Some bounds for the absorption coefficient of an isotropic nonconducting medium

Frederick W. King
Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, Wisconsin, 54701
(Received 20 August 1981)

Lower bounds are derived for the quantities $\max[\omega^{-1/2}\kappa(\omega)]$ and $\max[\omega^{-1}\kappa(\omega)]$, where $\kappa(\omega)$ is the absorptive part of the generalized refractive index and $\omega\in[0,\infty)$. An upper bound is obtained for $\min[\kappa(\omega)]$ where ω lies in the finite spectral range $[\omega_1,\omega_2]$ (ω_1 and ω_2 arbitrary). The results are restricted to a nonconducting isotropic medium, and no specific assumptions on the nature of the medium are employed.

The determination of the sharpest bounds $\theta_{\min},\theta_{\max}$ for any medium for the optical constant $O(\omega)$, i.e.,

$$\theta_{\min}\le O(\omega)\le\theta_{\max}\ ,\quad \omega\in(\omega_1,\omega_2) \tag{1}$$

where the spectral range (ω_1,ω_2) may be finite (arbitrary ω_1,ω_2) or infinite, is clearly a problem of great practical significance. This is particularly so if the results are not based on restrictive assumptions specific for a particular material. Any knowledge of $\theta_{\min}$ and $\theta_{\max}$ would be extremely useful in testing the quality of experimental data and would potentially be a powerful adjunct procedure to the standard techniques of optical data analysis using the well known sum rule approach.[1] Unfortunately, very few general relations exist, and these are essentially obvious results which follow directly from the definition of the appropriate optical constants.

The purpose of this Report is to point out the existence of some bounds on $\theta_{\min}$ and $\theta_{\max}$ when $O(\omega)$ is $\omega^{-1}\kappa(\omega)$, $\omega^{-1/2}\kappa(\omega)$, and $\kappa(\omega)$, respectively, where $\kappa(\omega)$ is the extinction coefficient (absorptive part of the generalized refractive index). For the bounds on $\theta_{\max}$, the infinite spectral range is employed, whereas for the bound on $\theta_{\min}$ a finite frequency interval $[\omega_1,\omega_2]$ is employed.

The underlying assumptions used in the derivation of the bounds presented below are as follows. The approach taken makes direct use of some sum rules derived from the Kramers-Kronig relations. The optical constant under consideration is therefore assumed to be a part of a generalized optical constant which is an analytic function in an appropriate frequency domain. The free electron gas model is assumed to be valid to determine the high frequency behavior of the optical constant in question. It is to be emphasized that no assumptions on the specific nature of the medium are made, except that it is nonconducting, and our treatment, has for reasons of simplicity, been restricted to isotropic medium.

If $\theta_{\max}$ denotes the maximum value of $\omega^{-1}\kappa(\omega)$ for $\omega\in[0,\infty)$ and $f(\omega)$ is a weight function, decreasing on $[0,\infty)$, then it follows that[2]

$$\int_0^\infty \omega^{-1}\kappa(\omega)f(\omega)d\omega\le\theta_{\max}\int_0^{\omega'} f(\omega)d\omega\ , \tag{2}$$

where the optimum value of ω' is

$$\omega'=\frac{1}{\theta_{\max}}\int_0^\infty \omega^{-1}\kappa(\omega)d\omega\ . \tag{3}$$

Because $\kappa(\omega)\sim\omega^{-1/2}$ as $\omega\to 0$ for conductors, the integral in Eq. (2) may diverge [the integral in Eq. (3) does diverge], and we have accordingly restricted consideration to the case of nonconductors, for which the integrals in question are convergent. With an appropriate choice for the weight function, i.e., $f(\omega)=\exp(-\alpha^2\omega^2)$, $\alpha>0$, and the simple approximation $1-\alpha^2\omega^2<\exp(-\alpha^2\omega^2)$, then,

$$\int_0^\infty \omega^{-1}\kappa(\omega)(1-\alpha^2\omega^2)d\omega<\int_0^\infty \omega^{-1}\kappa(\omega)e^{-\alpha^2\omega^2}d\omega\le\frac{\theta_{\max}}{\alpha}\int_0^{\alpha\omega'} e^{-\omega^2}d\omega<\frac{\theta_{\max}}{\alpha}\int_0^\infty e^{-\omega^2}d\omega\ .$$

