Bilinear Expansions for Redistribution Functions

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We suggest here a method for construction of a bilinear expansion for an angle-averaged redistribution function. An eigenvalues and eigenvectors determination problem is formulated and the required matrices are found analytically, and numerical procedures for their computations are elaborated. A simple method for the accuracy evaluation of the numerical calculations is suggested. It is shown that a group of redistribution functions describing the light scattering process within the spectral line frequencies can be constructed if the eigenvalue problem is solved for the considered function. It becomes possible if various combinations of eigenvalues and eigenvectors with the basic functions are used.

1 The redistribution function $r_{II}(x', x)$

Let us first redefine the redistribution function $r(x', x)$ which has a rather simple physical meaning: the quantity $r(x', x)dx$ represents the probability that a photon with the dimensionless frequency x' will be absorbed by an atom and re-emitted then in the frequency interval $(x; x + dx)$. The introduced dimensionless frequencies show the distance of photon's frequency $\nu(\nu')$ from the line center frequency ν_0 in Doppler half widths $\left(x = \frac{\nu-\nu_0}{\Delta\nu_D}\right)$. This redistribution function differs from one defined by Hummer [1] by the constant factor $\left(\pi^{\frac{1}{4}}U(0,\sigma)\right)^{-1}$, where the function

$$U(x, \sigma) = \frac{\sigma}{\pi}\int_{-\infty}^{\infty}\frac{\exp(-t^2)}{(x-t)^2+\sigma^2}dt \qquad (1)$$

is the well known Voigt function and $\sigma = \frac{\Delta\nu_T}{\Delta\nu_D}$, where $\Delta\nu_T$ is the total half-width of the line caused by all the broadening mechanisms taken into account.

The redistribution function describing the photon scattering within the line frequencies of the model two-level atom the upper level of which is broadened due to radiation damping has been independently derived by Henyey [2], Unno [3] and Sobolev [4] assuming that in the atom's reference frame the scattering is coherent.

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V. Grinin et al. (eds) Radiation mechanisms of astrophysical objects. Yerevan: Edit Print, 2017, pp. 33–42.

Then, using also Hummer's [1] designation, one can represent it in the following form:

$$r_{II}(x',x) = \frac{1}{\pi U(0,\sigma)} \int_{\frac{|\overline{x}-\underline{x}|}{2}}^{\infty} \exp(-t^2) \left[\arctan \frac{\underline{x}+t}{\sigma} - \arctan \frac{\overline{x}-t}{\sigma}\right] dt. \tag{2}$$

In the expression (2) we used the following denotations: $\overline{x} = \sup(x',x)$ and $\underline{x} = \inf(x',x)$.

It is noteworthy that there has been known bilinear expansion for two out of four redistribution functions described in Hummer's paper [1], namely, $r_I(x',x)$ and $r_{III}(x',x)$ before their classification by him. This fact was rather important for solving the light scattering problems applying the Principle of Invariance (PI). However, up to nowadays no any "natural" bilinear expansion has been revealed for the function $r_{II}(x',x)$. Therefore, one might try to create such a bilinear expansion using some artificial procedures.

In order to construct numerically such an expansion, let us first introduce here another representation of $r_{II}(x',x)$ derived by Nikoghossian [5] (see also Heinzel's paper [6])

$$r_{II}(x',x) = \frac{\sigma}{\pi U(0,\sigma)} \int_{-\infty}^{\infty} \frac{r_I(x'+t,x+t)}{t^2+\sigma^2} dt. \tag{3}$$

From Eq. (3) one finds easily that the function $r_{II}(x',x)$ transforms into the $r_I(x',x)$ when $\sigma = 0$.

On the other hand, the function $r_I(x',x)$ allows the following bilinear expansion first derived by Unno [7]:

$$r_I(x',x) = \int_{|\overline{x}|}^{\infty} \exp(-t^2) dt = \sum_{k=0}^{\infty} \frac{\alpha_{2k}(x')\,\alpha_{2k}(x)}{2k+1}, \tag{4}$$

where

$$\alpha_k(x) = (2^k \pi^{\frac{1}{2}} k!)^{-\frac{1}{2}}\, H_k(x) \exp(-x^2) \tag{5}$$

and $H_k(x)$ are the Hermit polynomials.

