

The structure of equilibrium solutions of the one-dimensional Doi equation

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Abstract

We analyse the structure of steady state solutions of the one-dimensional Doi model for rod-like molecules. We prove that if the interaction strength parameter U is less than 4, then the constant solution is the only possible steady state solution. If U is larger than 4, then there is a new solution that corresponds to the nematic phase. All other non-constant solutions are obtained from this solution by translation. We prove further that the nematic solutions have period π instead of 2π , a property that signifies the fact the rods are symmetric, i.e. they have orientations but no directions.

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1. Introduction

The Doi model for rod-like molecules has been very successful in describing the properties of liquid crystal polymers in a solvent [3]. The basic object in the Doi model is the single molecule position-orientation distribution function. Interactions between molecules are modelled by a mean-field potential. Therefore, the Doi model can be regarded as a mean-field kinetic theory. Besides interaction with other rods, the rods are also interacting with the flow and are subject to Brownian force. If the interaction strength is sufficiently strong, compared with the Brownian force, or if the rod concentration is sufficiently high, then the system prefers to be in a nematic phase in which the rods tend to line up with each other. Otherwise the system is in an isotropic phase in which the orientation of the rods is completely random.

The mathematical structure of the Doi model is also very interesting. In the general case, the Doi model is a Fokker–Planck equation coupled with a Navier–Stokes-like equation for the hydrodynamics. The Fokker–Planck equation describes the convection, rotation and diffusion of the rods.

A basic feature of the Doi model is its ability to describe both the isotropic and nematic phases [4–7], Constantin *et al* [2] gave the first rigorous proof of the transition to the nematic

state as the intensity goes to infinity, and this is the property that we will concentrate on in this paper. We will consider the structure of steady state solutions of the one-dimensional Doi model in the absence of flow, in which case the model reduces to a non-local diffusion equation on the circle:

$$f_t = D_r[f_{\theta\theta} + (fV_\theta)_\theta], \quad t \in \mathbb{R}^+, \quad \theta \in \mathbb{R}. \quad (1.1)$$

Here $f(\theta, t)$ is the orientation (angle) distribution function, D_r is the rotational diffusivity, which, without loss of generality, will be set to 1; V is the mean-field interaction potential, the simplest of which is given by the Maier–Saupe potential [3, 8]:

$$V(f) = U \int_0^{2\pi} \sin^2(\theta - \theta') f(\theta', t) d\theta', \quad (1.2)$$

where U is a parameter that measures the interaction strength. Equations (1.1) and (1.2) are solved together with the normalization and boundary conditions:

$$\int_0^{2\pi} f(\theta, t) d\theta = 1 \quad \text{for any } t \geq 0, \quad (1.3)$$

$$f(\theta, t) = f(2\pi + \theta, t). \quad (1.4)$$

In physical terms, an isotropic phase corresponds to the case when $f = 1/2\pi$ and a nematic phase corresponds to the case when f is peaked at some particular angle.

Our main results are the following theorem.

Theorem 1.1. *If $U \leq 4$, then the only steady state solution of (1.1) is the constant solution $f(\theta) = 1/2\pi$.*

If $U > 4$, then besides the constant solution, all other steady state solutions are of the form $f(\theta) = f^(\theta + \theta_0)$, where θ_0 is arbitrary and f^* is a periodic function with period π .*

This result says that there is only one class of nematic solutions and the nematic solutions are symmetric on the circle. A typical form of f^* is shown in figure 1.

In a related work, Constantin *et al* [1, 2] gave an upper bound on the number of steady state solutions to the Doi equation with dimension up to 3. They also prove other interesting results on the dynamical behaviour of the solutions. However, in this paper we will concentrate on the structure of the one-dimensional steady state solutions.

Before ending this introduction, we mention an interesting fact regarding (1.1) and (1.2).

