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Abstract. For the case of finite lifetime broadening the standard Kubo formula for the optical conductivity tensor is rederived in terms of Green's functions by using contour integrations, whereby finite temperatures are accounted for by using the Fermi–Dirac distribution function. For zero lifetime broadening, the present formalism is related to expressions well known in the literature. Numerical aspects of how to calculate the corresponding contour integrals are also outlined.

1. Introduction

A general theory of linear response functions was formulated several decades ago [1–3] that became the basis of numerous studies of correlation functions, susceptibilities and transport properties in solid matter. Although early attempts have already been devoted within this theoretical framework to magneto-optical phenomena, i.e., the Faraday and the Kerr effect [2, 4], it was the rapid development of both band-structure methods and computational facilities that brought about the renaissance in this field from the end of the 1980s (see [5, 6] and references therein). This progress was built on the assumption that the original expression for the linear response functions, derived on the basis of a non-relativistic approach, is still valid when applying relativistic band-structure methods. Recently, this has been rigorously confirmed by Huhne and Ebert [7].

Within an independent-particle picture the interband part of the optical conductivity tensor at finite temperatures, $\Sigma_{\mu\nu}(\omega)$, is given by [1, 3]

$$\Sigma_{\mu\nu}(\omega) = \frac{\hbar}{iV} \sum_{m,n} \frac{f(\epsilon_n)(1 - f(\epsilon_m))}{\epsilon_n - \epsilon_m} \left\{ \frac{J_{nm}^{\mu} J_{mn}^{\nu}}{\hbar\omega + \epsilon_n - \epsilon_m + i\delta} + \frac{J_{nm}^{\nu} J_{mn}^{\mu}}{\hbar\omega + \epsilon_m - \epsilon_n + i\delta} \right\} \quad (1)$$

where ω is the frequency, $f(\epsilon)$ is the Fermi function, V is the volume of the system and the $J_{nm}^{\mu} = \langle n|J^{\mu}|m\rangle$ are the matrix elements of the current-density operator J^{μ} ($\mu = x, y, z$) with respect to the eigenfunctions $|n\rangle$ of the one-electron Hamiltonian corresponding to energy eigenvalues ϵ_n. Lifetime-broadening effects due to different scattering processes are partially accounted for by a finite value of $\delta = \hbar/\tau \sim 0.03$ Ryd, where τ can be associated with a relaxation time [5, 6]. Such a lifetime effect can be incorporated naturally into linear response theory either by assuming an adiabatic switching on of the external field $\phi(r, t) = \phi(r)e^{t/\tau}$ [8] or, equivalently, by convoluting the corresponding frequency-dependent conductivity for $\delta \to +0$ with a Lorentzian of finite halfwidth δ.

10451

Expression (1) is usually directly evaluated by applying standard band-structure methods for ordered bulk (three-dimensional translationally invariant) systems by associating the states $|n\rangle$ with (three-dimensional) Bloch functions [2, 5]. This kind of approach, however, cannot be extended easily to layered systems or systems with a surface, i.e., to systems with (at best) two-dimensional translational symmetry. Furthermore, it is totally unsuited to dealing with disorder such as interdiffusion effects in magnetic multilayer systems.

For zero lifetime broadening an alternative approach consists of splitting equation (1) into an absorptive and a dispersive part, which in turn are interrelated via the Kramers–Kronig relations [4, 6]. Thus it is sufficient to directly calculate the absorptive part only, the corresponding Kubo formula of which can be expressed in terms of Green's functions as was shown by Butler [9] for $\omega = 0$, and which was used recently by Banhart [10] for $\omega > 0$. Even much earlier, Luttinger [8] derived a general formula for the conductivity tensor which builds on the Green's function of the system. However, when using this method the corresponding energy integrals have to be taken along the real axis which makes a calculation of $\Sigma_{\mu\nu}(\omega)$ enormously tedious and also numerically hard to control.

In the present work a suitable extension of Luttinger's formula is given in terms of contour integrations that avoids the above-mentioned numerical difficulties, and is suitable for applications to magnetic multilayer systems and for treating alloying effects (interdiffusion etc) by means of the coherent potential approximation (CPA).