The obvious connection between functions $r_{II}(x',x)$ and $r_I(x',x)$ expressed by relation (3) allows suggesting the functions (5) as basic ones for constructing the eigenfunctions of $r_{II}(x',x)$. Taking into account this connection, one can search for the bilinear expansion of $r_{II}(x',x)$ in the following form:

$$r_{II}(x',x) = \sum_{k=0}^{\infty} \frac{\omega_{2k}(x',\sigma)\,\omega_{2k}(x,\sigma)}{\zeta_k(\sigma)}, \tag{6}$$

where

$$\omega_{2k}(x,\sigma) = \sum_{m=0}^{\infty} \gamma_{km}(\sigma)\,\alpha_{2k}(x). \tag{7}$$

The vector $\zeta_k(\sigma)$ and matrix $[\gamma_{km}(\sigma)]$ are, respectively, the eigenvalues and eigenfunctions of the following problem (see, for example, [8, 9]):

$$\sum_{m=0}^{\infty} [\gamma_{km}(a_{mn} - \zeta_k(\sigma) b_{mn})] = 0, \tag{8}$$

where

$$a_{mn} = \int_{-\infty}^{\infty} \alpha_{2m}(x)\, \alpha_{2n}(x) dx, \tag{9}$$

and

$$b_{mn} = \int_{-\infty}^{\infty} \alpha_{2m}(x) dx \int_{-\infty}^{\infty} r_{II}(x', x)\, \alpha_{2n}(x') dx'. \tag{10}$$

It is evident that calculating the matrices $[a_{mn}]$ and $[b_{mn}]$ and solving the eigenvalue problem (8) one can numerically construct the bilinear expansion (6).

2 Calculation of the relevant matrices

Using the integral forms for the Hermit polynomials, one can easily find the following presentation for the introduced above basic functions [10]:

$$\alpha_k(x) = (2^k \pi^{\frac{1}{2}} k!)^{-\frac{1}{2}} \frac{2}{\sqrt{\pi}} \operatorname{Re}(-2i)^k \int_0^{\infty} t^k \exp(-t^2 + 2ixt) dt. \tag{11}$$

Then, using the following expression for the δ function:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ixt) dt = \delta(t), \tag{12}$$

one finds directly

$$a_{mn} = (-1)^{m+n} \frac{(2m + 2n - 1)!!}{2^{m+n+\frac{1}{2}} \sqrt{(2m)!(2n)!}}. \tag{13}$$

For calculations of the matrix $[b_{mn}]$, one can suggest two different ways. One is the direct calculation of the threefold iterated integral (10) which is fraught with huge numerical difficulties arising due to the complicated behavior of the basic functions. Therefore, some simplifying analytical calculations before starting the numerical procedures would sufficiently facilitate the numerical procedures. One can find from Eq. (10) substituting Eq. (4) for the redistribution function $r_I(x', x)$ in the relation (3)

$$b_{mn} = \frac{\sigma}{\pi U(0, \sigma)} \sum_{k=0}^{\infty} \frac{1}{2k + 1} \int_{-\infty}^{\infty} \frac{g_{km}(t)\, g_{kn}(t)}{t^2 + \sigma^2} dt, \tag{14}$$

where

$$g_{km}(t) = \int_{-\infty}^{\infty} \alpha_{2k}(x + t)\, \alpha_{2m}(x) dx = N_{km}\, \alpha_{km}\left(\frac{t}{\sqrt{2}}\right), \tag{15}$$

and

$$N_{km} = \frac{\pi^{\frac{1}{4}}}{2^{k+m+\frac{1}{2}}} \sqrt{\frac{(2k+2m)!}{(2k)!(2m)!}}. \tag{16}$$

Thus, one finds finally

$$b_{mn} = \frac{1}{U(0,\sigma)} \sum_{k=0}^{\infty} \frac{N_{km} N_{kn}}{2k+1} c_{k+m,k+n}, \tag{17}$$

where

$$c_{mn} = \frac{\sigma}{\pi} \int_{-\infty}^{\infty} \frac{\alpha_{2m}\left(\frac{t}{\sqrt{2}}\right) \alpha_{2n}\left(\frac{t}{\sqrt{2}}\right)}{t^2+\sigma^2} dt. \tag{18}$$

As a matter of fact, the threefold iterated integral is given now by an infinite series where only a single integration appears. However, the integrand is again a vastly oscillating function making the direct numerical computation extremely inefficient especially for greater values of indexes. Also it is not difficult to realize that for the smaller damping parameters the computing error gets larger. But at the same time in the limiting case when $\sigma = 0$, the integral (18) can be taken analytically to find

$$c_{mn}|_{\sigma=0} = \alpha_{2m}(0)\, \alpha_{2n}(0). \tag{19}$$

In order to calculate the integral (18) for the values $\sigma > 0$, let us use the formulae (5) and the Hermit polynomials definition (see, for example, [10])

$$H_{2k}(x) = (2k)! \sum_{l=0}^{k} \frac{(-1)^l}{(l)!(2k-2l)!} (2x)^{2k-2l}, \tag{20}$$

to obtain

$$\alpha_{2n}\left(\frac{t}{\sqrt{2}}\right) = \exp\left(-\frac{t^2}{2}\right) \frac{\sqrt{(2n)!}}{\pi^{\frac{1}{4}}} \sum_{k=0}^{n} \frac{(-1)^k t^{2n-2k}}{2^k k!(2n-2k)!}. \tag{21}$$

