ON THE THEORY OF THE COMBINED INFLUENCE OF COLLISION AND DOPPLER BROADENING ON THE SHAPE OF SPECTRAL LINES

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The theory of collision broadening by Fano is extended to include the effect of translational motion of the radiating molecules. We derive an integral-equation for determining the shape of the spectral line. In the case of moving radiating molecules scattered by perturbing gas molecules in rest, this equation has been solved under simplifying assumptions. The resulting line shape shows a typical Dicke narrowing, caused by direction changing collisions.

1. Introduction

In recent years the problem of combined collision and Doppler broadening was treated repeatedly [1–5]. Often using a kinetic approach, it has been shown that the Voigt profile [6] must be replaced by a complicated line shape. The line width of this spectral shape goes through a minimum as a function of the density of the perturbing foreign gas molecules (perturbers), beginning with the Doppler width by the density zero.

The Dicke narrowing [7] was experimentally verified [8–11] and can be explained in the following way. The collisions of the perturbers with the radiating molecule (radiator) give rise to a broadening of the spectral shape. They also reduce the efficiency of the Doppler broadening mechanism based on free moving molecules, which radiate unperturbed. Therefore, in the range of small perturber densities (whereby the interaction results in succesive uncorrelated collisions between only one perturber and the radiator in each case) the line width can decrease below the Doppler width. In Section 2 we extend the theory of collision broadening by Fano [12] and include the motion of the radiators. As a result, we derive an integral equation for a function $a_q(\omega)$ determining, after an integration, the spectral shape. Section 3 is devoted to the discussion of the kernel of this integral

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equation and to some special cases. In Section 4 we consider a situation in which light radiators are scattered by heavy resting perturbers. The possibility of a partial wave expansion is briefly discussed. With these results we undertake in Section 5 a numerical and graphical analysis of a special situation containing only the s-wave scattering. This approximation means that we especially take into account direction changing collisions because of the directional independency of the scattering efficiency.

The results show the expected Dicke narrowing. In Section 6 we discuss the results and the approximations used to obtain these results.

2. *Application of the theory of Fano on the combined collision and Doppler broadening*

2.1. General formalism of the theory

In this paper we consider the problem of foreign gas broadening by assuming that the radiators are only perturbed by foreign gas molecules. The spectral shape of the light emitted by a radiator can be characterized by a function $F(\omega)$

$$F(\omega) = (-\pi)^{-1} \operatorname{Im} \operatorname{Tr} (e^{-i\mathfrak{k}\mathfrak{w}_R} x^+) (\omega - \mathfrak{L})^{-1} \varrho (e^{i\mathfrak{k}\mathfrak{w}_R} x), \tag{1}$$

resulting from a similar expression as in [12] and taking into account the translational motion of the radiator. Here $\mathfrak{w}_R$ and x are the position and the dipole moment operator of the radiator. $\mathfrak{k}$ and ω are the wave vector and the frequency of the emitted photon ($\omega = c|\mathfrak{k}|$, c — velocity of light). A small imaginary part $+i\varepsilon$ of ω describes how to circumvent the pole in $(\omega - \mathfrak{L})^{-1}$, and after all the calculations we must take the limit $\varepsilon \to 0$. The Liouville operator $\mathfrak{L}$ of the system "radiator plus perturbers" is defined by his action on any operator Q

$$\mathfrak{L}Q = [H, Q], \tag{2}$$

(H being the Hamiltonian of the system, $\hbar = 1$ is always assumed). ϱ is the density matrix in thermal equilibrium

$$\varrho = e^{-\beta H} / \operatorname{Tr} e^{-\beta H} \tag{3}$$

$\left(\beta = \frac{1}{k_B T},\ T \text{ temperature, } k_B \text{ Boltzmann constant}\right)$, and the trace Tr goes over all degrees of freedom of the system. H is equal to

$$H = H_R + H_P + V, \tag{4}$$

where $H_R(H_P)$ is the Hamiltonian of the radiator (perturbers) and V the interaction between radiator and perturbers. The meaning of the symbols $\mathfrak{L}_R$, $\mathfrak{L}_P$, $\mathfrak{L}_V$, Tr_R, Tr_P, ϱ_R, ϱ_P frequently used is analogous to $\mathfrak{L}$, Tr, ϱ and should not be explained further.

Following Fano [12] we write $F(\omega)$ in the form

$$F(\omega) = (-\pi)^{-1} \operatorname{Im} \operatorname{Tr}_R (e^{-i\mathfrak{k}\mathfrak{w}_R} x^+) \mathfrak{A}(\omega) (\varrho_R e^{i\mathfrak{k}\mathfrak{w}_R} x). \tag{5}$$

Here $\mathfrak{A}(\omega)$ is a super operator acting only on the radiator variables

$$\mathfrak{A}(\omega) = \mathrm{Tr}_P\,(\omega-\mathfrak{L})^{-1}\varrho\varrho_R^{-1}. \tag{6}$$