If we employ the well-known sum rules[3-7]

$$\int_0^\infty \omega^{-1}\kappa(\omega)d\omega=\frac{\pi}{2}[n(0)-1]\ , \tag{5}$$

$$\int_0^\infty \omega\kappa(\omega)d\omega=\frac{\pi}{4}\omega_p^2\ , \tag{6}$$

where $n(0)$ is the refractive index at zero frequency and ω_p is the plasma frequency, then Eq. (4) yields

$$\alpha\pi^{1/2}[n(0)-1-\tfrac{1}{2}\alpha^2\omega_p^2]<\theta_{\max} . \quad (7)$$

Optimizing Eq. (7) for the parameter α leads to the following bound:

$$\pi^{1/2}\{\tfrac{2}{3}[n(0)-1]\}^{3/2}/\omega_p<\max\{\omega^{-1}\kappa(\omega)\} , \quad \omega\in[0,\infty) . \quad (8)$$

Improvement of Eq. (7), at the expense of additional complexity, can be obtained by using suitable approximations for the integral $\int_0^{\alpha\omega'}\exp(-\omega^2)d\omega$ appearing in Eq. (4). If $\alpha\omega'<0.752\,763$, the approximation $\exp(-\omega^2)\leq(1+\omega^2)^{-1}$ gives satisfactory results; while for $\alpha\omega'$ greater than the aforementioned value, the approximation[8]

$$\int_0^{\beta}\exp(-\omega^2)d\omega\leq\tfrac{1}{2}\pi^{1/2}-\frac{\exp(-\beta^2)}{\beta+(\beta^2+2)^{1/2}} , \quad \beta>0 \quad (9)$$

is very satisfactory. Using these two approximations, the following improvements on Eq. (7) are obtained:

$$\tfrac{1}{2}\alpha\pi[n(0)-1-\tfrac{1}{2}\alpha^2\omega_p^2]<\theta_{\max}\tan^{-1}\beta , \quad (10)$$

$$\tfrac{1}{2}\alpha\pi[n(0)-1-\tfrac{1}{2}\alpha^2\omega_p^2]<\theta_{\max}\left[\tfrac{1}{2}\pi^{1/2}-\frac{\exp(-\beta^2)}{\beta+(\beta^2+2)^{1/2}}\right] , \quad (11)$$

where $\beta=\alpha\pi[n(0)-1]/2\theta_{\max}$. Optimum values of α in Eqs. (10) and (11) can be found by iterative solution of these equations.

The same approach may be employed to bound $\omega^{-1/2}\kappa(\omega)$. If $\bar{\theta}_{\max}$ denotes $\max[\omega^{-1/2}\kappa(\omega)]$ for $\omega\in[0,\infty)$, and we choose the weight function $f(\omega)=\omega^{-1/2}$, then

$$\int_0^{\infty}[\omega^{-1/2}\kappa(\omega)]\omega^{-1/2}d\omega\leq\bar{\theta}_{\max}\int_0^{\omega'}\omega^{-1/2}d\omega , \quad (12)$$

where

$$\omega'=\frac{1}{\bar{\theta}_{\max}}\int_0^{\infty}\omega^{-1/2}\kappa(\omega)d\omega . \quad (13)$$

From the Buniakowsky-Schwartz inequality, the following result is obtained using Eqs. (4) and (5),

$$\int_0^{\infty}\omega^{-1/2}\kappa(\omega)d\omega\leq2^{-5/4}\pi\omega_p^{1/2}[n(0)-1]^{3/4} . \quad (14)$$

