An Efficient Numerical Solution to the Stochastic Collection Equation

SHALVA TZIVION (TZITZVASHVILI)*, GRAHAM FEINGOLD AND ZEV LEVIN

Department of Geophysics and Planetary Sciences, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Ramat Aviv, 69978, Israel

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ABSTRACT

A new, accurate, efficient method for solving the stochastic collection equation (SCE) is proposed. The SCE is converted to a set of moment equations in categories using a new analytical form of Bleck's approach. The equations are written in a form amenable to solution and to a category-by-category analysis of drop formation and removal. This method is unique in that closure of the equations is achieved using an expression relating high-order moments to any two lower order moments, thereby restricting the need for approximation of the category distribution function only to integrals over incomplete categories. Moments in categories are then expressed in terms of complete moments with the aid of linear or cubic polynomials. The method is checked for the case of the constant kernel and a linear polynomial kernel. Results show that excellent approximation to the analytical solutions for these kernels are obtained. This is achieved without the use of weighting functions and with modest computing time requirements. The method conserves two or more moments of the spectrum (as required) and successfully alleviates the artificial enhancement of the collection process which is a feature of many schemes.

1. Introduction

Numerous attempts have been made at accurate, efficient solution to the stochastic collection equation (SCE). One such attempt (Berry, 1967; Berry and Reinhardt, 1974) converts the continuous spectrum to a discrete spectrum and solves for the distribution function at the grid points which separate the categories. Values of the function between grid points are interpolated using Lagrange polynomials. Gelbard and Seinfeld (1978) use collocation on finite elements and interpolate within elements using a cubic spline polynomial. Although the abovementioned methods ensure exact solutions at the grid points, they cannot ensure conservation of physical moments of the spectrum since moments are integral characteristics of a continuous spectrum and are not defined for a discrete spectrum.

In a different approach, Bleck (1970), Danielsen et al. (1972), and Soong (1974) solve the time dependent SCE in subcategories of the spectrum, assuming a mass-weighted mean value for the drop number density in each category. Since the equations are normalized for the mass density distribution function they conserve the liquid water content of the spectrum. A one moment solution of this kind cannot, however, ensure the conservation of additional physical moments of the spectrum (e.g., number density, N, or radar reflectivity, Z).

As a rule, numerical methods are usually tested and evaluated according to their ability to reproduce the few analytical solutions which exist for the SCE. Analytical solutions exist for the case of a constant kernel and the linear polynomial kernel (Golovin, 1963; Scott, 1968). For the case of the constant kernel with an initial gamma distribution, Bleck obtained satisfactory results using 90 categories. However, in the case of 30 or 60 categories, significant acceleration of the collection process was obtained. Acceleration was also obtained for Golovin's (1963) kernel, even when 90 categories were used. In order to suppress this acceleration, Bleck introduced power weighting functions which were specially designed to suit the initial distribution and kernel being considered. For the same purpose, Soong (1974) used exponential weighting functions. We wish to stress that acceleration is an artifact of all one moment approximations since they require the average mass of particles in each category to be constant and independent of time, with a value given by the mass of the category center. The introduction of weighting functions simply moves the position of this average mass but still keeps it constant with time. In reality, the av-

* Also affiliated with Israel Meteorological Service, Department for Research and Development, Bet Dagan, Israel.

erage mass in a category can change significantly with time, especially in the high categories which tend to be broad because of the logarithmically increasing mass scale. The inaccuracies of the one moment approximation can be smoothed by increasing the number of categories when using the constant kernel. In the case of Golovin's kernel, however, increasing the number of categories to 90 still does not produce satisfactory results and weighting functions are required. Since a good fit to the analytical solutions for the constant or Golovin's kernel does not guarantee good approximation to the solution for a real kernel, care should be taken before the method of weighting is generalized for all forms of initial distribution function and kernels.

To overcome these aforementioned problems we require, at least, a two moment approximation method. In this case, we will no longer require the average mass of particles in each category to be constant. A two moment approximation should also enable the approximation of the distribution function in each category to be expressed in terms of two parameters. In order for such an approach to succeed, the distribution function must be positive within the category. In the one moment approximation, this requirement is automatically fulfilled, but for the two moment approximation this is not necessarily the case. The first attempts at solving for two moments of the spectrum were proposed by Ochs and Yao (1978), Enukashvily (1980) and Tzivion (1980). The method of Ochs and Yao employs an adaptation of Egan and Mahoney's (1972) moment conserving approach to the advection problem. Its main limitation is that it requires an unreasonably short time increment (of the order of 0.1 sec) for the purely stochastic treatment of collection. For the time scales usually considered in numerical cloud models (of the order of 1 hour), this stochastic treatment is extremely costly in terms of computer time. The method proposed by Ochs and Yao is hybrid in nature, employing *stochastic* treatment for the interaction between drops of similar size and *continuous* treatment when the interacting drops differ greatly in size. Enukashvily (1980) conserves two moments of the distribution and uses a linear approximation to the distribution function. However, this function does not always satisfy the condition of positiveness throughout the interval. In order to overcome this, the zeroes of the approximation function must be found in each category (during each time step). Integration is then performed only in that part of the interval where the function is positive. Although good results are obtained for both the constant kernel and Golovin's kernel (with the aid of a power weighting function, in the case of the latter), this approach has proven to be prohibitive in terms of required computer time, rendering it unsuitable for dynamic cloud modeling purposes.

The present work is an extension and refinement of the method proposed by Tzivion (1980). It conserves two or more moments of the spectrum while minimizing use of the approximate distribution function. Closure is achieved with the aid of a dimensionless parameter connecting neighboring moments. This dimensionless parameter is a function of the category width only. The method is accurate, efficient (requiring less computing time than the Bleck algorithm) and easily adaptable for incorporation into numerical cloud models.

2. Equation for the moments

The time dependent SCE for a spectrum of drops may be written in the form:

$$\frac{\partial n(x,t)}{\partial t}=\frac{1}{2}\int_0^x n(x-y,t)n(y,t)K(x-y,y)dy - n(x,t)\int_0^\infty n(y,t)K(x,y)dy, \quad (1)$$

where $n(x, t)dx$ is the number of drops with masses between x and $x + dx$ per unit volume at time t. The kernel, $K(x, y)$, represents the probability of collection between drops having mass x and mass y per unit time per unit volume of air.

The overall drop spectrum is now subdivided into separate categories according to the expression:

$$x_{k+1}=px_k, \quad (2)$$

k being the number of the category, x_k and x_{k+1}, the lower and upper mass boundaries of the category, and p, a parameter designating the category width. Normally p takes on values of 2, $2^{1/2}$, $2^{1/3}$, etc.

