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Eigenvalues and Eigenfunctions of the Hilbert Operator

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The eigenvalues and eigenfunctions of the Hilbert operator have been evaluated as part of a technique for solving Boltzmann's equation for a gas model consisting of rigid spheres. The numerical method for their evaluation is presented as well as a small sample of the results.

1. INTRODUCTION

We have proposed (see [10, 12]) a new, very fast numerical method for solving Boltzmann's equation for a gas model consisting of rigid spheres by means of Hilbert's expansion. Using Hilbert's expansion, Boltzmann's equation reduces to a sequence of integral equations. The success of the method rests upon the simultaneous use of four judiciously chosen expansions; Hilbert's expansion for the distribution function, another expansion of the distribution function in terms of Hermite polynomials, the expansion of the kernel in terms of the eigenvalues and eigenfunctions of the Hilbert operator, and an expansion involved in solving a system of linear equations through a singular value decomposition. The time required to compute the eigenvalues and eigenfunctions is great, however, one need compute these only once; see [10, 12].

Boltzmann's equation describes the evolution of the one-particle distribution function $f = f(\mathbf{x}, \mathbf{u}, t)$, where $\mathbf{x}$ is the position vector, $\mathbf{u}$ is the velocity vector, and t is time. In the case of a gas model consisting of rigid spheres of diameter σ and in the absence of external forces it takes the form

$$\mathscr{D}f = \frac{\partial f}{\partial t} + (\mathbf{u} \cdot \nabla_x) f = \frac{\sigma^2}{2} \iint | \mathbf{V} \cdot \mathbf{e} | (f' f_1' - f f_1) \, d\mathbf{u}_1 \, d\omega, \tag{1}$$

where $\mathbf{V} = \mathbf{u} - \mathbf{u}_1$, ∇_x denotes the gradient operator with respect to the $\mathbf{x}$ variables, the primes refer to molecules which enter the element of volume after collision, and boldface type denotes vector quantities.

In solving Boltzmann's equation by means of Hilbert's expansion (see [6, 10, 12)] retaining only the first two terms, Boltzmann's equation reduces to the Boltzmann–Hilbert integral equation

$$-\frac{2\pi\mathscr{R}T}{\sigma^2\rho^2} \mathscr{D}f_0 = M(p) \, e^{-2p^2} \phi(\mathbf{p}) + \frac{e^{-p^2}}{\pi} \int \phi(\mathbf{p}_1) \, e^{-p_1^2} \left(R - \frac{2}{R} \, e^{\omega^2} \right) d\mathbf{p}_1 , \tag{2}$$

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where

$$f = f_0(1 + \phi), \qquad f_0 = \rho(2\pi\mathscr{R}T)^{-3/2}\, e^{-p^2}, \qquad \mathbf{p} = \mathbf{u}(2\mathscr{R}T)^{-1/2}, \tag{3}$$

$$M(p) = 1 + \left(2p + \frac{1}{p}\right) e^{p^2} \int_0^p e^{-z^2}\, dz, \qquad \omega = \frac{pp_1}{R} \sin\theta, \tag{4}$$

ρ denotes the density, T the temperature, $\mathscr{R}$ the universal gas constant, $R = |\mathbf{p}_1 - \mathbf{p}|$, and θ denotes the angle between $\mathbf{p}$ and $\mathbf{p}_1$. Successive terms in the Hilbert expansion are obtained by solving the integral equation with a different source term.

Let $\psi(\mathbf{p}) = e^{-p^2} M(p)^{1/2} \phi(\mathbf{p})$; then Eq. (2) may be written in the form

$$\begin{aligned} -(2\pi\mathscr{R}T/\sigma^2\rho^2)\, e^{p^2} M(p)^{-1/2}\, \mathscr{D}f_0 &= \psi(\mathbf{p}) + (1/\pi) \int K(\mathbf{p}, \mathbf{p}_1)\, \psi(\mathbf{p}_1)\, d\mathbf{p}_1 \\ &= \psi(\mathbf{p}) + (1/\pi)\, \mathscr{K}\psi, \end{aligned} \tag{5}$$

where

$$K(\mathbf{p}, \mathbf{p}_1) = (R - (2/R)\, e^{\omega^2})[M(p)\, M(p_1)]^{-1/2}, \tag{6}$$

and $\mathscr{K}$ denotes the Hilbert operator; see [9, 10].