2. Contour integrations

Following Luttinger [8], equation (1) can be rewritten as

$$\Sigma_{\mu\nu}(\omega) = \frac{\sigma_{\mu\nu}(\zeta) - \sigma_{\mu\nu}(0)}{\zeta} \tag{2}$$

where $\zeta = \omega + i\delta/\hbar$ and

$$\sigma_{\mu\nu}(\zeta) = \frac{i}{V} \sum_{m,n} \frac{f(\epsilon_n) - f(\epsilon_m)}{\hbar\zeta + \epsilon_n - \epsilon_m} J_{nm}^{\mu} J_{mn}^{\nu}. \tag{3}$$

For simplicity, in what follows, we denote $\sigma_{\mu\nu}(\zeta)$ as $\sigma_{\mu\nu}(\omega)$ [11], in whose calculation we will be careful to keep it in mind that we have a finite imaginary part of the denominator in equation (3). Consider a pair of eigenvalues ϵ_n and ϵ_m. For a suitable contour $\mathcal{C}$ in the complex-energy plane (see figure 1) the residue theorem implies

$$\oint_{\mathcal{C}} \mathrm{d}z \, \frac{f(z)}{(z - \epsilon_n)(z - \epsilon_m + \hbar\omega + i\delta)}$$
$$= -2\pi i \frac{f(\epsilon_n)}{\epsilon_n - \epsilon_m + \hbar\omega + i\delta} + 2i\delta_T \sum_{k=-N_2+1}^{N_1} \frac{1}{(z_k - \epsilon_n)(z_k - \epsilon_m + \hbar\omega + i\delta)} \tag{4}$$

where the $z_k = \epsilon_F + i(2k - 1)\delta_T$ (ϵ_F is the Fermi energy, k_B the Boltzmann constant, T the temperature and $\delta_T = \pi k_B T$) are the so-called Matsubara poles. In equation (4) it was supposed that the N_1 and N_2 Matsubara poles in the upper and lower semi-plane lie within the contour $\mathcal{C}$, respectively, i.e.,

$$(2N_1 - 1)\delta_T < \delta_1 < (2N_1 + 1)\delta_T \tag{5}$$

$$(2N_2 - 1)\delta_T < \delta_2 < (2N_2 + 1)\delta_T. \tag{6}$$

Equation (4) can be rearranged as

$$\mathrm{i}\frac{f(\epsilon_n)}{\hbar\omega + \epsilon_n - \epsilon_m + \mathrm{i}\delta} = -\frac{1}{2\pi}\oint_{\mathcal{C}}\mathrm{d}z\,\frac{f(z)}{(z-\epsilon_n)(z-\epsilon_m+\hbar\omega+\mathrm{i}\delta)}$$
$$+\mathrm{i}\frac{\delta_T}{\pi}\sum_{k=-N_2+1}^{N_1}\frac{1}{(z_k-\epsilon_n)(z_k-\epsilon_m+\hbar\omega+\mathrm{i}\delta)}. \tag{7}$$

Similarly, by choosing a contour $\mathcal{C}'$ as shown in figure 2, the following expression:

$$-\mathrm{i}\frac{f(\epsilon_m)}{\hbar\omega + \epsilon_n - \epsilon_m + \mathrm{i}\delta} = \frac{1}{2\pi}\oint_{\mathcal{C}'}\mathrm{d}z\,\frac{f(z)}{(z-\epsilon_m)(z-\epsilon_n-\hbar\omega-\mathrm{i}\delta)}$$
$$+\mathrm{i}\frac{\delta_T}{\pi}\sum_{k=-N_1+1}^{N_2}\frac{1}{(z_k-\epsilon_m)(z_k-\epsilon_n-\hbar\omega-\mathrm{i}\delta)} \tag{8}$$
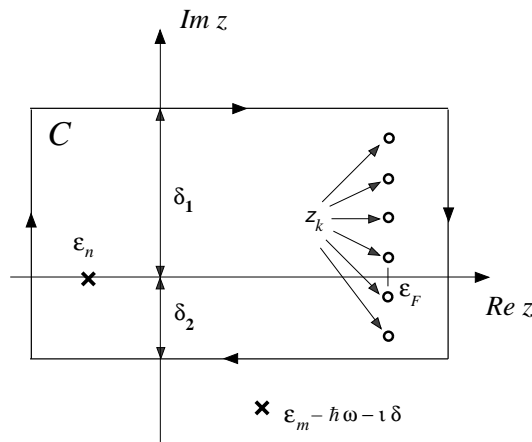

