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Analytical solutions of Smoluschowski's coagulation equation

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Received 13 August 1992, in final form 25 November 1991

Abstract. It is proven that Smoluchowski's coagulation equation with a kernel, $K_{ij} \le \alpha(i+j)$ for some constant α has a unique solution which is analytical for all $t \ge 0$.

1. Introduction

The general form of Smoluchowski's coagulation equation is

$$\dot{c}_{k} = \frac{1}{2} \sum_{j=1}^{k-1} K_{j,k-j} c_{j} c_{k-j} - c_{k} \sum_{j=1}^{\infty} K_{k,j} c_{j}$$
(1)

k = 1, 2, ... One of the intriguing properties of this equation is that the solution is not necessarily analytical for all $t \ge 0$. In fact, with the kernel $K_{i,j} = ij$, it is known from the exact solution that a singularity occurs at t = 1 [1-4]. Also, even though mass conservation is apparently built into equation (1), the solutions do not necessarily have conservation of mass as one can see from the above-mentioned exact solution. On the other hand, for $K_{i,j} = 1$ and $K_{i,j} = i+j$ one finds solutions which do have conservation of mass and no singularities [5, 6].

White [7] has proved that if $K_{i,j} \leq (i+j)$ for all *i* and *j* and all the moments are bounded at t = 0 then (1) will have at least one solution valid for all $t \geq 0$ and that any solution to (1) will have bounded moments on all bounded time intervals for $t \geq 0$. This implies conservation of mass for this class of kernel. In the present article this class of kernel will be studied further and it will be proven that it has a unique solution which is analytical along the positive *t*-axis and that all the moments are analytical too, thus excluding any kind of singular behaviour.

The proof is carried through using the initial condition at t = 0:

 $c_1 = 1 \qquad c_k = 0 \qquad \text{for } k \ge 2. \tag{2}$

However, the precise form of the initial distribution is not important. The only condition used is that the moments of the initial distribution are bounded appropriately.

The important assumption is that we can find a constant α , such that $K_{i,j} \leq \alpha(i+j)$ for all *i* and *j*. This condition can always be transformed to

$$K_{i,i} \leq (i+j)/2 \qquad i \geq 1 \qquad j \geq 1 \tag{3}$$

by a scaling of time.

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2. A bound on the moments

First we notice that the form of the kinetic equations (1) implies that if all concentrations are non-negative at t=0 then the concentrations stay non-negative at all later times (t>0) [2, 8].

Next, provided a solution of equation (1) exists at time t, we define moments $\mu_k(t)$ (k=0, 1, 2, ...) by

$$\mu_{k}(t) = \sum_{j=1}^{\infty} j^{k} c_{j}(t).$$
(4)

White [7] gives in connection with the proof of his lemma 4 bounds for the moments $m_k(t)$ (k = 1, 2, 3, ...). In our notation his bounds are given by:

$$m_1(t) = \mu_1(0) \tag{5a}$$

$$m_2(t) = e^t \mu_2(0)$$
 (5b)

$$m_{k}(t) = e^{kt/2} \left\{ \frac{1}{2} \int_{0}^{t} e^{-k\tau/2} \sum_{i=1}^{k-2} {k \choose i} m_{i+1}(\tau) m_{k-i}(\tau) \, \mathrm{d}\tau + \mu_{k}(0) \right\}.$$
(5c)

We shall prove that equations (5) imply (for $k \ge 1$)

$$m_k(t) \le \frac{(2(k-1))!}{2^{k-1}(k-1)!} e^{(k-1)t} \qquad t \ge 0$$
(6)

provided (6) holds for t = 0. Clearly, for k = 1 and k = 2 inequality (6) is identical with the bounds given by (5a) and (5b), respectively, if $\mu_1(0) = \mu_2(0) = 1$. With the initial condition given by (2) all moments are 1 for t = 0, which is certainly consistent with

$$\mu_k(0) = m_k(0) \le \frac{(2(k-1))!}{2^{k-1}(k-1)!}.$$
(7)