Then, taking into account that

$$t^{2k} = \frac{(2m)!}{2^{2m}} \sum_{j=0}^{m} \frac{H_{2j}(t)}{(2j)!\,(m-j)!}, \tag{22}$$

one can finally find

$$c_{mn} = \frac{\sqrt{(2m)!(2n)!}}{\pi^{\frac{1}{4}} 2^{2m+2n}} \sum_{k=0}^{m} \frac{(-2)^k}{k!\,(2m-2k)!} \sum_{l=0}^{n} \frac{(-2)^l}{l!\,(2n-2l)!}$$

$$\times\, (2m+2n-2k-2l)! \sum_{q=0}^{m+n-k-l} \frac{2^q \alpha_{2q}(0,\sigma)}{(m+n-k-l-q)!\sqrt{(2q)!}}, \tag{23}$$

where the following notation is introduced:

$$\alpha_{2q}(0,\sigma) = \frac{(-1)^q}{\pi^{\frac{1}{4}}\sqrt{(2q)!}} \sum_{p=0}^{\infty} \frac{2^p \sigma^{2p}}{(2p)!} \left[(2q+2p-1)!! - \frac{\sigma}{\sqrt{\pi}} \frac{2}{2p+1}(2q+2p)!!\right]. \quad (24)$$

The expression (23) obtained for description of elements of the required matrix, though explicit, is again rather complicated for direct numerical calculations. Therefore, any numerical procedure based on the ordinary accuracy of the used computer calculations cannot provide the required accuracy of the final results. These difficulties can be overcome only using methods of calculations based on the usage of a higher number of significant digits. For example, about one hundred twenty or more significant digits are needed to provide 15 correct digits for all the elements of the 100×100 matrix.

Nevertheless, it is possible to obtain a much simpler expression if one of the indexes of the matrix $[c_{mn}]$ is equal to zero (the first row or the first column). Then one out of the three sums disappears immediately and one obtains after some transformations

$$c_{0,n} = \frac{(-1)^n \sqrt{(2n)!}}{\pi^{\frac{1}{4}} 2^{2n}} \sum_{q=0}^{n} \frac{(-2)^q \, \alpha_{2q}(0,\sigma)}{(n-q)!\sqrt{(2q)!}} = c_{n,0}. \quad (25)$$

On the other hand, taking into account the relation of recurrence for the Hermit polynomials

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad (26)$$

one can derive the following recurrence relation for the required elements of the matrix $[c_{mn}]$:

$$c_{mn} = \sqrt{\frac{2n+1}{2m}} d_{m-1,n+1} + \sqrt{\frac{n}{m}} d_{m-1,n-1} - \sqrt{\frac{2m-1}{2m}} c_{m-1,n}, \quad (27)$$

where

$$d_{mn} = c_{m+\frac{1}{2},n+\frac{1}{2}}. \quad (28)$$

Further, in terms of the physical meaning of the redistribution function one might conclude that its integral over one of the arguments should give the profile of the absorption coefficient

$$\int_{-\infty}^{\infty} r_{II}(x',x)dx' = \alpha(x,\sigma) = \frac{U(x,\sigma)}{U(0,\sigma)}, \quad (29)$$

and bearing in mind (5)–(7), one finds

$$\sum_{k=0}^{\infty} \frac{\gamma_{k,0}}{\zeta_k} \, \omega_{2k}(x,\sigma) = \frac{U(x,\sigma)}{U(0,\sigma)}. \quad (30)$$

Here the following normalization relation is used:

$$\int_{-\infty}^{\infty} \alpha_m(x)\, \alpha_n(x) dx = \delta_{mn}, \tag{31}$$

where δ_{mn} is the Kronecker symbol. Integrating Eq. (34) over all frequencies, one obtains finally

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} r_{II}(x', x) dx' = \sum_{k=0}^{\infty} \frac{{\gamma_{k0}}^2}{\zeta_k} = \sqrt{\pi}, \tag{32}$$

which can be used for the normalization purposes.