Figure 1. The contour in the complex plane corresponding to the integration in equation (4).
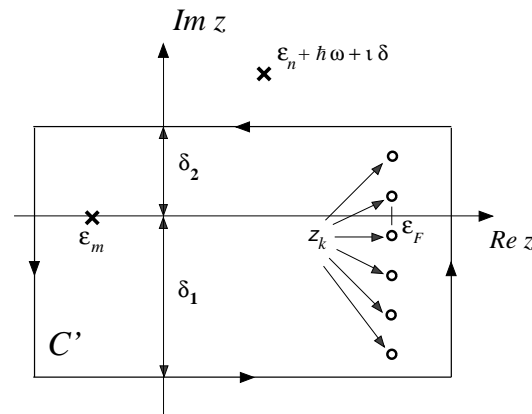

Figure 2. The contour in the complex plane corresponding to the integration in equation (8).

can be derived. On inserting equations (7) and (8) into equation (3) and closing the contours at ∞ and $-\infty$, $\sigma_{\mu\nu}(\omega)$ is given by

$$\sigma_{\mu\nu}(\omega) = -\frac{1}{2\pi V}\left\{\oint_C dz\, f(z)\sum_{m,n}\frac{J^\mu_{nm}J^\nu_{mn}}{(z-\epsilon_n)(z-\epsilon_m+\hbar\omega+\mathrm{i}\delta)}\right.$$

$$-\oint_{C'} dz\, f(z)\sum_{m,n}\frac{J^\mu_{nm}J^\nu_{mn}}{(z-\epsilon_m)(z-\epsilon_n-\hbar\omega-\mathrm{i}\delta)}\right\}$$

$$+\mathrm{i}\frac{\delta_T}{\pi V}\left\{\sum_{k=-N_2+1}^{N_1}\sum_{m,n}\frac{J^\mu_{nm}J^\nu_{mn}}{(z_k-\epsilon_n)(z_k-\epsilon_m+\hbar\omega+\mathrm{i}\delta)}\right.$$

$$+\sum_{k=-N_1+1}^{N_2}\sum_{m,n}\frac{J^\mu_{nm}J^\nu_{mn}}{(z_k-\epsilon_m)(z_k-\epsilon_n-\hbar\omega-\mathrm{i}\delta)}\right\}. \tag{9}$$

It is now straightforward to rewrite equation (9) in terms of the resolvent [12]:

$$G(z) = \sum_n \frac{|n\rangle\langle n|}{z-\epsilon_n} \tag{10}$$

such that

$$\sigma_{\mu\nu}(\omega) = -\frac{1}{2\pi V}\left\{\oint_C dz\, f(z)\,\mathrm{Tr}[J^\mu G(z+\hbar\omega+\mathrm{i}\delta)J^\nu G(z)]\right.$$

$$-\oint_{C'} dz\, f(z)\,\mathrm{Tr}[J^\mu G(z)J^\nu G(z-\hbar\omega-\mathrm{i}\delta)]\right\}$$

$$+\mathrm{i}\frac{\delta_T}{\pi V}\left\{\sum_{k=-N_2+1}^{N_1}\mathrm{Tr}[J^\mu G(z_k+\hbar\omega+\mathrm{i}\delta)J^\nu G(z_k)]\right.$$

$$+\sum_{k=-N_1+1}^{N_2}\mathrm{Tr}[J^\mu G(z_k)J^\nu G(z_k-\hbar\omega-\mathrm{i}\delta)]\right\} \tag{11}$$

where Tr denotes the trace of an operator. By using the quantity given below, originally introduced by Butler [9]:

$$\widetilde{\sigma}_{\mu\nu}(z_1, z_2) = -\frac{1}{2\pi V}\,\mathrm{Tr}[J^\mu G(z_1)J^\nu G(z_2)] \tag{12}$$

for which the following symmetry relations apply:

$$\widetilde{\sigma}_{\nu\mu}(z_2, z_1) = \widetilde{\sigma}_{\mu\nu}(z_1, z_2)$$
$$\widetilde{\sigma}_{\mu\nu}(z_1^*, z_2^*) = \widetilde{\sigma}_{\nu\mu}(z_1, z_2)^* = \widetilde{\sigma}_{\mu\nu}(z_2, z_1)^* \tag{13}$$

