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Complete redistribution in the transfer of resonance radiation

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The assumption of complete redistribution in frequency used in the theory of transport of resonance radiation, when Doppler broadening is important, is shown to predict the correct number densities in the excited levels at large optical depth. The line shape, however, is not a Doppler distribution in the wings but decreases like $\exp(-u^2)/u$.

I. INTRODUCTION

In the theory of radiative transfer in spectral lines under conditions such that Doppler broadening[1] determines the spectral line shape, a fundamental role is played by the assumption that the line shape of the radiation emitted by the excited atoms is proportional to the absorption coefficient $\mathfrak{L}(u) \propto k(u)$. This assumption, known in astrophysics as the assumption of complete redistribution in frequency, has been discussed extensively by Holstein.[2] He has argued that the assumption is reasonable at large optical thickness. In astrophysics,[3] it has been shown that, on this basis, models can be constructed for radiative transfer problems which give reasonable agreement with physical reality much better than with the previous assumption of so-called "monochromatic scattering."[4] When the assumption is adopted, it is not difficult for the stationary state of a radiating plasma immersed in an electron gas to derive the equation

$$A(2,1)n_2(\vec{r}) + n_2(\vec{r})n_e K(2,1) = n_1 n_e K(1,2) + A(2,1)\int_V K(|\vec{r}-\vec{r}'|)n_2(\vec{r}')\,d\vec{r}', \quad (1)$$

$$K(|\vec{r}-\vec{r}'|) = \int_0^\infty \mathfrak{L}(u)k(u)\frac{\exp(-k(u)|\vec{r}-\vec{r}'|)}{4\pi|\vec{r}-\vec{r}'|^2}\,du.$$

Here $A(2,1)$ is the Einstein coefficient for spontaneous emission $2\to 1$ and n_2, n_e, and n_1 are the densities of excited atoms, electrons, and ground state atoms, respectively. For the sake of simplicity it has been assumed that n_e, n_1, and the electron temperature are independent of position. $K(2,1)$ and $K(1,2)$ are the rate constants for deexcitation and excitation, $\mathfrak{L}(u)$ is the line shape, $k(u) = k_0\mathfrak{L}(u)$ is the absorption coefficient, and

$$\mathfrak{L}(u) = \exp(-u^2)/\pi^{1/2}, \quad u = 2(\nu-\nu_0)/\Delta\nu_D, \ \Delta\nu_D$$

is Doppler breadth. The integration extends over a certain volume V.

Equation (1) can be solved with the aid of the solutions of the following eigenvalue problem[5]:

$$\tilde{A}(2,1)\psi(\vec{r}) = A(2,1)\psi(\vec{r}) - A(2,1)\int_V K(|\vec{r}-\vec{r}'|)\psi(\vec{r}')\,d\vec{r}'. \quad (2)$$

Here $\tilde{A}(2,1)$ is an eigenvalue and $\psi(\vec{r})$ an eigenfunction. For the analysis of Eq. (2) at large optical thickness, only the behavior of $\mathfrak{L}(u)$ in the far wings is important.[2,5] More precisely, let the volume V be a slab of thickness L. Define the dimensionless frequency $u_0(k) > 0$ as the solution of $\mathfrak{L}(u_0) = (k_0L/2k)^{-1}$ when $k_0L\to\infty$. For a Doppler profile we have $u_0(k) = (\ln k_0L/2k\pi^{1/2})^{1/2}$. The eigenvalues and eigenfunctions of Eq. (2) are determined by the behavior of the Fourier transform of the kernel near $k/k_0L = 0$.[5,6] For this behavior the following formula has been derived[5]:

$$\int K(r)e^{i\vec{k}\cdot\vec{r}}\,d\vec{r} \sim 1 - \frac{\pi}{2}\frac{k_0L}{k}\int_{u_0(k)}^\infty \mathfrak{L}^2(u)\,du, \quad |\vec{k}|/k_0L \to 0. \quad (3)$$

It follows that the solutions of Eq. (2) are determined by the behavior of $\mathfrak{L}(u)$ for frequencies of the order of and larger than u_0, the far wings of the spectral line; u_0 is precisely the frequency at which a photon has a mean free path of the order of[7] $\frac{1}{2}L$, so that for frequencies $|u| \geq u_0$, the slab is optically thin. The following criticism can now be raised: Irrespective of whether the assumption $\mathfrak{L}(u) \propto k(u)$ is valid in some frequency range or other, it is highly doubtful that it is valid in the far wings of the line, where the loss of photons is substantial. If this is true, then the assumption breaks down precisely where we need it, and the whole theory is invalid.

It will be shown that this criticism is basically correct; we shall obtain an equation for the line shape and prove that for $k_0L\to\infty$ it approaches the Doppler line for frequencies[8] $|u| \leq u_0$. For frequencies $|u| \geq u_0$, however,[8] it becomes proportional to $u_0e^{-u^2}/u$ and is even anisotropic in that frequency range. Nevertheless, and rather surprisingly, our analysis yields the same eigenvalues and eigenfunctions[9,10] as Eq. (2) for $k_0L\to\infty$, which means that the number densities in the excited levels, the total production of radiation, etc., as calculated from Eq. (1), are correct. The line shape of the emitted radiation is not correct. The differences may be sizeable in the far wings of the line, but, fortunately, this is not the part of the line in which one is usually most interested. The reason is essentially the following: Suppose that Eqs. (1)-(3) remain valid in the correct theory, in the sense that we need only insert the correct line shape everywhere. This is not absolutely true, but may be assumed to be fairly close to the truth.[11] In first-order asymptotic theory for $k_0L\to\infty$, it does not matter then whether e^{-u^2} or $u_0e^{-u^2}/u$ is used in the integral in Eq. (3) because the exponential determines its behavior for $u_0\to\infty$.

The plan of the paper is as follows: In Sec. II the general equation of radiative transfer for a stationary problem is reduced to a set of linear integral equations. The set is analysed in Sec. III, where the line shape of the excited atoms is obtained and where it is shown that the eigenvalues obtained from Eq. (2) are correct for large optical depth.

The manner in which the problem is dealt with is likely to be applicable to more difficult situations where the assumption of complete redistribution certainly fails; for instance, when natural broadening is of importance in addition to Doppler and/or Lorentz broadening.[10]

II. REDUCTION OF TRANSPORT EQUATION

We shall work in a simple geometry, namely, the slab

$$V=(-\tfrac{1}{2}L\leqslant x\leqslant\tfrac{1}{2}L,\quad -\infty<y,\quad z<+\infty).$$

The analysis can be extended to other geometries (e.g., an infinite cylinder) at the expense of somewhat more complicated formulas. The results, however, remain essentially the same. There will be present in V electrons whose density is designated by n_e (independent of position) which excite and deexcite atoms. The atoms in the ground state, density n_1 independent of position, will have a Maxwellian velocity distribution such that the absorption coefficient $k(u)$ is Doppler: ' $=k_0e^{-u^2}\pi^{-1/2}$, and atoms excited by electrons en their radiation into the radiation field according to the Doppler distribution. Our starting point will be the Milne-Edington equation for the intensity of radiation $I(\vec{r},u,\vec{s})$ in V. $I(\vec{r},u,\vec{s})\,du\,d\Omega$ represents the energy transported per cm^2 and per second at position $\vec{r}$ in the direction denoted by the unit vector $\vec{s}$ at frequency u, within the element of solid angle $d\Omega$. The angle between $\vec{s}$ and the positive x direction is denoted by ϑ. The angle between the projection of $\vec{s}$ on the yz plane and the positive y direction is φ and will be measured counterclockwise. Since n_1 and n_e are independent of position and the density of excited atoms n_2 is at most a function of x (and not of y and z), $I(\vec{r},u,\vec{s})$ will be a function of x, u, and ϑ only. We then have the following transport[12] equation in V:

$$\cos\vartheta\frac{\partial}{\partial x}I(x,u,\vartheta)+k(u)I(x,u,\vartheta)=(1-\epsilon)S(u)+\frac{k_0(1-\epsilon)}{4\pi}\int_{-\infty}^{+\infty}\int_{\Omega'}R(u,\vec{s};u',\vec{s}\,')I(x,u',\vartheta')\,du'\,d\Omega', \qquad (4)$$

where

$$1-\epsilon=A(2,1)[A(2,1)+n_eK(2,1)]^{-1}$$

represents the fraction of the primary excitations [by the radiation field $I(x,u,\vartheta)$ or by sources $S(u)$ independent of $I(x,u,\vartheta)$] that is emitted into the radiation field and where

$$4\pi S(u)=h\nu n_1n_eK(1,2)\mathcal{L}(u)$$

is the energy per cm^3 and per second produced by the electron gas in creating excited atoms. The fraction $(1-\epsilon)S(u)$ is emitted into the radiation field, the emission being isotropic. Finally,[12]

$$R(u,\vec{s};u',\vec{s}\,')=(\pi\sin\gamma)^{-1}\exp[(-u^2-u'^2+2uu'\cos\gamma)/\sin^2\gamma]. \qquad (5)$$

$R(u,\vec{s};u',\vec{s}\,')$ gives the frequency u of the photons absorbed from $I(x,u',\vec{s}\,')$ and reemitted in the direction $\vec{s}$ ($\cos\gamma=\vec{s}\cdot\vec{s}\,'$) when (a) natural line broadening is negligible compared to Doppler broadening and (b) the atom does not change its velocity during the absorption-emission event. The aim is to solve Eq. (4). However, since $I(x,u,\vartheta)$ is a function of three independent variables, a direct treatment of Eq. (4) seems hopeless. We therefore try to decompose Eq. (4) into a set of (coupled) equations for functions with fewer independent variables. These functions are constructed such that $I(x,u,\vartheta)$ and the density of excited atoms and the line shape of the emitted radiation, which are even more interesting, can be calculated from them. We shall do this by reducing Eq. (4) to a set of linear integral equations.

The principle of this reduction will be demonstrated first be approximating $R(u,\vec{s};u',\vec{s}\,')$ by $\exp[-u^2-u'^2]/\pi$, the product of two Doppler distributions [assumption of complete redistribution; the reemitted radiation is assumed to have a line shape proportional to the absorption profile, and $\mathcal{L}(u) \propto k(u)$].

The result will be the Biberman-Holstein integral equation, Eq. (1). Next, using an expansion of $R(u, \vec{s}; u', \vec{s}')$ to be derived in Appendix A, we derive in essentially the same way the required set of integral equations which will be analyzed in Sec. III.

