TWO-PARAMETER METHOD OF SUMMING EQUIVALENT SPECTRAL LINEWIDTHS IN THE CURTIS–GOODSON APPROXIMATION

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An expression is found, within the framework of a random band model, for the spectral-line intensity distribution density in application to the problem of IR radiation transfer in an inhomogeneous molecular-gas volume.

A great deal of attention has recently been spent on investigating the radiation of heated volumes of molecular gases in the IR spectrum range and the transfer of this radiation in earth's atmosphere. Taking account of the exact dependence of the absorption coefficient on the frequency in such problems should be performed in a band formed by a large number of spectral lines, which complicates the analysis considerably and usually without justification. In this connection, a number of authors proposed approximate methods permitting taking the average of the band fine structure. One of the most effective methods, called the statistical or random band model, was developed by Goody [1] and assumes no correlation between the spectral line intensity and the frequency of its center. Within the framework of this model, the average with respect to the passband, to whose calculation the solution of the spectral radiation transport equation actually reduces, turns out to be proportional to the exponental of the sum of the equivalent widths of all the band lines.

The sum of the equivalent widths V is calculated most simply for homogeneous optical paths, if it is here assumed that the band is representable with a sufficient degree of accuracy in the form of a set of nonoverlapping lines having an identical Lorentz contour:

$$V = \int_0^\infty dS P(S)\, W(S), \tag{1}$$

where the equivalent width of an individual line is determined by the relationship

$$W(S) = \int_{-\infty}^{+\infty} d\nu \left[1 - \exp\left(-\frac{Sl}{\pi}\,\frac{\gamma}{\nu^2+\gamma^2}\right)\right]. \tag{2}$$

Here P(S)dS is the probability that the intensity of a given spectral line is in the interval between S and S + dS. The form of the distribution density P(S) is ordinarily sufficiently arbitrary and selected from both the requirement of correspondence of the computation to experimental data and from considerations of convenience, for instance, $S_0^{-1}\exp(-S/S_0)$ or S_0/S [2]. Giving the mean with respect to the line-intensity spectrum S_0 turns out to be sufficient for a good approximation of their real distribution.

However, the extension of similar, relatively simple methods to the more complex case of inhomogeneous optical paths is of special interest. In particular, in an approximation proposed independently by Curtis [3] and Goodson [4] for the random band model, it is assumed that the passage of an inhomogeneous gas layer can be approximated well by the passage of a certain homogeneous layer of the same gas if it is demanded that the equivalent widths of each line, taken individually, of the model homogeneous layer agree with the true widths in the weak and strong line limit cases. This requirement results in the parameters γ and S in (2) being replaced by $\langle\gamma\rangle$ and $\langle S\rangle$ characterizing the model optical path, where

$$\begin{cases} \langle S \rangle = \dfrac{1}{l}\displaystyle\int_0^l S(x)\,dx, \\ \langle \gamma \rangle = \dfrac{1}{\langle S \rangle}\,\dfrac{1}{l}\displaystyle\int_0^l S(x)\,\gamma(x)\,dx, \end{cases} \tag{3}$$

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i.e., $\langle\gamma\rangle$ and $\langle S\rangle$ can be understood to be special means along the optical path. Here (1), which yields the method of evaluating the sum V, also remains valid, except that the parameter S_0 in P(S) is now averaged twice, with respect to the spectrum and with respect to the inhomogeneous layer.

It is here necessary to investigate the correctness of summing equivalent widths in the form (1) with a previously assigned distribution function P(S). The fact is that for noticeable temperature fluctuations along the optical path, the population of high-lying energy levels of the absorbing (emitting) gas molecules grows substantially in the high-temperature sections. In turn, this results in the necessity to take into account both the "cold" as well as the "hot" lines formed because of transitions from the high-energy levels, and which are ordinarily ignored in computations. Taking such lines into account should generally change not only the mean intensity over the band S_0 but also the form of the distribution density P(S). Hence, to avoid errors associated with discarding the "hot" lines, a change in the summation procedure is proposed in [5], whereupon the spectral-line distribution density in two parameters is introduced: in the energy of the lowest level of the transition under consideration ε and the normalized line intensity, i.e., the intensity corresponding to the transition from the level ε if its population were equal the Loschmidt number. In this case, it will be more convenient for us to modify the second parameter somewhat and consider it equal to the product of the square of the matrix element of the dipole transition moment D^2_{nk} by the multiplicity of lowest-level degeneration g_k:

