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The Index of Refraction in the Neighbourhood of an Isolated Stark Broadened Spectral Line

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ABSTRACT

The index of refraction in the neighbourhood of a Stark broadened spectral line has been calculated using the Kronig-Kramers relation between the absorption coefficient and the index of refraction. For the absorption coefficient, the function $j_r(x, \alpha)$ given by Griem has been used. A discussion of the results as they apply to the hook method of measuring oscillator strengths is given, and it is shown that errors of the order of 5% can occur in the oscillator strength if the conventional formula for anomalous dispersion is used.

INTRODUCTION

The parallelism between the index of refraction and the absorption coefficient represented mathematically by the Kronig-Kramers dispersion relation is often exploited experimentally to measure plasma quantities by using the refractivity when these same quantities could have been measured by absorption or emission experiments. For instance, electron density measurements of plasmas are often obtained by using the behaviour of the index of refraction in wavelength regions distant from spectral lines. The analogous absorption coefficient experiment measures the continuum intensity in such spectral regions but is subject to errors due to scattered light. More relevant is that the index of refraction in the regions near spectral lines is used to obtain oscillator strengths (or, equivalently, number densities in excited states) by means of the hook method. The analogous absorption coefficient measurement would measure equivalent widths of spectral lines.

Because of this close relationship between the two quantities, any processes which modify the shape of the absorption coefficient of a spectral line (such as Doppler broadening, pressure broadening, etc.) also disturb the index of refraction. However, the effect of these processes on the index of refraction is not known for many important cases. For instance, the effect of quasistatic microelectric fields on the absorption coefficient after the treatment of Griem, Baranger, Kolb and Oertel[2] is shown in Figure 1; the figure illustrates that the cores of the line are reasonably Lorentzian, but the wing behavior deviates from Lorentzian with the deviation increasing with distance from the center of the spectral line. However, it is just in this far spectral region that the hook method samples the refractive index to determine the oscillator strength. If anomalies in the shape of the refractive index exist, that is, if the refractivity is not represented by the ordinary dispersion profile, then the oscillator strength determination will be erroneous correspondingly. In the following discussion, the shape of the index of refraction will be derived using the quasistatic approximation of reference 2 and an analysis of the errors introduced into the hook method oscillator strengths will be given.

THEORY

For tenuous media, the index of refraction and the absorption coefficient can be calculated from the real and imaginary parts of a complex function, i.e.,

$$f(\omega) = n(\omega) - 1 + i\,\kappa(\omega) \qquad (1)$$

where $\kappa(\omega)$ is related to the ordinary absorption coefficient by the relation

$$\kappa(\omega) = \frac{k(\omega)c}{2\omega} \qquad (2)$$

Here c is the velocity of light, ω is the angular frequency being considered and $k(\omega)$ is the ordinary absorption coefficient. In this extended range of the definition of $\kappa(\omega)$, the relationship between the positive and the negative frequency regions is

$$\kappa(\omega) = -\kappa\ (-\omega) \tag{3}$$

Then integrating equation 1 around a closed contour gives (if $f(\omega)$ has no poles above the positive real axis),

$$\text{Re } f(\omega) = \frac{1}{\pi} \ P \int_{-\infty}^{+\infty} \frac{\text{Im } f(\omega)}{\omega' - \omega} \tag{4}$$

where P indicates the Cauchy principle value of the integral; i.e., the integral can be written

$$n(\omega) - 1 = \frac{1}{\pi} \ P \int_{-\infty}^{+\infty} \frac{\kappa(\omega')}{\omega' - \omega} \tag{5}$$

or with the aid of equation 3, the Kronig-Kramers equation can be obtained

$$n(\omega) - 1 = \frac{2}{\pi} \ P \int_{0}^{\infty} \frac{\omega' \kappa(\omega')}{\omega'^2 - \omega^2} \, d\omega' \tag{6}$$

With the assumption of tenuous media, the refractivity can be expressed as a sum of terms; one term is the atomic and ionic contribution, another term is the contribution from the electrons, and the last term is due to the contribution from the nearby spectral line (all other spectral line contributions are assumed negligible)[3].

$$n-1 = (n-1)_A + (n-1)_e + (n-1)_\lambda \tag{7}$$

The first two terms of this expression come from the "continuum" refractive index, and the last term, the contribution to the refractivity by the spectral line, will be the term discussed in the following sections.

