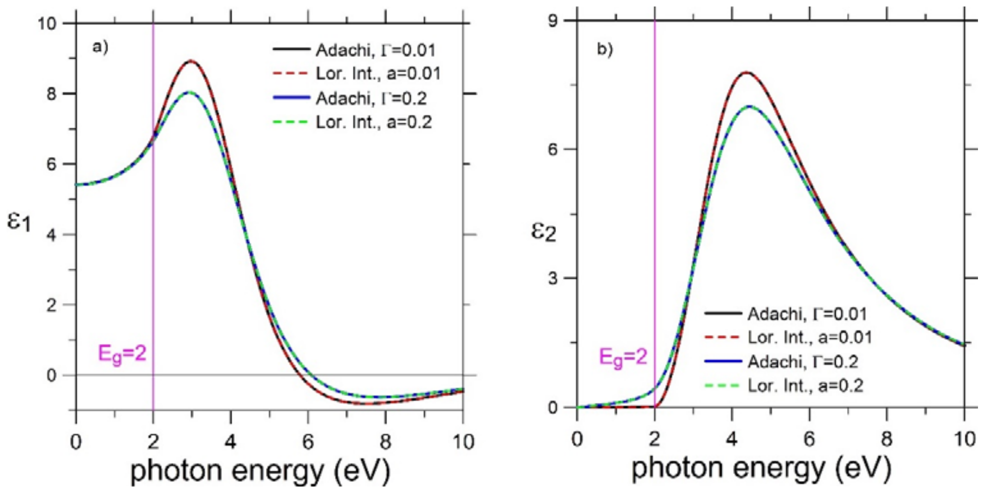

Fig. 4. TL model dielectric function [a) ε_1, b) ε_2] once analyticized both with Adachi and with Lorentzian integration procedure. Two shift parameters were used: $\Gamma=a=0.01$ eV and 0.2 eV. The model parameters used are given in Table 1.

Let us now apply Adachi procedure on a popular optical model: the Tauc-Lorentz (TL) model [21], which was derived to model the optical constants of amorphous semiconductors and insulators. ε_2 in TL model is non-null at energies larger than a certain bandgap energy E_g and it turns null below this energy. Figure 4 displays the two analyticizing procedures applied to the TL model. To apply Adachi model, the expression obtained in [21] for ε_1 was used. This procedure had already been turned analytic with the Lorentzian integration procedure [6] and here it is seen how it can be turned analytic with Adachi procedure too. The two procedures result in the same dielectric function for $\Gamma=a$. The parameters used in this example of TL model, as defined in [21] and [6], are given in Table 1.

The Lorentzian integration procedure had been also applied to the Cody-Lorentz (CL) and Cody-Lorentz-Urbach (CLU) models [7], which were derived to model the optical constants of amorphous semiconductors. This model, which was developed by Ferlauto et al. [22], involves two functionalities for ε_2: a sort of Lorentz behaviour above some energy E_t close to the material bandgap E_g, and an Urbach tail below that energy. This model is then a good example of a piecewise function with two functionalities. The two ranges altogether extend to the full spectrum. The Urbach-tail part in CLU model had been slightly modified in [7] to avoid a divergence at E=0, and this modification is used here.

Figure 5 displays the analyticized CLU model with the function developed in [7] compared with Adachi procedure: again, the two procedures are coincident. As a reminder, Adachi's procedure has been applied separately to each ε_1 term that was obtained with each of the two functionalities of ε_2, and the two have been later added. The Lorentzian integration procedure can be directly used on the two contributions to CLU model at a time. The parameters used in this example of CLU model, as defined in [22] and [7] are shown in Table 1.

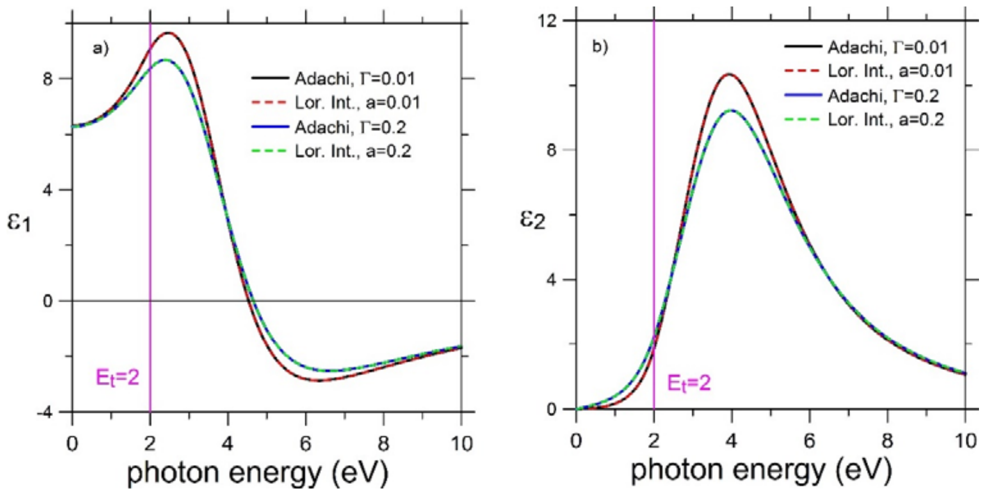

Fig. 5. CLU model dielectric function [a) ε_1, b) ε_2] once analyticized both with Adachi and with the Lorentzian integration procedure. Two shift parameters were used: $\Gamma=a=0.01$ eV and 0.2 eV. The model parameters used are given in Table 1.