Define a free energy

$$A(f) = \int_0^{2\pi} \left[f(\theta) \ln f(\theta) + \frac{1}{2} f(\theta) V(f(\theta)) \right] d\theta \quad (1.5)$$

and the chemical potential μ

$$\mu = \frac{\delta A}{\delta f} = \ln f + V; \quad (1.6)$$

then (1.1) can be written as

$$f_t + (fv)_\theta = 0, \quad v = -D_r \mu_\theta, \quad (1.7)$$

which is in the usual form of Fick's law. By definition, equilibrium solutions are steady state solutions with constant chemical potential, $\mu = \text{constant}$. In this case, the solutions can be expressed in a Gibbs form:

$$f(\theta) = \frac{1}{Z} e^{-V(\theta)}. \quad (1.8)$$

This is a nonlinear equation in f since V still depends on f .

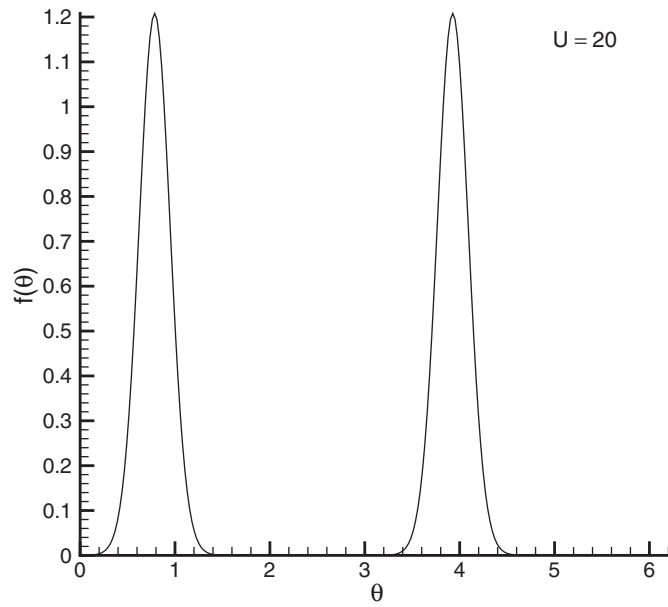


Figure 1. Numerically computed steady state function $f(\theta)$ when $U = 20$.

2. Proof of the theorem

We begin by translating the steady state equations,

$$f_{\theta\theta} + (fV_{\theta})_{\theta} = 0, \tag{2.1}$$

$$f(0) = f(2\pi), \quad f_{\theta}(0) = f_{\theta}(2\pi) \tag{2.2}$$

into a Fourier form. Writing

$$f(\theta) = \frac{1}{2\pi} + \sum_{k=1}^{\infty} [a_k \cos k\theta + b_k \sin k\theta], \tag{2.3}$$

then (2.1) changes to

$$\begin{aligned} -k^2 a_k + \frac{1}{2} k \pi U (a_2 a_{k-2} - b_2 b_{k-2} - b_2 b_{k+2} - a_2 a_{k+2}) &= 0, & k \geq 3, \\ -k^2 b_k + \frac{1}{2} k \pi U (a_2 b_{k-2} + b_2 a_{k-2} + b_2 a_{k+2} - a_2 b_{k+2}) &= 0, & k \geq 3, \\ (U - 4) a_2 + \pi U (-b_2 b_4 - a_2 a_4) &= 0, \\ (U - 4) b_2 + \pi U (b_2 a_4 - a_2 b_4) &= 0, \\ -a_1 + \frac{1}{2} \pi U (-b_2 b_3 - a_2 a_3 + b_2 b_1 + a_2 a_1) &= 0, \\ -b_1 + \frac{1}{2} \pi U (b_2 a_3 - a_2 b_3 + b_2 a_1 - a_2 b_1) &= 0. \end{aligned} \tag{2.4}$$