Since a spectral line is peaked in a narrow wavelength region, ω_o, the following approximations can be made in equation 6

$$\kappa(\omega') \approx \frac{c}{2\omega_o} k(\omega')$$
$$\omega'^2 - \omega^2 \approx 2\omega_o (\omega' - \omega) \qquad (8)$$

where ω_o is the central frequency of the spectral line. These approximations will introduce errors of the order of w/ω_o, where w is the width of the spectral line; such errors will normally be less than 0.1% for spectral lines in the visible region of the spectra whose width is less than 5Å. With these approximations, the refractivity can be written

$$n(\omega) - 1 = \frac{c}{2\pi\omega_o} \int_0^\infty \frac{k(\omega')}{\omega' - \omega} d\omega' \qquad (9)$$

where the absorption coefficient for the spectral line is given by the usual equation

$$k(\omega) = 2\pi^2 r_o c \, f_{mn} N_n L(\omega), \qquad (10)$$

where r_o is the classical radius of the electron, f_{mn} is the oscillator strength of the spectral line, N_n is the density of atoms in the state n, and $L(\omega)$ is the shape parameter normalized such that

$$\int_{-\infty}^{+\infty} L(\omega) \, d\omega = 1 \qquad (11)$$

At this point, the equation 9 is parameterized in the manner of Griem, Baranger, Kolb and Oertel[2]; that is, the electron impact widths and shifts are introduced as the measure of frequency from the center of the spectral line

$$x = -\frac{\omega-\omega_o-d}{w} = \frac{\lambda-\lambda_o-d_\lambda}{w_\lambda} \tag{12}$$

where d is the electron impact shift and w is the electron impact width. d_λ and w_λ are the same quantities measured in units of wavelength. Also, the reduced shape factor is defined

$$L(\omega) = \frac{1}{w} \; j_r \; (x) \tag{13}$$

which allows equation 9 to be written

$$n(\omega)-1 = \frac{\pi^2 r_o c^2}{\omega_o} \; f_{mn} \; N_n \; \frac{R_r(x)}{w} \tag{14}$$

and the reduced refractivity is defined'

$$R_r \; (x) = -\frac{1}{\pi} \; P \int_{-\infty}^{+\infty} \frac{j_r(x)'}{x'-x} \, dx' \tag{15}$$

This quantity carries all the information on shapes and electric field dependence of the refractive index through the function $j_r(x)$. Furthermore, the shape of the absorption coefficient is given in reference 5 as

$$j_r(x,\alpha) = \frac{1}{\pi} \int_0^\infty \frac{d\beta \, W_r(\beta)}{1 + (x-\alpha^{4/3}\beta^2)^2} \tag{16}$$

where β is the low frequency component of the electric field (measured in units of the normal field strength), $W_r(\beta)$ is the probability distribution of the electric fields including correlations, r is the ratio of the mean distance between the ions and the Debye radius, and α is the quasistatic broadening parameter. For many spectral lines of light elements, α and w are given by Griem;[4] for other lines α and w can be calculated using the formulae that he gives. The plasma parameter, r, is given by

$$r = \sqrt[6]{36\pi N} \quad \left(\frac{e^2}{kT}\right)^{\frac{1}{2}} \tag{17}$$

where N is the ion density of the plasma.

When relation (16) is substituted for $j_r\ (x,\alpha)$, the orders of integration in equation (15) can be interchanged to give for the reduced refractivity,

$$R_r(x,\alpha) = \frac{1}{\pi} \int_0^\infty d\beta\ W_r(\beta) \quad \frac{x-\alpha^{4/3}\beta^2}{1+\ (x-\alpha^{4/3}\beta^2)^2} \tag{18}$$

This formula was used to calculate figures 2 and 3 with values of $W_r\ (\beta)$ taken from Mozer and Baranger[5]. Since, even for relatively large values of r, the value of $R_r\ (x,\alpha)$ does not differ significantly from the Holtsmark value, $R_H\ (x,\alpha)$, (the value for r =0.0) the subsequent discussion will be devoted to the reduced refractivity calculated in the Holtsmark approximation, i.e., the curves shown in figure 3. The striking aspect of these curves, however, is that the large deviations which occurred in the wings for the absorption coefficient are not present in the index of refraction. In appendix A, asymptotic forms for the reduced refractivity are obtained, and it can be seen that indeed the leading term is always the ordinary dispersion term.