Assuming the inequality (6) to hold for k = 1, 2, ..., n-1, equation (5c) yields for k = n

$$m_n(t) \leq e^{nt/2} \left\{ \frac{2}{n-2} \left(e^{(n/2-1)t} - 1 \right) \left(2^{-n} \sum_{i=1}^{n-2} \binom{n}{i} \frac{(2i)!}{i!} \frac{(2(n-i-1))!}{(n-i-1)!} + \frac{(2(n-1))!}{2^{n-1}(n-1)!} \right\} \right\}$$

The sum can be evaluated (see (A.4) in the appendix) and we find

$$m_n(t) \le e^{nt/2} 2^{1-n} \left\{ \frac{1}{n-2} \left(e^{(n/2-1)t} - 1 \right) \right.$$
$$\times \left(2 \frac{(2(n-1))!}{(n-2)!} - n \frac{(2(n-1))!}{(n-1)!} \right) + \frac{(2n-2)!}{(n-1)!} \right\}.$$

From this the inequality (6) is easily obtained for k = n. The inequality (6) has thus been proven by induction and we have:

Lemma 1. If the kernel satisfies (3) and the initial concentrations are non-negative and the moments satisfy (7) at t = 0 then for $k \ge 1$ a solution of (1) will necessarily satisfy

$$\mu_k(t) \leq \frac{(2(k-1))!}{2^{k-1}(k-1)!} e^{(k-1)t} \qquad t \geq 0.$$
(8)

The fact that the moments are bounded has several important consequences. First one concludes from (3) that

$$\sum_{j=1}^{\infty} c_j K_{i,j}$$

is bounded for all *i* and $t \ge 0$ and that $c_i(t)$ consequently is a continuous and differentiable function for all *i* and $t \ge 0$. Also, from (8)

$$c_i(t) \leq \frac{(2(k-1))!}{i^k 2^{k-1}(k-1)!} \exp[(k-1)t_0] \qquad 0 \leq t \leq t_0$$
(9)

valid for all $k \ge 1$. This bound with $k \ge j+2$ implies that the convergence of the partial sums for $\mu_j(t)$ is uniform for $0 \le t \le t_0$. The uniform convergence together with the continuity of the partial sums imply the continuity of $\mu_j(t)$. The bound (9) can also be used to prove the uniform convergence of the sums defining $d\mu_j(t)/dt$, which implies that $\mu_j(t)$ is a differentiable function of t.

3. Bounds on the derivatives

The purpose of this section is to establish bounds similar to (8) and (9) for the derivatives of the concentrations. Throughout the section we shall work at some definite time $t (\geq 0)$. We shall assume the concentrations to be given at this time and that the moments satisfy

$$\mu_0 \le 1 \qquad \mu_k \le 2\beta^k (2(k-1))! / (k-1)! \qquad \text{for } k \ge 1 \tag{10}$$

where β is some constant (which we in view of (8) may take to be e'/2). We write

$$a(i,0) = c_i(t) \tag{11}$$

and define formally for n > 0

$$a(i, n) = \sum_{l=0}^{n-1} {\binom{n-1}{l}} \times \left[\frac{1}{2} \sum_{j=1}^{i-1} K_{j,i-j} a(j,l) a(i-j, n-1-l) - a(i,l) \sum_{j=1}^{\infty} K_{i,j} a(j, n-1-l) \right].$$
(12)

Our aim is of course to identify a(i, n) with the *n*th derivative of c_i for all *n* and not just for n = 1 where (12) is identical to (1). In order to do this we also introduce moments $\eta(n, m)$:

$$\eta(0, m) = \mu_m$$

$$\eta(n, m) = \sum_{k=1}^{\infty} k^m |a(k, n)|.$$
(13)

The following lemma will now be established by induction on n, and thus the proof simultaneously justifies definition (12) by induction.

Lemma 2. If at some time t the moments satisfy the inequalities (10) then the numbers $\eta(n, m)$ defined by equations (11)-(13) satisfy

$$\eta(n,m) \le 2 \, 3^n \beta^{n+m} (2n+2m-2)! / (n+m-1)! \tag{14}$$

for $n \ge 0$ and $m \ge 0$, except for (n, m) = (0, 0).