We first show that $a_k = 0, b_k = 0$ if k is odd. To prove this observe that if $f = f(\theta)$ is a steady state solution, then $\tilde{f}(\theta) = f(\theta + \theta_0)$ is also a steady state solution for any θ_0 . Furthermore, if

$$\tilde{f}(\theta) = \frac{1}{2\pi} + \sum_{k=1}^{\infty} [\tilde{a}_k \cos k\theta + \tilde{b}_k \sin k\theta], \tag{2.5}$$

then

$$\begin{pmatrix} \tilde{a}_k \\ \tilde{b}_k \end{pmatrix} = \begin{pmatrix} \cos(k\theta_0) & \sin(k\theta_0) \\ -\sin(k\theta_0) & \cos(k\theta_0) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}. \quad (2.6)$$

Therefore, without loss of generality we can assume that (a_2, b_2) is of the form $(-r_2, 0)$, where $r_2 = \sqrt{a_2^2 + b_2^2} \geq 0$. Then (2.4) can be written as

$$\begin{aligned} a_{k+2} &= \frac{2k}{r_2\pi U} a_k + a_{k-2}, & k \geq 3, \\ b_{k+2} &= \frac{2k}{r_2\pi U} b_k + b_{k-2}, & k \geq 3, \\ a_4 &= \frac{4-U}{r_2\pi U} a_2, & a_2 = -r_2, \\ b_4 &= \frac{4-U}{r_2\pi U} b_2, & b_2 = 0, \\ a_3 &= \left(\frac{2}{r_2\pi U} + 1 \right) a_1, \\ b_3 &= \left(\frac{2}{r_2\pi U} + 1 \right) b_1 \end{aligned} \quad (2.7)$$

and it is easy to see $b_{2m} = 0$ for all m .

Consider first the case for k odd. In this case, $(2/r_2\pi U) + 1 > 0$. If $a_1 > 0$ (< 0), we see that $a_{2m+1} > 0$ (< 0) for all m . Therefore, we have

$$a_{2m+3} > \frac{2(2m+1)}{r_2\pi U} a_{2m+1}, \quad \left(a_{2m+3} < \frac{2(2m+1)}{r_2\pi U} a_{2m+1} \right).$$

Hence $|a_{2m+1}|$ goes to infinity. The same argument can be used for b_{2m+1} . Thus, in this case, the only solution is for $a_{2m+1} = 0$, $b_{2m+1} = 0$.

As a consequence, we have shown that steady state solutions of (2.1) are periodic with period π .

Now we can express (2.4) in the form

$$\begin{aligned} a_{2m+2} &= \frac{4m}{r_2\pi U} a_{2m} + a_{2m-2}, & m > 1, \\ a_4 &= \frac{4-U}{r_2\pi U} a_2, & a_2 = -r_2. \end{aligned} \quad (2.8)$$

The recursion relation for the coefficients is described also in [2]. We define $\tilde{a}_m = a_{2m}$, now \tilde{a}_m satisfies the following recursion formula:

$$\begin{aligned} \tilde{a}_{m+1} &= \lambda m \tilde{a}_m + \tilde{a}_{m-1}, & m > 1, \\ \tilde{a}_2 &= \sigma \tilde{a}_1, & \tilde{a}_1 = -r_2, \end{aligned} \quad (2.9)$$

where $\lambda = 4/r_2\pi U$, $\sigma = (4-U)/r_2\pi U$.

Consider first the case when $U < 4$. In this case $\sigma = (4-U)/\pi r_2 U > 0$. Since $\tilde{a}_1 < 0$ and $\lambda > 0$, we see that $\tilde{a}_m < 0$ for all m . Therefore, we have

$$\tilde{a}_{m+1} < \lambda m \tilde{a}_m.$$

Hence $|\tilde{a}_m|$ goes to infinity. Thus in this case, there are no solutions with $r_2 > 0$. The only solution is for $r_2 = 0$ and this is the constant solution.

The same argument also holds for the case when $U = 4$, even though in this case $\sigma = 0$ and $\tilde{a}_2 = 0$.

Now let us consider the case when $U > 4$. In this case $\sigma < 0, \tilde{a}_1 < 0, \tilde{a}_2 > 0$.