$$m = g_k D^2_{nk}\,. \tag{4}$$

Then the sum of the equivalent band linewidths takes the following form when the two-parameter density $f(\varepsilon, m)$ is used (summation over the energies is later replaced everywhere by integration in the standard manner):

$$V = \int_0^\infty d\varepsilon \int_0^\infty dm f(\varepsilon, m) W(\varepsilon, m), \tag{5}$$

where $W(\varepsilon, m)$ is easily obtained from W(S) (formula (3)) if it is taken into account that the local line intensity S(x) is expressed as follows in terms of ε and m [6]:

$$S(x) = \frac{8\pi^2\bar{\nu}N}{3hcQ(T)}\left(1-\exp\left(-\frac{h\bar{\nu}}{kT}\right)\right) g_k D^2_{nk} \exp\left(-\frac{\varepsilon}{kT}\right) \equiv \lambda(T) m \exp(-\beta\varepsilon).$$

Here $Q(T) = \sum\limits_k g_k \exp(-\varepsilon_k/kT)$ is the statistical sum of the molecules, and in addition, the following notation is introduced:

$$\lambda(T) \equiv \frac{8\pi^2\bar{\nu}N}{3hcQ(T)}\left(1-\exp\left(-\frac{h\bar{\nu}}{kT}\right)\right),\quad \beta \equiv \frac{1}{kT}.$$

Returning to the examination of radiation propagation along an inhomogeneous optical path, we can write an expression for the equivalent linewidth in new variables in the form

$$W(\varepsilon, m) = \int_{+\infty}^{-\infty} d\nu \left[1 - \exp\left(-\int_0^l dx \,\frac{\lambda(x)}{\pi}\,\frac{\gamma(x)}{\nu^2+\gamma(x)^2}\, m \exp(-\beta(x)\varepsilon)\right)\right].$$

Utilizing the theorem of the mean, we reduce the integral $I(\varepsilon, m)$ in the exponent of the exponential to the form

$$I(\varepsilon, m) = \frac{ml\Phi(\varepsilon)}{\pi}\,\frac{\langle\gamma\rangle}{\nu^2+\langle\gamma\rangle^2},$$

where

$$\Phi(\varepsilon) = \frac{1}{l}\int_0^l dx\lambda(x)\exp(-\beta(x)\varepsilon). \tag{6}$$

The Curtis–Goodson requirement of agreement between the exact equivalent width $W(\varepsilon_0, m_0)$ of each individual line within the strong and weak absorption limits and the equivalent width of this same line (ε_0, m_0) in the model homogeneous gas layer is satisfied if

$$\langle\gamma\rangle = \Phi(\varepsilon_0)^{-1}\frac{1}{l}\int_0^l dx\lambda(x)\gamma(x)\exp(-\beta(x)\varepsilon_0).$$

It is now easy to see that such averaging over an inhomogeneous optical path results in a standard Curtix-Goodson mean (see (3)); for this it is sufficient to take into account how $\lambda(x)$ and $\beta(x)$ are related to $S(x)$ in the last expression and to introduce $\langle S \rangle$ in the form

$$\langle S \rangle = m\Phi(\varepsilon). \tag{7}$$

The function P(S) can be determined as follows from the known two-parameter density $f(\varepsilon, m)$. If it is considered that the total number of lines in the band equals n_b, then the number of lines whose intensity is within the interval from S to $S + \Delta S$ equals $n_b P(S)\Delta S$. On the other hand, the number of lines of intensity S formed by transitions from levels in the energy interval from ε to $\varepsilon + \Delta\varepsilon$ is $n_b f(\varepsilon, S\Phi(\varepsilon)^{-1})\Delta\varepsilon\Delta m(\varepsilon)$, where $\Delta m(\varepsilon) = \Delta S\Phi(\varepsilon)^{-1}$, as follows from (7). Then the total number of lines with intensity S in the interval ΔS is found by summing $n_b f(\varepsilon, S\Phi(\varepsilon)^{-1}\Delta\varepsilon[\Delta S/\Phi(\varepsilon)]$ over all possible values of the energy. Furthermore, by equating the sum to $n_b P(S)\Delta S$ and canceling identical factors, we have

$$P(S) = \int_0^\infty \frac{d\varepsilon}{\Phi(\varepsilon)} f\left(\varepsilon, \frac{S}{\Phi(\varepsilon)}\right). \tag{8}$$

As should have been expected, the introduction of the mean line intensity S_0 is insufficient to take account of averaging over the inhomogeneous optical path. We see that taking more accurate account of the gas layer inhomogeneity results in a change in the functional dependence of the line intensity distribution density in the band.

