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An information–theoretical lineshape: general case

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Abstract. Following Powles and Carazza, the information–theoretical method is used to obtain the most probable spectral distribution given only a knowledge of a finite number of moments of the line. An approximate method is given to obtain Lagrange undetermined multipliers. Examples of application of the method are given.

1. Introduction

Powles and Carazza (1970) applied the information–theoretical method to the problem of the absorption lineshape in nuclear magnetic resonance. Assuming that a finite number of moments of the line is given they obtained a most probable lineshape in the form

$$p(x) = Z^{-1} \exp\left(-\sum_{k=1}^{2n} \lambda_k x^k\right), \tag{1}$$

where x denotes the frequency, and Z is the normalization constant

$$Z = Z(\lambda_1, \ldots, \lambda_{2n}) = \int_{-\infty}^{+\infty} \exp\left(-\sum_{k=1}^{2n} \lambda_k x^k\right) \mathrm{d}x. \tag{2}$$

$\lambda_1, \ldots, \lambda_{2n}$ are Lagrange undetermined multipliers which can be calculated from the equation

$$M_k = -\frac{\partial \ln Z}{\partial \lambda_k}, \qquad k = 1, \ldots, 2n, \tag{3}$$

where M_k are moments of the line. The difficulty consists now in the calculation of the λ_k's from equation (3). Powles and Carazza gave a method for obtaining λ_2 and λ_4 for a symmetrical lineshape:

$$p(x) = Z^{-1} \exp(-\lambda_2 x^2 - \lambda_4 x^4) \tag{4}$$

for M_2 and M_4 only known (in this case $M_1 = M_3 = 0$). In what follows we give an approximate method of calculation of the λ_k's for the general case of the distribution (1), that is for $M_1, M_2, \ldots, M_{2n}$ lines ($n = 2, 3, \ldots$; for $n = 1$ one obtains the gaussian distribution). In particular, approximate formulae for $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ for M_1, M_2, M_3, M_4 lines and $\lambda_2, \lambda_4, \lambda_6$ for M_2, M_4, M_6 lines are given. For M_2, M_4 lines the results are compared with those of Powles and Carazza.

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2. Calculation of Lagrange undetermined multipliers

Following Powles and Carazza we assume that a nuclear magnetic resonance absorption lineshape $p(x)$ is a probability distribution in frequency x. The kth moment of the lineshape is defined as

$$M_k = \int_{-\infty}^{+\infty} x^k p(x)\,dx, \qquad k = 1, 2, \ldots. \tag{5}$$

The line is called symmetric when all odd moments vanish (for the detailed physical discussion cf, eg, Powles and Carazza). Assume that a finite number of moments $M_1, \ldots, M_{2n}$ is known. There exists, in general, a set of distributions $p(x)$ satisfying the relations (5):

$$K = K(M_1, \ldots, M_{2n}) = \left\{ p(x) \in W : \int_{-\infty}^{+\infty} x^k p(x)\,dx = M_k, \qquad k = 1, \ldots, 2n \right\} \tag{6}$$

where

$$W = : \left\{ p(x) : p(x) \geqslant 0, \qquad \int_{-\infty}^{+\infty} p(x)\,dx = 1 \right\}.$$

The set K will be called a macrostate. The notion of a macrostate was introduced in the so called information thermodynamics (cf Ingarden and Urbanik 1962, see also, eg, Kossakowski 1969, Ingarden 1973). Suppose that there exists a distribution $p_K(x) \in K$ (called the most probable distribution or the representative distribution of K) such that

$$S(p_K) = -\int_{-\infty}^{+\infty} p_K(x) \ln p_K(x)\,dx = \sup_{p \in K} \left(-\int_{-\infty}^{+\infty} p(x) \ln p(x)\,dx \right). \tag{7}$$