2. Eigenvalues and Eigenfunctions

The eigenvalues and eigenfunctions of the linearized Boltzmann collision operator for a Maxwellian gas have been extensively studied by Burnett [2, 3], Mott-Smith [8], and Wang-Chang and Uhlenbeck [13]. It has been shown that the eigenfunctions are

$$\Phi_{rl}(\mathbf{p}) = N_{rl} P_l(\cos\theta)\, p^l L_r^{l+1/2}(p^2), \tag{7}$$

where

$$N_{rl} = \left[\frac{r!\,(l + \frac{1}{2})}{\pi\Gamma(l + r + \frac{1}{2})}\right]^{1/2}$$

is a normalization factor with respect to the weight e^{-p^2}, $L_r^{l+1/2}$ denotes the associated Laguerre polynomial and P_l the Legendre polynomial; see [7]. Dependence on the azimuthal angle ϕ can be included by replacing $P_l(\cos\theta)$ by $e^{im\phi} P_l^m(\cos\theta)$, and the eigenvalues are independent of m.

We determine the eigenvalues λ_{rl} and the eigenfunctions ψ_{rl} satisfying the integral equation

$$\psi_{rl}(\mathbf{p}) = (\lambda_{rl}/\pi) \int K(\mathbf{p}, \mathbf{p}_1)\, \psi_{rl}(\mathbf{p}_1)\, d\mathbf{p}_1 . \tag{8}$$

Equation (8) is solved using a method introduced by Wang-Chang and Uhlenbeck

[13] and also by Pekeris *et al.* [9]; expand ψ (dropping the subscripts) in a complete set of orthonormal functions $\{h_i(p)\}$, i.e.,

$$\psi(p) = \sum_{i=0}^{\infty} a_i h_i(\mathbf{p}), \tag{9}$$

following the Galerkins method, in which we require that the error term be orthogonal to these functions h_i ; see [4]. Upon substitution of (9) into (8) we obtain

$$\sum_{i=0}^{\infty} a_i \left[(\lambda/\pi) \int K(\mathbf{p}, \mathbf{p}_1)\, h_i(\mathbf{p})_1\, d\mathbf{p}_1 - h_i(\mathbf{p})\right] = 0. \tag{10}$$

The sum in (10) has to be orthogonal to each base function $h_k(\mathbf{p})$, thus

$$\sum_{i=0}^{\infty} a_i \left[(\lambda/\pi) \iint K(\mathbf{p}, \mathbf{p}_1)\, h_i(\mathbf{p}_1)\, h_k(\mathbf{p})\, d\mathbf{p}_1\, d\mathbf{p} - \int h_i(\mathbf{p})\, h_k(\mathbf{p})\, d\mathbf{p}\right] = 0. \tag{11}$$

Equation (11) represents a system of linear equations, the vanishing of whose determinant yields the eigenvalues λ_{rl} and the eigenvectors $\mathbf{a}_{rl}$ for the expansion in (11).

For orthogonal family we choose $\{\exp(-p^2)M(p)^{1/2}\Phi_{rlm}(\mathbf{p})\}$, i.e.,

$$h_{rlm}(\mathbf{p}) = \exp(-p^2)M(p)^{1/2}\Phi_{rlm}(\mathbf{p}) \tag{12}$$

where Φ_{rlm} is given by (7). Thus

$$\psi_{rlm}(p) = \exp(im\phi)\, P_l^m(\cos\theta) \exp(-p^2)\, M(p)^{1/2}\, p^l \sum_{k=0}^{\infty} a_{rlk} L_k^{l+1/2}(p^2). \tag{13}$$

Upon the explicit substitution of (13) into (11) we obtain

$$\sum_{r',l'=0}^{\infty} a_{r'l'} \left\{(\lambda/\pi) \iint (R - (2/R)\, e^{\omega^2}) \exp(-p^2 - p_1^2)\, \Phi_{r'l'}(\mathbf{p}_1)\, \Phi_{rl}(\mathbf{p})\, d\mathbf{p}_1\, d\mathbf{p} \right.$$
$$\left. - \int \exp(-2p^2)\, M(p)\, \Phi_{r'l'}(\mathbf{p})\, \Phi_{rl}(\mathbf{p})\, d\mathbf{p}\right\} = 0, \tag{14}$$

where Φ_{rl} denotes Φ_{rl0}, for when $\mathscr{K}$ is applied to a function of the form $g(p^2)$ $P_l^m(\cos\theta)\, e^{im\phi}$ the result is of the form $g_l(p^2)\, P_l^m(\cos\theta)\, e^{im\phi}$, where $g_l(p^2)$ does not depend on m, see [13].