Proof. For n = 0, m > 0 the inequality (14) is identical to (10). If (14) has been established for n = 0, 1, ..., n'-1 then the bound (3) on $K_{i,j}$ implies the absolute convergence of all the sums

$$\sum_{j=1}^{\infty} K_{i,j} a(j, n-1-l)$$

involved in the definition (12) of a(i, n') (i = 1, 2, ...). Furthermore, the absolute convergence of all the sums involved in the computation of $\eta(n', m')$ when (12) is substituted into (13) is also established by the boundedness of $\eta(n, m)$ for n < n' and $m \le m'+1$. It is thus clear how the inductive proof of (14) simultaneously justifies definitions (12) and (13).

If (12) is substituted into (13) and the numerical signs are moved inside the sums and (3) is used we get for $n \ge 1$

$$\eta(n,m) \leq \frac{1}{2} \sum_{k=1}^{\infty} k^m \left\{ \sum_{l=0}^{n-1} \binom{n-1}{l} \left[\frac{1}{2} k \sum_{j=1}^{k-1} |a(j,l)| |a(k-j,n-1-l)| + |a(k,l)| \sum_{j=1}^{\infty} (k+j)|a(j,n-1-l)| \right] \right\}.$$

If we rearrange the sums (which is legal because of the absolute convergence) we get

$$\eta(n,m) \leq \frac{1}{2} \sum_{l=0}^{n-1} {\binom{n-1}{l}} \left[\frac{1}{2} \sum_{j=1}^{\infty} |a(j,l)| \sum_{k=1}^{\infty} (k+j)^{m+1} |(a(k,n-1-l))| + \sum_{j=1}^{\infty} j^m |a(j,l)| \sum_{k=1}^{\infty} (k+j) |a(k,n-1-l)| \right].$$

In the last line we use $j^m < (k+j)^m$ to obtain (for $n \ge 1$)

$$\eta(n,m) \leq \frac{3}{4} \sum_{l=0}^{n-1} {\binom{n-1}{l}} \sum_{i=0}^{m+1} {\binom{m+1}{i}} \eta(l,i) \eta(n-1-l,m+1-i).$$
(15)

In the appendix it is shown that if one defines coefficients v(n, m) for $n \ge 0$, $m \ge 0$ by

$$\nu(0,0) = 1$$

$$\nu(n,m) = 2(2n+2m-2)!/(n+m-1)! \qquad ((n,m) \neq (0,0))$$
(16)

then they satisfy the recurrence relation

$$\nu(n,m) = \frac{1}{4} \sum_{l=0}^{n-1} {\binom{n-1}{l}} \sum_{i=0}^{m+1} {\binom{m+1}{i}} \nu(l,i) \nu(n-1-l,m+1-i)$$
(17)

for $n \ge 1$ and $(n, m) \ne (1, 0)$; for (n, m) = (1, 0) the right-hand side is 1 while the left side is 2. Using (17) it is easily seen by induction on n that (15) implies (14) thus concluding the proof of lemma 2.

Combining lemma 1 and lemma 2 it is seen that the right-hand side of (12) converges uniformly on bounded intervals $0 \le t \le t_0$ and that (11) and (12) thus define a(i, n) as continous functions of t. We are therefore justified in identifying a(i, n) with the nth derivative of c_i and conclude that $c_i(t)$ has continuous time-derivatives to all orders and (in view of the bound (14)) that they are bounded by

$$\left|\frac{d^{(n)}c_i(t)}{dt^n}\right| \leq \frac{3^n(2n+2k-2)!}{i^k 2^{n+k-1}(n+k-1)!} \exp[(n+k)t_0]$$
(18)

for $0 \le t \le t_0$ and all $k \ge 1$.