A. Complete redistribution

We make the assumption of complete redistribution, i.e., (without proper justification) we insert in Eq. (4)

$$R(u, \vec{s}; u', \vec{s}') = \mathcal{L}(u)\mathcal{L}(u') = \pi^{-1} e^{-u^2 - u'^2}. \tag{6}$$

After perfroming the integration over φ, Eq. (4) becomes

$$\cos\vartheta \frac{\partial}{\partial x} I(x,u,\vartheta) + k(u) I(x,u,\vartheta) = (1-\epsilon) S(u) + \tfrac{1}{2}(1-\epsilon)\mathcal{L}(u) \int_{-\infty}^{+\infty} k(u') \int_0^{\pi} I(x,u',\vartheta') \sin\vartheta' \, d\vartheta' \, du'.$$

The right-hand side of this equation is independent of ϑ and proportional to $\mathcal{L}(u)$. We formally put

$$(1-\epsilon)\left(S(u) + \tfrac{1}{2}\mathcal{L}(u) \int_{-\infty}^{+\infty} k(u') \int_0^{\pi} I(x,u',\vartheta') \sin\vartheta' \, d\vartheta' \, du' \right) = (h\nu/4\pi) A(2,1) n_2(x) \mathcal{L}(u). \tag{7}$$

This formula defines $n_2(x)$, which can be interpreted as the density of excited atoms at position x. We thus have

$$\cos\vartheta \frac{\partial}{\partial x} I(x,u,\vartheta) + k(u) I(x,u,\vartheta) = (h\nu/4\pi) A(2,1) n_2(x) \mathcal{L}(u).$$

This is a first-order differential equation. When no radiation is incident from the outside on the planes $x = \pm\frac{1}{2}L$, the solution is

$$I(x,u,\vartheta) = \begin{cases} \dfrac{h\nu}{4\pi} A(2,1) \dfrac{\mathcal{L}(u)}{\cos\vartheta} \displaystyle\int_{-L/2}^{x} \exp\left(\frac{k(u)}{\cos\vartheta}(x'-x)\right) n_2(x')\,dx', & 0<\vartheta<\tfrac{1}{2}\pi \\ \dfrac{h\nu}{4\pi} A(2,1) \dfrac{\mathcal{L}(u)}{\cos\vartheta} \displaystyle\int_{L/2}^{x} \exp\left(\frac{k(u)}{\cos\vartheta}(x'-x)\right) n_2(x')\,dx', & \tfrac{1}{2}\pi<\vartheta<\pi . \end{cases}$$

Multiply both sides of this equation by $k(u)\sin\vartheta\, d\vartheta\, du$ and integrate over ϑ from 0 to π and over u from $-\infty$ to $+\infty$. Making use of Eq. (7), and the definitions of $S(u)$ and $1-\epsilon$, we obtain

$$\begin{aligned} &A(2,1)n_2(x) + n_2(x) n_e K(2,1) = n_1 n_e K(1,2) + A(2,1) \int_{-L/2}^{L/2} K(|x-x'|) n_2(x')\,dx', \\ &K(|x|) = \frac{1}{2}\int_{-\infty}^{+\infty} \mathcal{L}(u) k(u) \int_0^{\pi/2} \exp\left(-\frac{k(u)|x|}{\cos\vartheta}\right) \tan\vartheta \, d\vartheta \, du . \end{aligned} \tag{8}$$

Equation (1) reduces to Eq. (8) if n_2 is taken independent of y and z and the integration over these variables is carried out. The analysis leading to Eq. (8) is very well known. It has been given because essentially the same treatment applies in the general case to which we now turn.

B. General theory

The approximation of Eq. (6) is the first term ($n = m = l = 0$) of the expansion (to be derived in Appendix A).

$$R(u,\vec{s};u',\vec{s}') = \sum_{n=0}^{\infty} \sum_{m=-n}^{+n} \sum_{l=0}^{\infty} \frac{(n+\frac{1}{2})}{\pi^{1/2}} \frac{(n-m)!}{(n+m)!} \frac{P_n^m(\cos\vartheta) P_n^m(\cos\vartheta') e^{im(\varphi-\varphi')} e^{-u^2-u'^2}}{l!\,\Gamma(l+n+\frac{3}{2}) 2^{4l+2n}} H_{2l+n}(u) H_{2l+n}(u') . \tag{9}$$

$P_n^m(\cos\vartheta)$ is an associated Legendre polynomial[13] and $H_{2l+n}(u)$ is a Hermite polynomial.[13] Equation (9) is substituted into Eq. (4). Since the intensity $I(x,u,\vartheta)$ is independent of φ, the integration over this variable yields $2\pi\delta_{m,0}$. The function $n_2(x,u,\cos\vartheta)$ is introduced as follows:

$$(1-\epsilon)\left(S(u) + e^{-u^2} \sum_{n,l=0}^{\infty} \frac{(n+\frac{1}{2}) P_n(s) H_{2l+n}(u)}{l!\,\Gamma(l+n+\frac{3}{2}) 2^{4l+2n+1}} \int_{-\infty}^{+\infty} k(u') H_{2l+n}(u') \int_0^{\pi} P_n(\cos\vartheta') I(x,u',\vartheta') \sin\vartheta' \, d\vartheta' \, du' \right)$$

$$= (h\nu/4\pi) A(2,1) n_2(x,u,s) , \tag{10}$$

where $s=\cos\vartheta$, and where $n_2(x,u,s)$ can be interpreted as the density of excited atoms at position x which emit photons at frequency u in the direction defined by the angle ϑ. According to this definition, Eq. (4) becomes

$$\cos\vartheta\frac{\partial}{\partial x}I(x,u,\vartheta)+k(u)I(x,u,\vartheta)=(h\nu/4\pi)A(2,1)n_2(x,u,s)\,. \quad (11)$$

The quantity $n_2(x,u,s)$ will in general be neither purely Doppler nor isotropic (and even if it were, we would want to prove it and not assume it). Therefore the following expansion of $n_2(x,u,s)$ is introduced in terms of the Legendre and Hermite polynomials:

$$n_2(x,u,s)=\frac{e^{-u^2}}{\pi^{1/2}}\sum_{n,l=0}^{\infty}(2n+1)P_n(s)H_{2l+n}(u)n_{2,l,n}(x)\,. \quad (12)$$

Note that if $n_2(x,u,s)$ were isotropic and Doppler, only the term $n=l=0$ in Eq. (12) would be different from zero (apply the orthogonality relations[13] for the Legendre and Hermite polynomials). The terms with $n, l\neq 0$ apparently describe the deviations from the Doppler distribution and the anisotropy which $n_2(x,u,s)$ may exhibit. $S(u)$ in Eq. (10) is proportional to e^{-u^2} and independent of ϑ. Its expansion in Legendre and Hermite polynomials contains only one term,[13] namely,

$$S(u)=\tfrac{1}{2}Se^{-u^2}P_0(s)H_0(u)\,,\qquad S=(h\nu/2\pi^{3/2})n_1n_eK(1,2)\,. \quad (13)$$

Equations (12) and (13) are substituted into Eq. (10). Since the Legendre and Hermite polynomials are mutually orthogonal[13] (the latter with respect to the weight function e^{-u^2}), the terms in the expansions must separately equal one another. We have

$$(1-\epsilon)\left(S\delta_{n,0}\delta_{l,0}+\int_{-\infty}^{+\infty}k(u')H_{2l+n}(u')\int_0^{\pi}\frac{P_n(\cos\vartheta')I(x,u',\vartheta')\sin\vartheta'}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n+1}}d\vartheta'\,du'\right)=\frac{h\nu}{2\pi^{3/2}}A(2,1)n_{2,l,n}(x)\,. \quad (14a)$$

We now proceed as in the case of complete redistribution (Sec. II A). The solution of Eq. (11) is

$$I(x,u,\vartheta)=\begin{cases}\dfrac{h\nu}{4\pi}\dfrac{A(2,1)}{s}\displaystyle\int_{-L/2}^{x}\exp\left(\frac{k(u)(x'-x)}{s}\right)n_2(x',u,s)\,dx'\,, & 0\leq s\leq 1\\[2ex] \dfrac{h\nu}{4\pi}\dfrac{A(2,1)}{s}\displaystyle\int_{L/2}^{x}\exp\left(\frac{k(u)}{s}(x'-x)\right)n_2(x',u,s)\,dx'\,, & -1\leq s\leq 0\,.\end{cases}$$

Both sides of this equation are multiplied by

$$k(u)H_{2l+n}(u)P_n(\cos\vartheta)\sin\vartheta\,d\vartheta\,du/[l!\,\Gamma(l+n+\tfrac{3}{2})2^{4l+2n+1}]$$

and integrated with respect to u and ϑ from $-\infty$ to $+\infty$ and from 0 to π, respectively. By means of Eq. (14a) we obtain ($s=\cos\vartheta$)

$$\frac{4\pi}{h\nu A(2,1)}\left(\frac{h\nu}{2\pi^{3/2}}A(2,1)(1-\epsilon)^{-1}n_{2,l,n}(x)-S\delta_{n,0}\delta_{l,0}\right)$$
$$=\int_{-\infty}^{+\infty}\int_0^1\int_{-L/2}^{x}\frac{k(u)H_{2l+n}(u)P_n(s)\exp[(k(u)/s)(x'-x)]}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n+1}}n_2(x',u,s)\,du\frac{ds}{s}dx'$$
$$+(-1)^n\int_{-\infty}^{+\infty}\int_0^1\int_x^{L/2}\frac{k(u)H_{2l+n}(u)P_n(s)\exp[(k(u)/s)(x-x')]}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n+1}}n_2(x',u,-s)\,du\frac{ds}{s}dx'\,.$$

Equation (12), with the indices of summation changed into n' and l', is substituted into the right-hand side of this equation. We then note that only for even values of $n+n'$ are the integrals obtained different from zero, because for $n+n'$ odd, $H_{2l+n}(u)H_{2l'+n'}(u)$ is odd while the rest of the integrand is an even function of u. Using the definition of

$$1-\epsilon=A(2,1)[A(2,1)+n_eK(2,1)]^{-1}$$

and of S, we obtain after some simplifications the following system of linear integral equations for the functions $n_{2,l,n}(x)(l,n=0,1,\ldots)$:

$$[A(2,1)+n_eK(2,1)]n_{2,l,n}(x)-n_1n_eK(1,2)\delta_{l,0}\delta_{n,0}=A(2,1)\sum_{l',n'=0}^{\infty}\int_{-L/2}^{L/2}K_{l,n,l',n'}(|x-x'|)n_{2,l',n'}(x')\,dx',\tag{14b}$$

$$K_{l,n,l',n'}(|x-x'|)=(n'+\tfrac{1}{2})\int_{-\infty}^{+\infty}\int_0^1\exp\left(-\frac{k(u)}{s}|x-x'|\right)\frac{e^{-u^2}k(u)H_{2l+n}(u)P_n(s)H_{2l'+n'}(u)P_{n'}(s)}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n+1}}\frac{ds}{s}\,du.$$

Note that the term $l=n=l'=n'=0$ is precisely the Biberman-Holstein integral equation, Eq. (8). Because the kernels are actually zero for $n+n'$ odd, Eq. (14b) separates into two sets of equations for n,n' both odd and n,n' both even. The inhomogeneous term for the odd set is zero, and therefore its solution will be zero. Hence only the solutions of Eq. (14b) for n,n' both even need be analyzed. We do not want to use $2n$ and $2n'$ as subscripts and therefore change the notation a little bit. In the following, we denote $n_{2,l,2n}(x)$ by $n_{2,l,m}(x)$ and $K_{1,2n,l',2n'}(|x-x'|)$ by $K_{l,m,l',m'}(|x-x'|)$. Equation (14b) for $l,m=0,1,\ldots$, becomes

$$[A(2,1)+n_eK(2,1)]n_{2,l,m}(x)-n_1n_eK(1,2)\delta_{l,0}\delta_{m,0}=A(2,1)\sum_{l',m'=0}^{\infty}\int_{-L/2}^{L/2}K_{l,m,l',m'}(|x-x'|)\times n_{2,l',m'}(x')\,dx'.\tag{15}$$

The expression for $K_{l,m,l',m'}(|x-x'|)$ is obtained from the corresponding one for $K_{l,2n,l',2n'}(|x-x'|)$ replacing n and n' by m and m' everywhere in Eq. (14b). Equation (15) is perfectly general and applies both at low and high optical thickness. It has the advantage over Eq. (4) in that it has been formulated in terms of functions of one variable only, but this has been achieved at the expense of the fact that we need to solve an infinite set. This price, however, will turn out not to be too high, at least if we restrict ourselves to the important case of large optical thickness. We shall show this in Sec. III.

III. ANALYSIS OF PROBLEM

In the analysis of Eq. (14b), Fourier techniques play an important role. We first briefly demonstrate the principle[14] in the particular case obtained by truncating Eq. (14b) at order zero (the Biberman-Holstein integral equation). The solution of this equation will be needed later for comparison with the solution of the complete set of equations given in Eq. (14b).