We first show that if f is a solution to (2.1), then \tilde{a}_m has to have alternating signs. Suppose this is not the case and \tilde{a}_l and \tilde{a}_{l+1} have the same sign for some l , then it can easily be seen from the recursion relation that \tilde{a}_m also has the same sign for all $m > l + 1$. We can then use the same argument as above to show that $|\tilde{a}_m|$ goes to infinity and hence such a solution does not exist.

For solutions with alternating signs, let $c_m = (-1)^m \tilde{a}_m$, then $c_m > 0$. The recursion formula for c_m is

$$c_2 = -\sigma c_1, \quad c_{m+1} = -\lambda m c_m + c_{m-1}, \quad m \geq 2. \tag{2.10}$$

Let $F_m = c_m/c_{m-1}, m \geq 2$, then

$$F_2 = -\sigma, \quad F_{m+1} = -\lambda m + \frac{1}{F_m}, \quad m \geq 2,$$

i.e.

$$F_m = \frac{1}{\lambda m + F_{m+1}}, \quad m \geq 2.$$

We write F_2 in a compact form:

$$F_2 = [2\lambda, 3\lambda, 4\lambda, \dots] = g(\lambda). \tag{2.11}$$

Our problem now reduces to solving the equation

$$g(\lambda) = -\sigma.$$

To study the properties of $g(\lambda)$, let us define:

$$g_m(\lambda) = [2\lambda, 3\lambda, 4\lambda, \dots, m\lambda], \quad g(\lambda) = \lim_{m \rightarrow \infty} g_m(\lambda),$$

where

$$[2\lambda, 3\lambda, \dots, m\lambda] = \frac{1}{2\lambda + \frac{1}{3\lambda + \frac{1}{\dots + \frac{1}{m\lambda}}}}.$$

Lemma 2.1. *For any given $\lambda_0 > 0$, the sequence $\{g_m(\lambda)\}$ is uniformly convergent for $\lambda > \lambda_0$, and so the limiting function $\{g(\lambda)\}$ is continuous for $\lambda > 0$.*

Proof. Let

$$g_{m,\sigma}(\lambda) = [2\lambda, 3\lambda, \dots, m\lambda + \epsilon],$$

where $\epsilon > 0$. Simple calculation yields

$$|g_m(\lambda) - g_{m,\sigma}(\lambda)| < \frac{\epsilon}{(m!\lambda^{m-1})^2}.$$

So $\forall p \in \mathbb{N}$

$$|g_m(\lambda) - g_{m+p}(\lambda)| < \frac{1}{(m!\lambda^{m-1})^2} \frac{1}{(m+1)\lambda}. \tag{2.12}$$

Thus, the sequence $\{g_m(\lambda)\}$ is uniformly convergent for $\lambda > \lambda_0$ and so the limiting function $\{g(\lambda)\}$ is continuous for $\lambda > 0$. \square

A picture of $g(\lambda)$ is shown in figure 2. Figure 2 suggests the following lemma.

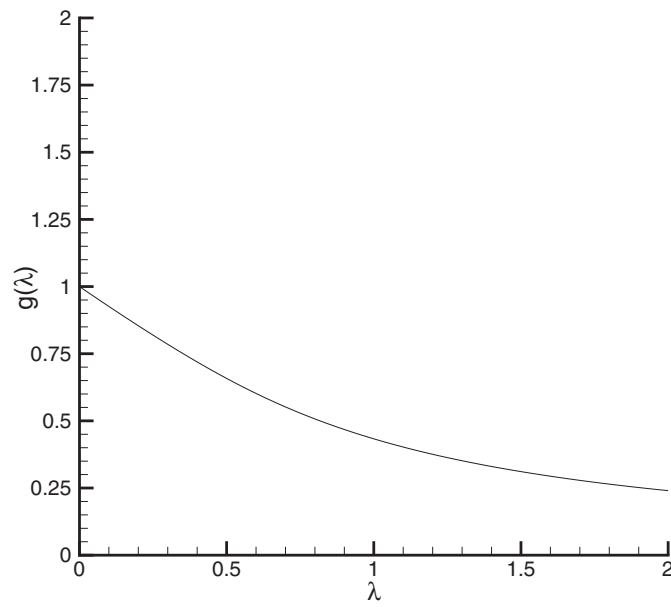


Figure 2. $g(\lambda)$.

