INVERSE FIRST MOMENT FOR THE WEIGHTED MAGNETOREFLECTION

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Received 27 February 1978

A rigorous dispersion theoretic derivation of the inverse first moment of the magnetoreflection weighted by the normal reflection is presented. Schnatterly's formula for the zeroth moment of the magnetoreflection is briefly discussed.

1. Introduction

Some time ago, Schnatterly [1] proposed that the zeroth moment of the magnetoreflection could be expressed as

$$\int_0^\infty [R_+(\omega) - R_-(\omega)]\,d\omega = -\omega_c, \tag{1}$$

where $R_+(\omega)$ and $R_-(\omega)$ are the reflectivities for left and right circularly polarized light, and ω_c is the cyclotron frequency eH/mc. The argument leading to eq. (1) centers on the assumption that the applied magnetic field causes a small perturbation on the electronic energy levels, and hence

$$R_+(\omega) - R_-(\omega) \approx [\partial R(\omega)/\partial\omega]\,\omega_c, \tag{2}$$

where $R(\omega)$ is the normal reflectivity in the absence of the field. Eq. (1) follows directly on integration over the interval $(0, \infty)$, and the case $R(0) = 1$ has been assumed.

In a recent paper, Smith [2] applied the above argument to the phase, and obtained the zeroth moment

$$\int_0^\infty [\theta_+(\omega) - \theta_-(\omega)]\,d\omega = \pi\omega_c. \tag{3}$$

Smith also showed that this result could be derived rigorously using dispersion theoretic methods. It was suggested that it may not be possible to derive the corresponding magnetoreflection moment, eq. (1), via dispersion theoretic procedures.

Since magnetoreflection measurements offer a potentially useful probe of molecular structure, particularly for solids with high absorption, knowledge of any of the moments of this quantity would serve as a valuable check on the quality of experimental data. In addition, Schnatterly suggested that eq. (1) may be a useful way to determine the cyclotron mass factor.

2. Theory

A large amount of work has appeared in the past few years in which the zeroth and higher moments of many optical properties have been given explicitly [2–10]. For the reflectivity (both normal and magneto-) however, the moments are not known. The reason for this situation is connected with a fundamental distinction between the generalized reflectance and other generalized optical properties such as the dielectric constant, refractive index, etc. The real and imaginary parts of the generalized optical properties of the latter group can be written as Hilbert transform pairs. For the generalized reflectance, no Hilbert transform pair can be written between $R(\omega)$ and $\theta(\omega)$. If such a relationship did exist, the zeroth moment could be obtained directly from a dispersion theory analysis. For this reason, a proof of eq. (1) using dispersion theory directly is not possible. The simplest dispersion relations that exist for the reflectance involve the quantity $\ln R(\omega)$.

A quantity of direct experimental interest is the magnetoreflection weighted by the normal reflectance

$$\mathcal{R}(\omega) = \frac{\Delta R(\omega)}{R(\omega)} = \frac{2[R_+(\omega) - R_-(\omega)]}{R_+(\omega) + R_-(\omega)} . \quad (4)$$

An analytic result is now derived for the inverse first moment of the quantity $\mathcal{R}(\omega)$. The generalized reflectance for left and right polarized modes is

$$\ln \tilde{r}_\pm(\omega) = \tfrac{1}{2} \ln R_\pm(\omega) + i\theta_\pm(\omega). \quad (5)$$

If we write

$$R_+(\omega) = R(\omega) + \tfrac{1}{2}\Delta R(\omega), \quad (6)$$

$$R_-(\omega) = R(\omega) - \tfrac{1}{2}\Delta R(\omega), \quad (7)$$

then

$$\ln \frac{\tilde{r}_+(\omega)}{\tilde{r}_-(\omega)} = \tfrac{1}{2} \ln\left[\frac{R(\omega) + \frac{1}{2} R(\omega)}{R(\omega) - \frac{1}{2} R(\omega)}\right] + i\Delta\theta(\omega), \quad (8)$$

where

$$\Delta\theta(\omega) = \theta_+(\omega) - \theta_-(\omega). \quad (9)$$

Eq. (8) can be expanded to obtain

$$\ln[\tilde{r}_+(\omega)/\tilde{r}_-(\omega)] = [\tfrac{1}{2}\mathcal{R}(\omega) + \tfrac{1}{24}\mathcal{R}^3(\omega) + \tfrac{1}{160}\mathcal{R}^5(\omega) + ...] + i\Delta\theta(\omega), \quad (10)$$

provided $-1 < \mathcal{R} < 1$.