We define the Chapman brackets $[rl, r'l]$ by

$$[rl, r'l] = \sigma^2 \left\{\pi^{-2} \iint d\mathbf{p}\, d\mathbf{p}_1\, K(\mathbf{p}, \mathbf{p}_1)[M(p)\, M(p_1)]^{1/2} \exp(-p^2 - p_1^2)\, \Phi_{r'l}(\mathbf{p}_1)\, \Phi_{rl}(\mathbf{p}) \right.$$
$$\left. + \pi^{-1} \int d\mathbf{p} \exp(-2p^2)\, M(p)\, \Phi_{r'l}(p)\, \Phi_{rl}(p)\right\}. \tag{15}$$

TABLE

Eigenvalues λ_{rl} and Coefficients of the Expansion a_{rlk} in

l	0	0	0	0
r	0	1	2	3
Eigenvalue	-1.00000000 00	-1.00000000 00	-1.57971633 00	-2.13148483 00
Coefficient k				
0	-1.23105631 -01	2.24622114 -01	1.85468841 -02	-1.05490921 -02
1	-1.74633757 -01	-5.80200252 -02	5.16782156 -02	-2.76991339 -01
2	0.	0.	1.85265673 -01	-7.42274434 -02
3	0.	0.	-1.90086175 -02	-1.79391206 -01
4	0.	0.	-4.86154072 -03	3.60149896 -02
5	0.	0.	-1.80348774 -03	8.86770647 -03
6	0.	0.	-7.77615594 -04	3.31439714 -03
7	0.	0.	-3.65746476 -04	1.44412287 -03
8	0.	0.	-1.82671270 -04	6.83833948 -04
9	0.	0.	-9.55486179 -05	3.42037854 -04
10	0.	0.	-5.19195077 -05	1.78209107 -04
11	0.	0.	-2.91547182 -05	9.59937056 -05
12	0.	0.	-1.68549791 -05	5.32239471 -05
13	0.	0.	-1.00026427 -05	3.02923580 -05
14	0.	0.	-6.07856424 -06	1.76646364 -05
15	0.	0.	-3.77441030 -06	1.05387214 -05
16	0.	0.	-2.39008582 -06	6.42424599 -06
17	0.	0.	-1.54072249 -06	3.99634193 -06
18	0.	0.	-1.00944185 -06	2.53370287 -06
19	0.	0.	-6.71196751 -07	1.63506431 -06
20	0.	0.	-4.52334524 -07	1.07257776 -06
21	0.	0.	-3.08604103 -07	7.14289559 -07
22	0.	0.	-2.12923421 -07	4.82313642 -07
23	0.	0.	-1.48431065 -07	3.29826023 -07
24	0.	0.	-1.04460592 -07	2.28176310 -07
25	0.	0.	-7.41642427 -08	1.59536429 -07
26	0.	0.	-5.30854374 -08	1.12634197 -07
27	0.	0.	-3.82869470 -08	8.02345572 -08
28	0.	0.	-2.78101567 -08	5.76278465 -08
29	0.	0.	-2.03347905 -08	4.17078078 -08

The Chapman brackets were evaluated by Mott-Smith [8], yielding

$$[rl, r'l'] = \delta_{ll'} \frac{\sigma^2(2\pi)^{1/2}\,(2l)!}{\Gamma(l+\frac{3}{2})\,2^{r+r'+3l}} \sum_{n=0}^{\min(r,r')} \sum_{m=0}^{l} \frac{4^n \Gamma(l-m+r+r'-2n-1/2)}{(r-n)!\,(r'-n)!\,(l-m)!} B_m{}^n \tag{16}$$

where

$$\begin{aligned} B_m{}^n &= 0, && m = n = 0 \\ &= \frac{(m+2n+1)!}{(2n+1)!\,m!} - \frac{2^{m-1}(m+n+1)!}{n!\,m!}, && \text{otherwise.} \end{aligned} \tag{17}$$

Upon substitution of (15) into (14) we obtain

$$\sum_{r',l'=0}^{\infty} a_{r'l'} \left\{(\lambda\pi/2)[rl, r'l] - (\lambda+1)\int \exp(-2p^2)\, M(p)\, \Phi_{r'l}(p)\, \Phi_{rl}(\mathbf{p})\, d\mathbf{p}\right\} = 0. \tag{18}$$