The jth moment of the distribution function $n(x, t)$ in category k, is given by

$$M_k^j=\int_{x_k}^{x_{k+1}} x^j n_k(x,t)dx. \quad (3)$$

Using Eqs. (3) and (1), we obtain a system of equations with respect to the moments in each category:

$$\frac{dM_k^j(t)}{dt}=\frac{1}{2}\int_{x_k}^{x_{k+1}} x^j dx\int_{x_1}^{x} n(x-y,t)n(y,t)K(x-y,y)dy - \sum_{i=1}^{I}\int_{x_k}^{x_{k+1}} x^j n_k(x,t)dx\int_{x_i}^{x_{i+1}} n_{i(y,t)}K_{k,i}(x,y)dy, \quad (4)$$

where I is the total number of categories and x_1, the lowest mass considered. The first double integral in (4) is transformed by dividing the area of integration into separate subareas (i, k) in which the functions in the integrand belong to a certain category k (for details, see Appendix A or, Bleck, 1970, Danielsen et al., 1972 and Soong, 1974). Using this approach, and after some transformations, yields the following set of equations (for the special case of $p = 2$):

$$\frac{dM_k^j(t)}{dt}=\sum_{i=1}^{k-1}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k}^{x_{k+1}-y}(x+y)^jK_{k,i}(x,y)n_k(x,t)dx+\sum_{i=1}^{k-2}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k-y}^{x_k}(x+y)^jK_{k-1,i}$$
$$\times(x,y)n_{k-1}(x,t)dx+\frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy\int_{x_{k-1}}^{x_k}(x+y)^jn_{k-1}(x,t)K_{k-1,k-1}(x,y)dx$$
$$-\sum_{i=1}^{I}\int_{x_k}^{x_{k+1}} x^jn_k(x,t)dx\int_{x_i}^{x_{i+1}} n_i(y,t)K_{k,i}(x,y)dy, \quad (5)$$

where $n_k(x, t)$ is the distribution function in category k and $K_{i,k}$, the probability of coagulation between particles in class i with those in class k.

Two problems must be overcome before the set of equations can be solved: First, the set of equations is not closed (even for the simple case of $K_{k,i}$ = constant), since moments of order greater than j appear in the equation for moment j. Second, in Eq. (5), terms 1 and 2 cannot be expressed in terms of moments because the domain of integration does not span the whole category. Consequently, an approximation to $n_k(x, t)$ is required. There are two possible ways of solving the set of Eq. (5). The first uses an approximation to $n_k(x, t)$ in each term of the equation. This ensures closure of the system of equations. For example, using a one moment approximation, Bleck (1970) and Soong (1974) obtained and solved an equation for the mass-weighted average number density, and, using a two-moment linear approximation, Enukashvily (1980) solved two equations for the number and mass concentrations. The second approach to the problem, and the one adopted here, is to close the set of equations and to restrict approximation of $n_k(x, t)$ only to those internal integrals over incomplete category intervals, thereby expressing incomplete moments in terms of complete moments. One of the advantages of such a method is that it uses an approximation only when absolutely necessary.

3. Solution of the equations

a. Closure

We wish to close the set of equations using a new approach. Long (1974), using Bleck's method, showed that excellent results can be obtained if a polynomial approximation to the collection kernel ($K_{k,i}$) is used instead of the actual kernel in each category. The order of the polynomial used determines the accuracy of the approximation. Soong (1974) adopted this method and used a zero order polynomial. If Long's approximation is employed, we note that the general form of the moment equations is still conserved. However, on the right-hand side of Eq. (5), moments of order greater than j appear. To close the equations, the latter must be expressed in terms of moments of order not exceeding j. To accomplish this, a nondimensional parameter, ξ_p is introduced:

$$\xi_p=\frac{\int_{x_k}^{x_{k+1}} x^{j+1}n_k(x,t)dx\cdot\int_{x_k}^{x_{k+1}} x^{j-1}n_k(x,t)dx}{\left[\int_{x_k}^{x_{k+1}} x^jn_k(x,t)dx\right]^2}. \quad (6)$$

Using the Schwarz inequality, it can be shown (see appendix B) that

$$1\leqslant\xi_p\leqslant\frac{(p+1)^2}{4p}. \quad (7)$$

For values of p = 2, $2^{1/2}$ and $2^{1/3}$ we note that ξ_p lies between 1 and 1.125, 1.030 and 1.013, respectively. Using the mean value of ξ_p ($\bar{\xi}_p$), the relationship between three neighboring moments of the distribution function can be expressed in the form:

$$M_k^{j+1}=\bar{\xi}_p\bar{x}_k^jM_k^j \quad (8a)$$

where,

$$\bar{x}_k^j=\frac{M_k^j}{M_k^{j-1}}. \quad (8b)$$

By decreasing the parameter p, i.e., the width of the categories, it is possible, in principle, to approximate moments of order greater than j by moments of order not exceeding j, to the required degree of accuracy. Use of the parameter $\bar{\xi}_p$ does not depend appreciably on the shape of the distribution function.

b. Solution

We wish to solve the system of Eq. (5) for two moments, M_k and N_k:

$$\frac{dN_k(t)}{dt}=\left[\frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy\int_{x_{k-1}}^{x_k}K_{k-1,k-1}(x,y)n_{k-1}(x,t)dx+\sum_{i=1}^{k-2}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k-y}^{x_k}K_{k-1,i}(x,y)n_{k-1}(x,t)dx\right]$$
$$-\left[\frac{1}{2}\int_{x_k}^{x_{k+1}} n_k(y,t)dy\int_{x_k}^{x_{k+1}}K_{k,k}(x,y)n_k(x,t)dx+\sum_{i=1}^{k-1}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_{k+1}-y}^{x_{k+1}}K_{k,i}(x,y)n_k(x,t)dx\right]$$
$$-\left[\frac{1}{2}\int_{x_k}^{x_{k+1}} n_k(y,t)dy\int_{x_k}^{x_{k+1}}K_{k,k}(x,y)n_k(x,t)dx+\sum_{i=k+1}^{I}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k}^{x_{k+1}}K_{k,i}(x,y)n_k(x,t)dx\right] \quad (9a)$$

$$\frac{dM_k(t)}{dt}=\left[\frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy\int_{x_{k-1}}^{x_k}(x+y)K_{k-1,k-1}(x,y)n_{k-1}(x,t)dx\right.$$
$$\left.+\sum_{i=1}^{k-2}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k-y}^{x_k}(x+y)K_{k-1,i}(x,y)n_{k-1}(x,t)dx\right]$$
$$-\left[\frac{1}{2}\int_{x_k}^{x_{k+1}} n_k(y,t)dy\int_{x_k}^{x_{k+1}}(x+y)K_{k,k}(x,y)n_k(x,t)dx+\sum_{i=1}^{k-1}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_{k+1}-y}^{x_{k+1}}(x+y)K_{k,i}(x,y)n_k(x,t)dx\right]$$
$$+\left[\sum_{i=1}^{k-1}\int_{x_i}^{x_{i+1}} yn_i(y,t)dy\int_{x_k}^{x_{k+1}}K_{k,i}(x,y)n_k(x,t)dx-\sum_{i=k+1}^{I}\int_{x_i}^{x_{i+1}} n_i(y,t)dy\int_{x_k}^{x_{k+1}}xK_{i,k}(x,y)n_k(x,t)dx\right]. \quad (9b)$$