A further simplification is possible when the function $f(\varepsilon, m)$ is successfully expressed in explicit form for some specific molecule models. Let us note that, in contrast to P(S), the two-parameter density is independent of thermodynamic quantities, i.e., of the state of the gas, and is determined completely by the characteristics of the molecules.

Let us consider some discrete energy spectrum without degeneration, and moreover, we will consider the number of levels to be a single quantum number. Let $\varepsilon = \vartheta(n)$, $m = \Omega(n, q)$, and let the system make the transition from the level n to $k = n + q$; hence, the meaning of q is clear. Then $f(\varepsilon, m)$ can be represented in the form

$$f(\varepsilon, m) = a \sum_{q=1}^{\infty} \frac{\partial G(\varepsilon)}{\partial \varepsilon} \delta(m - \Omega[G(\varepsilon), q]), \tag{9}$$

where $G(\varepsilon)$ denotes the function reciprocal to $\vartheta(n)$. Formula (9) is obtained if it is taken into account that for a fixed q the number of spectral lines formed by transitions from levels whose energy is less than ε equals

$$R(\varepsilon, q) = n - q = G(\varepsilon) - q,$$

and, therefore, the distribution density of such lines is proportional to

$$\frac{\partial R(\varepsilon, q)}{\partial \varepsilon} = \frac{\partial G(\varepsilon)}{\partial \varepsilon}.$$

Taking account of (8) and (9) we obtain for the distribution density P(S):

$$P(S) = a \int_0^\infty \frac{d\varepsilon}{\Phi(\varepsilon)} \sum_{q=1}^{\infty} \frac{\partial G(\varepsilon)}{\partial \varepsilon} \delta\left(\frac{S}{\Phi(\varepsilon)} - \Omega[G(\varepsilon), q]\right) = \frac{a}{S} \sum_{q=1}^{\infty} \sum_i \frac{\left.\dfrac{\partial G(\varepsilon)}{\partial \varepsilon}\right|_{\eta_{qi}(S)}}{\left|\dfrac{\partial}{\partial \varepsilon} \ln(\Phi(\varepsilon)\Omega[G(\varepsilon), q])|_{\eta_{qi}(S)}\right|}, \tag{10}$$

where the functions $\eta_{qi}(S)$ are roots of the equation

$$S = \Phi(\eta_{qi})\Omega[G(\eta_{qi}), q], \tag{11}$$

and the sum over i in (10) corresponds to summation over all the roots of (11).

We write these formulas for the case of a weakly inhomogeneous layer, although it is not of independent value but clarifies their meaning. In a first approximation it is always possible to limit oneself to the first term in the sum over q since the remaining transitions are usually attenuated strongly by the selection rules. Then

$$\frac{\partial}{\partial \varepsilon} \ln \frac{1}{l} \int_0^l dx \lambda(x) \exp(-\beta(x)\varepsilon) \cong -\frac{1}{l} \int_0^l dx \beta(x) \equiv -\langle \beta \rangle.$$

Introducing the temperature $T \equiv (k\langle\beta\rangle)^{-1}$ characteristic for the whole layer for clarity, we write

$$S = \langle \lambda \rangle \exp\left(-\frac{\eta_i(S)}{kT}\right) \Omega[G(\eta_i(S))] \tag{12}$$

and

$$P(S) = \frac{akT}{S} \sum_i \frac{\left.\dfrac{\partial G(\varepsilon)}{\partial \varepsilon}\right|_{\eta_i(S)}}{\left| 1 - kT \dfrac{\partial}{\partial \varepsilon} \ln \Omega[G(\varepsilon)]|_{\eta_i(S)} \right|} . \tag{13}$$

The greatest and least line intensities can be determined from (12) from the known frequency boundaries of the band under investigation, namely, $S^{\max}$ and $S^{\min}$. Then the line intensity distribution density for our band takes the form

$$P(S) = \begin{cases} 0, & S < S^{\min}, \\ \dfrac{kT}{S} \sum\limits_i Z(\eta_i(S), T), & S^{\min} \leqslant S \leqslant S^{\max}, \\ 0, & S^{\max} < S, \end{cases}$$

where

$$Z(\varepsilon, T) = a \left(\left| 1 - kT \frac{\partial}{\partial \varepsilon} \ln \Omega[G(\varepsilon)] \right| \right)^{-1} \frac{\partial G(\varepsilon)}{\partial \varepsilon} .$$