A. Complete redistribution

Equation (14b) truncated at order zero reads for $|x|\le\frac{1}{2}L$

$$A(2,1)\left(n_2(x)-\int_{-L/2}^{+L/2}K(|x-x'|)n_2(x')\,dx'\right)+n_2(x)n_eK(2,1)=n_1n_eK(1,2).\tag{16}$$

For brevity we have set $n_2(x)=n_{2,0,0}(x)$ and $K(|x-x'|)=K_{0,0,0,0}(|x-x'|)$. Equation (16) would be correct if we could argue that (e.g., for $k_0L\gg1$) the line shape of the excited atoms is Doppler, because then all $n_{2,l,m}(x)$ in Eq. (14b) vanish for $l,m\ge1$, as follows from Eq. (12). We introduce in Eq. (16) the new variables $\frac{1}{2}\xi L=x$, $\frac{1}{2}\xi' L=x'$ and obtain for $|\xi|\le1$

$$A(2,1)\left(n_2(\xi)-\tfrac{1}{2}L\int_{-1}^{+1}K(\tfrac{1}{2}L|\xi-\xi'|)n_2(\xi')\,d\xi'\right)+n_2(\xi)n_eK(2,1)=n_1n_eK(1,2).$$

For the application of Fourier analysis, it is most unpleasant that the integration extends over a finite interval. Actually this causes no difficulty because the number densities n_2, n_1, and n_e are zero outside $[-1,+1]$. It is, however, necessary to make this fact more transparent in the mathematics. We introduce a function $P(\xi)$ defined as follows: $P(\xi)=1$ for $|\xi|\le1$, $P(\xi)=0$ for $|\xi|>1$. We then have

$$A(2,1)P(\xi)\left(n_2(\xi)-\tfrac{1}{2}L\int_{-\infty}^{+\infty}K(\tfrac{1}{2}L|\xi-\xi'|)P(\xi')n_2(\xi')\,d\xi'\right)+P(\xi)n_2(\xi)n_eK(2,1)=P(\xi)n_1n_eK(1,2).$$

After applying Fourier transformation to both sides, the equation becomes (n_e and n_1 are assumed to be independent of position)

$$A(2,1)\left(\hat{n}_2(k)-(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\hat{K}(k')\hat{n}_2(k')\,dk'\right)+\hat{n}_2(k)n_eK(2,1)=n_1n_eK(1,2)\hat{P}(k),\tag{17}$$

where

$$\hat{n}_2(k) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} e^{ik\xi} P(\xi) n_2(\xi)\, d\xi \,,$$

$$\hat{K}(k) = \tfrac{1}{2}L \int_{-\infty}^{+\infty} e^{ik\xi} K(\tfrac{1}{2}L\xi)\, d\xi \,,$$

$$(2\pi)^{-1/2}\hat{P}(k) = (2\pi)^{-1} \int_{-\infty}^{+\infty} e^{ik\xi} P(\xi)\, d\xi = \frac{1}{\pi}\frac{\sin k}{k} \,.$$

In connection with Eq. (17), the following eigenvalue problem is of importance:

$$\hat{\psi}_j(k) - (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \hat{P}(k-k')\hat{K}(k')\hat{\psi}_j(k')\, dk' = \frac{\tilde{A}_j(2,1)}{A(2,1)} \hat{\psi}_j(k') \,. \quad (18)$$

Assume that this equation has been solved. It can be proved that the eigenfunctions constitute a complete, orthonormal set. After having normalized them to unity, we expand $\hat{n}_2(k)$ as follows:

$$\hat{n}_2(k) = \sum_{j=0}^{\infty} a_j \hat{\psi}_j(k), \quad a_j = \int_{-\infty}^{+\infty} \hat{n}_2(k)\hat{\psi}_j(k)\, dk \,.$$

Substitution of this expression into Eq. (17) immediately yields the following soulution:

$$\hat{n}_2(k) = n_1 n_e K(1,2) \sum_{j=0}^{\infty} \frac{\psi_j(k)}{\tilde{A}_j(2,1) + n_e K(2,1)} \times \int_{-\infty}^{+\infty} \hat{P}(k')\hat{\psi}_j(k')\, dk' \,. \quad (19)$$

If desired, inverse Fourier transformation can be applied to yield the solution in ordinary ξ space. We shall not do this since we are only interested in the form of the solution given in Eq. (19). The eigenvalue problem defined in Eq. (18) is therefore of crucial importance to us. Widom[6] has proved that for $k_0 L \gg 1$ both the eigenvalues and the eigenfunctions of Eq. (18) can be derived from the behavior of $\hat{K}(k)$ near $k=0$. It is shown in Appendix B that we have

$$\hat{K}(k) \sim 1 - \frac{\pi}{2}\frac{k}{k_0 L}\left(\ln \frac{k_0 L}{2k\pi^{1/2}}\right)^{-1/2}, \quad \frac{|k|}{k_0 L} \to 0 \quad (20)$$

and Widom[6] has proved that in that case

$$\frac{\tilde{A}_j(2,1)}{A(2,1)} \sim \frac{\pi}{2}\frac{\lambda_j^{1}}{k_0 L}\left(\ln \frac{k_0 L}{2\pi^{1/2}}\right)^{-1/2}, \quad k_0 L \gg 1 \quad (21)$$

where the λ_j are the eigenvalues of a certain integral equation which also yields the eigenfunctions $\hat{\psi}_j(k)$. The integral equation is determined *completely by the exponent* (=1) *of* k in the second term of Eq. (20). In the sequel we shall need this fact only, and not the actual form of the integral equation or the actual form of its solutions λ_j and $\hat{\psi}_j(k)$. This brings the analysis of the Biberman-Holstein integral equation to a close.

B. General theory--preliminaries

The analysis of Eq. (15) is difficult because we have to solve for the $n_{2,l,m}(x)$ all at once. The problem resides in the off-diagonal kernels $K_{l,m,l',m'}(|x-x'|), l \neq l', m \neq m'$, because if these were zero, there would remain only the task of separately solving a set of independent integral equations. Using the theory of Subsection III A this would be simple, and actually, because the inhomogeneous term contains only one nonvanishing expression ($l=m=0$), we would retrieve the Biberman-Holstein integral equation. The idea is now to calculate the functions $n_{2,p,q}(x)$, these being a linear superposition of the functions $n_{2,l,m}(x)$ and integral kernels $K_{p,q,p',q'}(|x-x'|)$, being a linear superposition of the kernels $K_{l,m,l',m'}(|x-x'|)$, such that when Eq. (15) is reformulated in terms of these quantities, the resulting set is diagonal, at least in good approximation for $k_0 L \gg 1$. The resulting inhomogeneous term possesses nonvanishing expressions for all values of p and q, so that we have to solve separately a great number of independent integral equations. It will be proved, however, that from the $n_{2,p,q}(x)$ under nonequilibrium conditions, the one with $p=q=0$ dominates the others for $k_0 L \gg 1$. We shall obtain an expression for $n_{2,p,q}(x)$, $p=q=0$, and compare it with the corresponding solution of the Biberman-Holstein integral equation. Furthermore, the line shape of the excited atoms will be calculated.

It is convenient to formulate the problem in Fourier space. By applying the steps used in transforming Eq. (16) into Eq. (17), Eq. (15) becomes, for both $l,m=0,1,\ldots$,

$$A(2,1)\left(\hat{n}_{2,l,m}(k) - (2\pi)^{-1/2} \sum_{l',m'=0}^{\infty} \int_{-\infty}^{+\infty} \hat{P}(k-k')\hat{K}_{l,m,l',m'}(k')\hat{n}_{2,l',m'}(k')\, dk'\right) + \hat{n}_{2,l,m}(k) n_e K(2,1) = \delta_{l,0}\delta_{m,0} n_1 n_e K(1,2)\hat{P}(k) \,. \quad (22)$$

The definition of the various symbols is, *mutatis mutandis*, equal to that given under Eq. (17). In Appendix B it is proved that

$$\hat{K}_{l,m,l',m'}(k') = \frac{(2m'+\frac{1}{2})2^{-4l-4m}}{l!\,\Gamma(l+2m+\frac{3}{2})}(g(k')h_{l,m}, g(k')h_{l',m'}),$$

where

$$h_{l,m} \equiv \exp(-\tfrac{1}{2}u^2)H_{2l+2m}(u)P_{2m}(s),$$

$g(k')$ designates

$$g(k';u,s) = [1+4k'^2s^2/k^2(u)L^2]^{-1/2},$$

and the inner product is defined as

$$(g(k')h_{l,m}, g(k')h_{l',m'}) = \int_{-\infty}^{+\infty}\int_0^1 g^2(k';u,s)e^{-u^2}H_{2l+2m}(u)H_{2l'+2m'}(u) \times P_{2m}(s)P_{2m'}(s)\,ds\,du.$$

We shall use this inner-product notation from now on. It is understood that the integration is always over u and s and that the addition of k means that the inner product is parametrically dependent on k.

How can Eq. (22) be transformed into diagonal form? Suppose that the interval of integration in Eq. (15) were $-\infty, +\infty$ instead of $-\frac{1}{2}L, +\frac{1}{2}L$. Applying Fourier transformation, we would obtain an equation similar to Eq. (22), the only difference being that $(2\pi)^{-1/2}\hat{P}(k-k')$ is replaced by $\delta(k-k')$. After integrating over k', we obtain for fixed k a simple set of linear equations for the $\hat{n}_{2,l,m}(k)$. The set can be transformed into diagonal form if we can calculate the eigenvalues and eigenvectors of the matrix $\hat{K}_{l,m,l',m'}(k)$ for any fixed k. This is what we shall do. Although the volume is actually finite and $(2\pi)^{-1/2}\hat{P}(k-k')$ not a δ function, we hope that the error introduced will decrease sufficiently fast for $k_0L\to\infty$. We shall derive an expression for this error and prove it to be small. The calculation of the eigenvectors and eigenvalues of a matrix can in general be reduced to solving an eigenvalue problem for an integral equation.[15] Sometimes (e.g. in our case) the latter problem is simpler. We shall now define such an abstract eigenvalue problem and study its properties. In Sec. III C it will be shown that with the aid of its solutions, Eq. (22) can be diagonalized. Let us define for fixed k and $p,q = 0,1\ldots$ the following eigenvalue problem [where $h_{l,m}(u,s) = e^{-u^2/2}H_{2l+2m}(u)P_{2m}(s)$]:

$$\mu_{p,q}(k)f_{p,q}(k;u,s) = \int_{-\infty}^{+\infty}\int_0^1 \tilde{R}(k;u,s,u',s') \times f_{p,q}(k;u's')\,du'\,ds',$$

$$\tilde{R}(k;u,s,u',s') = g(k;u,s)g(k;u',s') \times \sum_{l,m=0}^{\infty}\frac{(4m+1)h_{l,m}(u,s)h_{l,m}(u',s')}{l!\,\Gamma(l+2m+\frac{3}{2})2^{4l+4m+1}},$$

$$g(k;u,s) = (1+4k^2s^2/k^2(u)L^2)^{-1/2},$$

which in common operator notation reads

$$\mu_{p,q}(k)f_{p,q}(k) = \tilde{R}(k)f_{p,q}(k). \tag{23}$$

$\tilde{R}(k)$ is the operator with kernel $\tilde{R}(k;u,s,u',s')$.

The eigenvalues $\mu_{p,q}(k)$ and the eigenfunctions $f_{p,q}(k;u,s)$ depend *parametrically* on k [k is *no* integration variable in Eq. (23)]. In the following, it is necessary to keep the dependence on k explicit in the formulas. We shall be interested only in those $f_{p,q}(k;u,s)$ which are real and even functions of u and s. Equation (23) admits solutions for zero and nonzero eigenvalues, and these solutions together constitute a complete, orthogonal set. We impose the normalization condition on the $f_{p,q}(k)$ with $\mu_{p,q}(k)\neq 0$, $p,q = 0,1,\ldots,$

$$(f_{p,q}(k), f_{p',q'}(k)) = \delta_{p,p'}\delta_{q,q'}. \tag{24}$$

The following is proved in Appendix C: The solutions of Eq. (23) associated with the nonzero eigenvalues are given by (in first approximation for $k/k_0L\to 0$)

$$f_{p,q}(k;u,s) \sim \begin{cases} C_{p,q}\,g(k;u,s)\,e^{-u^2/2}H_{2p+2q}(u)P_{2q}(s), & |u| \le u_0(k,s) = (\ln k_0L/2sk\pi^{1/2})^{1/2}, \quad 0\le s\le 1 \\ \dfrac{C_{p,q}}{\mu_{p,q}}g(k;u,s)\dfrac{e^{-u^2/2}}{u}P_{2q}(s)\displaystyle\int_0^{u_0}P_{2q}\!\left(\frac{t}{u}\right)H_{2p+2q}(t)\,dt, & |u| \ge u_0(k,s), \quad 0\le s\le 1. \end{cases} \tag{25}$$

The neglected terms in Eq. (25) are of order

$$(k_0L/k)^{-1}[\ln(k_0L/2k\pi^{1/2})]^{p+q-1/2}$$

near $u=0$ and of order $[\ln(k_0L/2k\pi^{1/2})]^{-1}$ for $|u| \gtrsim u_0(k,s)$.