Now let us briefly consider the physical situation when both energetic levels are broadened. Heinzel [6] has shown that the redistribution function derived by Hummer [1] for description of this process is not correct and obtained a new expression allowing the following notation:

$$r_V(x', x) = \frac{{\sigma_i}^2}{\pi^2} \int_{-\infty}^{\infty} \frac{dt}{t^2 + {\sigma_i}^2} \int_{-\infty}^{\infty} \frac{r_{II}(x' + t, x + u)}{u^2 + {\sigma_i}^2} du. \tag{33}$$

Then, using Eq. (6), one will find a bilinear expansion for this function as well. Putting Eq. (6) into Eq. (33), one obtains

$$r_V(x', x) = \sum_{k=0}^{\infty} \frac{\omega_{2k}(x', \sigma_i, \sigma_j)\, \omega_{2k}(x, \sigma_i, \sigma_j)}{\zeta_k(\sigma_j)}, \tag{34}$$

where the functions

$$\omega_{2k}(x, \sigma_i, \sigma_j) = \sum_{m=0}^{\infty} \gamma_{km}(\sigma_j)\, \alpha_{2m}(x, \sigma_i) \tag{35}$$

depend on damping parameters of both energetic levels. The functions $\alpha_{2k}(x, \sigma)$ are defined by the relation

$$\alpha_k(x, \sigma) = (2^k \pi^{\frac{1}{2}} k!)^{-\frac{1}{2}} \frac{2}{\sqrt{\pi}} \mathrm{Re}(-2i)^k \int_0^{\infty} t^k \exp(-t^2 - 2\sigma t + 2ixt) dt. \tag{36}$$

Thus, constructing a bilinear expansion for the function $r_{II}(x', x)$ as described above, one arrives at a conclusion that this method provides a tool for constructing similar expansions for all the applicable redistribution functions. It can be done immediately, if one obtains the eigenfunctions $\gamma_{km}(\sigma)$ and eigenvalues $\zeta_k(\sigma)$ and also uses an appropriate numerical procedure for computing the functions $\alpha_k(x, \sigma)$. Then the corresponding redistribution functions could be constructed by the same procedure using the various values of the parameters σ_i and σ_j. It is easy to see that $r_V(x', x) = r_{III}(x', x)$, if $\sigma_j = 0$, $r_V(x', x) = r_{II}(x', x)$ for $\sigma_i = 0$ and, at last, $r_V(x', x) = r_I(x', x)$, if both damping parameters are equal to zero – $\sigma_j = \sigma_i = 0$.

3 The auxiliary functions $\alpha_k(x,\sigma)$

Obviously, besides the eigenvalue problem (8) one should overcome the second key computational difficulties for the eventual construction of the redistribution functions. That is the problem of the numerical evaluation of the corresponding auxiliary functions. The functions $\alpha_{2m}(x,\sigma)$ defined by Eq. (36) have been introduced and studied by Hummer [1], and a rather effective method for their calculation was suggested by him in the same paper. In order to simplify the initial expression (36), the exponent $\exp(-2\sigma t)$ is replaced by its power series. Then one should compute several terms of that series to provide the required accuracy of auxiliary functions. Following the Hummer's procedure in general, Harutyunian [11] has separated from each other the even and odd functions appearing in the derived series to obtain the following relation:

$$\alpha_k(x,\sigma) = (2^k\pi^{\frac{1}{2}}k!)^{-\frac{1}{2}} \sum_{m=0}^{\infty} \frac{(i\sigma)^m}{(2m)!}\left[M_{k+2m}(x) + \frac{\sigma}{2m+1}N_{k+2m+1}(x)\right], \tag{37}$$

where

$$M_k(x) = \frac{2}{\sqrt{\pi}}\,\mathrm{Re}(-2i)^k \int_0^\infty t^k \exp(-t^2+2ixt)dt \tag{38}$$

and

$$N_k(x) = \frac{2}{\sqrt{\pi}}\,\mathrm{Im}(-2i)^k \int_0^\infty t^k \exp(-t^2+2ixt)dt \tag{39}$$

are the Hermit functions of the first and second kinds [10].

From Eqs. (38) and (39) one can easily find the following recurrent formulas well known from the mathematical textbooks (see, for example, [10]):

$$M_{k+1}(x) = 2xM_k(x) - 2kM_{k-1}(x) \tag{40}$$

for the first kind functions and similarly

$$N_{k+1}(x) = 2xN_k(x) - 2kN_{k-1}(x) \tag{41}$$

for the second kind functions. The first functions to be used for recurrent relations are defined as follows:

$$M_0(x) = \exp(-x^2), \quad M_1(x) = 2xM_0(x), \tag{42}$$

$$N_0(x) = \frac{2}{\sqrt{\pi}}, \quad N_1(x) = 2xN_0(x) - \frac{2}{\sqrt{\pi}}. \tag{43}$$

Here

$$F(x) = \int_0^\infty \exp(-t^2)\sin 2xt\,dt = \exp(-x^2)\int_0^x \exp(t^2)dt \tag{44}$$

is the Dawson function connected with the error function of an imaginary argument and represents the solution of the following Cauchy problem:

$$F'(x) = 1 - 2xF(x) \tag{45}$$

with the initial condition $F(0) = 0$.