Therefore, evaluation of P(S) for a specific gas reduces to finding the functions $\eta_i(S)$ and $Z(\varepsilon, T)$. For instance, let us consider the spectrum of diatomic molecules. Since we are interested in the IR range, we will consider just the vibrational–rotational transitions without changing the electron configuration of the molecule. Then the problem about the relative motion of two nuclei reduces, as is known, to the problem of particle motion in a field with effective potential which has the following form in a first approximation [7]:

$$U(r) = U_e + BK(K+1) + \frac{m_e \omega_e^2}{2} (r - r_e)^2 .$$

The third term here corresponds to a one-dimensional harmonic oscillator; consequently, we write for the energy

$$\varepsilon = U_e + BK(K+1) + \hbar\omega_e \left(n + \frac{1}{2}\right) .$$

It can here be considered that the weak anharmonicity of the oscillator term that appears in the next order of the expansion of the potential in a small parameter will permit resolution of the line with respect to frequency, but cannot be taken into account in a first approximation in the calculation of $G(\varepsilon)$ and $\Omega[G(\varepsilon)]$.

Let us find $g_s D_{sp}^2$ for the transition n → n + 1, K → K − 1 (P is a branch of the spectrum band)

$$g_{(nK)} D^2_{(nK)(n+1,\, K-1)} = g_K \frac{1}{g_{K-1}} \sum_{M, M'} |\langle n+1, K-1, M' | er | n, K, M \rangle|^2 \cong \frac{e^2 \hbar w}{2 m_e \omega_c} K(n+1).$$

In the case of the transition K → K + 1 (R is a branch), the quantity K is replaced by K + 1 in the last formula. Then by fixing n we have

$$G(\varepsilon, n) = \frac{1}{2} [\sqrt{1 + 4B^{-1}(\varepsilon - E(n))} - 1], \tag{14}$$

$$\Omega[G(\varepsilon, n)] = \frac{e^2 \hbar w}{2 m_e \omega_e} (n+1) G(\varepsilon, n), \tag{15}$$

where $E(n) = U_e + \hbar\omega_e[n + (1/2)]$.

Taking account of the explicit form of the function $\Omega[G(\varepsilon, n)]$, Eq. (12) for $\eta_i(S)$ is written as follows:

$$S = \langle \lambda \rangle \exp\left(-\frac{\eta_i}{kT}\right) \frac{e^2 \hbar w}{2 m_e \omega_e} \frac{n+1}{2} [\sqrt{1 + 4B^{-1}(\eta_i - E(n))} - 1], \tag{16}$$

and we obtain the following iteration equations for the two roots of this transcendental equation:

$$\eta_{1,j+1} \cong \frac{BS^2}{4\mu(n)^2} \exp\left(\frac{2\eta_{1,j}}{kT}\right) + E(n)$$

and

$$\eta_{2,j+1} \cong \frac{kT}{2} \ln\left[\frac{4\mu(n)^2}{BS^2}(\eta_{2,j} - E(n))\right],$$

where $\mu(n) = \langle\lambda\rangle(n + 1)e^2\hbar w(4m_e\omega_e)^{-1}$.

For fixed n we obtain for the line intensity distribution

$$P_n(S) \cong \frac{akT}{2S\sqrt{B}} \sum_{i=1}^{2} \frac{\sqrt{\eta_i(S) - E(n)}}{\left|\eta_i(S) - E(n) - \frac{1}{2}kT\right|}, \qquad (17)$$

Then the total distribution density P(S) can be written in the form

$$P(S) = \sum_{n=0}^{\infty} \Theta(S_n^{\max} - S)\,\Theta(S - S_n^{\min})\,P_n(S). \qquad (18)$$

where $\Theta(z)$ is the Heaviside function and the limits of variation of $P_n(S)$ are obtained from the following considerations: the upper limit is determined by the maximal value of the right side of (16), and the lower by the frequency range under consideration. A simple estimate yields

$$S_n^{\max} \sim \mu(n)\left(\frac{kT}{B}\right)^{1/2} \exp\left(-\frac{E(n)}{kT}\right),$$

$$S_n^{\min} \sim \mu(n)\left(\frac{4\Delta_P\hbar}{B}\right)^{1/2} \exp\left(-\frac{E(n) + \Delta_P\hbar}{kT}\right).$$

Calculations were also performed for the R-branch of the spectrum band. Finally, the normalizing factor equals

$$a = \left(\int_0^{\infty} dS P(S)\right)^{-1}.$$

It should be noted that in practical calculations it is always possible to limit oneself to the first three to four terms of the sum over n in (18). Computations can analogously be performed for strongly inhomogeneous media also with the sole difference that (12) and (13) determining the functions $\eta_i(S)$ and P(S) should be replaced, respectively, by (11) and (10).