As is well known the distribution $p_K(x)$ (if it exists) has the form (1) with (2) and (3). Now we calculate the Lagrange multipliers. Denoting $M_0 = 1$ and $\lambda_0 = \ln Z$ we may rewrite the equations (3) and the normalization condition of $p(x)$ in the form

$$M_i = \int_{-\infty}^{+\infty} x^i \exp\left(-\sum_{j=0}^{2n} \lambda_j x^j \right) dx \qquad i = 0, 1, \ldots, 2n. \tag{8}$$

Now we make use of the well known quadrature formula. Let $f(x)$ be a continuous function and assume that the integral $\int_{-\infty}^{+\infty} \exp(-x^2) f(x)\,dx$ exists. Then

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx = \sum_{k=1}^{m} A_k^{(m)} f(x_k) + R(f), \tag{9}$$

where

$$A_k^{(m)} = \frac{2^{m+1} m! \sqrt{\pi}}{H_m'^2(x_k)}, \qquad R(f) = \frac{m!}{2^m (2m)!} f^{(2m)}(\eta), \tag{10}$$

$-\infty < \eta < +\infty$, $H_m(x)$ are Hermite polynomials:

$$H_m(x) = (-1)^m e^{x^2} \frac{d^m}{dx^m} e^{-x^2}, \tag{11}$$

and $x_1, \ldots, x_m$ are zeros of the polynomial $H_m(x)$. The coefficients $A_k^{(m)}$ are tabulated (cf, eg, Krylov 1967, pp 141–2). Suppose that functions $f(x), f'(x), \ldots, f^{(2m)}(x)$ are finite so that $R(f) \to 0$ for $m \gg 1$. For example, for $m = 5$ we have $R(f) \sim 10^{-6} f^{(10)}(\eta)$.

Neglecting the term $R(f)$ and substituting

$$C_{ik} = A_k^{(m)} \exp(x_k^2) x_k^i = w_k x_k^i, \qquad i = 0, 1, \ldots, 2n; \qquad k = 1, \ldots, m; \tag{12}$$

$$f_k = f(x_k) = \exp\left(- \sum_{j=0}^{2n} \lambda_j x_k^j \right), \tag{13}$$

we rewrite equations (8) in the form

$$M_i = \sum_{k=1}^{m} C_{ik} f_k. \tag{14}$$

The function $f(x)$ in (13) has at most n maxima. Our approximation will be good for $f(x)$ attaining their maximal values in the interval $(-x_m, x_m)$. If $m = 2n + 1$, then (14) becomes a system of $2n + 1$ linear equations for $2n+1$ unknowns $f_1, \ldots, f_{2n+1}$ which can be easily solved by the Cramer's formulae, namely

$$f_k = \frac{d_k \exp(-x_k^2)}{A_k^{(m)} V_{2n+1}}, \tag{15}$$

where d_k denotes the determinant

$$d_k = \begin{vmatrix} 1 & 1 \ldots 1 & 1 & 1 \ldots 1 \\ x_1 & x_2 \ldots x_{k-1} & M_1 & x_{k+1} \ldots x_{2n+1} \\ \vdots & & & \vdots \\ x_1^{2n} & x_2^{2n} \ldots x_{k-1}^{2n} & M_{2n} & x_{k+1}^{2n} \ldots x_{2n+1}^{2n} \end{vmatrix} \tag{16}$$

and V_{2n+1} is the Vandermond determinant

$$V_{2n+1} = \prod_{\substack{k,l=1 \\ k>l}}^{2n+1} (x_k - x_l). \tag{17}$$

Note that all f_k's ($k = 1, \ldots, 2n+1$) have to be positive with respect to (13), so that the method referred to can be applied if the prescribed moments $M_1, \ldots, M_{2n}$ satisfy the relations

$$d_k = d_k(M_1, \ldots, M_{2n}) > 0. \tag{18}$$

Suppose it is satisfied. Then, substituting $B_k = -\ln f_k$, we obtain a set of linear equations for the Lagrange multipliers $\lambda_0, \lambda_1, \ldots, \lambda_{2n}$:

$$B_k = \sum_{j=0}^{2n} \lambda_j x_k^j, \qquad k = 1, \ldots, 2n+1. \tag{19}$$

The solution of (19) has the form

$$\lambda_j = \frac{\Delta_j}{V_{2n+1}}, \qquad j = 0, 1, \ldots, 2n, \tag{20}$$

where Δ_j denotes the determinant

$$\Delta_j = \begin{vmatrix} 1 & x_1 & x_1^2 & \dots x_1^{j-1} & B_1 & x_1^{j+1} & \dots & x_1^{2n} \\ 1 & x_2 & x_2^2 & \dots x_2^{j-1} & B_2 & x_2^{j+1} & \dots & x_2^{2n} \\ \vdots & & & & & & & \vdots \\ 1 & x_{2n+1} & x_{2n+1}^2 & \dots x_{2n+1}^{j-1} & B_{2n+1} & x_{2n+1}^{j+1} & \dots & x_{2n+1}^{2n} \end{vmatrix}. \tag{21}$$

For the polynomial $H_{2n+1}(x)$, $x_{n+1} = 0$, so that (20) yields

$$\lambda_0 = \ln Z = B_{n+1} = -\ln f_{n+1}. \tag{22}$$

One can calculate the Lagrange multipliers $\lambda_0, \lambda_1, \dots, \lambda_{2n-2}$ from (20) and the remaining λ_{2n-1} and λ_{2n} from the equations

$$\sum_{k=1}^{2n} k\lambda_k M_k = 1; \qquad \sum_{k=1}^{2n} k\lambda_k M_{k-1} = 0, \tag{23}$$

which can be easily verified by integration by parts. In particular, for symmetric lineshapes one obtains

$$\begin{aligned} &2\lambda_2 M_2 = 1 \qquad \text{for } n = 1, \\ &4\lambda_4 M_4 + 2\lambda_2 M_2 = 1 \qquad \text{for } n = 2, \\ &6\lambda_6 M_6 + 4\lambda_4 M_4 + 2\lambda_2 M_2 = 1 \qquad \text{for } n = 3, \text{ etc.} \end{aligned} \tag{24}$$

The last two relations were given by Powles and Carazza (cf equations (22) and (52) of Powles and Carazza 1970). Integrating by parts the expression

$$M_{2n+s} = Z^{-1} \int_{-\infty}^{+\infty} x^{2n+s} \exp\left(- \sum_{k=1}^{2n} \lambda_k x^k \right) dx$$

one obtains the recurrence formula

$$M_{2n+s} = (2n\lambda_{2n})^{-1} \left((s+1)M_s - \sum_{k=1}^{2n-1} k\lambda_k M_{k+s} \right). \tag{25}$$

3. Examples

For illustration of the method consider two examples.

3.1. M_1, M_2, M_3, M_4 lineshape

Here we have $n = 2$ and

$$\begin{aligned} &x_3 = 0 && A_3 = 0{\cdot}945 \\ &x_4 = -x_2 := b = 0{\cdot}959 && A_2 = A_4 = 0{\cdot}393 \\ &x_5 = -x_1 := a = 2{\cdot}02 && A_1 = A_5 = 0{\cdot}020 \end{aligned} \tag{26}$$

and

$$A_1 \exp(x_1^2) =: w_1 = 1{\cdot}282, \qquad A_2 \exp(x_2^2) =: w_2 = 0{\cdot}987, \tag{26}$$

(cf, eg, Krylov 1967, p 141, see also Abramowitz and Stegun 1965, p 924). From (15) one obtains

$$\begin{aligned}
f_1 &= \frac{(M_4 - b^2M_2) - a(M_3 - b^2M_1)}{w_1 2a^2(a^2 - b^2)}, \\
f_2 &= \frac{(a^2M_2 - M_4) + b(M_3 - a^2M_1)}{w_2 2b^2(a^2 - b^2)}, \\
f_3 &= \frac{M_4 - (a^2 + b^2)M_2 + a^2b^2}{a^2b^2A_3}, \\
f_4 &= \frac{(a^2M_2 - M_4) - b(M_3 - a^2M_1)}{w_2 2b^2(a^2 - b^2)}, \\
f_5 &= \frac{(M_4 - b^2M_2) + a(M_3 - b^2M_1)}{w_1 2a^2(a^2 - b^2)}.
\end{aligned} \tag{27}$$