To get a quantity which can be developed in powers of the density we define (see also [12, 13])

$$\mathfrak{B}(\omega) = \mathrm{Tr}_P(\omega-\mathfrak{L}_R-\mathfrak{L}_P)^{-1}\varrho\varrho_R^{-1} \tag{7}$$

and make the following "Ansatz":

$$\mathfrak{A}(\omega) = (\mathfrak{B}(\omega)^{-1}-\mathfrak{C}(\omega))^{-1}. \tag{8}$$

Then $\mathfrak{C}(\omega)$ is determined by

$$\mathfrak{C}(\omega) = (1+\mathfrak{M}(\omega)\mathfrak{B}(\omega))^{-1}\mathfrak{M}(\omega) \tag{9}$$

with

$$\mathfrak{M}(\omega) = \mathfrak{B}(\omega)^{-1}(\mathfrak{A}(\omega)-\mathfrak{B}(\omega))\mathfrak{B}(\omega)^{-1}. \tag{10}$$

Because we are only interested in low densities we approximate ϱ by $\varrho \approx \varrho_R \cdot \varrho_P$. From this it follows

$$\mathfrak{B}(\omega) = (\omega-\mathfrak{L}_R)^{-1}. \tag{11}$$

Moreover we develop $\mathfrak{C}(\omega)$ in powers of the density, and retain only terms up to first order. The result is

$$\mathfrak{C}(\omega) \approx \mathfrak{M}(\omega) \approx \mathfrak{M}_1(\omega) = N_0\,\mathrm{Tr}_P\,(\mathfrak{L}_v+\mathfrak{L}_v(\omega-\mathfrak{L}_R-\mathfrak{L}_P-\mathfrak{L}_v)^{-1}\mathfrak{L}_v)\varrho_P, \tag{12}$$

where N_0 is the number of perturbers in the quantization volume V_0, and v is the interaction Hamiltonian between the radiator and one of the perturbers, $\mathfrak{L}_v$ the corresponding Liouville-operator. If the radiators are in rest, the expressions (12), (8), (5) are easily obtained [12] giving the Lorentz profile of collisional broadening in a good approximation.

In the case of moving radiators, $\mathfrak{M}_1(\omega)$ is nondiagonal in the "eigenstates" of $\mathfrak{L}_R$ and a solution cannot be found directly. Therefore, we first construct an integral equation whose solution can be used to determine $F(\omega)$.

2.2. Derivation of the integral equation

Let us define a complete set of eigenfunctions of H_R,

$$H_R|i\mathfrak{q}\rangle = (H_t+H_r)\,|i\mathfrak{q}\rangle = \left(\frac{\mathfrak{q}^2}{2m_R}+\varepsilon_i\right)|i\mathfrak{q}\rangle$$

$$|i\mathfrak{q}\rangle = |i\rangle\,\frac{1}{\sqrt{V_0}}\,e^{i\mathfrak{q}\mathfrak{r}_R}, \tag{13}$$

where H_t, H_r are the Hamiltonians for the translational motion of the radiator ($|\mathfrak{q}\rangle$ eigenstate, $\frac{1}{2m_R}\mathfrak{q}^2$ eigenvalue, m_R mass of the radiator and $\mathfrak{q}$ eigenvalue of the momentum operator) and the internal degrees of freedom ($|i\rangle$ eigenstate, ε_i eigenvalue). Now we can write $F(\omega)$ in the following form

$$F(\omega) = (-\pi)^{-1} \operatorname{Im} \sum_{ij} \sum_{\mathfrak{q}} c_{\mathfrak{q}}^{ij} \mathfrak{A}_{\mathfrak{q}}^{ij}(\omega) \tag{14}$$

with

$$\mathfrak{A}_{\mathfrak{q}}^{ij}(\omega) = \mathrm{Tr}_R(e^{-i\mathfrak{k}\mathfrak{r}_R} x^+)\mathfrak{A}(\omega)\, |i\mathfrak{q}\rangle \langle j\mathfrak{q}-\mathfrak{k}| \tag{15}$$

$$c_{\mathfrak{q}}^{ij} = \langle i\mathfrak{q}|\varrho_R e^{i\mathfrak{k}\mathfrak{r}_R} x|j\mathfrak{q}-\mathfrak{k}\rangle = x_{ij}\varrho^{(i)}(e^{-\frac{\beta\mathfrak{q}^2}{2m_R}}/\mathrm{Tr}_t e^{-\beta H_t}). \tag{16}$$

$\varrho^{(i)}$ describes the probability of finding the radiator in the internal state $|i\rangle (\sum_i \varrho^{(i)} = 1)$. Utilizing the identity

$$\mathfrak{A}(\omega) = \mathfrak{B}(\omega) + \mathfrak{A}(\omega)\mathfrak{C}(\omega)\mathfrak{B}(\omega) \tag{17}$$

we get a coupled system of equations for $\mathfrak{A}_{\mathfrak{q}}^{ij}(\omega)$:

$$\mathfrak{A}_{\mathfrak{q}}^{ij}(\omega) = \mathfrak{B}_{\mathfrak{q}}^{ij}(\omega)\, [1 + \sum_{kl} \sum_{\mathfrak{p}} \mathfrak{M}_{\mathfrak{q}\mathfrak{p}}^{ijkl} \mathfrak{A}_{\mathfrak{p}}^{kl}(\omega)] \tag{18}$$