The function $\ln[\tilde{r}_+(\omega)/\tilde{r}_-(\omega)]$ is analytic in the upper half complex frequency plane. To obtain the desired moment, we consider the following function

$$F(\omega) = \ln[\tilde{r}_+(\omega)/\tilde{r}_-(\omega)]/(\omega^2 - \omega_0^2) \quad (11)$$

and perform a contour integration of $F(\omega)$ on a semicircle contour that includes the real axis indented at $\omega = \pm\omega_0$ (into the upper half plane) and around the semicircle arc in the upper half plane. The result is

$$P\int_{-\infty}^{\infty} \frac{\ln[\tilde{r}_+(\omega)/\tilde{r}_-(\omega)]}{(\omega^2 - \omega_0^2)} d\omega = \frac{\pi i}{2\omega_0} \ln\left[\frac{\tilde{r}_+(\omega_0)\tilde{r}_-(-\omega_0)}{\tilde{r}_-(\omega_0)\tilde{r}_+(-\omega_0)}\right]. \quad (12)$$

Employing the crossing relations (for real ω)

$$\tilde{r}_\pm^*(\omega) = \tilde{r}_\mp(-\omega), \quad (13)$$

$$\Delta\theta(-\omega) = \Delta\theta(\omega), \quad (14)$$

$$\mathcal{R}(-\omega) = -\mathcal{R}(\omega) \quad (15)$$

simplifies eq. (12) to yield

$$P\int_0^\infty \frac{\Delta\theta(\omega)}{\omega^2 - \omega_0^2} d\omega = (\tfrac{1}{4}\pi/\omega_0)\mathcal{R}(\omega_0) \times [1 + \tfrac{1}{12}\mathcal{R}^2(\omega_0) + \tfrac{1}{80}\mathcal{R}^4(\omega_0) + ...]. \quad (16)$$

For many situations of physical interest, $|\Delta R(\omega)|/R(\omega) \approx 10^{-4}$–$10^{-6}$, and it is therefore possible to truncate the series expansion at the first term in eq. (16) without introducing any significant error. Therefore

$$P\int_0^\infty \frac{\Delta\theta(\omega)}{\omega^2 - \omega_0^2} d\omega = (\tfrac{1}{4}\pi/\omega_0)\mathcal{R}(\omega_0). \quad (17)$$

Eq. (17) is now integrated over the range $(0, \infty)$, to give

$$\tfrac{1}{4}\pi \int_0^\infty \omega_0^{-1}\mathcal{R}(\omega_0)\, d\omega_0 = \int_0^\infty d\omega_0\, P\int_0^\infty \frac{\Delta\theta(\omega)}{\omega^2 - \omega_0^2} d\omega, \quad (18)$$

which simplifies on interchanging the order of integration and noting the result [8]

$$\mathrm{P}\int_0^\infty \frac{d\omega_0}{\omega^2-\omega_0^2} = -\tfrac{1}{4}\pi^2\,\delta(\omega), \tag{19}$$

to yield

$$\int_0^\infty \omega^{-1}\mathcal{R}(\omega)\,d\omega = 0. \tag{20}$$

Eq. (20) is the simplest moment formula to be expected for the weighted magnetoreflectivity. The reason for this is not hard to see. If we employ a generalization of $F(\omega)$ of the form

$$F(\omega) = \omega^m \ln[\tilde{r}_+(\omega)/\tilde{r}_-(\omega)], \tag{21}$$

where m is a nonnegative integer, then the above argument leads to the result

$$\mathrm{P}\int_0^\infty \frac{\omega^m}{\omega^2-\omega_0^2}\{\tfrac{1}{2}\mathcal{R}(\omega)[1+(-1)^{m+1}] + i\Delta\theta(\omega)[1+(-1)^m]\}\,d\omega$$
$$= \tfrac{1}{2}\pi i\,\omega_0^{m-1}\{\tfrac{1}{2}\mathcal{R}(\omega_0)[1+(-1)^m] + i\Delta\theta(\omega_0)[1+(-1)^{m+1}]\}. \tag{22}$$

The terms of interest for generating moments of the magnetoreflection are obtained from eq. (22) for even values of m. The number of convergent moments for a specific material is determined by the asymptotic behavior of $\mathcal{R}(\omega)$ as $\omega \to \infty$. The most important situation is

$$\lim_{\omega\to\infty} \mathcal{R}(\omega) \simeq 1/\omega. \tag{23}$$

With this constraint on the asymptotic behavior, eq. (22) is restricted to $m = 0$, which leads to the inverse first moment given in eq. (20). Higher negative moments diverge due to the singularity at $\omega = 0$.

Eq. (20) is an exact result for any medium, subject to the usual assumptions needed to employ dispersion theory, and the validity of the series truncation in eq. (16). In contrast to the Schnatterly formula, eq. (20) does not provide a method for determining the cyclotron mass factor. Eq. (20) can serve as useful *necessary* criterion on the quality of magnetoreflectance data expressed via the function $\mathcal{R}(\omega)$.

Finally, we remark that eq. (20) may be derived from the dispersion relation for the derivative of the normal reflection,

$$\frac{1}{R(\omega)}\frac{\partial R(\omega)}{\partial\omega} = \frac{4\omega}{\pi}\,\mathrm{P}\int_0^\infty \frac{\partial\theta(\omega')}{\partial\omega'}[(\omega')^2-\omega^2]^{-1}\,d\omega, \tag{24}$$

combined with eq. (2). This alternative derivation of eq. (20) should not, however, be used to support the credibility of eq. (1).

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