Suppose that the inequalities $f_k > 0$, $k = 1, \ldots, 5$, and $f_3 < 1$, are satisfied. Denoting $B_k = -\ln f_k$ one obtains from (20)–(22) the following formulae for $\lambda_0, \lambda_1, \ldots, \lambda_4$:

$$\begin{aligned}
\lambda_0 &= B_3 = -\ln f_3, \\
\lambda_1 &= \frac{-a^3(B_2 - B_4) + b^3(B_1 - B_5)}{2ab(a^2 - b^2)}, \\
\lambda_2 &= \frac{a^4(B_2 + B_4 - 2B_3) - b^4(B_1 + B_5 - 2B_3)}{2a^2b^2(a^2 - b^2)}, \\
\lambda_3 &= \frac{a(B_2 - B_4) - b(B_1 - B_5)}{2ab(a^2 - b^2)}, \\
\lambda_4 &= \frac{-a^2(B_2 + B_4 - 2B_3) + b^2(B_1 + B_5 - 2B_3)}{2a^2b^2(a^2 - b^2)}.
\end{aligned} \tag{28}$$

Substituting the values (26) one obtains

$$\begin{aligned}
\lambda_0 &= 1{\cdot}266 - \ln h_3, \\
\lambda_1 &= \frac{1}{12{\cdot}24}\{-8{\cdot}24(\ln h_4 - \ln h_2) + 0{\cdot}88(\ln h_5 - \ln h_1)\}, \\
\lambda_2 &= \frac{1}{23{\cdot}7}\{2(6{\cdot}17 + 15{\cdot}8 \ln h_3) - 16{\cdot}65(\ln h_2 + \ln h_4) + 0{\cdot}85(\ln h_1 + \ln h_5)\} \\
\lambda_3 &= \frac{1}{12{\cdot}24}\{2{\cdot}02(\ln h_4 - \ln h_2) - 0{\cdot}96(\ln h_5 - \ln h_1)\}, \\
\lambda_4 &= \frac{1}{23{\cdot}7}\{2(0{\cdot}08 - 3{\cdot}16 \ln h_3) + 4{\cdot}08(\ln h_2 + \ln h_4) - 0{\cdot}92(\ln h_1 + \ln h_5)\},
\end{aligned} \tag{29}$$

where

$$\begin{aligned} h_1 &= M_4 - 2{\cdot}02M_3 - 0{\cdot}92M_2 + 1{\cdot}86M_1, \\ h_2 &= -M_4 + 0{\cdot}96M_3 + 4{\cdot}08M_2 - 3{\cdot}92M_1, \\ h_3 &= M_4 - 5M_2 + 3{\cdot}75, \\ h_4 &= -M_4 - 0{\cdot}96M_3 + 4{\cdot}08M_2 + 3{\cdot}92M_1, \\ h_5 &= M_4 + 2{\cdot}02M_3 - 0{\cdot}92M_2 - 1{\cdot}86M_1. \end{aligned} \tag{29'}$$

The conditions $0 < f_k$ and $f_3 < 1$ are equivalent to

$$0 < h_1, h_2, h_4, h_5; \qquad 0 < h_3 < 3{\cdot}54. \tag{30}$$

For symmetric lineshapes $M_1 = M_3 = 0$, so that $h_1 = h_5$ and $h_2 = h_4$ and the relations (29) take the form

$$\begin{aligned} \lambda_0 &= 1{\cdot}266 - \ln h_3, \\ \lambda_1 &= \lambda_3 = 0, \\ \lambda_2 &= \frac{1}{11{\cdot}85}(6{\cdot}17 + 0{\cdot}85 \ln h_1 - 16{\cdot}65 \ln h_2 + 15{\cdot}8 \ln h_3), \\ \lambda_4 &= \frac{1}{11{\cdot}85}(0{\cdot}08 - 0{\cdot}92 \ln h_1 + 4{\cdot}08 \ln h_2 - 3{\cdot}16 \ln h_3), \end{aligned} \tag{31}$$