Numerical procedures for calculation of the Dawson function are considered in Hummer's paper [12]. Some earlier references could be found in the mentioned above review by Hummer [1]. Among the relatively recent studies one might refer to the papers [13–14]. The most efficient procedure for calculation of the Dawson function can be carried out using the power series [10]

$$F(x) = \sum_{n=0}^{\infty} \frac{(-1)^n\, 2^n}{(2n+1)!!} x^{2n+1}, \tag{46}$$

which converges for all values of the argument. However, one should take care for the accuracy issues when applying the relation (46) for numerical computations. Obviously, for the smaller values of the argument ($x \leq 1$) the series (46) converges rather rapidly and no big difficulties can arise. However, for the larger values of the argument, the need in much higher digit numbers for calculations grows up very rapidly. For instance, for $x = 12$ one can easily provide around 35 correct digits of the Dawson function if uses 120 significant digits for calculations. Nonetheless, the usage of the same number of significant digits provides only 12 correct digits in the final result if the argument reaches to the value $x = 15$. Many correct significant digits are very important not only for computing the Dawson function itself. The point is that the recurrent formula themselves are a perilous source of the error accumulation and therefore one needs to calculate the Dawson function with a bigger number of correct significant digits. Actually, the problem is absolutely the same that we encountered considering the matrix $[c_{mn}]$ in the previous paragraph.

Of course, on the other hand, one can find an asymptotic series for the larger arguments of the Dawson function which can be rather useful for the practical applications [10]

$$F(x) \approx \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n+1}\, n!\, x^{2n+1}}. \tag{47}$$

This asymptotic relation, as opposed to the series (46), is a diverging one. Nevertheless, a few first terms of this series will provide an applicable accuracy for various asymptotic estimates. Indeed, starting with the relations (42)–(43) and using the relation (47), one obtains for $x \to \infty$ the following asymptotic form:

$$N_k(x) \approx \frac{(-1)^k}{\sqrt{\pi} x^{k+1}} \sum_{n=0}^{\infty} \frac{(2n+k)!}{2^{2n}\, n!\, x^{2n}}, \tag{48}$$

which can be used in the series (37). It is easy to see that due to the exponentially decreasing behavior of the first kind Hermit functions for larger values of the argument they are falling much faster than the second kind functions. Therefore, one finds the asymptotic relation

$$\alpha_k(x,\sigma) = \frac{\sigma}{x^{k+2}\sqrt{\pi}}(2^k\pi^{\frac{1}{2}}k!)^{-\frac{1}{2}}\sum_{n=0}^{\infty}\frac{(2n+k+1)!}{x^{2n}}\sum_{m=0}^{n}\frac{(-1)^m\sigma^{2m}}{2^{2(n-m)}(2m+1)!(n-m)!}, \tag{49}$$

which turns into the known asymptotic expression for the Voigt function [15]

$$U(x,\sigma) = \frac{\sigma}{x^2\sqrt{\pi}}\sum_{n=0}^{\infty}\frac{(2n+1)!}{x^{2n}}\sum_{m=0}^{n}\frac{(-1)^m\sigma^{2m}}{2^{2(n-m)}(2m+1)!(n-m)!}. \tag{50}$$

These asymptotic forms coupled with the exact formulas derived above provide one with all the necessary tools for building the bilinear expansions of redistribution functions and their usage for the practical purposes.

Preliminary calculations show that these numerical procedures easily can be performed on modern PC. Elaborated specially for these purposes software package HAHMATH allows one to perform computations with the needed number of significant digits when high accuracy calculations are required. However, extraordinary accuracies are needed only when the matrix $[c_{mn}]$ or Dawson function and its derivatives are calculated. Once calculated the matrix $[c_{mn}]$ can be used for building the matrix $[b_{mn}]$ and to continue all other computations with the ordinary accuracy of computers. There is no need for using the extremely long numbers when solving the corresponding eigenvalue problem. Calculated once the eigenvalues and eigenfunctions for the given damping factor might be used for further calculations.

Acknowledgments. Two of the authors (H.H. and G.A.) thank the Armenian SCS and French CNRS for the financial support given during the joint project implementation.

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