which in the limit $V_0 \to \infty$ goes over into a system of integral equations with $\mathfrak{q}$ and $\mathfrak{p}$ as continuous variables. $\mathfrak{B}_{\mathfrak{q}}^{ij}(\omega)$ and $\mathfrak{M}_{\mathfrak{q}\mathfrak{p}}^{ijkl}$ may be derived from

$$\mathfrak{B}_{\mathfrak{q}}^{ij}(\omega) = x_{ij}^* \left(\omega - \omega_{ij} - \frac{1}{2m_R} [\mathfrak{q}^2 - (\mathfrak{q}-\mathfrak{k})^2] \right)^{-1} \tag{19}$$

$$\omega_{ij} = \varepsilon_i - \varepsilon_j.$$

$$\mathfrak{M}_{\mathfrak{q}\mathfrak{p}}^{ijkl} = \langle k\mathfrak{p}|\, \{\mathfrak{M}_1(\omega)\, |i\mathfrak{q}\rangle \langle j\mathfrak{q}-\mathfrak{k}|\}\, |l\mathfrak{p}-\mathfrak{k}\rangle. \tag{20}$$

In (20) $\mathfrak{M}_1(\omega)$ at first acts on $|i\mathfrak{q}\rangle\langle j\mathfrak{q}-\mathfrak{k}|$, and from the resulting operator one must take the matrix element between $\langle k\mathfrak{p}|$ and $|l\mathfrak{p}-\mathfrak{k}\rangle$. We are interested mainly in the influence of the translational motion on the spectral shape. Therefore, we consider only the shape of an isolated spectral line resulting from the transition between two nondegenerate internal states $|i\rangle$ and $|j\rangle$. The resulting equation for $F(\omega)$ is

$$F(\omega) = (-\pi)^{-1} \varrho^{(i)} |x_{ij}|^2 \operatorname{Im} \sum_{\mathfrak{q}} \frac{e^{-\frac{\beta\mathfrak{q}^2}{2m_R}}}{\mathrm{Tr}_t\, e^{-\beta H_t}} a_{\mathfrak{q}}(\omega), \tag{21}$$

where $a_{\mathfrak{q}}(\omega)$ means a solution of the integral equation

$$a_{\mathfrak{q}}(\omega) = a_{\mathfrak{q}}^0(\omega)\, [1 + \sum_{\mathfrak{p}} K_{\mathfrak{q}\mathfrak{p}} a_{\mathfrak{p}}(\omega)], \tag{22}$$

with

$$a_{\mathfrak{q}}^0(\omega) = \left(\omega - \omega_{ij} - \frac{1}{2m_R} [\mathfrak{q}^2 - (\mathfrak{q}-\mathfrak{k})^2] \right)^{-1}, \tag{23}$$

and

$$K_{\mathfrak{q}\mathfrak{p}} = \mathfrak{M}^{ijij}_{\mathfrak{q}\mathfrak{p}}. \tag{24}$$

These are the basic equations which we shall discuss in the next section in more detail.

3. *Investigation of the integral equation*

3.1. The kernel of the integral equation

Instead of $\mathfrak{M}^{ijij}_{\mathfrak{q}\mathfrak{p}}$ first we consider a slightly more general expression

$$\mathfrak{M}(\mathfrak{q}, \mathfrak{p}|\mathfrak{q}', \mathfrak{p}') = \langle i\mathfrak{p}|\{\mathfrak{M}_1(\omega)|i\mathfrak{q}\rangle\langle j\mathfrak{q}'|\}|j\mathfrak{p}'\rangle. \tag{25}$$

Besides, we assume that the perturbers are structureless particles which only have translational degrees of freedom. Denoting by h_p, $\mathfrak{w}_p$, m_p, and $|\mathfrak{a}\rangle$ the Hamiltonian, position, mass, and eigenstate of h_p with the momentum $\mathfrak{a}$ of one perturber, we can write

$$h_p|\mathfrak{a}\rangle = \frac{\mathfrak{a}^2}{2m_p}|\mathfrak{a}\rangle, \qquad |\mathfrak{a}\rangle = \frac{1}{\sqrt{V_0}}e^{i\mathfrak{a}\mathfrak{w}_p}. \tag{26}$$

If we define the product states

$$|\mathfrak{a}i\mathfrak{p}\rangle = \frac{1}{V_0}e^{i(\mathfrak{a}\mathfrak{w}_p+\mathfrak{p}\mathfrak{w}_R)}|i\rangle, \tag{27}$$

we can express (25) in the form

$$\mathfrak{M}(\mathfrak{q}, \mathfrak{p}|\mathfrak{q}', \mathfrak{p}') = N_0\sum_{\mathfrak{a}\mathfrak{b}}\varrho^{\mathfrak{b}}_p\langle\mathfrak{a}i\mathfrak{p}|$$

$$\otimes\{[\mathfrak{L}_v+\mathfrak{L}_v(\omega-\mathfrak{L}_R-\mathfrak{L}_p-\mathfrak{L}_v)^{-1}\mathfrak{L}_v]\,|\mathfrak{b}i\mathfrak{q}\rangle\,\langle\mathfrak{b}j\mathfrak{q}'|\}\,|\mathfrak{a}j\mathfrak{p}'\rangle, \tag{28}$$

with

$$\varrho^{\mathfrak{b}}_p = e^{-\frac{\beta\mathfrak{b}^2}{2m_p}}\Big/\sum_{\mathfrak{b}}e^{-\frac{\beta\mathfrak{b}^2}{2m_p}}, \tag{29}$$