$\sigma_{\mu\nu}(\omega)$ can be written as

$$\sigma_{\mu\nu}(\omega) = \oint_C dz\, f(z)\widetilde{\sigma}_{\mu\nu}(z+\hbar\omega+\mathrm{i}\delta, z) - \oint_{C'} dz\, f(z)\widetilde{\sigma}_{\mu\nu}(z, z-\hbar\omega-\mathrm{i}\delta)$$

$$-2\mathrm{i}\delta_T\left\{\sum_{k=-N_2+1}^{N_1}\widetilde{\sigma}_{\mu\nu}(z_k+\hbar\omega+\mathrm{i}\delta, z_k) + \sum_{k=-N_1+1}^{N_2}\widetilde{\sigma}_{\mu\nu}(z_k, z_k-\hbar\omega-\mathrm{i}\delta)\right\}$$

$$\tag{14}$$

which, because of the reflection symmetry for the contours $\mathcal{C}$ and $\mathcal{C}'$ (see figures 1 and 2) and the relations in equation (13), can be transformed to

$$
\sigma_{\mu\nu}(\omega) = \oint_{\mathcal{C}} \mathrm{d}z \; f(z)\widetilde{\sigma}_{\mu\nu}(z + \hbar\omega + \mathrm{i}\delta, z) - \left(\oint_{\mathcal{C}} \mathrm{d}z \; f(z)\widetilde{\sigma}_{\mu\nu}(z - \hbar\omega + \mathrm{i}\delta, z)\right)^{*}
$$

$$
- 2\mathrm{i}\delta_{T} \sum_{k=-N_{2}+1}^{N_{1}} \{\widetilde{\sigma}_{\mu\nu}(z_{k} + \hbar\omega + \mathrm{i}\delta, z_{k}) + \widetilde{\sigma}_{\mu\nu}(z_{k} - \hbar\omega + \mathrm{i}\delta, z_{k})^{*}\}. \tag{15}
$$

Equation (15) displays the central result of the present work: it compactly expresses the optical conductivity tensor in terms of contributions of a contour integral and those due to Matsubara poles. The quantities occurring of the type $\widetilde{\sigma}_{\mu\nu}(z_{1}, z_{2})$ are now exactly of the form for which substitutional disorder (CPA) for layered systems [13, 14] can be treated. It should be noted that in the case of site-diagonal terms—see [14]—in principle for the evaluation of the contour integrals the 'irregular' part of the Green's function also has to be included. Since the inhomogeneous CPA for semi-infinite systems and the corresponding Kubo–Greenwood approach to electric transport are discussed at length in [14], no further discussion with respect to layered systems is needed.

3. Integration along the real axis: the limit of zero lifetime broadening

In this section we give the relationship of equation (15) to formulations existing in the literature. For this reason the contour $\mathcal{C}$ is deformed to the real axis such that the contributions from the Matsubara poles vanish. On using the relations in equation (13), equation (15) reduces to

$$
\sigma_{\mu\nu}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; f(\epsilon)[\widetilde{\sigma}_{\mu\nu}(\epsilon + \hbar\omega + \mathrm{i}\delta, \epsilon + \mathrm{i}0) - \widetilde{\sigma}_{\mu\nu}(\epsilon + \hbar\omega + \mathrm{i}\delta, \epsilon - \mathrm{i}0)]
$$

$$
- \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; f(\epsilon)[\widetilde{\sigma}_{\mu\nu}(\epsilon - \mathrm{i}0, \epsilon - \hbar\omega - \mathrm{i}\delta) - \widetilde{\sigma}_{\mu\nu}(\epsilon + \mathrm{i}0, \epsilon - \hbar\omega - \mathrm{i}\delta)]. \tag{16}
$$

That is,

$$
\sigma_{\mu\nu}(\omega) = -\frac{1}{2\pi V} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; f(\epsilon) \, \mathrm{Tr}\{J^{\mu} G(\epsilon + \hbar\omega + \mathrm{i}\delta) J^{\nu}\{G^{+}(\epsilon) - G^{-}(\epsilon)\}
$$

$$
+ J^{\mu}\{G^{+}(\epsilon) - G^{-}(\epsilon)\}J^{\nu} G(\epsilon - \hbar\omega - \mathrm{i}\delta)\} \tag{17}
$$

where we have introduced upper and lower limits for the resolvents [12]. On taking the limit $\delta \to 0$, equation (17) becomes equivalent to equation (5.15) of reference [8] for $q = 0$:

$$
\sigma_{\mu\nu}(\omega) = -\frac{1}{2\pi V} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; f(\epsilon) \, \mathrm{Tr}\{J^{\mu} G^{+}(\epsilon + \hbar\omega) J^{\nu}\{G^{+}(\epsilon) - G^{-}(\epsilon)\}
$$

$$
+ J^{\mu}\{G^{+}(\epsilon) - G^{-}(\epsilon)\}J^{\nu} G^{-}(\epsilon - \hbar\omega)\}. \tag{18}
$$