where

$$h_1 = M_4 - 0{\cdot}92M_2; \qquad h_2 = -M_4 + 4{\cdot}08M_2. \tag{31'}$$

We can also use the relations (23) or (24), respectively. We tested our method for some M_2, M_4 and M_1, M_2, M_3, M_4 lines. The results are given in table 1. The exact values for λ_2 and λ_4 were obtained by the method of Powles and Carazza. Namely

$$\lambda_2 = xy, \qquad \lambda_4 = \tfrac{1}{2}y^2 \tag{32}$$

where

$$y = \frac{M_2}{2M_4}[-x + \{x^2 + 2(M_4/M_2^2)\}^{1/2}].$$

Table 1. Coefficients $\lambda_0, \lambda_2, \lambda_4$ for some M_2, M_4 lineshapes.

			λ_0		λ_2		λ_4		$x = \lambda_2/(2\lambda_4)^{1/2}$	
	M_2	M_4	Exact	Approx.	Exact	Approx.	Exact	Approx.	Exact	Approx.
1	1	1·79	1·43	1·88	−0·75	−1·14	0·35	0·46	−0·9	−1·2
2	1	1·93	1·29	1·65	−0·42	−0·89	0·24	0·36	−0·6	−1
3	1	2·51	1·181	1·043	0·228	0·281	0·041	0·054	1	0·7
4	1·24	3·50	1·205	1·140	0·106	0·106	0·064	0·064	0·3	0·3
5	1·22	3·50	1·219	1·126	0·150	0·200	0·045	0·036	0·5	0·7

The parameter x was obtained from the relation

$$\frac{M_4}{M_2^2} := g(x) = 3\frac{D_{-5/2}(x)D_{-1/2}(x)}{D^2_{-3/2}(x)}, \tag{33}$$

$D_q(x)$ being the so called parabolic cylinder functions:

$$D_q(x) = \frac{\exp(-\frac{1}{4}x^2)}{\Gamma(-q)}\int_0^\infty \exp(-xs-\tfrac{1}{2}s^2)s^{-q-1}\,ds, \qquad (\mathrm{Re}\, q < 0),$$

(cf also Powles and Carazza 1970, equation (32)). Some values of $g(x)$ are given in table 2.

Table 2

x	0	0·1	0·2	0·3	0·4	0·5
$g(x)$	2·19	2·23	2·29	2·30	2·33	2·35
$g(-x)$	2·19	2·15	2·10	2·07	2·02	1·98
x	0·6	0·7	0·8	0·9	1·0	1·1
$g(x)$	2·40	2·43	2·46	2·48	2·51	2·53
$g(-x)$	1·93	1·88	1·84	1·79	1·75	1·70

The exact value for λ_0 was found from the relation

$$\lambda_0 = \ln Z = \ln\left\{(2\lambda_4)^{-1/4}\pi^{1/2}\exp\left(\frac{\lambda_2^2}{8\lambda_4}\right)D_{-1/2}\left(\frac{\lambda_2}{(2\lambda_4)^{1/2}}\right)\right\}.$$

The functions $D_q(x)$ are tabulated (cf, eg, Abramowitz and Stegun 1965, p 686).