(here $\mathfrak{L}_p$ means the Liouville-operator of one perturber). Now we assume v to be a function of $|\mathfrak{w}_R-\mathfrak{w}_p|$ only, and introduce new coordinates $\mathfrak{w}$ and $\mathfrak{R}$ by

$$\mathfrak{w} = \mathfrak{w}_R-\mathfrak{w}_p, \qquad \mathfrak{R} = \frac{1}{M}(m_R\mathfrak{w}_R+m_p\mathfrak{w}_p)$$

$$M = m_R+m_p, \qquad m = \frac{m_R\cdot m_p}{m_R+m_p}, \qquad \overline{m}_R = \frac{m_R}{M}, \qquad \overline{m}_p = \frac{m_p}{M}, \tag{30}$$

describing the relative motion and the motion of the center of mass. In the Hilbert space of the relative motion we define states $|\ldots)$ by

$$|\mathfrak{a}i\mathfrak{p}\rangle = \frac{1}{V_0}e^{i(\mathfrak{a}\mathfrak{w}_p+\mathfrak{p}\mathfrak{w}_R)}|i\rangle = \frac{1}{V_0}e^{i((\mathfrak{a}+\mathfrak{p})\mathfrak{R}+(\overline{m}_p\mathfrak{p}-\overline{m}_R\mathfrak{a})\mathfrak{w})}|i\rangle$$

$$= \frac{1}{V_0}e^{i(\mathfrak{a}+\mathfrak{p})\mathfrak{R}}|i\overline{m}_p\mathfrak{p}-\overline{m}_R\mathfrak{a}), \tag{31}$$

and obtain

$$\mathfrak{M}(\mathfrak{q},\mathfrak{p}|\mathfrak{q}',\mathfrak{p}') = \frac{N_0}{V_0}\sum_{\mathfrak{ab}}\frac{1}{V_0}\,\delta_{\mathfrak{a}+\mathfrak{p},\mathfrak{b}+\mathfrak{q}}\delta_{\mathfrak{b}+\mathfrak{q}',\mathfrak{a}+\mathfrak{p}'}\varrho_p^{\mathfrak{b}}$$

$$\otimes(i\overline{m}_p\mathfrak{p}-\overline{m}_R\mathfrak{a}|\left\{\left[\mathfrak{L}_v+\mathfrak{L}_v\left(\omega-\mathfrak{L}_h-\frac{1}{2M}[(\mathfrak{b}+\mathfrak{q})^2-(\mathfrak{b}+\mathfrak{q}')^2]\right)^{-1}\mathfrak{L}_v\right]\right.$$

$$\left.\otimes|i\overline{m}_p\mathfrak{q}-\overline{m}_R\mathfrak{b})\,(j\overline{m}_p\mathfrak{q}'-\overline{m}_R\mathfrak{b}|\right\}|j\overline{m}_p\mathfrak{p}'-\overline{m}_R\mathfrak{a}). \tag{32}$$

Here $\delta_{\mathfrak{a}+\mathfrak{p},\mathfrak{b}+\mathfrak{q}}$ is a Kronecker symbol and $h = -\frac{1}{2m}\nabla_{\mathfrak{w}}^2+h_r+v(|\mathfrak{w}|)$ is the Hamiltonian of the relative motion, $\mathfrak{L}_h$ the corresponding Liouville-operator. From (32) we can easily find an expression for $K_{\mathfrak{qp}}$ in which we make a further approximation and ignore the wave vector $\mathfrak{k}$ of the photon

$$K_{\mathfrak{qp}} = n\sum_{\mathfrak{ab}}\frac{1}{V_0}\,\delta_{\mathfrak{a}+\mathfrak{p},\mathfrak{b}+\mathfrak{q}}\varrho_p^{\mathfrak{b}}(i\overline{m}_p\mathfrak{p}-\overline{m}_R\mathfrak{a}|\,\{\mathfrak{T}(\omega)$$

$$\otimes|i\overline{m}_p\mathfrak{q}-\overline{m}_R\mathfrak{b})\,(j\overline{m}_p\mathfrak{q}-\overline{m}_R\mathfrak{b}|\}\,|j\overline{m}_p\mathfrak{p}-\overline{m}_R\mathfrak{a}). \tag{33}$$

Here $n = \frac{N_0}{V_0}$ is the density of the perturbers, and $\mathfrak{T}(\omega)$ is the superoperator $\mathfrak{T}(\omega) = \mathfrak{L}_v+\mathfrak{L}_v(\omega-\mathfrak{L}_h)^{-1}\mathfrak{L}_v$, which is analogously constructed as the T-matrix operator belonging to the Hilbert space of the relative motion $v+v(\omega-h)^{-1}v$.