Note that the equations have been written in a form so as to make their physical sense easily understood. In Eq. (9a), the first two terms represent autoconversion of particles to interval k as a result of the coagulation between particles in category $k-1$ with one another (term 1), and, with those in categories less than $k-1$ (term 2). Terms 3 and 4 describe autoconversion from class k to class $k+1$ as a result of coagulation between particles in category k with one another (term 3), and, with those in categories less than k (term 4). The last two terms represent the decrease in the number of particles in category k due to coagulation of particles in category k with one another (term 5), and, with those in categories larger than k. The terms in the equation for mass are analogous to those in Eq. (9a) except that they represent mass transfer rather than number transfer. The fifth and sixth terms respectively describe the increase or decrease in mass in category k due to coagulation between particles in k and all those less than k, or, greater than k.

With the kernel $K_{k,i}$, approximated by integer order polynomials (the coefficients of which may be removed from the integrals), it is necessary to solve integrals of the form:

$$\int_{x_{k+1}-y}^{x_{k+1}} x^j n_k(x,t)dx. \quad (10)$$

We define a linear distribution function to approximate $x^j n_k(x, t)$:

$$x^j n_k(x,t)=x_k^j f_k\left(\frac{x_{k+1}-x}{x_k}\right)+x_{k+1}^j\psi_k\left(\frac{x-x_k}{x_k}\right), \quad (11)$$

where f_k and ψ_k are the values of n_k at $x=x_k$ and x_{k+1} respectively. The integral given by (10) can be solved to obtain:

$$\int_{x_{k+1}-y}^{x_{k+1}} x^j n_k(x,t)dx=x_{k+1}^j\psi_k y-\frac{x_k^j}{2x_k}(2^j\psi_k-f_k)y^2. \quad (12)$$

Functions f_k and ψ_k must now be expressed in terms of moments M_k^j. This is easily done using the definition for M_k^j Eq. (3). Substituting (11) into (3) we obtain

$$f_k=\frac{2N_k}{x_k}\left(2-\frac{\bar{x}_k}{x_k}\right) \quad (13a)$$

$$\psi_k=\frac{2N_k}{x_k}\left(\frac{\bar{x}_k}{x_k}-1\right). \quad (13b)$$

Alternatively, f_k and ψ_k may be expressed in terms of higher order moments such as M_k and Z_k (the second moment, or, radar reflectivity). Using Eqs. (3), (11), (B11) and (B12) we obtain

$$f'_k=\frac{N_k}{x_k}\left[2+\frac{\bar{x}_k}{x_k}-\left(\frac{\bar{x}_k}{x_k}\right)^2\right] \quad (14a)$$

$$\psi'_x=\frac{N_k}{2x_k}\left[\left(\frac{\bar{x}_k}{x_k}\right)^2+\frac{\bar{x}_k}{x_k}-2\right]. \quad (14b)$$

This will be necessary when high-order integrals (j greater than 1) of the form given by Eq. (10) must be solved. Note that the proposed approximate distribution function is positive in the interval (x_k, x_{k+1}) as long as $x_k \leqslant \bar{x}_k \leqslant x_{k+1}$. In the event that this condition does not hold (due to numerical inaccuracies), we require that

$$f_k=2\frac{N_k}{x_k};\quad \psi(k)=0,\quad \text{if}\quad \bar{x}_k<x_k \quad (15a)$$

$$f_k=0;\quad \psi(k)=2\frac{N_k}{x_k},\quad \text{if}\quad \bar{x}_k>x_{k+1}. \quad (15b)$$

This guarantees positiveness of the approximation distribution function throughout the category.

To investigate the accuracy of the linear approximation to $x^j n_k(x, t)$ we can use instead a cubic polynomial. The difference between the results obtained by these two approximations would indicate the degree of accuracy of the linear approximation. A comparison between these two approximations will be presented in section 4d. The cubic polynomial is given by

$$x^j n_k(x,t)=x_k^j f_k\left[\frac{x_{k+1}-x}{x_k}\right]\left[\frac{x-x_k}{x_{k-1}}-1\right]^2$$
$$+x_{k+1}^j\psi_k\left[\frac{x-x_k}{x_k}\right]\left[\frac{x-x_k}{x_{k-1}}-1\right]^2$$
$$+4\phi_k\left[\frac{x_{k+1}+x_k}{2}\right]^j\left[\frac{x_{k+1}-x}{x_k}\right]\left[\frac{x-x_k}{x_k}\right], \quad (16)$$

where ϕ_k is the value of $n_k(x, t)$ at $x = (x_k + x_{k+1})/2$. If f_k, ψ_k and ϕ_k are positive at all times, then Eq. (16) ensures positiveness of the function in the interval $(x_k; x_{k+1})$ at any time. f_k, ψ_k and ϕ_k can now be found in terms of the first three moments N_k, M_k and Z_k. Using (3) and (16) we get

$$f_k = \frac{6N_k}{x_k}\left[2\frac{Z_k}{N_k x_k^2} - 7\frac{\bar{x}_k}{x_k} + 6\right] \quad (17a)$$

$$\psi_k = \frac{6N_k}{x_k}\left[2\frac{Z_k}{N_k x_k^2} - 5\frac{\bar{x}_k}{x_k} + 3\right] \quad (17b)$$

$$\phi_k = \frac{6N_k}{x_k}\left[3\frac{\bar{x}_k}{x_k} - \frac{Z_k}{N_k x_k^2} - 2\right]. \quad (17c)$$