We therefore must have $[\ln(k_0L/2k\pi^{1/2})] \gg 1$ if Eq. (25) is to be a valid approximation. The constant $C_{p,q}$ in Eq. (25) is determined by the normalization condition Eq. (24). We have for $k/k_0L\to 0$

$$C_{p,q}^{-2} \sim \pi^{1/2}(4q+1)^{-1}2^{2p+2q}\Gamma(2p+2q+1). \tag{26}$$

The approximate eigenfunctions in Eq. (25) are not exactly orthogonal. It is possible to show that for $p \neq p', q \neq q'$

$$(f_{p,q}(k), f_{p',q'}(k)) = O\left[\frac{k}{k_0 L}\left(\ln\frac{k_0 L}{2k\pi^{1/2}}\right)^{p+p'+q+q'-1/2}\right],$$

i.e., they are orthogonal in very good approximation. For the eigenvalues we have for $k/k_0 L \to 0$

$$\mu_{p,q} \sim \frac{\pi^{1/2}\Gamma(2p+2q+1)}{p!\,\Gamma(p+2q+\frac{3}{2})} 2^{-2p-2q-1} + O\left[\frac{k}{k_0 L}\left(\ln\frac{k_0 L}{2k\pi^{1/2}}\right)^{p+q-1/2}\right]. \tag{27}$$

The first term is always smaller than 1 except if $p = q = 0$. In that case, we shall need the explicit form of the 0 term.

It is proved in Appendix C that

$$\mu_{0,0}(k) \sim 1 - \frac{\pi}{2}\frac{k}{k_0 L}\left(\ln\frac{k_0 L}{2k\pi^{1/2}}\right)^{-1/2}, \quad \frac{k}{k_0 L} \to 0. \tag{28}$$

The two different expressions for $f_{p,q}(k; u, s)$ in Eq. (25) fit continuously at $|u| = u_0(k, s) \gg 1$; we have[13]

$$H_{2p+2q}(u) \sim 2^{2p+2q} u^{2p+2q}, \quad |u| \gg 1.$$

The integral can be evaluated to yield[13]

$$2^{2p+2q} u_0^{2p+2q+1} \int_0^1 P_{2q}(t)\, t^{2p+2q}\, dt = u_0^{2p+2q+1} \frac{\pi^{1/2}\Gamma(2p+2q+1)}{2p!\,\Gamma(p+2q+\frac{3}{2})} \sim 2^{2p+2q} u_0^{2p+2q+1} \mu_{p,q}.$$

We shall prove below that the eigenfunctions with vanishing eigenvalues are of no interest to us. The integral operator $\tilde{D}(k)$ with kernel $D(k; u'', s'', u, s)$ is defined as

$$\tilde{D}(k; u'', s'', u, s) = g(k; u'', s'') g^{-1}(k; u, s) \times \sum_{l,m=0}^{\infty} \frac{(4m+1) h_{l,m}(u'', s'') h_{l,m}(u, s)}{\pi^{1/2}\Gamma(2l+2m+1) 2^{2l+2m}}.$$

It is easily verified from Eq. (23) and the orthogonality relations of the Hermite and Legendre polynomials in our notation, these being[13]

$$(h_{l,m}, h_{l',m'}) = \pi^{1/2} \frac{\Gamma(2l+2m+1)}{(4m+1)} 2^{2l+2m} \delta_{l,l'} \delta_{m,m'}, \tag{29}$$

that for the $f_{p,q}(k)$ with $\mu_{p,q}(k) \neq 0$ (in usual operator notation), we have

$$\tilde{D}(k) f_{p,q}(k) = f_{p,q}(k). \tag{30}$$

Equation (30) shows that as far as the $f_{p,q}(k)$ with $\mu_{p,q}(k) \neq 0$ are concerned, the integral kernel $D(k; u'', s''; u, s)$ acts like $\delta(u'' - u)\delta(s'' - s)$. The integral kernel $\tilde{D}(k; u'', s''; u, s)$, however, is not a representation of $\delta(u'' - u)\delta(s'' - s)$, for if we let $\tilde{D}(k)$ operate on functions of the type

$$g(k; u, s)\, e^{-u^2/2} P_{2q}(s) H_{2p}(u), \quad p < q, \ q = 1, 2, \ldots,$$

this yields zero, while these functions are clearly not identically zero. The reader will easily convince himself that this means that the solutions of Eq. (23) with $\mu_{p,q}(k) \neq 0$ cannot constitute a complete set and that there must be nonzero eigenfunctions associated with vanishing eigenvalues. We shall need the Fourier transform of $n_2(\xi, u, s)$ introduced in Eq. (10) ($\xi = 2x/L$, $s = \cos\vartheta$)

$$\hat{n}_2(k, u, s) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} e^{ik\xi} P(\xi) n_2(\xi, u, s)\, d\xi. \tag{31}$$

Analogously to Eq. (12), we have, where $h_{l,m}(u, s) \equiv e^{-u^2/2} H_{2l+2m}(u) P_{2m}(s)$, the expansion

$$\hat{n}_2(k, u, s) = \frac{e^{-u^2/2}}{\pi^{1/2}} \sum_{l,m=0}^{\infty} (4m+1) h_{l,m}(u, s) \hat{n}_{2,l,m}(k). \tag{32}$$

We have used this such that the odd terms in Eq. (32) are zero, as stated at the end of Sec. II. We may also expand $\hat{n}_2(k, u, s)$ to obtain

$$\hat{n}_2(k, u, s) = g^{-1}(k; u, s) e^{-u^2/2} \sum_{p,q} f_{p,q}(k; u, s) \hat{n}_{2,p,q}(k). \tag{33}$$

The sum extends over the eigenfunctions with $\mu_{p,q}(k) \neq 0$ ($p, q = 0, 1, \ldots$) and those with $\mu_{p,q}(k) = 0$. These two sets of eigenfunctions together constitute a complete set. We now prove that the $f_{p,q}(k)$ associated with $\mu_{p,q}(k) = 0$ can be omitted from the sum in Eq. (33).

Let H_1 and H_2 be the spaces of functions consisting of all linear combinations of functions

$$g(k; u, s) e^{-u^2/2} H_{2l}(u) P_{2m}(s)$$

with $l \geq m$ and with $l < m$, respectively. H_1 and H_2 together span the space of square integrable functions which are even in both variables u and s, because the set of functions $e^{-u^2/2} H_{2l}(u) P_{2m}(s)$, $l, m = 0, 1$ is complete.[13] It is readily verified from the definition of the operator $\tilde{D}(k)$ that $\tilde{D}(k)$ acts as the identity operator in H_1 but yields zero in H_2. Since $\tilde{D}(k)$ also acts as the identity operator for the $f_{p,q}(k)$ with $\mu_{p,q}(k) \neq 0$, these $f_{p,q}(k)$ must be situated entirely in H_1. It follows from Eq. (32) that $g(k; u, s)\hat{n}_2(k, u, s)$ is in H_1, so that the sum in Eq. (33) cannot contain functions in H_2, i.e., the summation is only over these $f_{p,q}(k)$ with $\mu_{p,q}(k) \neq 0$. We therefore need only the solutions stated in Eq. (25). Applying the orthogonality relations of Eqs. (24) and (29), we express the $\hat{n}_{2p,q}(k)$ in terms of the $\hat{n}_{2,l,m}(k)$ and vice versa,

$$\hat{n}_{2,p,q}(k)=\pi^{-1/2}\sum_{l,m=0}^{\infty}(4m+1)(f_{p,q}(k),g(k)h_{l,m})\times\hat{n}_{2,l,m}(k)\,,$$
$$\hat{n}_{2,l',m'}(k)=\frac{2^{-2l'-2m'}}{\Gamma(2l'+2m'+1)}\times\sum_{p,q=0}^{\infty}(h_{l',m'},g^{-1}(k)f_{p',q'}(k))\hat{n}_{2,p',q'}(k)\,. \qquad (34)$$

A last thing remains to be done before we can proceed to the analysis of Eq. (15) in the form given by Eq. (22). By using the fact that the inverse Fourier transform of $\hat{P}(k)$ is $P(\xi)$ and $P^2(\xi)=P(\xi)$ [since $P(\xi)=1$, $|\xi|\le 1$ and $P(\xi)=0$, $|\xi|>1$], it is easy to prove from Eq. (31) that

$$(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\hat{n}_2(k,u,s)\,dk=\hat{n}_2(k',u,s)\,.$$

Each of the functions $\hat{n}_{2,l,m}(k)$ in Eq. (32) has exactly this same property because the $h_{l,m}(u,s)$ are independent of k and are mutually orthogonal. The $f_{p,q}(k;u,s)$ in Eq. (33) are dependent on k, but according to Eq. (25) this dependence is very weak. They can be removed under the integral sign and we therefore have approximately, as for the $\hat{n}_{2,l,m}(k)$,

$$(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k'-k)\hat{n}_{2,p,q}(k)\,dk=\hat{n}_{2,p,q}(k')\,. \qquad (35)$$

C. Solution and interpretation

We multiply both sides of Eq. (22) by

$$\pi^{-1/2}(4m+1)(f_{p,q}(k),g(k)h_{l,m})\,,$$

sum over all l and m, and substitute for $\hat{n}_{2,l',m'}(k)$ the second expansion of Eq. (34) in Eq. (22). Using the definitions of Eqs. (23), (30), and the first expression of Eq. (34), we obtain for $p,q=0,1,\ldots$

$$A(2,1)\left(\hat{n}_{2,p,q}(k)-(2\pi)^{-1/2}\sum_{p',q'=0}^{\infty}\int_{-\infty}^{+\infty}\hat{P}(k-k')\hat{K}_{p,q,p'q'}(k')\hat{n}_{2,p',q'}(k')\,dk'\right)+\hat{n}_{2,p,q}(k)n_eK(2,1)$$
$$=\pi^{-1/2}n_1n_eK(1,2)\,\hat{P}(k)(f_{p,q}(k),g(k)h_{0,0})\,,$$
$$\hat{K}_{p,q,p',q'}(k)=(f_{p,q}(k),\tilde{R}(k)g^{-1}(k)g(k')\tilde{D}(k')f_{p',q'}(k'))\,. \qquad (36)$$

The terms on the left-hand side of the inner product have the following meaning: First $\tilde{D}(k')$ operates on $f_{p',q'}(k')$ resulting in some function of the variables u and s [it is actually $f_{p',q'}(k',u,s)$ itself]. This function is multiplied by

$$(1+4k^2s^2/k^2(u)L^2)^{1/2}(1+4k'^2s^2/k^2(u)L^2)^{-1/2}\,,$$

and the result is operated on by $\tilde{R}(k)$. We now use the fact that $\tilde{R}(k)$ is symmetric, and then from Eqs. (23), (30), and (24), we obtain

$$\hat{K}_{p,q,p',q'}(k')n_{2,p',q'}(k')=\mu_{p,q}(k)[n_{2,p',q'}(k)\delta_{p,p'}\delta_{q,q'}-(f_{p,q}(k),f_{p',q'}(k))n_{2,p',q'}(k)+(f_{p,q}(k),g^{-1}(k)g(k')f_{p',q'}(k'))n_{2,p',q'}(k')]\,.$$