3.2. Special cases

We consider some examples characterized by the ratio of the perturber mass to the radiator mass:

a) $m_R \to \infty$

In this limit of very heavy radiators we obtain $\overline{m}_p = 0$, $\overline{m}_R = 1$, $a_{\mathfrak{q}}^0(\omega) = (\omega-\omega_{ij})^{-1}$ and

$$K_{\mathfrak{qp}} = n\sum_{\mathfrak{ab}}\frac{1}{V_0}\,\delta_{\mathfrak{a}+\mathfrak{p},\mathfrak{b}+\mathfrak{q}}\varrho_p^{\mathfrak{b}}(i-\mathfrak{a}|\,\{\mathfrak{T}(\omega)\,|i-\mathfrak{b})\,(j-\mathfrak{b}|\}\,|j-\mathfrak{a}). \tag{34}$$

The Eq. (22) for $a_{\mathfrak{q}}(\omega)$ may be solved with a $\mathfrak{q}$-independent "Ansatz", and the resulting $F(\omega)$ is

$$F(\omega) = (-\pi)^{-1}\varrho^{(i)}|x_{ij}|^2\,\mathrm{Im}\,a(\omega), \tag{35}$$

with

$$a(\omega) = (\omega-\omega_{ij}-K)^{-1} \tag{36}$$

and

$$K = n \sum_{\mathfrak{a}\mathfrak{b}} \frac{1}{V_0} \varrho_p^{\mathfrak{b}}(i\mathfrak{a}| \{\mathfrak{T}(\omega)\,|i\mathfrak{b})\,(j\mathfrak{b}|\}\,|j\mathfrak{a}). \tag{37}$$

This is the well known result of pressure broadening mentioned in Section 2.1. Approximating $\mathfrak{T}(\omega)$ by $\mathfrak{T}(\omega_{ij})$, $F(\omega)$ describes a Lorentz profile with a line width proportional to Im $K \sim n$.

b) $m_p \to \infty$
Now the radiators are scattered by resting perturbers. Using $\bar{m}_p = 1$, $\bar{m}_R = 0$, $K_{\mathfrak{q}\mathfrak{p}}$ is given by

$$K_{\mathfrak{q}\mathfrak{p}} = n\,\frac{1}{V_0}\,(i\mathfrak{p}|\,\{\mathfrak{T}(\omega)\,|i\mathfrak{q})\,(j\mathfrak{q}|\}\,|j\mathfrak{p}). \tag{38}$$

Finally, we go over to operators in the Hilbert space of the relative motion. Then (38) may be written approximately in the form [14]

$$K_{\mathfrak{q}\mathfrak{p}} = n\left[t^{ii}_{\mathfrak{q}\mathfrak{q}}\delta_{\mathfrak{q},\mathfrak{p}} - t^{jj*}_{\mathfrak{q}\mathfrak{q}}\delta_{\mathfrak{q},\mathfrak{p}} + \frac{1}{V_0}\,2\pi i t^{ii}_{\mathfrak{p}\mathfrak{q}} t^{jj*}_{\mathfrak{p}\mathfrak{q}}\,\delta\left(\frac{1}{2m}\,[\mathfrak{p}^2-\mathfrak{q}^2]\right)\right], \tag{39}$$

with

$$t^{ii}_{\mathfrak{p}\mathfrak{q}} = (i\mathfrak{p}|v + v\left(\varepsilon_i + \frac{\mathfrak{q}^2}{2m} - h + i\varepsilon\right)^{-1} v|i\mathfrak{q}) = -\frac{2\pi}{m} f_{i,i}(\mathfrak{p},\mathfrak{q}). \tag{40}$$

$f_{i,i}(\mathfrak{p},\mathfrak{q})$ is the quantum mechanical scattering amplitude describing the $\mathfrak{q} \to \mathfrak{p}$ scattering process without changing the internal state $|i\rangle$ [15]. The above result is exact in the case of $\omega = \omega_{ij}$. Physically the approximation (39) means that we take into account only complete scattering processes. All scattering amplitudes in $K_{\mathfrak{q}\mathfrak{p}}$ are without alteration of the internal state $|i\rangle$, $|j\rangle$, the first and the second term describe forward scattering processes only. These may be taken over into $d^0_{\mathfrak{q}}(\omega)$ of (22).