In this paper we limit ourselves to solution of the equations for N_k and M_k only. Therefore, Z_k will be found in terms of N_k and M_k using (B11) and (B12). Following this procedure and substituting into (17), we get

$$f_k = \frac{6N_k}{x_k}\left[\left[\frac{\bar{x}_k}{x_k}\right]^2 - 4\frac{\bar{x}_k}{x_k} + 4\right] \quad (18a)$$

$$\psi_k = \frac{6N_k}{x_k}\left[\left[\frac{\bar{x}_k}{x_k}\right]^2 - 2\frac{\bar{x}_k}{x_k} + 1\right] \quad (18b)$$

$$\phi_k = \frac{3N_k}{x_k}\left[3\frac{\bar{x}_k}{x_k} - \left[\frac{\bar{x}_k}{x_k}\right]^2 - 2\right]. \quad (18c)$$

When calculated in this way f_k, ψ_k and ϕ_k are positive at all times, as long as $\bar{x}_k$ lies in the interval $(x_k; x_{k+1})$. If, as a result of numerical inaccuracies, $\bar{x}_k$ lies outside of these bounds, then we require that

$$f_k = \frac{6N_k}{x_k}; \quad \psi_k = 0 \quad \text{and} \quad \psi_k = 0 \quad \text{if} \quad \bar{x}_k < x_k \quad (19a)$$

$$f_k = 0; \quad \psi_k = 6\frac{N_k}{x_k} \quad \text{and} \quad \phi_k = 0 \quad \text{if} \quad \bar{x}_k > x_{k+1}. \quad (19b)$$

The set of equations (9a, b) can now be solved using either linear or cubic polynomials. We emphasize that the approximation to the distribution function is only used in inner integrals of the form given by (10). All other integrals are expressed in terms of moments M_k^j. These are in turn expressed in terms of N_k and M_k using the relation connecting moments [Eq. (8a)].

The above method offers a novel approach to solution of the SCE and other related problems. First, the set of moment equations is closed using a relation connecting high order moments with those of lower order. With closure ensured the solution to the equations can be obtained using a two or three parameter approximation to the distribution function in integrals over incomplete categories. The distribution function chosen here is positive in the region $(x_k; x_{k+1})$. The set of equations can be solved for two or more moments of any order j (real or integer) and is not limited to solution of the SCE alone. The method is easily adaptable to other microphysical processes such as breakup and condensation/evaporation or other related problems where moment solutions are required to integrals over incomplete categories and/or where closure poses a problem.

4. Results and discussion

Tests of the above method have been carried out using three kernels, namely, the constant kernel [$K(x, y)$ = const], Golovin's kernel [$K(x, y) = C(x + y)$] and a hydrodynamic kernel. In the first two cases, comparisons are made with the analytical solution and Bleck's (1970) solution. An exponential initial distribution is used. No weighting functions are used in the case of Bleck's method. Use of weighting functions amounts to a fine tuning of the results for a specific initial distribution and kernel and should be avoided in these numerical experiments in order to preserve the generality of the discussion. The spectrum is divided into 36 categories with mass doubling every category ($p = 2$). The minimum drop size is 3.125 μm (diameter) and we use a simple forward scheme with a time increment of 10 seconds to solve Eq. (9). Empty categories (i.e., categories for which $\bar{x}_k < x_k$) are prevented from entering into coagulation with other categories (they can only acquire mass through autoconversion from lower categories).

a. The constant kernel

Figure 1a, b show the results for the case of $K(x, y) = 10^{-4}$ cm^3 s^{-1}, a liquid water content of 1 g m^{-3} and an initial number concentration of 300 cm^{-3}. After 1 hour of collection time, we see that the method proposed here follows the analytical solution very closely for both the number and mass distribution functions and alleviates the common problem of accelerated collection growth which results in the premature production of precipitation particles. Also shown in Fig. 1a is Bleck's solution which is seen to deviate from the analytical solution and tends to accelerate the process. Our method conserves both liquid water content and number concentration while Bleck's method conserves LWC only.

b. Golovin's kernel

The case of Golovin's kernel is an interesting one in that its mass dependence somewhat resembles that of the hydrodynamic kernel. The analytical solution for this kernel therefore provides the best known test of the performance of a numerical method for a given initial distribution. Figure 2a, b show the evolution of a spectrum through collection after 30 min and after 50 min for the case of $K(x, y) = 1500(x + y)$, a LWC

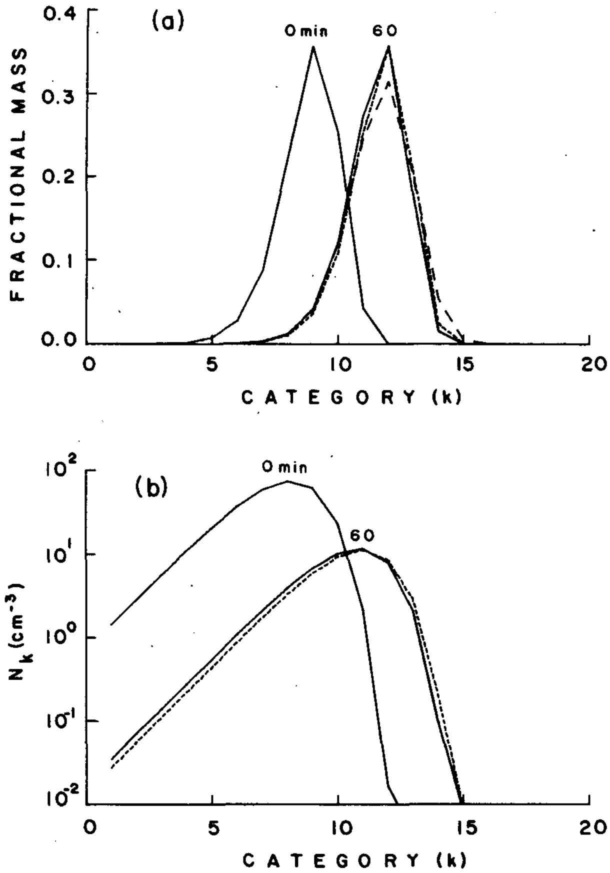

FIG. 1. A comparison of stochastic collection computations for the constant kernel [$K(x, y) = 1.10^{-4}$ cm^{-3} s^{-1}] after 60 minutes of collection for (a) fractional mass (M_k/LWC) and (b) category number concentration (N_k). The analytical solutions are represented by solid lines, Bleck's (1970) method by long dashed lines (– – –), and the proposed method by short dashed lines (-----). The initial exponential distribution is indicated at left by a solid line.

of 1 g m^{-3} and an initial drop concentration of 300 cm^{-3}. Once again this method provides an excellent approximation to both the category mass and number distributions. The differences between this method and Bleck's method are even more marked than those observed in the case of the constant kernel. Using Bleck's method, anomalous spreading towards the large-drop end of the spectrum is very significant and a weighting function would be required to produce satisfactory results.