Table 1. Parameters used in TL and CLU models plotted in Figs. 4 and 5.

Tauc-Lorentz		Cody-Lorentz-Urbach	
A	120 eV	A	60 eV
E_0	4 eV	E_0	4 eV
C	4 eV	Γ (CL)	4 eV
E_g	2 eV	E_g	1 eV
		E_t	2 eV
		E_p	2 eV
$\varepsilon_{1,\infty}$	1	$\varepsilon_{1,\infty}$	1
$\Gamma=a$	0.01, 0.2 eV	$\Gamma=a$	0.01, 0.2 eV

Each of the above models involves at least one branch cut. Figure 6 displays the behaviour of the dielectric function at significant energies close to or in the branch cut of functions F1, TL, and CLU.

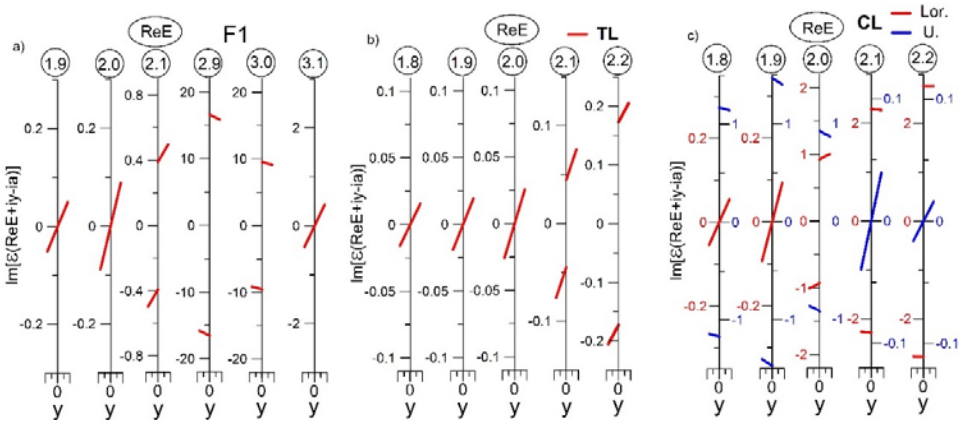

Fig. 6. $Im[\tilde{\varepsilon}(ReE + iy - ia)]$ vs. y for various values of ReE (the real part of energy) at or near the edge of the branch cut. Plots correspond to Adachi F1 (a), and to TL (b) and CLU (c) models. Calculations were performed with Γ=a=0.2 eV and with the same parameters of functions plotted in Figs. 2, 4, and 5 and Table 1. The imaginary part of energy was shifted by -ia for the discontinuity to appear centered at y=0. For CLU model, red (blue) color stands for the branch cut originated in the Lorentzian (Urbach tail) contribution to the dielectric function.

To display the branch cut, the real axis is intercepted with vertical scans (y variable) at different real values of the complex photon energy: E=ReE+i(y-a). The -ia shift is included for all discontinuities to be centered at y=0. It has to be noted that the analyticized function does not keep the branch cut on the real axis, but shifts it to C^-, so that the modified function is already analytic on the real axis. The edge of the branch cut is seen to be the limit of the discontinuity, and no discontinuity is seen away from the branch cut. For F1, the discontinuity is located between E_g (2 eV) and E_c (3 eV). TL branchcut is located at $E>E_g$. CLU is defined with two functionalities, so that it involves two branch cuts for positive real energies separated at E_t=2 eV which altogether span the full spectrum. The two contributions in CLU model, the Lorentzian and the Urbach tail ones, are plotted in different colors, so that it can be observed that the Lorentzian branch cut extends to $E>E_t$=2eV, whereas the Urbach tail branch cut extends to $E<E_t$. In all cases, the branch cut extension is coincident with the non-null definition of ε_2. The plotted discontinuity is for $Im[\tilde{\varepsilon}(E)]$, according to what was said in section 2 about the discontinuity of the logarithm at the branch cut. $Re[\tilde{\varepsilon}(E)]$ does not present any discontinuity.

5. Conclusions

Adachi procedure to avoid divergences in optical-constant models, which had been phenomenologically applied on many materials, has been rigorously analysed and the mathematical fundaments that support it have been established, along with the conditions for it to apply. Adachi procedure, which consists in shifting ε_1 to imaginary photon energies, has been seen to originate in that ε_2 is defined as a piecewise function with some range where ε_2 is null. The shift can be performed from real energies where ε_2 is null. The fact that ε_2 is piecewise implies that the dielectric function has a branch cut in the spectral range where ε_2 is non-identically null. The branch cut involves a discontinuity at the imaginary part of the dielectric function. The above can be generalized to any piecewise function.

One condition for Adachi procedure to apply is that the energy range on the real axis from where the shift to C^+ is applied be analytic in an open subset. The other conditions to enable Adachi procedure are that the function extended to C^+ is analytic with no poles and is square integrable on any line parallel to the real axis in C^+.

Adachi procedure has been proved to be equivalent to a former procedure to analyticize optical models which is based on a convolution of the dielectric function with a Lorentzian function. The equivalence is exemplified with three functions used by Adachi and with two popular models based on piecewise functions: Tauc-Lorentz and Cody-Lorentz-Urbach.

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Disclosures

The authors declare no conflicts of interest.

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