In the limit $V_0 \to \infty$ we obtain after performing the integration with respect to $|\mathfrak{p}|$

$$a(\omega, |\mathfrak{q}|, \Omega_{\mathfrak{q}}) = b(\omega, |\mathfrak{q}|, \Omega_{\mathfrak{q}})\,[1 + n \int d\Omega_{\mathfrak{p}} \Phi(|\mathfrak{q}|, \Omega_{\mathfrak{q}}, \Omega_{\mathfrak{p}}) a(\omega, |\mathfrak{q}|, \Omega_{\mathfrak{p}})] \tag{41}$$

where

$$a(\omega, |\mathfrak{q}|, \Omega_{\mathfrak{q}}) = a_{\mathfrak{q}}(\omega)$$

and

$$b(\omega, |\mathfrak{q}|, \Omega_{\mathfrak{q}}) = \left(\omega - \omega_{ij} - \frac{1}{2m_R}\,[\mathfrak{q}^2 - (\mathfrak{q}-\mathfrak{k})^2] - n(t^{ii}_{\mathfrak{q}\mathfrak{q}} - t^{jj*}_{\mathfrak{q}\mathfrak{q}})\right)^{-1} \tag{42}$$

$$\Phi(|\mathfrak{q}|, \Omega_{\mathfrak{q}}, \Omega_{\mathfrak{p}}) = \left(\frac{1}{2\pi}\right)^3 2\pi i m |\mathfrak{q}|\,(t^{ii}_{\mathfrak{p}\mathfrak{q}} t^{jj*}_{\mathfrak{p}\mathfrak{q}})_{|\mathfrak{p}|=|\mathfrak{q}|}. \tag{43}$$

$|\mathfrak{q}|$ and $\Omega_{\mathfrak{q}}$ denote the absolute value and the direction of the vector $\mathfrak{q}$. These formulae are basic for the investigation of the case in which the perturbers are in rest.

4. *Scattering by resting perturbers*

The integral equation derived at the end of the last section shows, that mathematical complications are due to the direction changing collisions. The solution of this integral equation is determined by the structure of $f_{i,i}$ $(\mathfrak{p}, \mathfrak{q})$ and $f_{j,j}$ $(\mathfrak{p}, \mathfrak{q})$. In the following we consider special cases.

(a) Forward scattering only

Assuming that the scattering amplitudes are different from zero mainly in forward direction, we can extract $a(\omega, |\mathfrak{q}|, \Omega_\mathfrak{p})$ out of the integral with $\Omega_\mathfrak{q}$ instead of $\Omega_\mathfrak{p}$ in (41) and obtain

$$a(\omega, |\mathfrak{q}|, \Omega_\mathfrak{q})$$

$$= \left(\omega-\omega_{ij}-\frac{1}{2m_R}\left[\mathfrak{q}^2-(\mathfrak{q}-\mathfrak{k})^2\right]-n\left(t_{\mathfrak{q}\mathfrak{q}}^{ii}-t_{\mathfrak{q}\mathfrak{q}}^{jj*}+\int d\Omega_\mathfrak{p}\Phi(|\mathfrak{q}|, \Omega_\mathfrak{q}, \Omega_\mathfrak{p})\right)\right)^{-1}. \tag{44}$$

The resulting line shape is a velocity dependent Voigt profile [4]. In the case when $f_{i,i}$ $(\mathfrak{p}, \mathfrak{q})$ and $f_{j,j}$ $(\mathfrak{p}, \mathfrak{q})$ are further independent on $|\mathfrak{q}|$, the line shape is the well known Voigt profile [4, 6], the half width of which increases monotonically with increasing density of the perturbers n.

(b) Partial wave analysis

The scattering amplitudes may be analysed in terms of partial waves. When this is done we can convert the integral equation in an infinite system of ordinary coupled equations. By truncating the partial wave expansion at $l = l_0$, one gets a finite system of $2l_0+1$ equations to be solved. In this paper we consider only the case $l_0 = 0$.

(c) s — wave scattering

In this case which corresponds to $l_0 = 0$ the scattering is isotropic and direction changing collisions are of considerable influence. Therefore, we expect a pronounced departure from the Voigt profile especially here. Then the integral kernel of (43) is independent on any direction ($\Phi \approx \Phi^0(|\mathfrak{q}|)$).

After performing the integration with respect to $\Omega_\mathfrak{q}$ in (41) we obtain

$$\int d\Omega_\mathfrak{q} a(\omega, |\mathfrak{q}|, \Omega_\mathfrak{q}) = \frac{\int d\Omega_\mathfrak{q} b(\omega, |\mathfrak{q}|, \Omega_\mathfrak{q})}{1-n\Phi^0(|\mathfrak{q}|)\int d\Omega_\mathfrak{q} b(\omega, |\mathfrak{q}|, \Omega_\mathfrak{q})}, \tag{45}$$

and finally

$$F(\omega) = (-\pi)^{-1}\varrho^{(i)}|x_{ij}|^2 \operatorname{Im} \frac{\int_0^\infty |\mathfrak{q}|^2 d|\mathfrak{q}| e^{-\frac{\beta|\mathfrak{q}|^2}{2m_R}} \int d\Omega_\mathfrak{q} a(\omega, |\mathfrak{q}|, \Omega_\mathfrak{q})}{\int d^3\mathfrak{q} e^{-\frac{\beta\mathfrak{q}^2}{2m_R}}}. \tag{46}$$