c. *The hydrodynamic kernel*

The hydrodynamic kernel may be expressed in the form:

$$K(x,y)=\left[\frac{9}{16}\pi\right]^{1/3}[x^{1/3}+y^{1/3}]^2E(x,y)|V_x-V_y|, \quad (20)$$

where, $E(x, y)$ is the collection efficiency (approximated by a method suggested by Long, 1974) and V_x and V_y, the terminal fall velocities of drops with mass x and y (Gunn and Kinzer, 1949 and Beard, 1976). $K(x, y)$ is approximated here using a first order polynomial in each category as follows:

$$K_{k,i}(x,y)=A_{k,i}(x+y) \quad (21)$$

where,

$$A_{k,i}=\left[\frac{1}{(x_{k+1}-x_k)(x_{i+1}-x_i)}\right]\int_{x_i}^{x_{i+1}}dy \times\int_{x_k}^{x_{k+1}}\frac{K_{k,i}(x,y)}{(x+y)}dx. \quad (22)$$

The solutions to the SCE for this kernel are shown in Fig. 3. Clearly, the collection process calculated using Bleck's algorithm artificially doubles the growth of the particles as compared with the method proposed here.

From a comparison of the results for the constant,

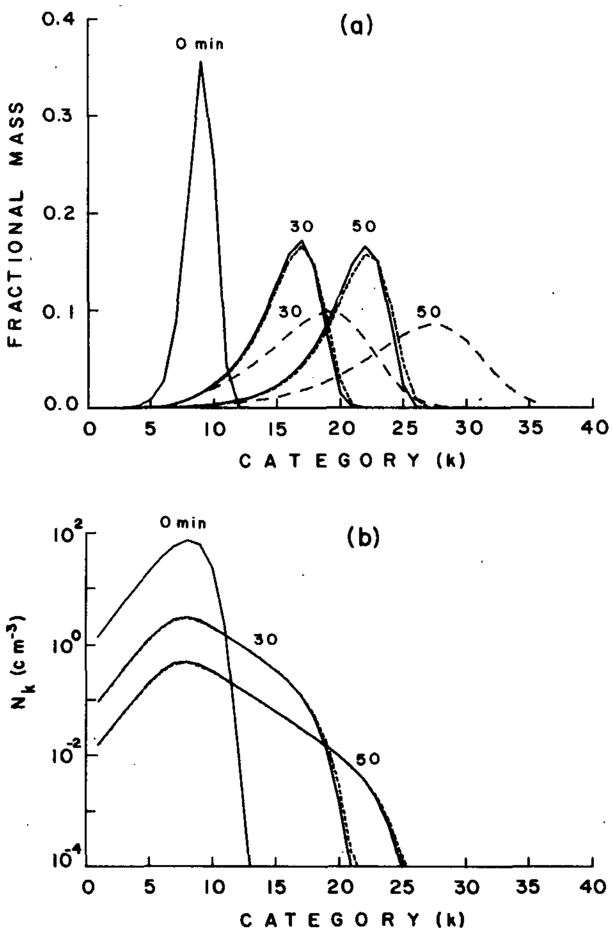

FIG. 2. Same as Fig. 1 but for Golovin's kernel ($K(x, y) = 1500(x + y)$ cm^{-3} s^{-1}). Solutions are shown for 30 min and 50 min collection time. Note the excellent fit obtained by the proposed method for both mass and number concentration and the tendency for the Bleck solution to accelerate the collection process.

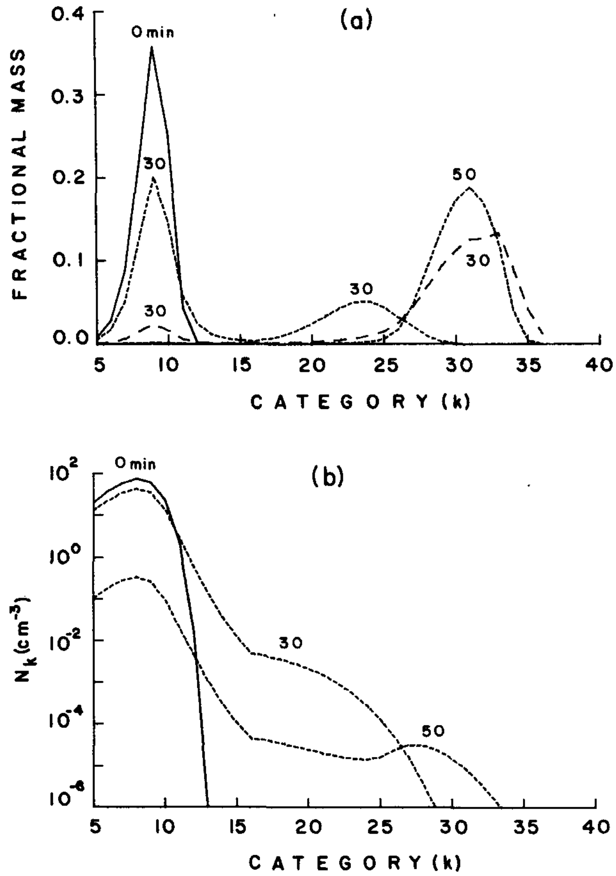

FIG. 3. As in Fig. 1 but for a "real" kernel (see Long, 1974). Evidently, the Bleck method enhances collection by a factor of about two compared with this method.

linear polynomial and hydrodynamic kernels, there seems to be a definite tendency for the accelerating effect of Bleck's method to increase with increasing mass dependence of the kernel. This seems to stem from the averaging of the distribution function in the category $[n_k(x, t)]$. The assumption of a constant value of $n_k(x, t)$ for the whole category becomes unrealistic in the case of a mass dependent kernel (especially at the large-drop end of the spectrum where category width is large) and results in an artificial forward transfer of mass. Application of weighting functions of the form x^{-n} (where n is chosen according to the kernel at hand) simply retards the process and amounts to a form of parameterization for a specific kernel and initial distribution. Use of a two moment approximation appears to alleviate the need for an additional parameter in the form of a weighting function.