APPLICATION OF THE STARK REFRACTIVITY TO OSCILLATOR STRENGTH MEASUREMENTS BY THE HOOK METHOD

The hook method of measuring oscillator strengths uses a two-beam interferometer to define the position at which the derivative of the refractivity is equal to some constant, K.[6] Since the derivative assumes this value, K, on either side of the spectral line, i.e., at the position of the hooks, then the separation of these points is measured to obtain a number related to the oscillator strength. In quantitative terms, the central equation of the hook method is:

$$\frac{d}{d\lambda}(n-1)\Big|_{\lambda\pm} = -K \tag{19}$$

If the refractivity given by equation 14 is expressed in wavelength units, the derivative can be written

$$\frac{d(n-1)}{d\lambda} = \frac{1}{w_\lambda}\frac{d}{dx}(n-1) = \frac{\lambda_o^3}{4w_\lambda{}^2}\, r_o\, f_{mn}\, N_n \frac{dR}{dx} \tag{20}$$

and the hooks occur at positions x+ and x- such that

$$\frac{dR}{dx}\Big|_{x\pm} = -K\left(\frac{\lambda_o^3}{4w_\lambda{}^2}\, r_o\, f_{mn}\, N_n\right)^{-1} \tag{21}$$

If there were no quasistatic electric fields, then in the asymptotic limit, the derivative would be written

$$\frac{dR}{dx} = -\frac{1}{\pi}\,\frac{1}{x^2} \tag{22}$$

and the roots of equation (21) would be

$$x\pm = \pm\sqrt{\frac{r_o^3\lambda^3}{4\pi w_\lambda{}^2}\,\frac{f_{mn}\, N_n}{K}} \tag{23}$$

or in terms of the separations of the hooks,

$$(x+ - x-) = 2\sqrt{\frac{r_o\lambda^3}{4\pi w_\lambda^2} \frac{f_{mn}N_n}{K}} \tag{24}$$

In this form, it seems that the hook positions depend on the width of the spectral line, but this is illusory, since (24) can be rewritten in the form

$$(\lambda+ - \lambda-)^2 K = \frac{1}{\pi} \lambda^3 r_o f_{mn} N_n \tag{25}$$

which is identical with Foster's equation 4.35[6] (with the present K equal to his k/d).

The presence of the quasistatic Stark fields causes equation (22) to be modified. After the asymptotic form of the derivative of the reduced refractivity is taken from the appendix, Eq. A-15, then the analysis can be simplified by writing the derivatives of the Stark refractivity as deviations from the ordinary anomalous dispersion equations, viz. for $x/\alpha >> 0$

$$-\frac{1}{\pi} \frac{1}{(x_+ + \epsilon_+)^2} = -\frac{1}{\pi |x+|^2} \left(1 - \frac{3}{x+^2}\right) - \frac{105}{32\sqrt{\pi}} \frac{\alpha}{|x+|^{11/4}} \tag{26}$$

or the deviations, ϵ_+ can be written as

$$\epsilon_+ = \frac{3}{2x+} + \frac{105\alpha}{64} \sqrt{\frac{\pi}{2}}\ x^{\frac{1}{4}} \approx \frac{1.5}{x_+} - 2.05\ \alpha\ x^{\frac{1}{4}} \tag{27}$$

Similarly the deviation for $x/\alpha << 0$ can be written

$$\epsilon_- = \frac{3}{2|x_-|} + \frac{105\alpha}{64} \sqrt{\pi}\ |x_-|^{\frac{1}{4}} \approx \frac{1.5}{|x_-|} + 2.9|\alpha|x_-|^{\frac{1}{4}} \tag{28}$$

so that the hook separation can be shown to be

$$\Delta = \frac{\lambda_+ - \lambda_-}{w} = x_+ + \epsilon_+ + (|x_-| + \epsilon_-)$$
$$= 2x + \frac{3}{x} + .86\alpha\ |x|^{\frac{1}{4}} \tag{29}$$

where the identification $|x_+| \approx |x_-| \approx |x|$ has been made.