For the case M_1, M_2, M_3, M_4 lineshape we considered the shape

$$p(x) = Z^{-1}\exp\{-\lambda(x^4-2x^3+1{\cdot}5x^2-0{\cdot}5x)\} \sim \exp\{-\lambda(x-0{\cdot}5)^4\}. \tag{34}$$

We took $\lambda = 0{\cdot}12$. Then

$$\lambda_0 = 1{\cdot}125, \quad \lambda_1 = -0{\cdot}05, \quad \lambda_2 = 0{\cdot}18, \quad \lambda_3 = -0{\cdot}24, \quad \lambda_4 = 0{\cdot}12$$

and

$$M_1 = 0{\cdot}5, \qquad M_2 = 1{\cdot}25, \qquad M_3 = 1{\cdot}63, \qquad M_4 = 3{\cdot}64. \tag{35}$$

From (29) we obtain the approximate values

$$\lambda_0 = 1{\cdot}135, \quad \lambda_1 = -0{\cdot}058, \quad \lambda_2 = 0{\cdot}24, \quad \lambda_3 = -0{\cdot}166 \quad \lambda_4 = 0{\cdot}11.$$

3.2. M_2, M_4, M_6 *lineshape*

Suppose that moments M_2, M_4, M_6 of the line are given and $M_1 = M_3 = M_5 = 0$. The most probable lineshape will have the form

$$p(x) = Z^{-1}\exp(-\lambda_2x^2-\lambda_4x^4-\lambda_6x^6) = \exp(-\lambda_0-\lambda_2x^2-\lambda_4x^4-\lambda_6x^6). \tag{36}$$

We calculate the parameters $\lambda_0, \lambda_2, \lambda_4, \lambda_6$ using the method of § 2. Here we have $n = 3$, that is, $m = 2n+1 = 7$ and

$$\begin{aligned} x_4 &= 0 & A_4 &= 0{\cdot}810 \\ x_5 &= -x_3 =: c = 0{\cdot}816 & w_3 &= 0{\cdot}829 \\ x_6 &= -x_2 =: b = 1{\cdot}674 & w_2 &= 0{\cdot}897 \\ x_7 &= -x_1 =: a = 2{\cdot}652 & w_1 &= 1{\cdot}137 \end{aligned} \tag{37}$$

(cf, eg, Abramowitz and Stegun 1965, p 924). From (15) and (16) we have

$$\begin{aligned} f_1 = f_7 &= \frac{1}{2a^2 w_1} \frac{M_6 - (b^2+c^2)M_4 + b^2c^2M_2}{(a^2-b^2)(a^2-c^2)}, \\ f_2 = f_6 &= \frac{1}{2b^2 w_2} \frac{-M_6 + (a^2+c^2)M_4 - a^2c^2M_2}{(a^2-b^2)(b^2-c^2)}, \\ f_3 = f_5 &= \frac{1}{2c^2 w_3} \frac{M_6 - (a^2+b^2)M_4 + a^2b^2M_2}{(a^2-c^2)(b^2-c^2)}, \\ f_4 &= \frac{1}{w_4} \frac{-M_6 + (a^2+b^2+c^2)M_4 - (a^2b^2+a^2c^2+b^2c^2)M_2 + a^2b^2c^2}{a^2b^2c^2}. \end{aligned} \tag{38}$$

Suppose that $f_k > 0$, $k = 1, \ldots, 4$, and $f_4 < 1$. Then, substituting $B_k = -\ln f_k$ one obtains from (20)–(22):

$$\begin{aligned} \lambda_0 &= B_4 = -\ln f_4 \\ \lambda_2 &= A^{-1}\{a^4b^4(a^2-b^2)(B_3-B_4) + b^4c^4(b^2-c^2)(B_1-B_4) - a^4c^4(a^2-c^2)(B_2-B_4)\}, \\ \lambda_4 &= A^{-1}\{-a^2b^2(a^4-b^4)(B_3-B_4) - b^2c^2(b^4-c^4)(B_1-B_4) + a^2c^2(a^4-c^4)(B_2-B_4)\}, \\ \lambda_6 &= A^{-1}\{a^2b^2(a^2-b^2)(B_3-B_4) + b^2c^2(b^2-c^2)(B_1-B_4) - a^2c^2(a^2-c^2)(B_2-B_4)\}, \end{aligned} \tag{39}$$