Furthermore, we have

$$(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\,dk'=\pi^{-1}\int_{-\infty}^{+\infty}\frac{\sin(k-k')}{k-k'}dk'=1\,,$$

so that Eq. (36) assumes the following form for $p,q=0,1,\ldots$:

$$A(2,1)[\hat{n}_{2,p,q}(k)-\mu_{p,q}(k)\hat{n}_{2,p,q}(k)+E_{p,q}(k)]+\hat{n}_{2,p,q}(k)n_eK(2,1)=\pi^{-1/2}n_1n_eK(1,2)\,\hat{P}(k)(f_{p,q}(k),g(k)h_{0,0})\,, \qquad (37)$$

$$E_{p,q}(k)=\mu_{p,q}(k)\Sigma_{p',q'}\left((2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')[(f_{p,q}(k),g^{-1}(k)g(k')f_{p',q'}(k'))\,\hat{n}_{2,p',q'}(k')]\,dk'-(f_{p,q}(k),f_{p',q'}(k))\hat{n}_{2,p',q'}(k)\right).$$

In order to put this into the form studied in Sec. III A, we multiply both sides by $(2\pi)^{-1/2}\hat{P}(k''-k)$, integrate over k, apply Eq. (35), and use the fact that in the same approximation as in the case of Eq. (35),

$$(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k'-k)\hat{P}(k)(f_{p,q}(k),g(k)h_{0,0})\,dk \approx (2\pi)^{-1/2}(f_{p,q}(k'),g(k')h_{0,0})\int_{-\infty}^{+\infty}\hat{P}(k'-k)\hat{P}(k)\,dk$$

$$=(f_{p,q}(k'),g(k')h_{0,0})\hat{P}(k') .$$

We then obtain our final equation for $p,q=0,1,\ldots,$

$$A(2,1)\left(\hat{n}_{2,p,q}(k)-(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\mu_{p,q}(k')\hat{n}_{2,p,q}(k')\,dk'+\epsilon_{p,q}(k)\right)+\hat{n}_{2,p,q}(k)n_eK(2,1)$$

$$=\pi^{-1/2}n_1n_eK(1,2)\,\hat{P}(k)(f_{p,q}(k),g(k)h_{0,0}) ,$$

$$\epsilon_{p,q}(k)=(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')E_{p,q}(k')\,dk' . \qquad (38)$$

We have achieved our purpose. If the error term $\epsilon_{p,q}(k)$ is small, then Eq. (38) constitutes a set of *independent* integral equations, all of which can be solved by Widom's theory expounded in Sec. III A [cf. Eq. (17)]. Before proceeding to its solution, let us explain the physical interpretation of Eq. (38). As we have seen, $n_2(\xi,u,s)$ represents the density of excited atoms which at the position ξ emit photons in the direction ϑ ($s=\cos\vartheta$) at the frequency u. The corresponding function $\hat{n}_2(k,u,s)$ in Fourier space is written as a superposition of modes $f_{p,q}(k;u,s)$, and the density in each of these modes is $\hat{n}_{2,p,q}(k)$. The electron gas produces excited atoms with a Doppler profile at a rate $n_1n_eK(1,2)$, and these excited atoms are distributed over the functions $\hat{n}_{2,p,q}(k)$ according to the term in the right-hand side of Eq. (38). The loss mechanisms are radiative loss at a rate $A(2,1)n_{2,p,q}(k)$, partially balanced by trapping represented by the integral [cf. Eqs. (17) and (16), and the physical interpretation of the integral in the latter equation] and loss due to deexciting collisions. Finally, the term $\epsilon_{p,q}(k)$ represents the loss or gain of excitation because the modes are coupled. For an infinite medium this coupling is zero; our procedure applies in this case, with the only exception that $(2\pi)^{-1/2}\hat{P}(k'-k)$ is to be replaced everywhere by $\delta(k'-k)$, as discussed under Eq. (22). It is verified from Eq. (37) that $E_{p,q}(k)$ and hence $\epsilon_{p,q}(k)$ vanish in that situation. The finiteness of the volume, therefore, introduces some coupling, but because the volume is also large ($k_0L\gg 1$), we hope that $\epsilon_{p,q}$ will turn out to be small compared to the other terms. We prove this in Appendix D.

We now proceed to the solution of Eq. (38), in which we put $\epsilon_{p,q}(k)=0$. Let us first consider the nonequilibrium case $A(2,1)\gg n_eK(2,1)$ and $p\neq 0$ or $q\neq 0$ (or both $\neq 0$.) Some calculation shows that

$$(f_{p,q}(k),g(k)h_{0,0})$$
$$=C_{p,q}\{\pi^{1/2}\delta_{p,0}\delta_{q,0}+O\{(k/k_0L)[\ln(k_0L/2k\pi^{1/2})]^{p+q-1/2}\}, \qquad (39)$$

where $C_{p,q}$ is the normalized constant introduced in Eq. (25). Hence the excitation rate of the density function $\hat{n}_{2,p,q}(k)$ of the mode $f_{p,q}(k;u,s)$ by the electron gas is small for $p\neq 0$ or $q\neq 0$ (or both $\neq 0$) as $k/k_0L\rightarrow 0$. Almost all excited atoms are produced in the $p=q=0$ mode.

It is observed that if $\epsilon_{p,q}$ can be neglected, Eqs. (38) are, for any value of p and q, of the same type as discussed in Sec. III A. They can therefore be solved in the same manner, and as shown in Sec. III A, we need the solutions of the following associated eigenvalue problem:

$$A(2,1)\left(\hat{\psi}_j(k)-(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\mu_{p,q}(k')\hat{\psi}_j(k')\,dk'\right)=\tilde{A}_j(2,1)\hat{\psi}_j(k) . \qquad (40)$$

Both $\hat{\psi}_j(k)$ and $\tilde{A}_j(2,1)$ depend on p and q, at least in principle. Applying Widom's theory as expounded in Sec. III A, we obtain the solutions of Eq. (40) by considering the first two terms in the expansion of $\mu_{p,q}(k)$, given in Eq. (27). We therefore have for $p\neq 0$ or $q\neq 0$ (or both $\neq 0$)

$$\frac{\tilde{A}_j(2,1)}{A(2,1)}\sim 1-\frac{\pi^{1/2}\Gamma(2p+2q+1)}{p!\,\Gamma(p+2q+\frac{3}{2})}2^{-2p-2q-1}+O\left[\frac{1}{k_0L}\left(\ln\frac{k_0L}{2\pi^{1/2}}\right)^{p+q-1/2}\right]. \qquad (41)$$

Because the second term in the right-hand side of the equation is less than 1, the eigenvalues $\tilde{A}_j(2,1)$ for $p,q\neq 0$ are all of the order of $A(2,1)$, i.e., the densities $\hat{n}_{2,p,q}(k)$ $p,q\neq 0$, all decay at a rate lower than, but in the same order of magnitude as, $A(2,1)$.[16] For $p,q\neq 0$, the solutions are therefore of order

$$\hat{n}_{2,p,q}(k)\approx\frac{n_1n_eK(1,2)\hat{P}(k)}{A(2,1)+n_eK(2,1)}\frac{1}{k_0L}\left(\ln\frac{k_0L}{2\pi^{1/2}}\right)^{p+q-1/2}$$

We shall show that under nonequilibrium conditions this is very small compared to $n_{2,0,0}(k)$. The amount of radiation produced by the functions $\hat{n}_{2,p,q}(k)$ is of the order of $A(2,1)n_{2,p,q}(k)$ and therefore, if $A(2,1) \gg n_e K(1,2)$, of the order of $(k_0L)^{-1}$ $(\ln k_0L/2\pi^{1/2})^{p+q-1/2}$ times the total number of excitations per second $n_1 n_e K(1,2)$,[17] hence negligible.

Let us now consider Eq. (38) for $p=q=0$. By comparing Eqs. (28) and (20), we see that the associated eigenvalue problem Eq. (40) has, rather surprisingly, exactly the same solutions as Eq. (18). Hence the solution of Eq. (38) for $p=q=0$ is exactly the same in form as that of the Biberman-Holstein integral equation. Using Eq. (39), we have for $p=q=0$

$$\hat{n}_{2,p,q}(k)=\pi^{-1/4}n_1 n_e K(1,2)\sum_{j=0}^{\infty}\left(\hat{\psi}_j(k)\int_{-\infty}^{+\infty}\hat{P}(k')\hat{\psi}_j(k')\,dk'\right)\Big/\left[\tilde{A}_j(2,1)+n_e K(2,1)\right],$$
$$\frac{\tilde{A}_j(2,1)}{A(2,1)}\sim\frac{\pi}{2}\frac{\lambda_j^{-1}}{k_0L}\left(\ln\frac{k_0L}{2\pi^{1/2}}\right)^{-1/2}. \tag{42}$$

In order to compare $\hat{n}_{2,0,0}(k)$ with $\hat{n}_{2,p,q}(k)$, $p,q\neq 0$, put $\tilde{A}_j(2,1)\approx\tilde{A}_0(2,1)$ in Eq. (42). Take $n_eK(2,1)$ to be of the same order as $\tilde{A}_0(2,1)$. Because $\Sigma\hat{\psi}_j(k)\hat{\psi}_j(k')=\delta(k-k')$, we see that $n_{2,p,q}$, $p,q\neq 0$ is of order $(k_0L)^{-2}$ $(\ln k_0L/2\sqrt{\pi})^{p+q-1}$ smaller than $n_{2,0,0}(k)$, and is therefore completely negligible. In the calculation of $\hat{n}_2(k,u,s)$ from Eq. (33), we need only retain the first term. We have from Eqs. (25) (the polynomials are equal to unity for $p=q=0$) and (26)

$$\hat{n}_2(k,u,s)=\mathcal{L}(u,s)n_1 n_e K(1,2)\sum_{j=0}^{\infty}\left(\hat{\psi}_j(k)\int_{-\infty}^{+\infty}\hat{P}(k')\hat{\psi}_j(k')\,dk'\right)\Big/\left[\tilde{A}_j(2,1)+n_e K(2,1)\right], \tag{43}$$

$$\mathcal{L}(u,s)\sim\begin{cases}\pi^{-1/2}e^{-u^2}, & |u|\leq u_0(k,s)=(\ln k_0L/2sk\pi^{1/2})^{1/2},\quad 0\leq s\leq 1\\ \pi^{-1/2}u_0(k,s)e^{-u^2}/u, & |u|\geq u_0(k,s),\quad 0\leq s\leq 1.\end{cases}$$

The precise meaning of $\mathcal{L}(u,\cos\vartheta)$ should be recalled here: $\mathcal{L}(u,\cos\vartheta)$ represents the fraction of photons which are emitted at the frequency u in the direction of the angle ϑ with the positive x axis. $\mathcal{L}(u,\cos\vartheta)$ is a function in Fourier space, but we shall show in a moment that the distribution function in ordinary space is obtained by putting $k=1$; $u_0=(\ln k_0L/2\pi^{1/2}\cos\vartheta)^{1/2}$ is precisely the frequency beyond which the slab is optically thin. In the far wings $|u|\geq u_0$, the loss of photons obliges the distribution function of the excited atoms to be non-Maxwellian and the line shape of the emitted photons to be non-Doppler. Note that parallel to the planes of the slab, i.e., for $\vartheta=\frac{1}{2}\pi$, there is no loss of photons and the line shape is purely Doppler. Equation (43) should be compared with the solution of the Biberman-Holstein integral equation, Eq. (19), by assumption to be multiplied by the normalized Doppler line $\pi^{-1/2}e^{-u^2}$ [see Eq. (12); $n_{2,l,m}(\xi)$, $l=m=0$, was abbreviated as $n_2(\xi)$ in Sec. III A]. The line shape is different, but the density in the excited state is the same. We mention that the rate at which the true line shape approaches the asymptotic one given in Eq. (43) is dependent on the frequency. For $u\approx 0$, the error is of the order $(k_0L)^{-1}(\ln k_0L/2\pi^{1/2})^{-1/2}$, and for $|u|\gtrsim u_0$, it is of the order $(\ln k_0L/2\pi^{1/2})^{-1}$, in agreement with our expectations. In the center, the line shape must be Doppler to a very good approximation. The solution in ordinary ξ space is obtained by applying an inverse Fourier transformation to $\hat{n}_2(k,u,\cos\vartheta)$ in Eq. (43) [cf. Eq. (31)]. Now it can be proved that the eigenfunctions $\hat{\psi}_j(k)$ in Eq. (43) are peaked in the neighborhood of $k=\lambda_j^{-1}$. On the other hand, $\mathcal{L}(u,\cos\vartheta)$ is a very slowly varying function of k/k_0L there. In the inverse Fourier transform, we may put $k=\lambda_j^{-1}\approx 1$ in $\mathcal{L}(u,\cos\vartheta)$ and then take it outside the integral sign. The remaining integral is exactly equal to the Biberman-Holstein solution in Eq. (19) transformed back to ordinary ξ space.