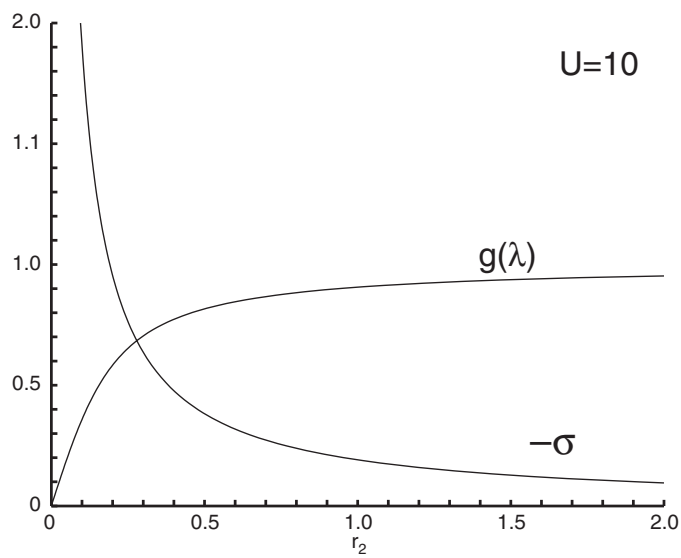


Figure 3. $g(\lambda)$ and $-\sigma$ as a function of r_2 when $U = 10$.

Lemma 2.2.

- (1) $g(\lambda)$ is a non-increasing continuous function;
- (2) $\lim_{\lambda \rightarrow 0^+} g(\lambda) > 0$;
- (3) $\lim_{\lambda \rightarrow \infty} g(\lambda) = 0$.

A rigorous proof of these properties can be found in the appendix. We now prove (see figure 3)

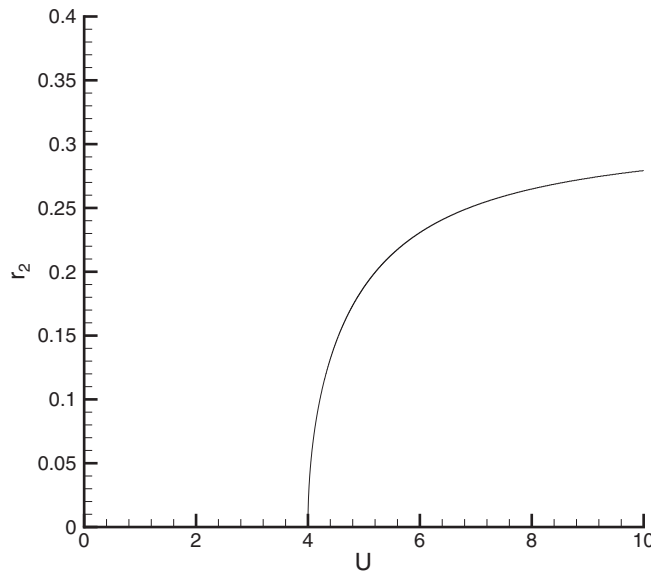


Figure 4. The figure of $r_2(U)$.

Lemma 2.3. *For any given $U > 4$, there is a unique $r_2 > 0$ such that $g(\lambda) = -\sigma$.*

Proof. For any given $U > 4$, from lemma 2.2 $g(\lambda)$ is a non-decreasing continuous function of r_2 . It is obvious that the right-hand side is a strictly decreasing continuous function of r_2 . Furthermore, when r_2 varies from 0 to ∞ , the left-hand side varies from 0 to a positive constant and the right-hand side varies from $+\infty$ to 0. Hence, there is a unique solution to $g(\lambda) = -\sigma$. \square

Denote this particular value of r_2 by $r_2 = r_2(U)$. A figure of r_2 is shown in figure 4. To prove that the Fourier series converges in this case, observe that we always have

$$F_m \leq \frac{1}{\lambda m}.$$

This implies that

$$F_m \leq \frac{1}{2}$$

if m is sufficiently large. Therefore, \tilde{a}_m decreases faster than exponential. Hence, the Fourier series must converge to an analytic function.