Note that by shifting in the second term of equation (18) the argument of the integration by $\hbar\omega$, the *Hermitian* part of $\sigma_{\mu\nu}(\omega)$ can be expressed as

$$
\sigma_{1,\mu\nu}(\omega) \equiv \frac{1}{2}(\sigma_{\mu\nu}(\omega) + \sigma_{\nu\mu}(\omega)^{*}) = -\frac{1}{4\pi V} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \; (f(\epsilon) - f(\epsilon + \hbar\omega))
$$

$$
\times \mathrm{Tr}\left\{J^{\mu}\{G^{+}(\epsilon + \hbar\omega) - G^{-}(\epsilon + \hbar\omega)\}J^{\nu}\{G^{+}(\epsilon) - G^{-}(\epsilon)\}\right\}. \tag{19}
$$

Since quite clearly $\sigma_{1,\mu\nu}(0) = 0$, from equation (2) we get

$$
\Sigma_{1,\mu\nu}(\omega) = \sigma_{1,\mu\nu}(\omega)/\omega
$$

as used in reference [10].

In order to obtain the correct zero-frequency formula, one has to take first the $\omega \to 0$ limit of equation (16) and then, after insertion into equation (2), the $\delta \to 0$ limit has to be performed. Making use of the analyticity of the Green's functions in the upper and lower complex semi-planes, this leads to [16]

$$
\Sigma_{\mu\nu}(0) = -\frac{\hbar}{2\pi V} \int_{-\infty}^{\infty} d\epsilon \; f(\epsilon)
$$
$$
\times \mathrm{Tr}\left\{ J^{\mu} \frac{\partial G^{+}(\epsilon)}{\partial \epsilon} J^{\nu}[G^{+}(\epsilon) - G^{-}(\epsilon)] - J^{\mu}[G^{+}(\epsilon) - G^{-}(\epsilon)]J^{\mu} \frac{\partial G^{-}(\epsilon)}{\partial \epsilon} \right\}
$$
(20)

which can be integrated by parts. The corresponding expression at $T = 0$ for the diagonal elements yields Butler's original formula [9]:

$$
\Sigma_{\mu\mu}(0)_{(T=0)} = -\frac{\hbar}{4\pi V} \mathrm{Tr}\{J^{\mu}[G^{+}(\epsilon_F) - G^{-}(\epsilon_F)]J^{\mu}[G^{+}(\epsilon_F) - G^{-}(\epsilon_F)]\}.
$$
(21)

4. Practical evaluation of the contour integrals

Returning to equation (15) we are left with the task of evaluating the contour integrals that occur, in a manner suitable for computational purposes. This is particularly demanding because, in principle, integrations from $-\infty$ to ∞ are involved. Recalling figure 1, it is essential to note that the integration paths can be chosen arbitrarily with the only constraint being that the one in the lower complex semi-plane should lie in the range $0 > \mathrm{Im}(z) > -\delta$. It is trivial to show that, if the contributions from the core states are not considered, the contour $\mathcal{C}$ can be closed at ϵ_b (the bottom of the valence band) which lies energetically just below the regime of valence states. Consequently, the integrals in equation (15) can be split up as follows:

$$
\oint_{\mathcal{C}} dz \; f(z)\widetilde{\sigma}_{\mu\nu}(z \pm \hbar\omega + i\delta, z)
$$
$$
= \int_{\epsilon_b+i0}^{\infty+i\delta_1} dz \; f(z)\widetilde{\sigma}_{\mu\nu}(z \pm \hbar\omega + i\delta, z) - \int_{\epsilon_b-i0}^{\infty-i\delta_2} dz \; f(z)\widetilde{\sigma}_{\mu\nu}(z \pm \hbar\omega + i\delta, z).
$$
(22)

Because of the fast decay of the Fermi function $f(z)$ for $\mathrm{Re}(z) > \epsilon_F$, the integrals on the rhs of equation (22) can be terminated at

$$
\epsilon_u = \epsilon_F + n\,k_BT \qquad (n \simeq 5\text{--}10).
$$

Finally, after manipulating the contributions from the Matsubara poles—see equation (15)—the optical conductivity (or rather the zero-wavenumber current–current correlation function [11]) can be written as

$$
\sigma_{\mu\nu}(\omega) = \sigma_{\mu\nu}^{1}(\omega) + \sigma_{\mu\nu}^{2}(\omega) + \sigma_{\mu\nu}^{3}(\omega)
$$
(23)