5. Numerical results in the s-wave scattering

Next we shall make some simplifying assumptions. The influence of the scattering process on $F(\omega)$ is contained in $(t^{ii}_{qq}-t^{jj*}_{qq})$ and $\Phi^0(|q|)$ which characterize the forward scattering and the direction changing processes, respectively. Because of our interest in the general behaviour of $F(\omega)$ we take them as constants independent of $|q|$

$$t^{ii}_{qq}-t^{jj*}_{qq} = -i\alpha \qquad (\alpha > 0)$$

$$\Phi^0(|q|) = \frac{i}{12}\gamma \qquad (\gamma > 0). \tag{47}$$

Real parts, which describe line displacements, are suppressed. The sign of α and γ is determined from general conclusions. The factor $\frac{1}{12}$ is introduced for practical purposes. Thus we can conclude $\alpha \geqslant K > \frac{3}{\pi} K \geqslant \gamma$ with $K = \frac{1}{2}\frac{|q|}{m}(\sigma_{ii}+\sigma_{jj})$, where $\sigma_{ii}(\sigma_{jj})$ is the total cross section for elastic scattering in the internal state $|i\rangle$ ($|j\rangle$).

In $b(\omega, |q|, \Omega_q)$ we disregard the term $\frac{1}{2m_R}k^2$ and finally we replace in $(1-n\Phi^0(|q|)\int d\Omega_q b(\omega, |q|, \Omega_q))\,|q|$ by its most probable value $|q|_w = \frac{1}{\sigma} = \left(\frac{2m_R}{\beta}\right)^{\frac{1}{2}}$. This somewhat crude approximation is possible because $(1-n\Phi^0(|q|)\int \Omega_q b(\omega, |q|, \Omega_q))$ is a smooth function of $|q|$. With these simplifying assumptions which, we think, do not influence the general behaviour of the line shape drastically, $F(\omega)$ may be expressed in terms of known functions. We introduce the abbreviations

$$\Delta = \frac{|\mathfrak{k}|}{\sigma m_R}, \qquad \bar{\omega} = \frac{\omega-\omega_{ij}}{\Delta}, \qquad \bar{\alpha} = \frac{\alpha}{\Delta}, \qquad \bar{\gamma} = \frac{\gamma}{\Delta} \tag{48}$$

and use the definition of the plasma dispersion function

$$Z(z) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty} e^{-t^2}(t-z)^{-1}dt, \tag{49}$$

and the definition of the Legendre polynomial of second kind

$$Q_0(z) = \tfrac{1}{2}\int_{-1}^{+1}(z-t)^{-1}dt. \tag{50}$$

Then $F(\omega)$ can be expressed in its final form by

$$F(\omega) = \pi^{-1}\varrho^{(i)}|x_{ij}|^2\frac{1}{\Delta}\,\mathrm{Im}\,\frac{Z(\bar{\omega}+in\bar{\alpha})}{1-in\bar{\gamma}\frac{4\pi}{12}Q_0(\bar{\omega}+in\bar{\alpha})}. \tag{51}$$

This line shape is symmetric in respect to ω_{ij}. It contains n, α, γ, and Δ as parameters in the dimensionless combinations $\bar{\omega}$, $n\bar{\alpha}$, and $n\bar{\gamma}$. n, α and γ characterize the density of perturbers, the phase changing and the direction changing collisions. Δ is the line width of the Doppler profile resulting from $n = 0$. It means the distance from the line centre

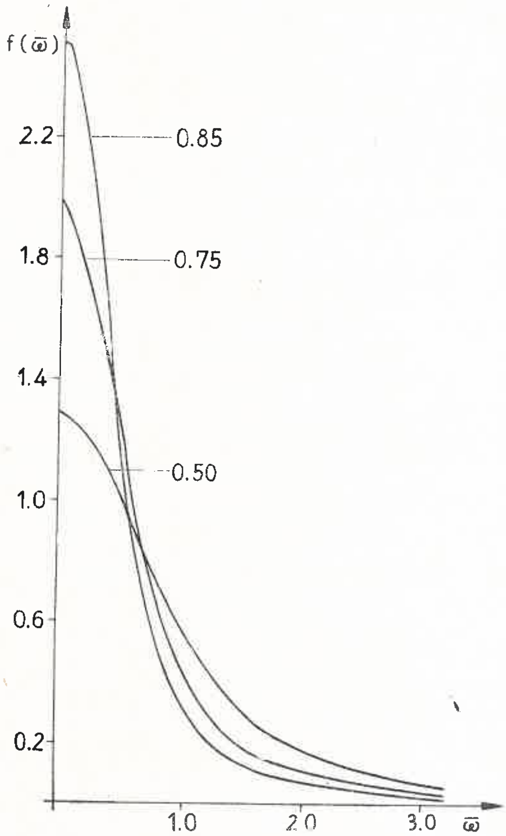

Fig. 1. $f(\bar{\omega})$ for $n\bar{\alpha} = 1.0$ and some selected values of $\bar{\gamma}/\bar{\alpha}$

at which $F(\omega)$ takes the value $e^{-1}F_{\max}$. (In this manner we also define the line width δ of the other profiles.)