where

$$A = a^2b^2c^2(a^2-b^2)(b^2-c^2)(a^2-c^2). \tag{39'}$$

With respect to (37) the formulae (39) can be written in the form

$$\begin{aligned} \lambda_0 &= 2{\cdot}3637 - \ln h_4, \\ \lambda_2 &= \tfrac{1}{781}(426 - 7{\cdot}4 \ln h_1 + 141 \ln h_2 - 1678 \ln h_3 + 1544 \ln h_4), \\ \lambda_4 &= \tfrac{1}{781}(-11 + 13{\cdot}8 \ln h_1 - 229 \ln h_2 + 820 \ln h_3 - 605 \ln h_4), \\ \lambda_6 &= \tfrac{1}{781}(1{\cdot}2 - 3{\cdot}98 \ln h_1 + 30{\cdot}2 \ln h_2 - 85{\cdot}2 \ln h_3 + 59 \ln h_4), \end{aligned} \tag{40}$$

where

$$\begin{aligned} h_1 &= M_6 - 3{\cdot}47M_4 + 1{\cdot}87M_2, \\ h_2 &= -M_6 + 7{\cdot}8M_4 - 4{\cdot}68M_2, \\ h_3 &= M_6 - 9{\cdot}93M_4 + 19{\cdot}71M_2, \\ h_4 &= -M_6 + 10{\cdot}6M_4 - 26{\cdot}26M_2 + 13{\cdot}12. \end{aligned} \tag{41}$$

The inequalities $0 < f_k, k = 1, 2, 3$, and $0 < f_4 < 1$ are equivalent to

$$0 < h_k, \qquad k = 1, 2, 3, \qquad 0 < h_4 < 10{\cdot}63. \tag{42}$$

Two examples are given below in tables 3 and 4. The moments are calculated for the lineshape $p(x) = Z^{-1} \exp(-\lambda x^6)$.

Table 3. $M_2 = 1{\cdot}273$, $M_4 = 3{\cdot}24$, $M_6 = 7{\cdot}15$

	Exact	Approximate
$\lambda_0 = \ln Z$	1·312	1·224
λ_2	0	0·70
λ_4	0	−0·146
λ_6	0·0156	0·0343

Table 4. $M_2 = 1{\cdot}21$, $M_4 = 2{\cdot}93$, $M_6 = 9{\cdot}14$

	Exact	Approximate
λ_0	1·286	1·552
λ_2	0	0·33
λ_4	0	−0·078
λ_6	0·0182	0·0202

4. Conclusions

An approximate method is given for calculating the parameters $\lambda_0, \lambda_1, \ldots, \lambda_{2n}$ of the most probable lineshape given moments $M_1, M_2, \ldots, M_{2n}$ ($M_0 = 1$). Conversely, for a lineshape of the type $\exp(-\Sigma_{j=0}^{2n}\lambda_j x^j)$ moments $M_1, M_2, \ldots$ can be calculated via relations (20)–(25). In particular parameters $\lambda_0, \lambda_1, \ldots, \lambda_4$, and $\lambda_2, \lambda_4, \lambda_6$ for M_1, M_2, M_3, M_4 and M_2, M_4, M_6 lineshapes are obtained. The results for M_2, M_4 lines agree, in general, with those of Powles and Carazza. The differences do not essentially change the lineshape, and the method gives at least the qualitative features of the line. Note that there is no limit for n, so that the method can also be applied, for example in lattice dynamics, where even 100 or more moments can be calculated (cf Isenberg 1970).

References

Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)

Ingarden R S 1973 *Acta Phys. Polon.* A **43** 3–14

Ingarden R S and Urbanik K 1962 *Acta Phys. Polon.* **21** 281–94

Isenberg C 1970 *J. Phys.* C: *Solid St. Phys.* **3** L179–82

Kossakowski A 1969 *Bull. Acad. Polon Sci., Sér. Sci. Math. Astron. Phys.* **17** 263–7

Krylov V I 1967 *Approximate Evaluation of Integrals* (in Russian) (Moscow: Gosfizmatizdat)

Powles J G and Carazza B 1970 *Proc. Int. Symp. on Electron and Nuclear Magnetic Resonance, Melbourne* 1969 (New York: Plenum) pp 133–61