Then the errors introduced into the oscillator strengths by reducing the data for the hook positions in terms of the anomalous dispersion formulae will be twice the errors in the hook positions, or

$$E = 2.\left\{\frac{\Delta-2x}{2x}\right\} = \frac{3}{x^2} + .86\alpha\, x^{-\frac{3}{4}} \qquad (30)$$

An idea of the size of the errors can be gained by the example of the Mg I λ5875 for an electron density of 10^{16} cm^{-3}. For this line at a temperature of 5000°K, Griem[4] gives α as .35 so that with a hook measurement at 10 halfwidths of the spectral line (x = 10), the error becomes

$$E = \frac{3}{100} + \frac{.86 \times .35}{5.6} \approx .08$$

DISCUSSION AND SUMMARY

The validity criteria of the refractivity relations given here will be the same as the validity criteria of the Stark broadening theory given in reference 7. The one remark which might be especially mentioned concerns the case where the Lorentzian width differs from that given by Griem. This would be the case if other broadening causes were operative, inaccuracies in the broadening theory were present,[7, 8], or effects such as Debye shielding should reduce the broadening[9]. Under these circumstances, the α given by Griem would still be an accurate quantity, but a new α should be calculated using the relation

$$\alpha' = \left(\frac{w}{w'}\right)^{\frac{3}{4}} \alpha \tag{31}$$

where the primes indicate the revised quantities and the unprimed numbers are those given by Griem.

In addition, mention should be made of the fact that the quasistatic theory presented here does not apply to spectral lines emitted by ions; of course, a similar analysis is possible, but the Holtsmark distribution used in the present context does not allow for the additional correlations produced in the neighbourhood of the ion.

The striking aspect of the refractivity curves presented is that indeed, they do approach the ordinary dispersion shape at large x. The strong deviation of the absorption coefficient from a Lorentzian in the wings of the spectral line seems to be replaced in the index of refraction by an anomalous behaviour in the cores of the spectral line. While it is difficult to find a physical explanation for this effect, it is tempting to regard it as an aspect of the nature of the Hilbert transform which can be expressed as an incomplete Fourier transform. The Fourier transform is known to give an inversion to the functions that it acts upon by transforming the wing behavior of the untransformed function into the cores of the transformed function. Because of this extraordinary behavior, the analysis of the refractivity is being continued with particular emphasis on the case where the ion perturbers are treated by the impact theory in the case of the absorption coefficient.

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APPENDIX

Asymptotic forms for R(x) can be derived by using the expression for the Holtsmark quasistatic field distribution

$$W_H(\beta) = \frac{2}{\pi}\beta \int_0^\infty y \sin \beta y \quad \exp\left\{-y^{3/2}\right\} dy \tag{A-1}$$

and following the procedure described in the appendix of reference [2]. When the relation (A-1) is substituted into equation (17), the refractivity can be expressed as

$$R_H(x,\alpha) = \frac{1}{\pi} \int_0^\infty d\beta \; \frac{x-\alpha^{4/3}\beta^2}{1+(x-\alpha^{4/3}\beta^2)^2} \int_0^\infty \frac{2\beta}{\pi} \; y \sin \beta y \quad \exp(-y^{3/2}) \; dy \tag{A-2}$$

If the orders of integration are interchanged, then the form results

$$R_H(x,\alpha) = \frac{2}{\pi^2} \int_0^\infty dy \quad \exp\,(-y^{3/2}) \quad (xI_1 - \alpha^{4/3} I_2) \tag{A-3}$$

where the integrals to be evaluated are:

$$I_1 = \int_0^\infty \frac{\beta \sin\beta y}{1+(x-\alpha^{4/3}\beta^2)^2} \; d\beta \tag{A-4}$$

$$I_2 = \int_0^\infty \frac{\beta^3 \sin\beta y}{1+(x-\alpha^{4/3}\beta^2)^2} \; d\beta = -\frac{\partial^2}{\partial y^2} I_1 \tag{A-5}$$