4. Analyticity

It is easily seen from (18) that we can define $c_i(t)$ by its Taylor expansion as an analytical function of t. To be precise we first define regions of the complex t-plane:

Definition 1.

$$A_1(r): |t-r| < e^{-r}/6 \tag{19}$$

$$A_2(r): 0 < \operatorname{Re}\{t\} < r, |\operatorname{Im}\{t\}| < \exp[-\operatorname{Re}\{t\}]/6.$$
(20)

Using Stirling's formula for large n in (14) with $\beta = e'/2$ we find

$$\eta(n,m)/n! \leq [6e^{i}]^{n}(n+m-1)^{m+3/2}\xi_{m}$$
(21)

where ξ_m is independent of *n*. If at some time $t = t_0$ the concentrations are given with moments which satisfy (8), and we define coefficients a(i, n) by equations (11) and (12) and then define functions $c_i(t)$ in $A_1(t_0)$ by

$$c_i(t) = \sum_{n=0}^{\infty} a(i, n)(t - t_0)^n / n!$$
(22)

then $c_i(t)$ satisfies (1) in $A_1(t_0)$, because of the absolute convergence of the involved sums implied by (21), and not only the concentrations, but also all the moments are analytic in $A_1(t_0)$.

With $t_0 = 0$ equation (22) defines an analytic solution of (1) for a given set of initial concentrations which satisfy (7) (for example the set given by (2)) in $A_1(0)$. Since the coefficients a(i, n) are uniquely given by (11) and (12) and an analytic function is uniquely given by its Taylor expansion there cannot be another analytic solution with the same initial concentrations. If we now choose t_1 inside $A_1(0)$ and use the values of $c_i(t_1)$ given by the expansion around t = 0 in (11) then (12) and (22) will define a solution of (1) in $A_1(t_1)$ which must be an analytic extension of the solution in $A_1(0)$. By repeated application of this procedure the solution can thus be analytically continued to $A_2(\infty)$. Since $A_1(0) A_2(\infty)$ is a simply connected region this continuation is unique.

The only remaining problem is then the possible existence of another solution which is not analytic along the whole positive *t*-axis. Normally, this type of uniqueness problem is solved by using a Lipschitz condition. But the right-hand side of (1) does not satisfy a Lipschitz condition unless we can find a constant K_0 such that $K_{i,j} \leq K_0$ for all *i* and *j* (see Melzak [9] for a proof in this case). Also, the uniqueness of the derivatives to all orders is not enough to ensure the uniqueness of the continuation. However, by (18) we also have uniform boundedness of the derivatives and that is sufficient.

To be specific, suppose that we had a second solution, $\hat{c}_i(t)$, to (1) which agreed with the analytic solution until the point $t = t_0$ (possibly $t_0 = 0$). Since the derivatives at t_0 are uniquely given by (11) and (12) then we can apply Taylor's theorem to show that for $t_0 < t' < t_1 < t_0 + \exp(-t_1)/6$

$$|c_i(t') - \hat{c}_i(t')| \le 2(3/2)^n \frac{(2n)!}{n!n!} \exp[(n+1)t_1]|t' - t_0|^n$$

where we have used (18) with k = 1 to bound the *n*th derivatives of $c_i(t)$ and $\hat{c}_i(t)$. With t_i as specified above, the right-hand side will approach zero as *n* goes to infinity. We have thus extended the uniqueness beyond t_0 . The result is summarized in the following theorem:

Theorem 3. If the kernel satisfies (3) and the initial concentrations have moments which satisfy (7) then (1) has a unique, analytic solution in $A_1(0) A_2(\infty)$. Also, all the moments are analytic functions in this region.

5. Truncated models

For a given model (defined by the kernel $K_{i,j}$, i = 1, 2, ..., j = 1, 2, ...) we define a sequence of truncated models, $K^{(N)}$ (N = 1, 2, ...):

$$K_{i,j}^{(N)} = \begin{cases} K_{i,j} & i \le N \text{ and } j \le N \\ 0 & i > N \text{ or } j > N. \end{cases}$$
(23)

This truncation was first suggested by Lushnikov and Piskunov [10]; it appears to be more natural to work with than the very similar truncation used by McLeod [8] and Leyvraz and Tschudi [2]. One advantage of the present truncation is that if the original kernel factorizes $(K_{i,j} = s_i s_j)$ then the truncation conserves this property. Another advantage is that it can be used to study the formation of a gel by considering the molecules which contains more than N monomer units as the gel fraction.