The formalism proposed here permits more accurate averaging of the band parameters for inhomogeneous molecular-gas layers and finding the line intensity distribution density in each specific case, although it certainly complicates the calculation procedure.

NOTATION

W, V, equivalent width and sum of the equivalent line widths; S, S_0, γ, line intensity, mean intensity over the spectrum, and half-width; $\langle\cdots\rangle$, symbol for taking the average over the optical path; l, optical path; ε, g_s, energy and multiplicity of level degeneration; D_{sp}^2, square of the matrix element of the dipole moment; ν, frequency; $\bar{\nu}$, frequency of the line center; ω_e, frequency of the normal molecule vibrations; Δ_P, frequency range in the domain of the band P-branch; n_b, number of lines in the band; N, number of molecules per unit volume; Q(T), statistical sum of the molecule; T, temperature; β, reciprocal temperature; $\delta(z)$, Dirac delta function; $\Theta(z) = 1$, $z \geqslant 0$, $\Theta(z) = 0$, $z < 0$, Heaviside function; $S^{\max}$, $S^{\min}$, line intensity limit values; B, a rotation constant; $h = 2\pi\hbar$, Planck's constant; k, Boltzmann constant; U(r), molecular potential; r_0, value of r minimizing U(r), $U_e \equiv U(r_0)$; x, coordinate along the optical path; m_e, reduced mass of the molecule; w, nucleus weight factor; P(S), f(ε, m), the one- and two-parameter line distribution densities; n, K, M, vibrational, rotational, and magnetic quantum numbers; c, velocity of light, a, normalizing factor; e, charge on the electron.

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THEORETICAL MODEL OF HIGH-CURRENT RELATIVISTIC ELECTRON-BEAM INTERACTION WITH A METAL OBSTACLE

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A method is described and results are presented for a numerical computation of crater and plasma-flare formation under the effect of a high-current relativistic electron beam on an aluminum obstacle.

During the interaction of high-current charged-particle beams, for example, relativistic electron beams (REB), with high power density and a metal obstacle, heating, evaporation, and rupture occur. The set of physical processes governing the dynamics of crater formation and the ejection of mass in the form of highly ionized target vapors differs substantially here from the sufficiently well-studied processes accompanying material treatment by particle beams at moderate energy-flux densities [1, 2]. Computations and experiments [2-4] show that for 10^6-10^7-A beam currents and 1-10-MeV electron energies the pressure in the action domain reaches 1-50 Mbar, the temperature 10-30 eV, and the velocity of the vapors being ejected 100 km/sec. A hydrodynamic model in which dissipative processes associated with charged-particle beam energy transfer to the target substance, target deformation and rupture under the effect of the shockwave, and energy transfer in the highly heated target vapors by the radiation diffusion mechanism are taken into account is applicable for the description of the dynamics of phenomena with such parameters.

Such a model is considered in this paper. It is here taken into account that the motion that occurs is axisymmetric and the target can be both finite and semiinfinite in thickness. We mention that in an analogous formulation, but without the spatial distribution of the energy liberation zone and the radiation diffusion of the energy in the vapor flare taken into account, the described problem was solved numerically in [4]; however, the results presented there do not afford the possibility of composing a sufficiently complete representation of the parameters of the motion that occurs.

Let us consider formulation of the problem. Energy is liberated in a certain volume of the target because of REB action, resulting in melting, evaporation, and ionization of the target material. Under the action of pressure forces the substance is set in motion, a plasma flare is formed, and a crater in the target. Since REB with electron energies above 0.1 MeV produce an interaction zone with quite definite volume nature in the target, we apply the method of multiple electron scattering in a substance to compute the zone by using angular distributions computed by Goudsmit–Sanderson theory. Preliminary computations of the energy liberation zone configuration in the 0.5-10-MeV electron energy range displayed good agreement with the results of computations by the successive collisions model [6], as well as with the experimental results [4, 6]. The density profiles in the interaction zone vary during the

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