Then, as in reference 2, it is convenient to introduce the following definitions

$$A_{+,-} = |\alpha|^{-\frac{2}{3}} \; (\delta \; |x| \pm i)^{\frac{1}{2}} \qquad \begin{array}{l} \delta = -1, \; x/\alpha < 0 \\ \delta = +1, \; x/\alpha > 0 \end{array}$$

$$R_{+,-} = \left[\pm \; \delta|x| + \sqrt{1+x^2}\,\right]^{\frac{1}{2}} / \sqrt{2}$$

$$A_+ + A_- = 2\ |\alpha|^{-\frac{2}{3}}\ R_+$$

$$R_+ + R_- = \tfrac{1}{2}\left[1+x^2 - \delta^2\ |x|^2\right]^{\frac{1}{2}} = \tfrac{1}{2}$$

With these definitions the integral can be rewritten in the form

$$I_1 = -\frac{|\alpha|^{-2}}{4R_-}\ \text{Im}\int_{-\infty}^{+\infty} d\beta\ \frac{e^{i\beta y}}{(\beta+iA_+)\ (\beta+iA_-)}\left[\frac{1}{\beta-iA_+} - \frac{1}{\beta-iA_-}\right] \qquad \text{(A-6)}$$

$$= \frac{\pi}{2}\ |\alpha|^{-4/3}\ \text{Im}\ \exp\left\{-A_-y\right\}$$

so that I_2 can now be written

$$I_2 = -\frac{\partial^2}{\partial y^2}\ I_1 = \text{Im}\ |\alpha|^{-4/3}\ (\delta|x|-i)\ I_1 \qquad \text{(A-7)}$$

and

$$I_2 = |\alpha|^{-4/3}\ \delta|x|\ I_1 - \text{Re}\ \frac{\pi}{2}\ |\alpha|^{-8/3}\ \exp\left\{-A_-y\right\} \qquad \text{(A-8)}$$

then if the relation

$$xI_1 - \alpha^{4/3}\ I_2 = \frac{\pi}{2}\ |\alpha|^{-4/3}\ \exp\left\{-|\alpha|^{-\frac{2}{3}}\ R_+y\right\}\ \cdot \qquad \text{(A-9)}$$

$$x\ \cos\ |\alpha|^{-\frac{2}{3}}\ R_-y$$

is noted, the refractivity can be rewritten

$$R_H(x,\alpha) = \frac{1}{\pi}\ |\alpha|^{-4/3}\int_0^{\infty} dy\ \exp\left\{-y^{3/2}\right\}\ \exp\left\{-|\alpha|^{-\frac{2}{3}}R_+y\right\}\ \cos|\alpha|^{-\frac{2}{3}}\ R_-y \qquad \text{(A-10)}$$

the expansion of the exponential

$$\exp\ (-y^{3/2}) = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{\Gamma(n)}\ y^{3/2(n-1)} \qquad \text{(A-11)}$$

allows Eq. A-10 to be integrated term by term with the help of the Fourier transform relation 15

$$\int_0^{\infty} x^{\nu-1}\ e^{-ax}\ \cos\ \eta x\ dx = \Gamma(\nu)\ (a^2+\eta^2)^{-\nu/2}\ \cos\ (\nu\text{Tan}^{-1}\eta/a) \qquad \text{(A-12)}$$

$$\text{Re}\ \nu>0,\ \text{Re}\ a>0$$

then the refractivity in the Holtsmark approximation is:

$$R_H(x,\alpha) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{\Gamma(\frac{3n+1}{2})}{\Gamma(n)} \frac{|\alpha|^{n-1}}{(1+x^2)} 3n+1/8 \cos\left[\frac{3n+1}{2} \mathrm{Tan}^{-1}(-\delta|x| + \sqrt{1+x^2})\right] \quad \text{(A-13)}$$

And, for large x, the asymptotic forms are

$$\frac{x}{\alpha} >> 0 \quad R(x) = \frac{1}{\pi|x|} (1-\frac{1}{x^2}) + \frac{15\alpha}{8\sqrt{2\pi}} |x|^{7/4} \quad \text{(A-14)}$$

$$\frac{x}{\alpha} << 0 \quad R(x) = -\frac{1}{\pi|x|} (1-\frac{1}{x^2}) + \frac{15\alpha}{8\sqrt{\pi}} |x|^{7/4}$$

for the index of refraction, and for the derivative of the reduced refractivity

$$\frac{x}{\alpha} >> 0 \quad \frac{dR}{dx} = -\frac{1}{\pi|x|^2} (1-\frac{3}{|x|^2}) - \frac{105}{32\sqrt{2\pi}} \frac{\alpha}{|x|^{11/4}} \quad \text{(A-15)}$$

$$\frac{x}{\alpha} << 0 \quad \frac{dR}{dx} = -\frac{1}{\pi|x|^2} (1-\frac{3}{|x|^2}) + \frac{105}{32\sqrt{\pi}} \frac{\alpha}{|x|^{11/4}}$$