Clearly, the kernel $K^{(N)}$ satisfies (3) if the original kernal does, and all the results of the preceding sections will therefore hold for the truncated models. We shall in this section only work with the initial condition (2) in order to avoid unnecessary complications. The solution of (1) with the kernel given by (23) and the initial condition (2) is denoted $c_k^{(N)}(t)$. With this initial condition it is easy to see that the solutions to the truncated models converge to the solution of the original model in $A_1(0)$ as $N \to \infty$. It follows from the fact that the Taylor expansion for $c_k^{(N)}(t)$ at t=0 agrees with the Taylor expansion of $c_k(t)$ for the first N terms. To be precise, if $0 < \rho < 1/6$, choose M such that

$$2\sum_{n=M}^{\infty} (3\rho/2)^n \frac{(2n-2)!}{n!(n-1)!} < \varepsilon/2.$$
(24)

Then by lemma 2 if N > M

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$$\sum_{i=1}^{\infty} |c_i(t) - c_i^{(N)}(t)| < \varepsilon \qquad \text{for } |t| \le \rho$$
(25)

which proves that convergence in the l^1 -norm is uniform in closed disks around the origin of the complex t-plane: $0 \le t \le \rho$ ($\rho < 1/6$).

In order to extend the uniform convergence to cover more of the positive t-axis we shall need to include uniform convergence of the derivatives. If we sharpen (24) to

$$2\sum_{n=M}^{\infty} (3/2)^n \rho^{n-m} \frac{(2n-2)!}{(n-m)!(n-1)!} < \varepsilon/2$$
(26)

then the convergence criterium (25) can be extended to the first *m* derivatives for N > M. We now formulate what we want to prove in a lemma:

Lemma 4. Let $t_0 > 0$, $m \ge 0$ and $\varepsilon > 0$ be given and choose $\rho < \exp(-t_0)/6$. Then we

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can determine M_0 such that if $N > M_0$ and $0 \le j \le m$:

$$\sum_{i=1}^{\infty} \left| \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^{j}} c_{i}(t) - \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^{j}} c_{i}^{(N)}(t) \right| < \varepsilon \qquad \text{for } |t - t_{0}| \leq \rho.$$
(27)

Proof. The proof is doen by induction on t_0 . We assume that the lemma has already be proven with t_1 in place of t_0 , where

$$0 \le t_1 \le t_0$$
 and $6(t_0 - t_1) \exp(t_1) \le 1$ (28)

i.e. t_0 is included in one of the disks around t_1 . We choose M such that

$$2\sum_{n=M}^{\infty} (3/2)^n \exp[nt_0] \rho^{n-m} \frac{(2n-2)!}{(n-m)!(n-1)!} < \varepsilon/4$$
⁽²⁹⁾

and then $M_0 > M$ such that for $t = t_0$ and j = 0, 1, 2, ..., M-1 and $N > M_0$ we have (this is possible because of the assumptions on t_1)

$$\sum_{i=1}^{\infty} \left| \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^j} c_i(t) - \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^j} c_i^{(N)}(t) \right| < \mathrm{e}^{-\rho} \times \varepsilon/2.$$
(30)

We have for $|t - t_0| \leq \rho$

$$\sum_{i=1}^{\infty} \left| \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^{j}} c_{i}(t) - \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^{j}} c_{i}^{(N)}(t) \right| \leq \sum_{i=1}^{\infty} \sum_{k=j}^{\infty} \frac{|t-t_{0}|k-j|}{(k-j)!} \left| \frac{\mathrm{d}^{(k)}}{\mathrm{d}t^{k}} c_{i}(t_{0}) - \frac{\mathrm{d}^{(k)}}{\mathrm{d}t^{k}} c_{i}^{(N)}(t_{0}) \right|.$$

If we interchange the order of the two summations we notice that in the sum over k the terms with k < M are bounded by (30) while the terms with $k \ge M$ are bounded by (29). Also, $|t - t_0|$ is bounded by ρ and we get

$$\sum_{i=1}^{\infty} \left| \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^j} c_i(t) - \frac{\mathrm{d}^{(j)}}{\mathrm{d}t^j} c_i^{(N)}(t) \right|$$

$$\leq \sum_{k=j}^{M-1} (\rho^{k-j}/(k-j)!) \varepsilon \, \mathrm{e}^{-\rho}/2 + \sum_{k=M}^{\infty} (\rho^{k-j}/(k-j)!)$$

$$\times 4(3/2)^k \exp(kt_0)(2k-2)!/(k-1)!$$

$$\leq \varepsilon/2 + 2\varepsilon/4 = \varepsilon.$$

This concludes the extension of the lemma from t_1 to t_0 . Since the lemma has been established for $t_0 = 0$ we have proved the lemma for all finite, non-negative values of t_0 .