So far we have identified a unique value of $r_2 = r_2(U)$ for the steady state solutions of the Doi equation. We next consider how these solutions are related to each other.

Lemma 2.4. *Let f and \tilde{f} be two solutions of (2.1). Then there exists a θ_0 such that*

$$\tilde{f}(\theta) = f(\theta + \theta_0)$$

for all θ .

Proof. Let $\{a_k, b_k\}$ and $\{\tilde{a}_k, \tilde{b}_k\}$ be the Fourier coefficients of f and \tilde{f} , respectively. From the argument above, we must have

$$a_2^2 + b_2^2 = \tilde{a}_2^2 + \tilde{b}_2^2.$$

Therefore, there exists a θ_0 such that

$$\begin{pmatrix} \tilde{a}_k \\ \tilde{b}_k \end{pmatrix} = \begin{pmatrix} \cos(2\theta_0) & \sin(2\theta_0) \\ -\sin(2\theta_0) & \cos(2\theta_0) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}. \quad (2.13)$$

Using (2.4) for $k = 2m$, we have

$$\begin{pmatrix} \tilde{a}_{2m} \\ \tilde{b}_{2m} \end{pmatrix} = \begin{pmatrix} \cos(2m\theta_0) & \sin(2m\theta_0) \\ -\sin(2m\theta_0) & \cos(2m\theta_0) \end{pmatrix} \begin{pmatrix} a_{2m} \\ b_{2m} \end{pmatrix} \quad (2.14)$$

for all m . Since we already know that $a_k = 0$, $b_k = 0$ and $\tilde{a}_k = 0$, $\tilde{b}_k = 0$ if k is odd, we thus conclude that

$$\tilde{f}(\theta) = f(\theta + \theta_0). \quad \square$$

3. Conclusion

In this paper, we have completely classified the steady state solutions of the one-dimensional Doi equation. We have shown that there are only isotropic solutions for $U \leq 4$ and there is only one class of nematic solutions for $U > 4$. We further prove that the nematic solutions are symmetric when considered on the circle. This is the mathematical statement that the director fields in nematic liquid crystals do not really have directions, i.e. \mathbf{n} is equivalent to $-\mathbf{n}$.

Extending these results to the sphere seems to be of considerable challenge. There one expects the nematic solutions to be axisymmetric. But a proof of this statement is yet to be found.

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Appendix. Proof of the properties of $g(\lambda)$

Let

$$G_n(\lambda) = 2\lambda + [3\lambda, \dots, (n+2)\lambda] \triangleq \frac{P_n(\lambda)}{Q_n(\lambda)}, \quad (A.1)$$

where $P_n(\lambda)$ and $Q_n(\lambda)$ are polynomials of λ with integer coefficients. We will prove $g(\lambda)$ is a non-increasing function. Since $G_{2m}(\lambda)$ converge to $G(\lambda) = \lim_{m \rightarrow \infty} G_{2m}(\lambda)$ uniformly and $g(\lambda)$ is the inverse of $G(\lambda)$, it is sufficient to prove $G_{2m}(\lambda)$ is a strictly increasing function of λ .

It can be easily verified that $P_n(\lambda)$ and $Q_n(\lambda)$ satisfy the following recursion relation ($n \geq 1$):

$$P_n(\lambda) = (n+2)\lambda P_{n-1} + P_{n-2}, \quad Q_n(\lambda) = (n+2)\lambda Q_{n-1} + Q_{n-2}, \quad (A.2)$$

where $P_{-2} = 0$, $P_{-1} = 1$, $Q_{-2} = 1$, $Q_{-1} = 0$.