I

Eq. (13) for the Eigenfunctions of the Hilbert Operator

ℓ	1	1	1	1
r	0	1	2	3
Eigenvalue	-1.00000000 00	-1.62519664 00	-2.17741228 00	-2.71692051 00
Coefficient k				
0	3.29918525 -01	-7.36282872 -02	-3.88397730 -02	2.41828476 -02
1	0.	-2.33375759 -01	-9.52260026 -02	5.53755023 -02
2	0.	2.66181162 -02	-1.80247805 -01	9.27265299 -02
3	0.	4.79475825 -03	3.97419952 -02	1.44984584 -01
4	0.	1.40884669 -03	7.24944098 -03	-4.83243446 -02
5	0.	5.06508115 -04	2.22605556 -03	-8.61713895 -03
6	0.	2.05059445 -04	8.26920710 -04	-2.70715533 -03
7	0.	9.01613924 -05	3.41139613 -04	-1.02520388 -03
8	0.	4.22369454 -05	1.50896408 -04	-4.27205654 -04
9	0.	2.08404543 -05	7.03270659 -05	-1.88820156 -04
10	0.	1.07485947 -05	3.42060120 -05	-8.69251791 -05
11	0.	5.76255266 -06	1.72659582 -05	-4.12658843 -05
12	0.	3.19739833 -06	9.01338362 -06	-2.00864770 -05
13	0.	1.82938709 -06	4.85497447 -06	-9.99289312 -06
14	0.	1.07585873 -06	2.69349488 -06	-5.07295269 -06
15	0.	6.48506622 -07	1.53668412 -06	-2.62662383 -06
16	0.	3.99653199 -07	9.00112335 -07	-1.38746418 -06
17	0.	2.51235923 -07	5.40400338 -07	-7.48296715 -07
18	0.	1.60783479 -07	3.31940865 -07	-4.12491527 -07
19	0.	1.04567851 -07	2.08221678 -07	-2.32661407 -07
20	0.	6.90054481 -08	1.33139417 -07	-1.34400124 -07
21	0.	4.61438949 -08	8.66216853 -08	-7.95556799 -08
22	0.	3.12308558 -08	5.72478906 -08	-4.82548647 -08
23	0.	2.13723032 -08	3.83744795 -08	-2.99750898 -08
24	0.	1.47751655 -08	2.60545102 -08	-1.90478644 -08
25	0.	1.03107685 -08	1.78960977 -08	-1.23631942 -08
26	0.	7.25825831 -09	1.24226111 -08	-8.18141629 -09
27	0.	5.15105600 -09	8.70664927 -09	-5.50942522 -09
28	0.	3.68342245 -09	6.15645019 -09	-3.76826194 -09
29	0.	2.65272558 -09	4.38888364 -09	-2.61313965 -09

We consider the integral

$$\int \exp(-2p^2)\, M(p)\, \Phi_{r'l}(\mathbf{p})\, \Phi_{rl}(\mathbf{p})\, d\mathbf{p};$$

by changing to spherical coordinates we obtain

$$\int \exp(-2p^2)\, M(p)\, \Phi_{r'l}(\mathbf{p})\, \Phi_{rl}(\mathbf{p})\, d\mathbf{p}$$

$$= \delta_{ll'} \frac{4\pi}{(2l+1)} \int_0^\infty \exp(-2p^2)\, M(p)\, p^{2l+2} L_r^{l+1/2}(p^2)\, L_{r'}^{l+1/2}(p^2)\, dp \qquad (19)$$

$$= -\delta_{ll'} b_{rr'}^l . \qquad (20)$$

The integral on the right in (19) can be evaluated numerically using the FORTRAN subroutine CADRE which uses cautious adaptive Romberg extrapolation; see Ref. [5].

Guassian quadrature is very poor since the integrand is very oscillatory. However, this can become very expansive as r and l increase.