So much for the discussion of the solution of the transport equation under nonequilibrium condition $A(2,1)\gg n_eK(2,1)$. In the opposite case, when $A(2,1)\ll n_eK(1,2)$, we neglect all radiative terms in Eq. (38). The solutions are, for all p,q,

$$\hat{n}_{2,p,q}(k)=\pi^{-1/2}n_1[K(1,2)/K(2,1)](f_{p,q}(k),g(k)h_{0,0})\hat{P}(k).$$

We substitute this into Eq. (33), use the completeness relation[18]

$$\sum_{p,q=0}^{\infty}f_{p,q}(k;u,s)f_{p,q}(k;u',s')=\delta(u-u')\delta(s-s')$$

and the fact that $h_{0,0}=e^{-u^2}/2$ to find

$$\frac{n_2(k,u,\cos\vartheta)}{n_1}=\frac{e^{-u^2}}{\pi^{1/2}}\frac{K(1,2)}{K(2,1)}\hat{P}(k)$$
$$=\frac{g_2}{g_1\pi^{1/2}}e^{-(u^2+h\nu/kT)}\hat{P}(k).$$

We have used detailed balance. Inverse Fourier transformation yields, as it should, $n_2/n_1=\pi^{-1/2}$

$g_2 g_1^{-1} e^{-u^2-h\nu/kT}$ for $|\xi| = |2x/L| \le 1$, and 0 for $|\xi| > 1$, i.e., the usual equilibrium solution.

IV. SUMMARY AND CONCLUSIONS

We have obtained an equation [Eq. (23)] of which the solution for $p=q=0$ has been shown to yield, under nonequilibrium conditions apart from the normalization, the line shape (or equivalently, the distribution function of the excited atoms) when Doppler broadening is dominant. The line shape appeared to be Doppler in the core of the line, and to decrease like e^{-u^2}/u in the far wings of the line. Strictly speaking, the assumption of complete redistribution is therefore incorrect. However, it has also been proved that the assumption yields correct number densities in the excited states if $k_0 L \gg 1$. In other situations, when natural broadening also plays an important role in addition to Doppler and/or Lorentz broadening, complete redistribution will be a poor approximation, because strong correlations between the frequencies of the emitted and absorbed photons may exist. Can the present analysis be applied in that case also?[10] We have considered a particular redistribution function, viz., Eq. (5), and its expansion in Hermite and Legendre polynomials, viz., Eq. (9), to derive Eq. (23). However, the attentive reader will have noticed that in the derivation, actually only the orthogonal properties of these functions mattered.

Other redistribution functions, e.g., the one corresponding with the case mentioned above, will have similar expansions in suitable orthogonal sets of functions. It seems that a derivation similar to the one given here must lead to an equation of the same type and the same meaning as Eq. (23). Now let us try for a moment to get rid of our mathematical inhibitions which forbid us to do things without proof. Let us conjecture how the general equation should look. The function $g(k; u, s)$ is essentially the Fourier transform of $\exp[-k(u)L|\xi|/2s]$ (see Appendix B). This exponential occurs always in transport problems of this kind, independent of the precise redistribution mechanism. It must therefore remain unmodified. The sum in Eq. (23) is clearly related to the redistribution function given in Eqs. (9) and (5) (integrated over φ and φ', because of the slab geometry), and it is this expression which needs modification.

Let us try some cases and see whether the right answers result. Take $R(u, \vec{s}; u', \vec{s}')$ as in Eq. (6) (complete redistribution). Comparison of Eqs. (6), (9), and (23) shows that the sum in Eq. (23) should be replaced by $[\mathcal{L}(u)\mathcal{L}(u')]^{1/2}$. Solving this equation is trivial. There is only one eigenfunction, $f(k; u, s) = g(k; u, s)\mathcal{L}^{1/2}(u)$. Substitution in Eq. (33) shows that the resulting line shape is Doppler. The corresponding eigenvalue is

$$\mu(k) = \frac{L}{2k}\int_{-\infty}^{+\infty} \mathcal{L}(u) k(u) \arctan\frac{2k}{k(u)L}\, du,$$

as it should be.[5] The same result applies if $\mathcal{L}(u)$ is a Lorentz or Voigt profile. Now consider the opposite case, when complete correlation exists between the emitted and absorbed frequencies, i.e.,

$$\begin{aligned} R(u, \vec{s}; u', \vec{s}') &= \delta(u-u')\mathcal{L}(u') \\ &= \mathcal{L}^{1/2}(u)\delta(u-u')\mathcal{L}^{1/2}(u') \\ &= \mathcal{L}^{1/2}(u)\mathcal{L}^{1/2}(u')\,\Sigma\varphi_n(u)\varphi_n(u'), \end{aligned}$$

with some complete set of eigenfunctions $\varphi_n(u)$ for which we may take[13] $\varphi_n(u) = N_n H_n(u) e^{-u^2/2}$, where $H_n(u)$ are the Hermite polynomials and N_n is a normalization factor. The representation of the redistribution function thus obtained is very similar to the one actually used in the paper. It is verified that the sum in Eq. (23) has to be replaced by $\Sigma\varphi_{2n}(u)\varphi_{2n}(u')$, which is equal to $\delta(u-u')$ because we only consider even functions $f_{p,q}(k; u, s)$. Solving the equation is again trivial. We have one eigenfunction $f(k; u, s) = g(k; u, s)$ multiplied by an undetermined function of u. The line shape is also undetermined, as it should, because in absence of a redistribution mechanism, it is determined by the outward sources. The corresponding eigenvalue is

$$\mu = [k(u)L/2k]\arctan[2k/k(u)L],$$

a well-know expression also occurring in one-speed neutron theory. It has thus been shown that Eq. (23) yields correct results also in cases for which it has not been derived explicitly. We therefore conjecture that Eq. (23), *mutatis mutandis*, has general validity and that is solution for $p=q=0$ will yield the line shape of the radiation emitted by the excited atoms.

It follows from the analysis in Appendix C that it is a good approximation to assume that the line shape is isotropic, thus considerably reducing the labor in solving Eq. (23). If the (isotropic) line shape of the excited atoms has been calculated, it is a straightforward matter to derive the transport equation (see Sec. II A) which can be solved in an equally straightforward manner by means of the theory in Sec. III A. Finally, it is recalled that for the calculation of number densities and radiative loss, we need not even calculate the line shape; for these purposes the eigenvalue $\mu_{0,0}(k)$ contains enough information.

APPENDIX A

In this appendix we prove the expansion given in Eq. (9) of this paper.

Let $\cos\gamma = \vec{s}\cdot\vec{s}'$, and further let

$$R(u,\vec{s};u'\vec{s}') = \frac{1}{\pi\sin\gamma}\exp\left(\frac{-u^2-u'^2+2uu'\cos\gamma}{\sin^2\gamma}\right) = \frac{1}{\pi\sin\gamma}\exp\left[-\left(\frac{u-u'}{2\sin\gamma/2}\right)^2-\left(\frac{u+u'}{2\cos\gamma/2}\right)^2\right].$$

The Fourier transform of $R(u,\vec{s};u',\vec{s}')$, defined as

$$\hat{R}(p,\vec{s};p',\vec{s}') = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp(ipu-ip'u')\times R(u,\vec{s};u',\vec{s}')\,du\,du',$$

can easily be calculated if the new variables $t=(u-u')/2\sin(\gamma/2)$ and $t'=(u+u')/2\cos(\gamma/2)$ are introduced. The Jacobi determinant of the transformation is $\sin\gamma$. We obtain

$$\hat{R}(p,\vec{s};p',\vec{s}') = (1/2\pi)\exp[\tfrac{1}{4}(-p^2-p'^2+2pp'\cos\gamma)]. \tag{A1}$$

We then have the following expansion[19]:

$$\exp(\tfrac{1}{2}pp'\cos\gamma) = (2\pi)^{1/2}\sum_{n=0}^{\infty}\frac{(n+\frac{1}{2})P_n(\cos\gamma)I_{n+1/2}(\frac{1}{2}pp')}{(\frac{1}{2}pp')^{1/2}}.$$

In this expression $P_n(\cos\gamma)$ is a Legendre polynomial. $I_{n+1/2}(\frac{1}{2}pp')$ is a modified spherical Bessel function.[20] We substitute this expression into Eq. (A1), write

$$\cos\gamma = \cos\vartheta\cos\vartheta' + \sin\vartheta\sin\vartheta'\cos(\varphi-\varphi'),$$

and apply the addition theorem for Legendre polynomials.[21] This yields

$$\hat{R}(p,\vec{s};p',\vec{s}') = \exp[-\tfrac{1}{4}(p^2+p'^2)](\tfrac{1}{2}pp')^{-1/2}(2\pi)^{-1/2}\times\sum_{n=0}^{\infty}\sum_{m=-n}^{+n}\frac{(n+\frac{1}{2})(n-m)!}{(n+m)!}P_n^m(\cos\vartheta)\times P_n^m(\cos\vartheta')e^{im(\varphi-\varphi')}I_{n+1/2}(\tfrac{1}{2}pp'). \tag{A2}$$

$R(u,\vec{s};u',\vec{s}')$ is found by applying inverse Fourier transformation,

$$R(u,\vec{s},u',\vec{s}') = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp(-ipu+ip'u')\times\hat{R}(p,\vec{s};p',\vec{s}')\,dp\,dp'.$$

We define

$$R_n(u,u') = \frac{1}{(2\pi)^{3/2}}\int_{-\infty}^{+\infty}e^{-(p^2+p'^2)/4}I_{n+1/2}(\tfrac{1}{2}pp')(\tfrac{1}{2}pp')^{-1/2}\times\exp(-ipu+ip'u')\,dp\,dp'. \tag{A3}$$

First, the series expansion[20] of the modified Bessel function is substituted into Eq. (A3). The integrals can all be expressed in terms of Hermite polynomials.[13] The result is

$$R_n(u,u') = \frac{e^{-u^2-u'^2}}{\pi^{1/2}}\sum_{l=0}^{\infty}\frac{H_{2l+n}(u)H_{2l+n}(u')}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n}}. \tag{A4}$$

A second representation is obtained if we use[22] the formula

$$e^{-(p^2+p'^2)/4}I_{n+1/2}(\tfrac{1}{2}pp') = 2\int_0^{\infty}e^{-t^2}J_{n+1/2}(pt)J_{n+1/2}(p't)\,t\,dt.$$

The integrals resulting when this expression is substituted into Eq. (A3) are all standard and can be obtained from existing tables.[23] We obtain

$$R_n(u,u') = \frac{2}{\sqrt{\pi}}\int_{\max(|u|,|u'|)}^{\infty}e^{-t^2}P_n\left(\frac{u}{t}\right)P_n\left(\frac{u'}{t}\right)dt. \tag{A5}$$