For the truncation introduced by McLeod [8] the convergence of the solutions of truncated models to the solution of the original model follows from the uniqueness of the solution proved in the preceding section combined with theorem 1 of Leyvraz and Tschudi [2].

6. Conclusion

The results obtained in this article are by no means surprising. The uniqueness of the solution and the convergence of the solutions of the truncated models might very well be true quite generally.

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McLeod [8] proved similar results for $|t| < v \le e^{-1}$ for a kernel which satisfies $K_{i,j} \le ij$ and initial conditions equal to (2). Melzak [9] also proved similar results valid for all positive times if the kernel is bounded by a constant $(K_{i,j} < K_0)$. Bak and Heilmann [11] recently proved the convergence of the solution of the truncated model (23) to the solution of the full model for the kernel $K_{i,j} = ij$. Kokholm [3] proved uniqueness of the known solution for the same model. It should be noticed that the two other kernels for which simple explicit solutions have been given $(K_{i,j} = 1$ and $K_{i,j} = i+j$) are covered by the present article.

Appendix

The purpose of the appendix is to derive two relations among binomial coefficients which are used in the article. We start from the Taylor expansions

$$(1-4x)^{-1/2} = \sum_{k=0}^{\infty} \frac{(2k)!}{k!k!} x^k$$
(A.1)

and

$$(1-4x)^{1/2} = 1-2\sum_{k=0}^{\infty} \frac{(2k)!}{k!(k+1)!} x^{k+1}.$$
 (A.2)

Multiplication and rearranging of the double sum yields

$$1 = \sum_{k=0}^{\infty} \frac{(2k)!}{k!k!} x^{k} - 2 \sum_{k=1}^{\infty} x^{k} \sum_{j=0}^{k-1} \frac{(2j)!}{j!(j+1)!} \frac{(2k-2j-2)!}{(k-j-1)!(k-j-1)!}$$

or

$$\sum_{i=0}^{k-1} \frac{(2k-2i-2)!(2i)!}{(k-i-1)!(k-i)!i!i!} = \frac{1}{2} \frac{(2k)!}{k!k!},$$
(A.3)

We need this in a slightly different form

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$$\sum_{i=1}^{k-1} \frac{(2k-2i-2)!(2i)!}{(k-i-1)!(k-i)!i!i!} = 2\frac{(2k-2)!}{(k-2)!k!}.$$
(A.4)

The second relation we want to derive is equation (17). From definition (16) it follows that

$$2 - (1 - 4x - 4y)^{1/2} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \nu(n, m) x^n y^m / (n!m!).$$
 (A.5)

Squaring the left-hand side of (A.5) we get

$$4[2-(1-4x-4y)^{1/2}]-3-4x-4y.$$

Squaring the right-hand side of (A.5) and rearranging the sums yields

$$\sum_{j=0}^{\infty} \frac{x^{j}}{j!} \sum_{k=0}^{\infty} \frac{y^{k}}{k!} \sum_{l=0}^{j} \binom{j}{l} \sum_{i=0}^{k} \binom{k}{i} \nu(l, i) \nu(j-l, k-i).$$

Equating equal powers of x and y in the two expressions we get for j+k > 1

$$\nu(j,k) = \frac{1}{4} \sum_{l=0}^{j} {j \choose l} \sum_{i=0}^{k} {k \choose i} \nu(l,i) \nu(j-l,k-i).$$
(A.6)

If we take j = n-1 and k = m+1 in (A.6) and use $\nu(n-1, m+1) = \nu(n, m)$, equation (17) obtains for $n \ge 1$, n+m > 1.

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