The integral (19) (or (20)) can be written in a closed form which enables efficient numerical computation for a large range of values of l, r, and r'; See [9, 10]. Using the notation of [9], (20) may be written as

$$b^l_{rr'} = A \sum_{k=0}^{r} \tau_k \sum_{\alpha=0}^{l+2r-2k} (\alpha + 1)\, \sigma_{\alpha k}\,, \tag{21}$$

where

$$A = \frac{2\pi\, 2^{1/2}\Gamma(l + r' + \frac{3}{2})}{(2l + 1)\, 2^{r+r'+l+1}}\,, \tag{22}$$

$$\tau_{k+1} = \frac{(\beta - 2k)(\gamma - k)}{2(k + 1)(\gamma + k)}\, \tau_k\,, \qquad \tau_0 = \frac{1}{r!\,(r' - r)!}\,, \tag{23}$$

$$\sigma_{\alpha+1,k} = \frac{2(\delta - 2k - \alpha)}{(2\gamma + 4k + 2\alpha + 1)}\, \sigma_{\alpha k}\,, \qquad \sigma_{0k} = \frac{1}{(2k + \gamma - \frac{3}{2})(2k + \gamma - \frac{1}{2})}\,, \tag{24}$$

$$\beta = 2(l + r) + 1, \qquad \gamma = r' - r + 1, \qquad \delta = l + 2r, \tag{25}$$

for $r \leqslant r'$. Interchange r and r' in (21)–(25) for $r' \leqslant r$. This computation was originally done by Pekeris *et al.* [9]. Equation (18) now takes the form

$$\sum_{r'=0}^{\infty} a_{r'l}\{(\lambda\pi/\sigma^2)[rl, r'l] + (\lambda + 1)\, b^l_{rr'}\} = 0, \qquad r, l = 0, 1,\ldots\,. \tag{26}$$

For a given value of l, the vanishing of the determinant of (26) determines the eigenvalues λ_{rl} of (8).

Writing, for a given value of l and r, $r' = 0, 1,\ldots, N < +\infty$,

$$A^l = (b^l_{rr'}), \tag{27}$$

$$B^l = -\left(\frac{\pi}{\sigma^2}\,[rl, r'l] + b^l_{rr'}\right), \tag{28}$$

$$\mathbf{a}^l = (a_{r'l}), \tag{29}$$

Eq. (26) becomes a generalized eigenvalue problem of order N, for each l,

$$A^l\mathbf{a}^l = \lambda B^l\mathbf{a}^l. \tag{30}$$

The matrices A^l and B^l are negative and positive definite, respectively. It is observed that the off-diagonal terms of A^l and B^l decay so rapidly that, for the expansion (13), $\mathbf{a}^l$ should be of order 30×1. Although N may be larger than 30, only the first 30 components of each eigenvector $\mathbf{a}^l$ need be retained for the expansion.

The method used to solve (30) consists of four parts: (1) Perform Cholesky decomposition of B^l into $L^l L^{lT}$, where L^l is lower triangular. The composition $L^{l-1} A^l L^{lT-1}$ is performed, resulting in a symmetric matrix. (2) Reduce the symmetric matrix obtained in (1) to a symmetric tridiagonal matrix using accumulating orthogonal similarity transforms. (3) Compute eigenvalues and eigenvectors of the symmetric tridiagonal matrix obtained in (2) by the implicit QL method. (4) Form eigenvectors of (30) by back transforming those obtained in (3); see [14].

The eigenvalues λ_{rl} and coefficients a_{rlk} have been computed for $l = 0, 1,..., 11$; $r = 0, 1,..., 56$; and $k = 0, 1,..., 29$; see [11]. The computing time was about 1 hour on a CDC 7600. Much of the computing time was used in evaluating the elements of the matrices A^l and B^l. This greatly expands the original table computed Pekeris *et al.* [1]. In Table I a sample of the eigenvalues and coefficients are presented for $l = 0, 1$; $r = 0, 1, 2, 3$; and $k = 0, 1,..., 29$.

The principal source of error in computing the eigenvalues and coefficients arises when the series in (26) is truncated to form a generalized eigenvalue problem of finite order, represented by (30). A disadvantage of this method is the difficulty in ascertaining its accuracy without repeating the complete calculation with a larger determinent. The successive determinant approach and the computation of the residual in (26) was used to determine the accuracy. For $l = 0, 1,..., 11$; $r = 0, 1,..., 56$; and $k = 0, 1,..., 29$ (and in Table I) the eigenvalues λ_{rl} are correct to $n + 8$ significant figures, where $10^{n-1} \leqslant |\lambda_{rl}| < 10^n$, and the coefficients are correct to nine significant figures.

The program as well as the computed eigenvalues and coefficients are on punched cards and are available from the author.

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