Putting everything together, we have the following expansions:

$$R(u,\vec{s};u',\vec{s}') = \sum_{n=0}^{\infty}\sum_{m=-n}^{+n}\frac{(n+\frac{1}{2})(n-m)!}{(n+m)!}P_n^m(\cos\vartheta)\times P_n^m(\cos\vartheta')e^{im(\varphi-\varphi')}R_n(u,u'),$$

$$R_n(u,u') = \frac{1}{\pi^{1/2}}e^{-u^2-u'^2}\sum_{l=0}^{\infty}\frac{H_{2l+n}(u)H_{2l+n}(u')}{l!\,\Gamma(l+n+\frac{3}{2})2^{4l+2n}} = \frac{2}{\pi^{1/2}}\int_{\max(|u|,|u'|)}^{\infty}e^{-t^2}P_n\left(\frac{u}{t}\right)P_n\left(\frac{u'}{t}\right)dt. \tag{A6}$$

The two expressions for $R_0(u,u')$ were first obtained by Unno.[24]

APPENDIX B

In this appendix we calculate the Fourier transforms of the kernels $K_{l,m,l',m'}$ as defined in Eq. (17). We have with $s=\cos\vartheta$,

$$\tfrac{1}{2}L\int_{-\infty}^{+\infty}e^{ik\xi}\exp\left(\frac{-k(u)L|\xi|}{2s}\right)d\xi = 2sg^2(k;u,s)k^{-1}(u),$$

$$g^2(k;u,s) = [1+4k^2s^2/k^2(u)L^2]^{-1},$$

so that

$$\hat{K}_{l,m,l',m'}(k)=\tfrac{1}{2}L\int_{-\infty}^{+\infty}e^{ik\xi}K_{l,m,l',m'}(\tfrac{1}{2}L|\xi|)d\xi$$
$$=\left(2m'+\frac{1}{2}\right)\int_{-\infty}^{+\infty}\int_0^1 e^{-u^2}\frac{H_{2l+2m}(u)H_{2l'+2m'}(u)P_{2m}(s)P_{2m'}(s)}{l!\Gamma(l+2m+\frac{3}{2})2^{4l+4m}}g^2(k;u,s)\,ds\,du.$$

For $l=m=l'=m'=0$, all the polynomials are equal to 1 and the integration over s can be carried out. Denoting $\hat{K}_{0,0,0,0}(k)$ by $\hat{K}(k)$ for simplicity, we have, upon introduction of new variables $t=k(u)L/2k$, $t_0=k_0L/2k\pi^{1/2}$,

$$\hat{K}(k)=1+\frac{2k}{k_0L}\int_0^{t_0}(t\arctan t^{-1}-1)\frac{dt}{(\ln t_0-\ln t)^{1/2}}.$$

If we expand the square root and subsequently extend the integral to infinity, we find

$$\hat{K}(k)\sim 1-\tfrac{1}{2}\pi(k/k_0L)(\ln k_0L/2k\pi^{1/2})^{-1/2},\quad k/k_0L\to 0.$$

This is the expression given in Eq. (20).

APPENDIX C

In this Appendix, we consider the eigenvalue problem defined in Eq. (23),

$$\mu_{p,q}(k)f_{p,q}(k;u,s)=\int_{-\infty}^{+\infty}\int_0^1\tilde{R}(k;u,s;u',s')f_{p,q}(k;u',s')\,du'\,ds',$$
$$\tilde{R}(k;u,s;u',s')=g(k;u,s)g(k;u',s')e^{-(u^2+u'^2)/2}\sum_{l,m=0}^{\infty}(4m+1)\frac{H_{2l+2m}(u)H_{2l+2m}(u')P_{2m}(s)P_{2m}(s')}{l!\Gamma(l+2m+\frac{3}{2})2^{4l+4m+1}},$$
$$g(k;u,s)=[1+4k^2s^2/k^2(u)L^2]^{-1/2}. \tag{C1}$$

An equivalent representation is obtained by carrying out the summation over l. We have by Eq. (A6)

$$\tilde{R}(k;u,s;u',s')=g(k;u,s)g(k;u',s')e^{(u^2+u'^2)/2}\sum_{m=0}^{\infty}(4m+1)P_{2m}(s)P_{2m}(s')\int_{\max(|u|,|u'|)}^{\infty}e^{-t^2}P_{2m}\left(\frac{u}{t}\right)P_{2m}\left(\frac{u'}{t}\right)dt. \tag{C2}$$

We need to consider Eq. (C1) in the limiting case $k/k_0L\to 0$ (i.e., $k_0L\to\infty$). The analysis of Eq. (C1) is tedious because we have to deal with functions of two variables. We shall therefore consider a simplified problem, in order to demonstrate the principle of the calculation. The corresponding results for Eq. (C1) are obtained in the same manner. Let us consider only those eigenfunctions which are in good approximation independent of s (i.e., those with $q=0$) [see Eq. (25)] and let us approximate them as follows: We put $\mu_{p,0}(k)=\mu_p(k)$ in Eq. (C1) and

$$g^{-1}(k;u,s)f_{p,0}(k;u,s)=g^{-1}(k;u)f_p(k;u)$$

where

$$g(k;u)=\left(\int_0^1 g^2(k;u,s)\,ds\right)^{1/2}$$
$$=\left(\frac{k_0Le^{-u^2}}{2k\pi^{1/2}}\arctan\frac{2k\pi^{1/2}}{k_0Le^{-u^2}}\right)^{1/2}. \tag{C3}$$

When these substitutions are made in Eq. (C1), we integrate both sides of the equation with respect to s from 0 to 1. By the orthogonality relations for the Legendre polynomials,[13] only the term with $m=0$ contributes, and we obtain

$$\mu_p(k)f_p(k;u)=\int_{-\infty}^{+\infty}\tilde{R}(k;u,u')f_p(k;u')\,du',$$
$$\tilde{R}(k;u,u')=g(k;u)g(k;u')e^{-(u^2+u'^2)/2}\sum_{l=0}^{\infty}\frac{H_{2l}(u)H_{2l}(u')}{l!\Gamma(l+\frac{1}{2})2^{4l+1}}$$
$$=g(k;u)g(k;u')e^{(u^2+u'^2)/2}\int_{\max(|u|,|u'|)}^{\infty}e^{-t^2}dt. \tag{C4}$$

It should be remarked that Eq. (C4) would replace Eq. (23) and its solutions $\mu_p(k)$, $f_p(k;u)$ would replace $\mu_{p,q}(k)$ and $f_{p,q}(k;u,s)$ everywhere in the paper, if we had assumed *a priori* that the redistribution function in Eqs. (5) and (9) may be replaced by its so-called isotropic approximation,[9,10] i.e., Eqs. (5) and (9) integrated over all angles.

Insight into the nature of the problem is afforded if, using an idea by Field,[4] we convert Eq. (C4) into the differential equation [where $F(u)=g^{-1}(k,u)f_p(u)$]

$$\frac{d^2F}{du^2}+\left[\frac{1}{\mu}\frac{k_0Le^{-u^2}}{k\pi^{1/2}}\arctan\left(\frac{2k\pi^{1/2}}{k_0Le^{-u^2}}\right)-(1+u^2)\right]F(u)=0. \tag{C5}$$

For $k_0Le^{-u^2}/2k\pi^{1/2} \gg 1$ and $\ll 1$, we replace the first term in the brackets by, respectively, $2\mu^{-1}$ (i.e., the first-order term for $k/k_0Le^{-u^2} \to 0$) and by $\pi k_0 Le^{-u^2}/2k\pi^{1/2}\mu$ (i.e., the first-order term for $k/k_0Le^{-u^2} \to \infty$). There result two differential equations of standard form,[25] which can be solved, requiring the solutions to be regular, and even at $u=0$, decreasing for $|u| \to \infty$, and to fit continuously at $|u| = [\ln(k_0L/2k\pi^{1/2})]^{1/2}$. We also find the eigenvalue in first order. The eigenvalue to second order in k/k_0L is obtained by pushing the perturbation theory one step further. Though the most elegant, the method cannot be easily generalized to be applicable to Eq. (C1).

We proceed, therefore, by a different method, namely, we verify that certain functions are actually solutions of Eq. (C4). Put

$$f_p(k;u) = g(k;u)\, e^{-u^2/2} H_{2p}(u),$$
$$|u| \le u_0(k) = (\ln k_0 L/2k\pi^{1/2})^{1/2}. \tag{C6}$$

In the interval $[-u_0, u_0]$, $g(k;u)$ in Eq. (C3) is approximated by 1. We have

$$\int_{-u_0}^{u_0} \tilde{R}(u,u') f_p(u')\, du' \approx g(k;u) e^{-u^2/2} \sum_{l=0}^{\infty} H_{2l}(u) \int_{-u_0}^{+u_0} \frac{H_{2l}(u') H_{2p}(u') e^{-u'^2/2}}{l!\,\Gamma(l+\frac{3}{2}) 2^{4l+1}}\, du'$$
$$\approx g(k;u) e^{-u^2/2} \sum_{l=0}^{\infty} H_{2l}(u) \int_{-\infty}^{+\infty} \frac{H_{2l}(u') H_{2p}(u') e^{-u'^2}}{l!\,\Gamma(l+\frac{3}{2}) 2^{4l+1}}\, du'$$
$$= g(k;u) e^{-u^2/2} H_{2p}(u) \frac{\pi^{1/2}\Gamma(2p+1)}{p!\,\Gamma(p+\frac{3}{2}) 2^{2p+1}}.$$

One can prove that the error is of order

$$\frac{(\ln k_0 L/2k\pi^{1/2})^{2p-1/2} k}{k_0 L}$$

near $u=0$ and of order $(\ln k_0L/2k\pi^{1/2})^{-1}$ near $u \approx u_0$, so that our guess in Eq. (C6) is correct. In addition, we have obtained μ_p in first order of $k/k_0L \to 0$, viz.,

$$\mu_p(k) \sim \mu_p^{(1)} = \pi^{1/2}\Gamma(2p+1)/p!\,\Gamma(p+\tfrac{3}{2}) 2^{2p+1} = (2p+1)^{-1}. \tag{C7}$$

Let us consider the second representation of $\tilde{R}(u,u')$ in Eq. (C4). We have

$$\mu_p(k) f_p(k;u) = 2g(k;u) e^{u^2/2} \left[\int_{|u|}^{\infty} e^{-t^2} dt \left(\int_0^{\infty} g(k;u') e^{u^2/2} f_p(k;u')\, du' - \int_{|u|}^{\infty} g(k;u') e^{u^2/2} f_p(k;u')\, du' \right) + \int_{|u|}^{\infty} g(k;u') e^{u^2/2} f_p(k;u') \int_{|u'|}^{\infty} e^{-t^2}\, dt\, du' \right]. \tag{C8}$$

We put for $|u| \ge u_0$

$$f_p(k;u) = \frac{C}{\mu_p} g(k;u) e^{u^2/2} \int_{|u|}^{\infty} e^{-t^2} dt,$$
$$C = 2\int_0^{\infty} g(k;u') e^{u^2/2} f_p(k;u')\, du', \tag{C9}$$

and verify that the second and third integrals in Eq. (C8) are small for $k/k_0L \to 0$ in the region $|u| \ge u_0$. The constant C in Eq. (C9) is evaluated to be[13]

$$C = 2^{2p+1}\mu_p^{(1)} [\ln(k_0 L/2k\pi^{1/2})]^{p+1/2}. \tag{C10}$$

It is verified that as a result the two representations of the eigenfunctions Eqs. (C6) and (C9) fit continuously at $|u| = u_0(k)$. The second order contribution to $\mu_p(k)$ is obtained by perturbation theory. Let us write $\mu_p(k) = \mu_p^{(1)} + \mu_p^{(2)}(k)$ and $f_p(k,u) = f_p^{(1)}(k;u) + f_p^{(2)}(k;u)$. Equation (C4) reads, in operator notation,

$$\mu_p(k) f_p(k) = \tilde{R}(k) f_p(k). \tag{C11}$$

We have

$$\mu_p(k) f_p^{(2)}(k) - \tilde{R}(k) f_p^{(2)}(k) = \tilde{R}(k) f_p^{(1)}(k) - \mu_p f_p^{(1)}(k).$$