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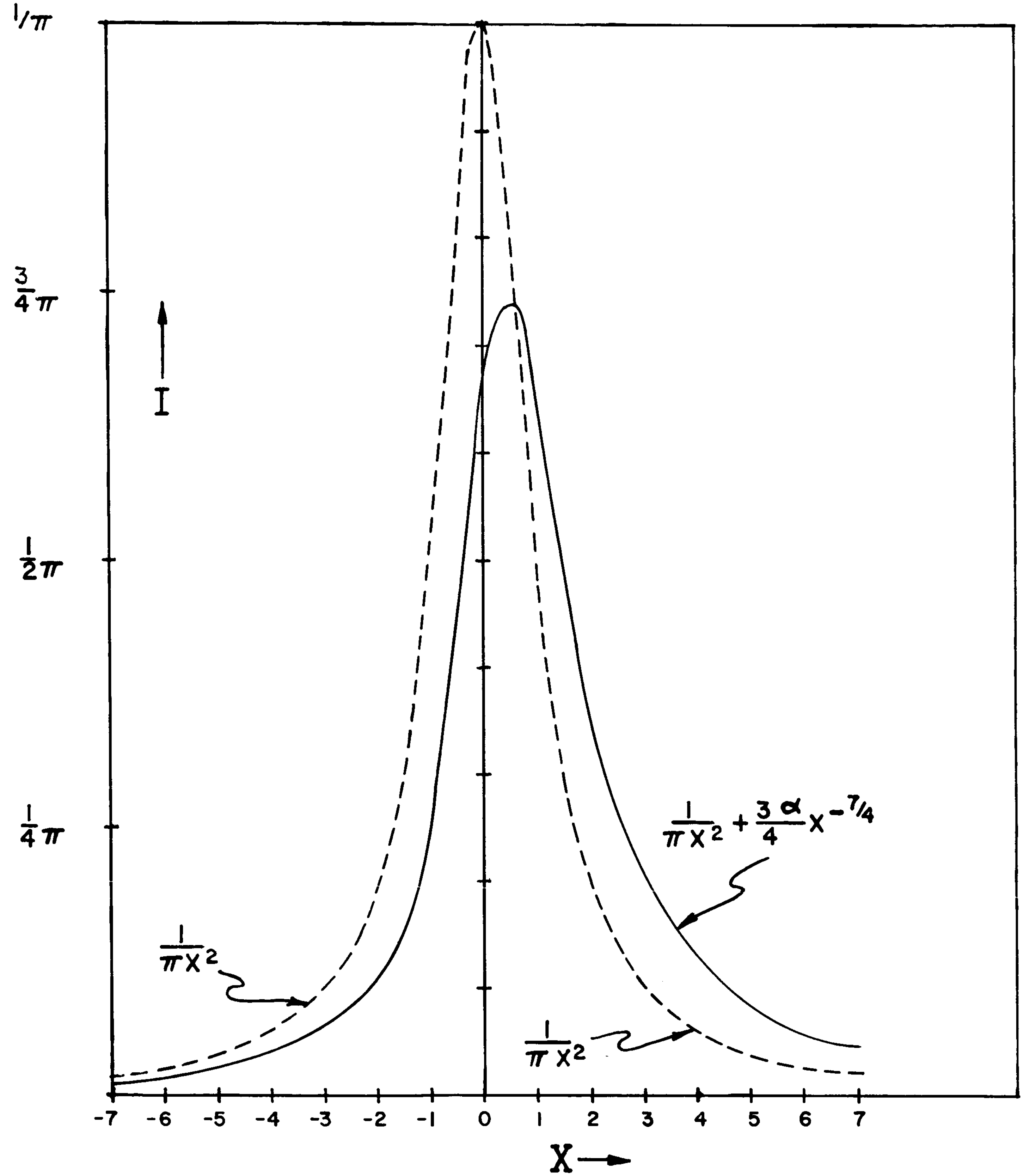
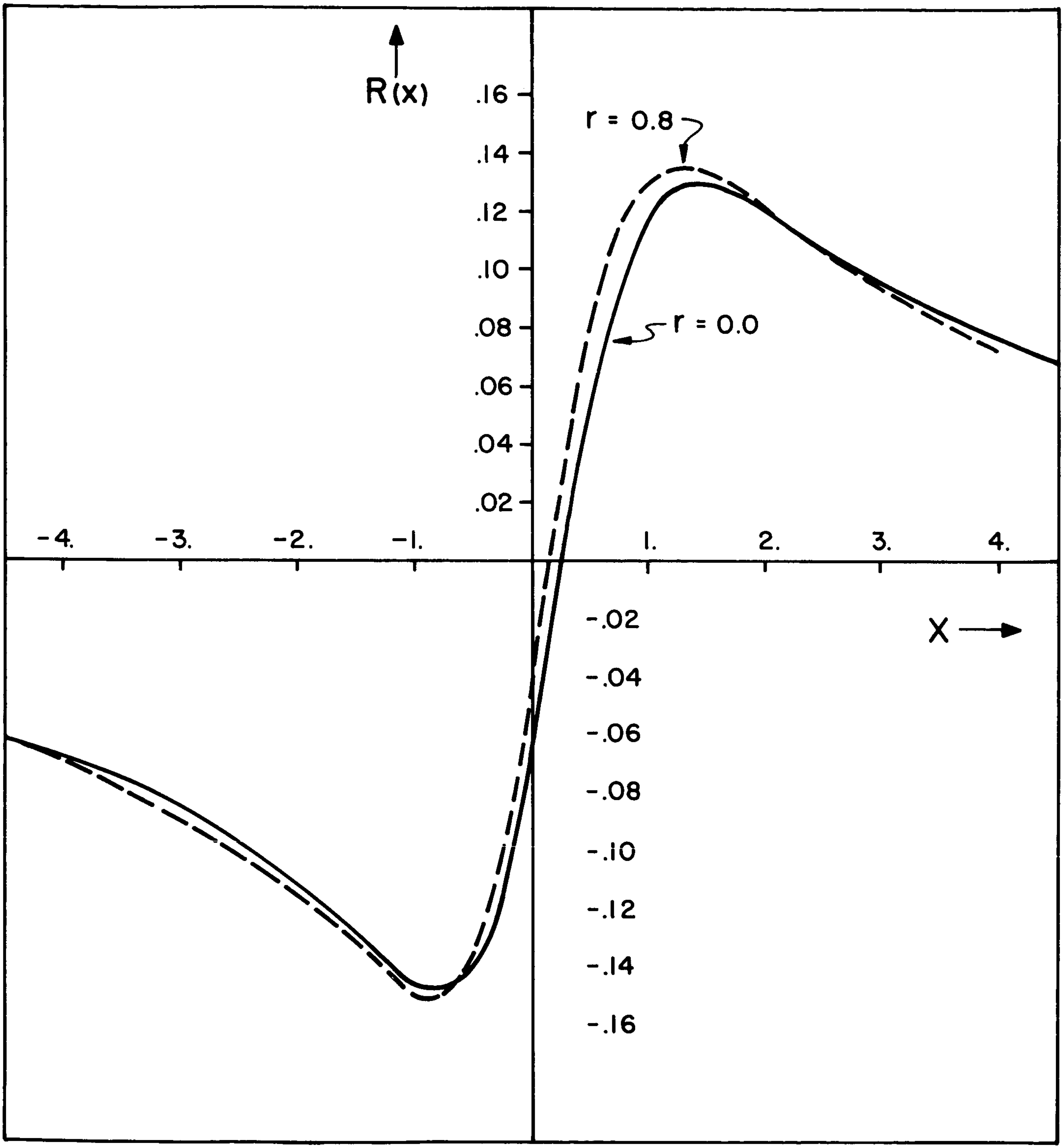