While there is no way of corroborating the results obtained for a "real" kernel with an analytical solution, some indication of the validity of the solution may be obtained by (i) checking to what extent mass is conserved and, (ii) decreasing the time step and observing the convergence properties of the solution (as was done by Ochs and Yao, 1978). The method of moments was found to conserve mass to an accuracy of 0.7% (after 50 min). In addition, the solution obtained using this method converges and is stable for the range of time increments from 0.1 sec to at least 30 sec.

d. Results for the cubic polynomial approximation

The above simulations were run using the cubic polynomial approximation to the distribution function [Eq. (16)] rather than the linear function [Eq. (11)]. Use of the cubic polynomial resulted in a very slight improvement in the results for the case of the constant kernel. For Golovin's kernel it was found that the cubic polynomial actually resulted in a slight retardation of collection when a time increment of 10 seconds was used. However, use of a 1-sec increment improved the results, bringing them even closer to the analytical solution than the results presented in Fig. 2. We feel however, that this improvement does not warrant use of a cubic polynomial unless computation time is not a limiting factor.

e. Stability of the method in the presence of other microphysical processes

In a detailed cloud model other processes such as nucleation, condensation, breakup or sedimentation are simultaneously treated. In order to test the durability of this method and its suitability for inclusion into such models, it is important to ascertain whether the solution remains stable when these processes are included. The latter may introduce sudden perturbations in the size spectrum which, in turn, could produce instabilities in subsequent computations. For example, nucleation could produce a "pulse" of small droplets in the spectrum at some stage in the spectral evolution. Figure 4 shows the results obtained when 10 drops per liter are introduced into category 13, or $D = 25$ μm, for the case of the hydrodynamic kernel. It can be seen that the introduction of these particles greatly enhances the collection rate. The perturbation produced by the pulse does not affect the stability of the solution. Moreover, the method of moments clearly resolves the effect of the pulse. This is in contrast to the results obtained using Bleck's method (also shown in Fig. 4). Although Bleck's solution is stable, its response to the introduction of these particles is almost non-existent since the artificial spread of the spectrum (as illustrated in Fig. 3) obscures the effect of the perturbation. It should be noted that the above trends were also obtained when the pulse was introduced at various stages of the collection process.

f. Computation time requirements

Another attractive feature of this method is that accurate results can be obtained with modest computation time requirements. In effect computation time is

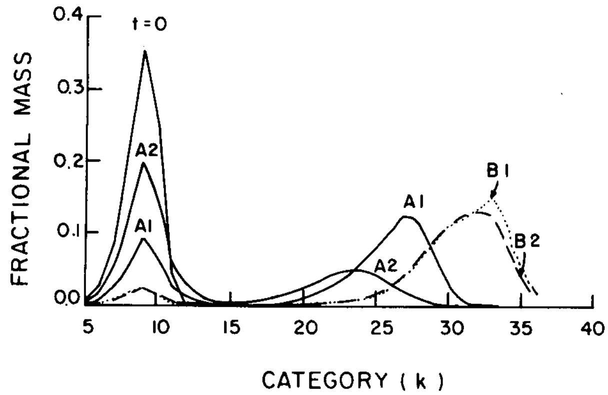

FIG. 4. An investigation of the resilience of the proposed solution to a sudden pulse in the initial spectrum for the case of the "real" kernel. Lines A1 and A2 represent, respectively, solutions for the proposed method with and without the pulse, after 30 min collection time. Lines B1 and B2 represent Bleck's solution for the same conditions. The perturbation introduced by the pulse does not affect the stability of the solutions in both the method of moments and Bleck's method. Notice, however, that the method of moments resolves the effect of the introduction of the pulse whereas in Bleck's method, the effect is obscured.

less than that required by the Bleck algorithm. This can been shown by taking into account that in order to obtain acceptable results, the Bleck algorithm would have to be modified to include about 90 categories (in the case of Golovin's kernel), and that if 90 categories were to be used, the time increment would have to be reduced somewhat (in order to maintain the present rate of collection). Even with these changes, the Bleck algorithm would still only conserve one moment, whereas the proposed method conserves two. Fifty minutes collection time (300 steps) requires 5.7 sec CPU time for Golovin's kernel and 3.0 sec for the constant kernel on the Tel Aviv University's CDC 7600 computer.

5. Summary

We have proposed an efficient accurate method for numerical solution of the SCE and other related problems. The SCE is reduced to a set of moment equations written in each category of the spectrum by an analytical version of a method proposed by Bleck (1970). We have written these equations in a form so as to make them amenable to a category by category analysis of drop formation and removal. This should assist in analyzing the evolution of natural drop size distributions. A set of equations is written for two moments (in this case, mass and number concentration) and is closed using a nondimensional parameter $\bar{\xi}_p$ which expresses high order moments in terms of two lower order moments. An approximation to the distribution function in a category is used only for integrals over an incomplete category. These integrals are expressed in terms of moments defined in a complete category. Results show that using this method, excellent approximations to the analytical solutions can be obtained for both the constant and Golovin's kernel, with full conservation of number and mass and without the use of weighting functions. The method is efficient, requiring less computation time than the Bleck algorithm. It is our belief that the proposed method will be very useful in the following areas of study:

(i) The accurate simulation of drop collection. The accuracy of this method should afford the possibility of studying the subtle effects of seeding clouds with CCN or IN on drop growth.

(ii) The simulation of other microphysical processes such as collisional breakup and condensation. The differences between this two moment scheme and Bleck's one moment scheme, as demonstrated here, suggest that simulation of the evolution of a drop spectrum with simultaneous collection and breakup may produce a rain drop spectrum different from that obtained using Bleck's method. Efforts to ascertain the degree of such differences are presently underway. The extension of this method to cloud scavenging and washout problems would have distinct advantages since the conservation of both the mass and number concentrations of drops and aerosols can be ensured.

(iii) Finally, since Eq. (5) can be solved for two or more moments (as required), this method is expected to be particularly useful for determining relations between the various moments of the spectrum (e.g., $Z - W$, $Z - \Sigma$, etc.). In addition, since more than two moments can be solved for, the implications for multiparameter remote sensing methods are far reaching.