Lemma A.1. *Let*

$$A_n(\lambda) = P'_n(\lambda)Q_n(\lambda) - P_n(\lambda)Q'_n(\lambda), \quad (A.3)$$

$$B_n(\lambda) = P'_{n-1}(\lambda)Q_n(\lambda) - P_n(\lambda)Q'_{n-1}(\lambda). \quad (A.4)$$

Then

$$A_n(\lambda) = (n + 2)(-1)^n + A_n$$

From (A.9) and (A.10), we get, respectively,

$$(2k+4)\alpha_{2k+1} - (2k+3)\alpha_{2k} = 3k^2 + 9k + 6, \quad (\text{A.14})$$

$$e_k - e_{k-1} = 3k^2 + 9k + 6. \quad (\text{A.15})$$

Therefore, (A.13) and (A.12) follow.

From (A.5) of lemma A.1, the induction assumption and (A.12), we have

$$A_{2k+2} \geq (2k+4)(2k+4)!\lambda^{4k+4} + (2k+4) + \alpha_{2k} + (2k+4)\lambda^2(-\beta_{2k+2} + \beta_{2k+1}). \quad (\text{A.16})$$

From (A.9), we have

$$\alpha_n = \alpha_{n-2} + (n+2). \quad (\text{A.17})$$

This implies

$$\alpha_{2k+2} \leq (2k+4) + \alpha_{2k}. \quad (\text{A.18})$$

Thus, from (A.16), (A.18) and (A.10) we obtain

$$A_{2k+2} \geq (2k+4)!\lambda^{4k+4} + \alpha_{2k+2}. \quad (\text{A.19})$$

From (A.6) of lemma A.1, the induction assumption and (A.19), we have

$$B_{2k+3} \geq (2k+5)!\lambda^{4k+5} + (2k+5)\lambda\alpha_{2k+2} - (2k+4)\lambda\alpha_{2k+1} + \beta_{2k+1}\lambda. \quad (\text{A.20})$$

Therefore, we have

$$B_{2k+3} \geq \{(2k+5)!\lambda^{4k+4} + \beta_{2k+3}\}\lambda \quad (\text{A.21})$$

if we prove

$$e_{k+1} \leq e_k + (2k+5)\alpha_{2k+2} - (2k+4)\alpha_{2k+1}. \quad (\text{A.22})$$

From (A.9) and (A.10), we have

$$(2k+5)\alpha_{2k+2} - (2k+4)\alpha_{2k+1} = 3(k+1)^2 + 9(k+1) + 6, \quad (\text{A.23})$$

$$e_{k+1} - e_k = 3(k+1)^2 + 9(k+1) + 6. \quad (\text{A.24})$$

Hence, (A.22) and (A.21) follow.

Similarly, from (A.5) of lemma A.1, the induction assumption, (A.12) and (A.21), we have

$$A_{2k+3} \geq (2k+5)(2k+5)!\lambda^{4k+6} - (2k+5) - \alpha_{2k+1} + (2k+5)\lambda^2(\beta_{2k+3} - \beta_{2k+2}). \quad (\text{A.25})$$

To prove

$$A_{2k+3} \geq (2k+5)!\lambda^{4k+6} - \alpha_{2k+3} \quad (\text{A.26})$$

it suffices to prove

$$\alpha_{2k+3} \geq \alpha_{2k+1} + (2k+5). \quad (\text{A.27})$$

Equation (A.27) is obviously true according to (A.17) for $n = 2k+3$. Thus, (A.26) is true.

In summary, (A.7) and (A.8) are also true for the cases $n = 2k+2$ and $n = 2k+3$. We have completed the proof of this lemma. \square

Now we can easily show that $G_{2m}(\lambda)$ is a strictly increasing function of λ since the derivative

$$\begin{aligned} G'_{2m}(\lambda) &= \frac{P'_{2m}Q_{2m} - P_{2m}Q'_{2m}}{Q_{2m}^2} \\ &= \frac{A_{2m}(\lambda)}{Q_{2m}^2} > 0. \end{aligned}$$

From the properties of $G_{2m}(\lambda)$ and lemma 2.1, lemma 2.2 follows.

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