where

$$
\sigma_{\mu\nu}^{1}(\omega) = \int_{\epsilon_b+i0}^{\epsilon_u+i\delta_1} dz \; f(z)\widetilde{\sigma}_{\mu\nu}(z + \hbar\omega + i\delta, z) - \left(\int_{\epsilon_b+i0}^{\epsilon_u+i\delta_1} dz \; f(z)\widetilde{\sigma}_{\mu\nu}(z - \hbar\omega + i\delta, z) \right)^{*}
$$
(24)

and

$$\sigma_{\mu\nu}^2(\omega) = \int_{\epsilon_b-\mathrm{i}0}^{\epsilon_u-\mathrm{i}\delta_2} \mathrm{d}z \, f(z)\widetilde{\sigma}_{\mu\nu}(z+\hbar\omega+\mathrm{i}\delta, z) - \left(\int_{\epsilon_b-\mathrm{i}0}^{\epsilon_u-\mathrm{i}\delta_2} \mathrm{d}z \, f(z)\widetilde{\sigma}_{\mu\nu}(z-\hbar\omega+\mathrm{i}\delta, z) \right)^* \tag{25}$$

and also

$$
\begin{aligned}
\sigma_{\mu\nu}^3(\omega) = &-2\mathrm{i}\delta_T \sum_{k=N_2+1}^{N_1} \{\widetilde{\sigma}_{\mu\nu}(\epsilon_F+\hbar\omega+\mathrm{i}[\delta+(2k-1)\delta_T], \epsilon_F+\mathrm{i}(2k-1)\delta_T) \\
&+ \widetilde{\sigma}_{\mu\nu}(\epsilon_F-\hbar\omega+\mathrm{i}[\delta+(2k-1)\delta_T], \epsilon_F+\mathrm{i}(2k-1)\delta_T)^*]\} \\
&- 2\mathrm{i}\delta_T \sum_{k=1}^{N_2} \{\widetilde{\sigma}_{\mu\nu}(\epsilon_F+\hbar\omega+\mathrm{i}[\delta+(2k-1)\delta_T], \epsilon_F+\mathrm{i}(2k-1)\delta_T) \\
&+ \widetilde{\sigma}_{\mu\nu}(\epsilon_F-\hbar\omega+\mathrm{i}[\delta+(2k-1)\delta_T], \epsilon_F+\mathrm{i}(2k-1)\delta_T)^* \\
&+ \widetilde{\sigma}_{\mu\nu}(\epsilon_F+\hbar\omega+\mathrm{i}[\delta-(2k-1)\delta_T], \epsilon_F-\mathrm{i}(2k-1)\delta_T) \\
&+ \widetilde{\sigma}_{\mu\nu}(\epsilon_F-\hbar\omega+\mathrm{i}[\delta-(2k-1)\delta_T], \epsilon_F-\mathrm{i}(2k-1)\delta_T)^*\}.
\end{aligned}
\tag{26}
$$

Preliminary calculations show that on choosing $\delta \simeq 0.05$ Ryd, $\delta_1 \simeq 0.1$–0.15 Ryd and using Gaussian quadrature, a total of 30–100 energy points (depending on $\hbar\omega$) is sufficient to sample the above energy integrals. Furthermore, since most of these energy points lie either below the valence band or far enough away from the real axis (the energy point closest to the real axis is at $z_1 = \epsilon_F + \mathrm{i}\delta_T$, where for $T = 300$ K, $\delta_T \simeq 6$ mRyd), the Brillouin-zone integrals occurring (see reference [14]) can be evaluated by using a sufficiently small set of k-points in the surface Brillouin zone, thus ensuring excellent numerical stability.

5. Summary

In the present paper, by using a finite lifetime broadening (or a finite adiabatic switch-on parameter) we reformulated the expression for the (linear response) optical conductivity tensor in terms of contour integrations such that Green's functions (resolvents) naturally appear and finite temperatures are represented by the Fermi–Dirac distribution function. For zero lifetime broadening the traditional expressions for the conductivity tensor in terms of the Green's function are recovered. Finally, a scheme for calculating the contour integrals that occur, in a numerically efficient way, is suggested. Although primarily applications to *ab initio* calculations of magneto-optical properties of ordered and disordered thin films in terms of the fully relativistic spin-polarized screened Korringa–Kohn–Rostoker method [14, 15] are currently under way, it should be noted that the present method can also be used to calculate other linear response functions, just as readily as it can easily be extended to the evaluation of non-linear response functions.

Acknowledgments

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