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APPENDIX A

Reduction of the SCE to a Set of Equations for Moments in Discrete Categories

We write the SCE in the form:

$$\frac{\partial n(x,t)}{\partial t} = \int_0^{x/2} n(x-y,t)n(y,t)K(x-y,y)dy - n(x,t)\int_0^{\infty} n(y,t)K(x,y)dy, \quad \text{(A1)}$$

where $n(x, t)$ is the distribution density function and $K(x, y)$, the collection kernel. The spectrum is divided into discrete categories according to the relation $x_{k+1} = px_k$, k being the category number, x_k and x_{k+1} the upper and lower mass boundaries of category k, and p a parameter designating the category breadth. From (A1) we can obtain a set of equations for moments in categories in the form:

$$\frac{dM_k^j(t)}{dt} = \int_{x_k}^{x_{k+1}} x^j dx \int_0^{x/2} n(x-y,t)n(y,t)K(x-y,y)dy - \sum_{i=0}^{I} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k}^{x_{k+1}} x^j n_k(x,t)K_{k,i}(x,y)dx, \quad \text{(A2)}$$

where

$$M_k^j(t) = \int_{x_k}^{x_{k+1}} x^j n_k(x,t)dx$$

the jth moment of the distribution function in category k, $K_{k,i}(x, y)$—the probability of coagulation between particles in category i with those in category k, and I—the total number of spectral intervals. The first term in (A2), the gain integral, must be reduced to a form pertaining to discrete categories. The first to do this was Bleck (1970), who proposed a *graphic* method for reducing the double gain integral to a sum of double integrals in categories. We use Bleck's approach, however, we adopt an *analytical* approach to this reduction. We write the gain integral in the form:

$$\int_{x_k}^{x_{k+1}} x^j dx \int_0^{x/2} K(x-y,y)n(x-y,t)n(y,t)dy = \int_{x_k}^{x_{k+1}} x^j dx \int_0^{x_k/2} K(x-y,y)n(x-y,t)n(y,t)dy + \int_{x_k}^{x_{k+1}} x^j dx \int_{x_k/2}^{x/2} K(x-y,y)n(x-y,t)n(y,t)dy. \quad \text{(A3)}$$

Using the fact that $\int_a^b dx \int_c^d F(x,y)\,dy = \int_c^d dy \int_a^b F(x,y)dx$, and temporarily introducing a variable $z = x - y$, (A3) can be written as

$$I1 = \int_0^{x_k/2} n(y,t)dy \int_{x_k-y}^{x_k} (x+y)^j K(x,y)\,n(x,t)dx + \int_0^{x_k/2} n(y,t)dy \int_{x_k}^{x_{k+1}} (x+y)^j K(x,y)n(x,t)dx - \int_0^{x_k/2} n(y,t)dy \int_{x_{k+1}-y}^{x_{k+1}} (x+y)^j K(x,y)n(x,t)dx. \quad \text{(A4)}$$

In order for the boundaries of an integral of the form $\int_0^{x_k/2} dy \int_{x_k-y}^{x_k} F(x,y)dx$ to encompass only category $k-1$ it is necessary that $\min(x_k - y) \geqslant x_{k-1}$, or $(x_k - x_k/2) \geqslant x_{k-1}$. This will be the case if $p \geqslant 2$. In this Appendix we restrict our analysis to the case of $p = 2$ (without loss of generality). In an analogous way we can obtain algorithms for $p > 2$ or for $1 < p < 2$, but in these cases, additional integrals are added. Therefore, assuming $p = 2$, we have (from A4):

$$I1 = \sum_{i=0}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \times \int_{x_k-y}^{x_k} (x+y)^j K_{k-1,i}(x,y)n_{k-1}(x,t)dx + \sum_{i=0}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k}^{x_{k+1}} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx - \sum_{i=0}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_{k+1}-y}^{x_{k+1}} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx. \quad \text{(A5)}$$

For the transformation of the second integral in (A3), we introduce a variable $z = 2y$ and use the expression $\int_a^b dx \int_a^x F(x,y)dy = \int_a^b dy \int_y^b F(x,y)dx$. This gives

$$I2 = \int_{x_k}^{x_{k+1}} x^j dx \int_{x_k/2}^{x/2} K(x-y,y)n(x-y,t)n(y,t)dy = \frac{1}{2}\int_{x_k}^{x_{k+1}} n\left(\frac{z}{2},t\right)dz \int_z^{x_{k+1}} x^j K\left(x-\frac{z}{2},\frac{z}{2}\right) \times n\left(x-\frac{z}{2},t\right)dx. \quad \text{(A6)}$$

Substituting $p = 2$ and a new variable, $\xi = x - (z/2)$ to facilitate integration, and, using $\int_y^{x_{k+1}-y} = \int_y^{x_{k+1}} - \int_{x_{k+1}-y}^{x_{k+1}}$ and the relation $\int_{x_{k-1}}^{x_k} dy \int_y^{x_k} F(x,y)dx = \frac{1}{2}\int_{x_{k-1}}^{x_k} dy \int_{x_{k-1}}^{x_k} F(x,y)dx$, $I2$ becomes

$$I2 = \frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy \times \int_{x_{k-1}}^{x_k} (x+y)^j K_{k-1,k-1}(x,y)n_{k-1}(x,t)dx + \int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy \int_{x_k}^{x_{k+1}} (x+y)^j K_{k-1,k}(x,y)n_k(x,t)dx - \int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy \int_{x_{k+1}-y}^{x_{k+1}} (x+y)^j K_{k,k-1}(x,y)n_k(x,t)dx. \quad \text{(A7)}$$

Combining (A5) and (A7) we obtain

$$I1 + I2 = \sum_{i=0}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k-y}^{x_k} (x+y)^j K_{k-1,i}(x,y)n_{k-1}(x,t)dx + \sum_{i=0}^{k-1} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k}^{x_{k+1}} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx + \frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy \int_{x_{k-1}}^{x_k} (x+y)^j K_{k-1,k-1}(x,y)n_{k-1}(x,t)dx - \sum_{i=0}^{k-1} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_{k+1}-y}^{x_{k+1}} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx. \quad \text{(A8)}$$

Combining terms 2 and 4 in (A8) we obtain for the gain integral:

$$\int_0^{x/2} K(x-y,y)n(x-y,t)n(y,t)dy = \sum_{i=0}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy$$

$$\times \int_{x_{k-y}}^{x_k} (x+y)^j K_{k-1,i}(x,y)n_{k-1}(x,t)dx$$

$$+ \sum_{i=0}^{k-1} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k}^{x_{k+1}-y} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx$$

$$+ \frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy \int_{x_{k-1}}^{x_k} (x+y)^j K_{k-1,k-1}$$

$$\times (x,y)n_{k-1}(x,t)dx. \quad \text{(A9)}$$

Substituting (A9) for the gain integral in (A2), we have a set of equations for moments of the category distribution function:

$$\frac{dM_k^j(t)}{dt} = \sum_{i=0}^{k-1} \int_{x_i}^{x_{i+1}} n_i(y,t)dy$$

$$\times \int_{x_k}^{x_{k+1}-y} (x+y)^j K_{k,i}(x,y)n_k(x,t)dx$$

$$+ \sum_{i=1}^{k-2} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_{k-y}}^{x_k} (x+y)^j K_{k-1,i}$$

$$\times (x,y)n_{k-1}(x,t)dx + \frac{1}{2}\int_{x_{k-1}}^{x_k} n_{k-1}(y,t)dy$$

$$\times \int_{x_{k-1}}^{x_k} (x+y)^j n_{k-1}(x,t)K_{k-1,k-1}(x,y)dx$$

$$- \sum_{i=0}^{I} \int_{x_i}^{x_{i+1}} n_i(y,t)dy \int_{x_k}^{x_{k+1}} x^j n_k(x,t)K_{k,i}(x,y)dx. \quad \text{(A10)}$$

The above method is an analytical approach to the reduction of the coagulation equation to a set of moment equations in categories for the case of $p = 2$. Using this approach, similar sets of equations can be obtained for any value of p.