Combining Eqs. (12) and (14) yields

$$\frac{\pi\{2[n(0)-1]\}^{5/4}}{16\omega_p}\leq\max[\omega^{-1/2}\kappa(\omega)] , \quad \omega\in[0,\infty) \quad (15)$$

An estimate for the upper bound on $\min[\kappa(\omega)]$ for the finite spectral range $[\omega_1,\omega_2]$ (arbitrary ω_1,ω_2) can be derived in the following manner. The starting point is the complementary Buniakowsky-Schwartz inequality[9]

$$m_1M_1\int_{\omega_1}^{\omega_2}g^2(\omega)d\omega+m_2M_2\int_{\omega_1}^{\omega_2}f^2(\omega)d\omega\leq(M_1M_2+m_1m_2)\int_{\omega_1}^{\omega_2}f(\omega)g(\omega)d\omega , \quad (16)$$

where

$$0\leq m_1\leq f(\omega)\leq M_1 , \quad 0\leq m_2\leq g(\omega)\leq M_2 \quad \text{for } \omega\in[\omega_1,\omega_2] . \quad (17)$$

There is considerable flexibility in choosing the weight function. Let $g(\omega)=\kappa(\omega)$ and take $f(\omega)=\omega-\omega_1$, then Eq. (16) simplifies to

$$\min[\kappa(\omega)]\leq\frac{\max[f(\omega)]\int_{\omega_1}^{\omega_2}\kappa(\omega)f(\omega)d\omega}{\int_{\omega_1}^{\omega_2}f^2(\omega)d\omega} , \quad (18)$$

which can be simplified using the inequality

$$\int_{\omega_1}^{\omega_2}\kappa(\omega)f(\omega)d\omega<\frac{\pi}{4}\omega_p^2 \quad (19)$$

to yield

$$\min[\kappa(\omega)]<\frac{3\pi\omega_p^2}{4(\omega_2-\omega_1)^2} \quad \text{for } \omega\in[\omega_2,\omega_1] . \quad (20)$$

The bounds derived in this Report only require information on the two asymptotic limits of the generalized refractive index as $\omega\to0$ and $\omega\to\infty$. A central equation used in this work, Eq. (6), is derived from the free electron gas model. If the free electron gas model is refined to yield an expression different from Eq. (6), this change can be readily incorporated into the bounds derived above.

The results obtained in this Report should prove to be a useful supplement to the standard techniques of optical data analysis. In the present investigation, lower bounds for $\max[\omega^{-1}\kappa(\omega)]$ and $\max[\omega^{-1/2}\kappa(\omega)]$ and an upper bound for $\min[\kappa(\omega)]$ have been obtained without making assumptions on the specific nature of the medium. For the purposes of data analysis, it would be of considerable value to obtain the corresponding upper and lower bounds for the aforementioned quantities, both for finite and infinite spectral ranges. Also of considerable interest is the question of how sharp the above bounds can be made. This problem is under investigation.

Acknowledgment is made to the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for support of this research.

---

[1]For a recent detailed application of the sum-rule approach to optical data analysis, see, E. Shiles, T. Sasaki, M. Inokuti, and D. Y. Smith, Phys. Rev. B 22, 1612 (1980).

[2]F. W. King, J. Math. Phys. 22, 1321 (1981).

[3]F. Stern, in *Solid State Physics,* edited by F. Seitz and D. Turnbull (Academic, New York, 1963), Vol. 15, p. 299.

[4]W. M. Saslow, Phys. Lett. A 33, 157 (1970).

[5]M. Altarelli, D. L. Dexter, H. M. Nussenzveig, and D. Y. Smith, Phys. Rev. B 6, 4502 (1972).

[6]A. Villani and A. H. Zimerman, Phys. Rev. B 8, 3914 (1973).

[7]F. W. King, J. Math. Phys. 17, 1509 (1976).

[8]*Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun, (Dover, New York, 1964), p. 298.

[9]J. B. Diaz and F. T. Metcalf, J. Math. Anal. Appl. 9, 278 (1964).