Because the exact eigenfunctions constitute a complete set, we may expand as follows:

$$f_p^{(2)}(k) = \sum_{p'=0}^{\infty} a_{p,p'} f_{p'}(k).$$

We substitute this expression into Eq. (C11), take the inner product with some eigenfunction $f_q(k)$, and use the fact that the eigenfunctions are orthogonal. We obtain

$$[\mu_p(k) - \mu_q(k)]a_{p,q}(f_q(k), f_q(k))$$
$$= (\tilde{R}(k)f_p^{(1)}(k) - \mu_p(k)f_p^{(1)}(k), f_q(k)).$$

For $p=q$ the left-hand side of the equation vanishes and the result yields an expression for $\mu_p^{(1)}(k)$, namely,

$$\mu_p^{(2)}(k) = (\tilde{R}(k)f_p^{(1)}(k) - \mu_p^{(1)}f_p^{(1)}(k), f_p(k))/(f_p^{(1)}(k), f_p(k))$$
$$\sim (\tilde{R}(k)f_p^{(1)}(k) - \mu_p^{(1)}f_p^{(1)}(k), f_p^{(1)}(k))/(f_p^{(1)}(k), f_p^{(1)}(k)). \quad \text{(C12)}$$

The procedure is well known in quantum mechanics.[26] The evaluation of the integrals in the right-hand side of Eq. (C12) is straightforward but tedious. The result for $k/k_0L \to 0$ and $p=0$ is

$$\mu_0(k) = \mu_0^{(1)} + \mu_0^{(2)}(k)$$
$$\sim 1 - \tfrac{1}{2}\pi(k/k_0L)(\ln k_0L/2k\pi^{1/2})^{-1/2}. \quad \text{(C13)}$$

The results given in Eqs. (25), (27), and (28) are obtained in similar fashion.

APPENDIX D

Here we estimate the error term $\epsilon_{p,q}(k)$ in Eq. (38),

$$\epsilon_{p,q}(k) = (2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')E_{p,q}(k')\,dk'. \quad \text{(D1)}$$

$E_{p,q}(k)$ has been defined in Eq. (37). The sum over p' and q' in that equation can be carried out by means of Eq. (33), and we have, where $h_{0,0}^{-1}$ represents $e^{(u^2/2)}$,

$$E_{p,q}(k) = \mu_{p,q}(k)\left((2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')(f_{p,q}(k), g^{-1}(k)g^2(k')h_{0,0}^{-1}\hat{n}_2(k'))\,dk' - (f_{p,q}(k), g(k)h_{0,0}^{-1}\hat{n}_2(k))\right). \quad \text{(D2)}$$

Here $\hat{n}_2(k)$ represents the function $\hat{n}_2(k;u,s)$. In Eq. (31) we can expand $e^{(ik\xi)}$ in powers of $ik\xi$. Because the integration is actually over the finite interval $[-1, 1]$ and the density of excited atoms $n_2(\xi, u, s)$ is certainly bounded, all integrals converge. It follows that $\hat{n}_2(k,u,s)$ is an analytic function of k. Furthermore, it is verified that $\hat{n}_2(k,u,s)$ is real for purely imaginary values of k and that $\hat{n}_2(k,u,s)$ does not increase faster than exponentially fast in the upper and lower parts of the complex plane[27] for $|k| \to \infty$. Since

$$(2\pi)^{-1/2}\hat{P}(k-k') = \pi^{-1}\sin(k'-k)/(k'-k)$$
$$= \operatorname{Im} e^{i(k'-k)}/\pi(k'-k),$$

we can calculate the integral over k' in Eq. (C1) by closing the integral in the upper part of the complex plane. We have

$$(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\hat{P}(k-k')\left(\frac{4k'^2s^2}{k^2(u)L^2}+1\right)^{-1}\hat{n}_2(k',u,s)\,dk'$$
$$= \left(\frac{4k^2s^2}{k^2(u)L^2}+1\right)^{-1}\hat{n}_2(k,u,s) - e^{-k(u)L/2s}\hat{n}_2\left(\frac{ik(u)L}{2s},u,s\right)\operatorname{Im}\frac{e^{-ik}}{2ks/k(u)L - i},$$

and obtain, by writing out the inner product

$$E_{p,q}(k) = \operatorname{Im}\mu_{p,q}(k)e^{-ik}\int_{-\infty}^{+\infty}\int_0^1 f_{p,q}(k;u,s)\frac{g^{-1}(k;u,s)\exp[-k(u)L/2s+\frac{1}{2}u^2]}{2ks/k(u)L - i}\,\hat{n}_2\left(\frac{ik(u)L}{2s},u,s\right)ds\,du. \quad \text{(D3)}$$

For $k_0L \to \infty$, $n_2[ik(u)L/2s, u, s]$ is given by Eq. (43). It can be proved[27] that under nonequilibrium conditions for $k = ik(u)L/2s = it$, $t \gg 1$, the sum over j becomes proportional to $I_1(t)/t$, where $I_1(t)$ is a modified Bessel function,[27] so that $n_2[ik(u)/2s, u, s]$ behaves like $\mathcal{L}(u,s)I_1(t)/t$.

We substitute in Eq. (C2) the expressions for $g^{-1}(k;u,s)f_{p,q}(k;u,s)$ from Eq. (25), $\mathcal{L}(u,s)$ from Eq. (43), and the first-order approximation to $\mu_{p,q}(k)$ from Eq. (27), which is a constant. It is readily verified that we have, apart from terms which are smaller by a factor $\ln(k_0L/2k\pi^{1/2})$

$$E_{p,q}(k) \sim \operatorname{Im} C e^{-ik}\int_0^1\int_0^\infty e^{-u^2}H_{2p+2q}(u)P_{2q}(s)$$
$$\times\frac{e^{-t}I_1(t)}{k-it}\,du\,ds,$$

$$t = k(u)L/2s; \quad t_0 = k_0L/2s\pi^{1/2}.$$

Changing the variable u into t everywhere and applying the asymptotic relations for the Hermite polynomials[13] yields

$$E_{p,q} \sim \mathrm{Im}\, C_1 e^{-ik} \int_0^1 s P_{2q}(s) \int_0^{t_0} \frac{e^{-t} I_1(t)}{k - it} dt\, ds$$

$$\sim \mathrm{Im}\, C_1 e^{-ik} \int_0^1 s P_{2q}(s) \int_0^{\infty} \frac{e^{-t} I_1(t)}{k - it} dt\, ds, \qquad \text{(D4)}$$

$$C_1 = 2^{2p+2q} \pi^{1/2} C (\ln k_0 L / 2\pi^{1/2})^{p+q-1/2} (k_0 L)^{-1},$$

i.e., $E_{p,q}$ is of the *same* order as the terms $(f_{p,q}(k), g(k)h_{0,0})$, $p, q \neq 0$, in Eq. (38) [cf. Eq. (39)] and of the same order for $p = q = 0$ as $1 - \mu_{0,0}(k)$ [cf. Eq. (28)]. However, this expression vanishes in Eq. (C1), since

$$\frac{\mathrm{Im}}{\pi} \int_{-\infty}^{+\infty} \frac{\sin(k - k')}{k - k'} \frac{e^{-ik}}{k - it} dk = 0,$$

as is shown by closing the path of integration in the lower part of the complex plane and observing that there is no singularity in that part. The treatment is somewhat unsatisfactory because, although it proves that $\epsilon_{p,q}$ may be neglected, it produces no precise estimate of this quantity, and suggests that $\epsilon_{p,q}$ is only of order $\ln k_0 L / 2\pi^{1/2}$ smaller than the expression in Eq. (C3). We have the feeling that $\epsilon_{p,q}$ is of the order of

$$(k_0 L)^{-2} (\ln k_0 L / 2\pi^{1/2})^{p+q-1/2},$$

and is therefore a factor $(k_0 L)^{-1}$ smaller. It if is true, this could possibly be proved by substituting the full expression of Eq. (C2) into Eq. (C1) and closing the path of integration in the lower part of the complex plane. The evaluation of the integral, however, requires a study of the functions $f_{p,q}(k; u, s)$ and the eigenvalues $\mu_{p,q}(k)$ for complex values of k, which is outside the scope of this paper.

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[1]J. Houtgast, thesis (University of Utrecht, 1942) (unpublished). The assumption has been made by many authors independently, sometimes without explicitly realizing it; cf. L. Spitzer, Astrophys. J. 99, 1 (1944); L. M. Biberman, Zh. Eksp. Teor. Fiz. 17, 416 (1947); H. Zanstra, Bull. Astron. Inst. Neth. 11, 1 (1949).

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[7]It is easy to prove that the mean free path is equal to $k^{-1}(u)$. A reasonable estimate is obtained by putting $k = 1$.

[8]The error is still dependent on u. For $u \approx 0$, it is of the order of $(k_0 L)^{-1} (\ln k_0 L)^{-1/2}$, but for $|u| \approx u_0$ and $|u| \geq u_0$, of the order of $(\ln k_0 L)^{-1}$. Therefore the assumption of complete redistribution is extremely good in the core of the line.

[9]Results of an essentially similar nature have been obtained in the so-called isotropic approximation by V. V. Ivanov, Bull. Astron. Inst. Neth. 19, 192 (1967); D. G. Hummer, Mon. Not. R. Astron. Soc. 145, 95 (1969).

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[11]It is true if the line shape is isotropic. It follows from the analysis presented here that this is a very good approximation.

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[13]A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. II; G. Szego, *Orthogonal Polynomials* (Am. Math. Soc., Providence, 1939).

[14]More details are given in Sec. II of C. van Trigt, J. Math. Phys. 14, 863 (1973).

[15]Consider the eigenvalue problem $\lambda a(m) = \Sigma \alpha(m, n) a(n)$, $\alpha(m, n) = \int g^2(x) X(m, x) X(m, x)\, dx$, with an orthogonal set of functions $X(m)$. Define $K(x, x') = g(x) g(x') \Sigma X(m, x) X(m, x')$ and $f(x) = g(x) \Sigma a(n) X(n, x)$. It is readily proved from the orthogonality relation that the matrix problem is equivalent, with $\lambda f = K f$ (in common operator notation). Note that the matrix elements $K(l, m, l', m')$ are of the type of the elements $\alpha(m, n)$ introduced here [see Eq. (22)].

[16]This means the following in a decay experiment: The distribution function of the exicted atoms tends to the dominant $p = q = 0$ mode. Initial deviations from this "equilibrium distribution" vanish within times of the order of $A^{-1}(2, 1)$. This fact was observed in Monte Carlo calculations by C. E. Klots and V. E. Anderson, J. Chem. Phys. 56, 120 (1972).

[17]This picture is correct only if the coupling term $\epsilon(p, q)$ in Eq. (38), describing the flow of excited atoms from the other modes into the p, q mode, is small compared to the direct excitation of the mode by the electron gas, at this stage still something to be proved (see Appendix D).

[18]The summation is over the eigenfunctions with zero and nonzero eigenvalues. The eigenfunctions of the first type yield zero in the inner product.

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[20]Reference 19, p. 5.

[21]Reference 19, pp. 183 and 250.

[22]Reference 19, p. 40.

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[24]W. Unno, Astrophys. J. 129, 388 (1959).

[25]Reference 19, p. 116.

[26]D. Bohm, *Quantum Theory* (Prentice-Hall, Englewood Cliffs, 1951).

[27]Under nonequilibrium circumstances, the solution in ordinary space behaves like $(1-\xi^2)^{1/2}$ at $\xi = \pm 1$ [see C. van Trigt, Phys. Rev. A 1, 1298 (1970), and A. G. Hearn, Proc. Phys. Soc. Lond. 88, 171 (1966), who observed this numerically]. The integral in Eq. (31) can be evaluated via Ref. 19, Vol. II, p. 81. The asymptotic behavior follows from Ref. 19, Vol. II, p. 86.