APPENDIX B

Relationship between Moments of the Distribution Function

We introduce a nondimensional parameter, $\xi_{p,j}$ in the form of an expression relating three contiguous moments of the distribution function $f(x)$:

$$\xi_{p,j} = \frac{\int_a^b x^{j+1}f(x)dx \cdot \int_a^b x^{j-1}f(x)dx}{\left[\int_a^b x^j f(x)dx\right]^2}$$

$$j = 1, 2, 3 \cdots, \quad p = b/a. \quad \text{(B1)}$$

Using the Schwarz inequality (e.g., see von Mises, 1964):

$$\int_a^b \rho(x)^2 g(x)dx \cdot \int_a^b \psi(x)^2 g(x)dx$$

$$\geqslant \left[\int_a^b \rho(x)\psi(x)g(x)dx\right]^2, \quad \text{(B2)}$$

where $\psi(x)$, $\rho(x)$ and $g(x) \geqslant 0$ in the interval (a, b), and assuming in (B2) that

$$\psi(x) = x^{(j+1)/2} f(x)^{1/2}, \quad \rho(x) = x^{(j-1)/2} f(x)^{1/2}$$

and, $g(x) = 1$ we have from (B1):

$$\xi_{p,j} \geqslant 1. \quad \text{(B3)}$$

We now introduce a new variable, $t = (x - a/b - a)$ where $f(x)dx = f(t)dt$. It can then easily be shown that:

$$\int_0^1 t^n f(t)dt = \frac{1}{(p-1)^n} \sum_{j=0}^{n} (-1)^j C_j^n \frac{M_{n-j}}{a^{n-j}} \quad \text{(B4)}$$

$$M_{j+1} = a^{j+1}\left[\sum_{l=0}^{j}\left[C_l^{j+1}(p-1)^l \int_0^1 t^l f(t)dt\right] + (p-1)^{j+1}\int_0^1 t^{j+1} f(t)dt\right], \quad \text{(B5)}$$

where $M_j = \int_a^b x^j f(x)dx$, is the jth moment in the spectral interval (a, b) and C_j^n, the binomial coefficients. Using (B4) and (B5) and the inequality $\int_0^1 t^{n+1} f(t)dt \leqslant \int_0^1 t^n f(t)dt$, we get:

$$M_{j+1} \leqslant \sum_{l=0}^{j-1} [C_l^{j+1} \sum_{i=0}^{l} (-1)^i C_i^l a^{j+i-l+1} M_{l-i}] + (j+p)\sum_{l=0}^{j} [(-1)^l C_l^j a^{l+1} M_{j-l}]. \quad \text{(B6)}$$

Substituting (B6) into (B1) and using (B3), we obtain, finally, a bounded inequality of the following form:

$$1 \leqslant \xi_{p,j} \leqslant \sum_{l=0}^{j-1}\left[C_l^{j+1} \sum_{i=0}^{l} (-1)^i a^{j+i-l+1} \frac{M_{l-i}M_{j-1}}{M_j^2}\right] + (j+p)\sum_{l=0}^{j} (-1)^l a^{l+1} c_l^j \frac{M_{j-l}M_{j-1}}{M_j^2}. \quad \text{(B7)}$$

Substituting $j = 1$ into (B7) we get:

$$1 \leqslant \xi_{p,1} \leqslant (p+1)\left(a\frac{N}{M}\right) - p\left(a\frac{N}{M}\right)^2, \quad \text{(B8)}$$

where N and M respectively denote the zeroth and first moments of the distribution function in interval (a, b). The right-hand side of the inequality (B8) has a maximum value at the point $N/M = (p + 1)/2ap$, equal to $(p + 1)^2/4p$. Therefore for $\xi_{p,1}$, we obtain

$$1 \leqslant \xi_p \leqslant \frac{(p+1)^2}{4p}. \quad \text{(B9)}$$

The inequality (B9) is valid for all positive distribution functions and demonstrates that the range of values of $\xi_{p,1}$ depends only on p. This expression enables us to find relationships between moments of a distribution function and to close a set of equations for moments in discrete spectral intervals. From (B9), it is clear that if $1 \leqslant p \leqslant 2$, then $\xi_{p,1}$ varies very little from the value 1. In this case, $\xi_{p,1}$ can be averaged with sufficient accuracy as follows:

$$\bar{\xi}_{p,1} = 0.5\left[1 + \frac{(p+1)^2}{4p}\right]. \quad \text{(B10)}$$

The deviation of $\xi_{p,1}$ from 1 for $p = 2, 2^{1/2}, 2^{1/3}$, is (respectively) 0.0625, 0.01524 and 0.0067. The deviation of $\xi_{p,1}$ will obviously be even smaller if we calculate this parameter according to (B8):

$$\bar{\xi}_{p,1} = 0.5\left[1 + (p+1)\left(\frac{a}{\bar{x}}\right) - p\left(\frac{a}{\bar{x}}\right)^2\right], \quad \bar{x} = \frac{M}{N}. \quad \text{(B11)}$$

Note that in order to use (B11), it is necessary that $a \leqslant \bar{x} \leqslant b$. In the event that this condition does not hold (because of inaccuracies associated with the numerical scheme), we require that $\bar{\xi}_{p,1}$ equal 1.

Using (B7), it can be shown that $\xi_{p,j+1} \leqslant \xi_{p,j}$. Therefore, for any $j \geqslant 1$, Eqs. (B8)–(B11) are still valid. Then, using (B1), (B6) and the fact that $\xi_{p,j+1} \leqslant \xi_{p,j}$ and $\xi_{p,j} \approx \bar{\xi}_{p,j}$, we get:

$$M_j = \bar{\xi}_{p,1}^{[j(j-1)]/2} \bar{x}^{j-1} M \quad j = 0, 1, 2, \cdots. \quad \text{(B12)}$$

Equation (B12) enables us to approximate any moment of order j in terms of the first and second moments of the spectrum, with accuracy depending only on the value of p. By decreasing the value of p, the required degree of accuracy can be obtained.

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