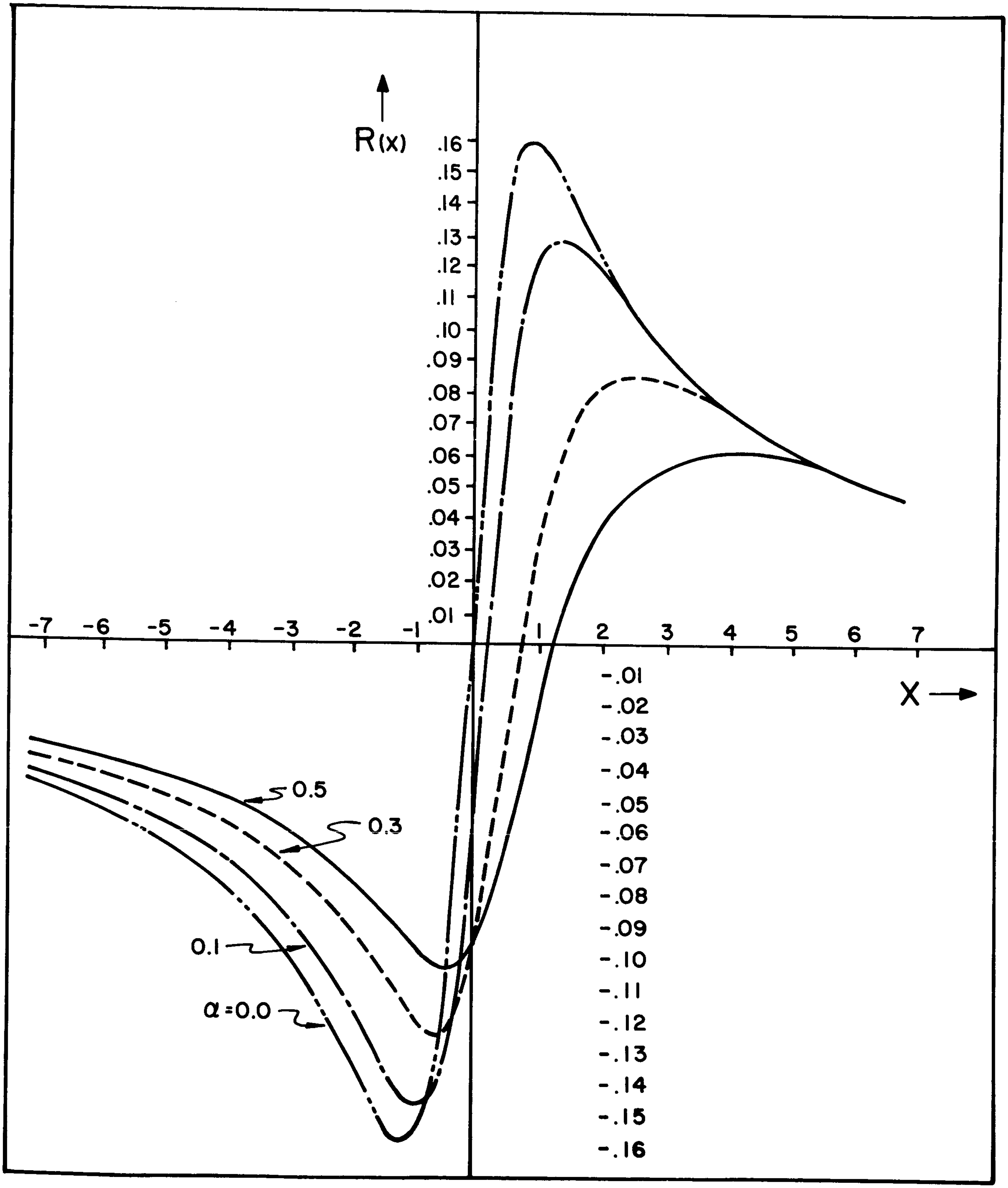
RELATIVE INTENSITY PLOTTED AGAINST REDUCED WAVELENGTH FOR A LORENTZIAN (DASHED LINE), AND A STARK BROADENED (SOLID LINE) PROFILE, $\alpha = .2$.

Figure 1



THE REDUCED REFRACTIVITY PLOTTED AGAINST THE REDUCED WAVELENGTH FOR $\alpha = .1$ WITH r AS A PARAMETER

Figure 2



THE REDUCED REFRACTIVITY PLOTTED AGAINST THE REDUCED WAVELENGTH WITH α AS A PARAMETER

Figure 3