$\frac{n\alpha}{\Delta}$ and $\frac{n\gamma}{\Delta}$ may be written in the form $\frac{\lambda}{l_\alpha}$ and $\frac{\lambda}{l_\gamma}$ respectively. Here l_α characterizes the mean free path of the radiators according to all collisions, and l_γ describes the mean free path connected only with direction changing collisions. The wave length λ is defined by $\lambda = \frac{2\pi}{|\mathfrak{k}|}$. The line shape $F(\omega)$ finally obtained contains as limiting cases the Doppler

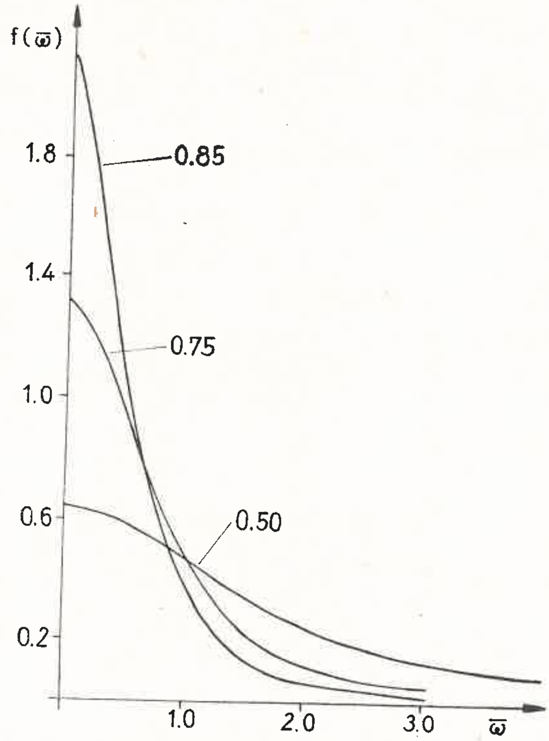

Fig. 2. $f(\bar{\omega})$ for $n\bar{\alpha} = 3.0$ and some selected values of $\bar{\gamma}/\bar{\alpha}$

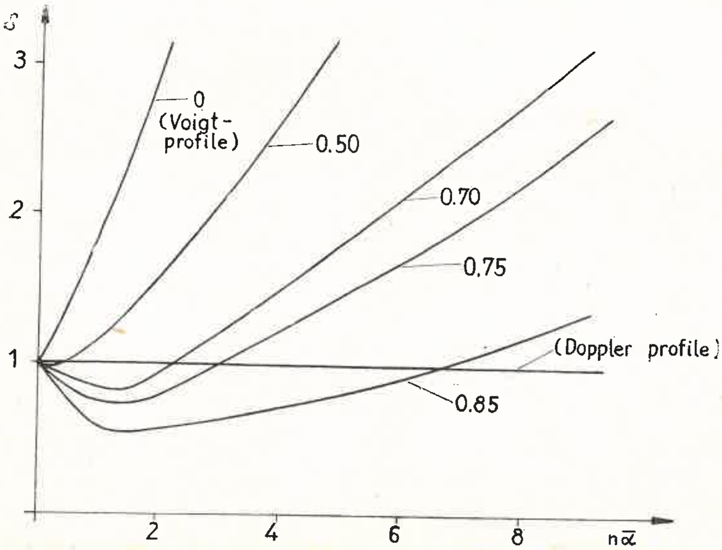

Fig. 3. Resulting line width δ as a function of $n\bar{\alpha}$ for some selected values of $\bar{\gamma}/\bar{\alpha}$

profile ($n = 0$), the Voigt profile ($\gamma = 0$) and in the case of large n the Lorentzian shape resulting from the above mentioned Voigt profile.

The results of the numerical calculations are shown partly in Figs 1 — 3. In Figs 1 — 2 we have plotted $f(\bar{\omega})$ defined by $F(\omega) = \pi^{-1}\varrho^{(i)}|x_{ij}|^2 \frac{1}{\Delta} f(\bar{\omega})$ for some selected values of $n\bar{\alpha}$ and $n\bar{\gamma}$. Fig. 3 shows the resulting line width δ as a function of the perturber density n (more exactly $n\bar{\alpha}$) for some values of $\bar{\gamma}/\bar{\alpha}$.

These Figs. show clearly that in the case of $\gamma \neq 0$ the resulting line shapes have line widths which go through a minimum regarded as a function of the density. The larger is the ratio $\bar{\gamma}/\bar{\alpha}$ which means that the influence of direction changing collisions becomes larger, the clearer this behaviour.

Summarizing the results we can say that we found the Dicke narrowing of spectral lines caused, in our model, by direction changing collisions.

6. *Discussion*

In this paper we have shown how to incorporate the influence of the radiators motion on the line shape in the framework of the Fano theory. As the resulting superoperator describing the scattering effects is not diagonal in the translational degrees of freedom of the radiators, it was necessary to go over to an integral equation as in kinetic theories. In our procedure the approximations at each stage of the calculation have a well defined meaning. The restriction on a situation with perturbers in rest and on s-wave scattering means that we consider such a case in which the Dicke narrowing is especially effective. The choice of completed scattering processes only and further approximations are of minor influence on the general line shape and may be relaxed in more involved calculations. The resulting line shape is a function of two characteristic parameters describing the ratio of the wave length of the photon to the mean free pathes for different scattering processes. The larger the influence of direction changing collisions, the clearer the resulting Dicke narrowing.

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