Travelling waves of a reaction-diffusion model for the acidic nitrate-ferroin reaction

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Abstract

In this paper we consider a reaction-diffusion system which describes the acidic nitrate-ferroin reaction. The existence of travelling wave solutions for this system is investigated. Our proofs are rigorous.

Key words: reaction-diffusion system; travelling wave; acidic nitrate-ferroin reaction

1 Introduction

Travelling waves in the acidic nitrate-ferroin reaction have drawn a lot of attention for many researchers; see, for example, [1]–[4]. In this paper we study the existence of travelling waves for the following reaction-diffusion system

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \frac{\partial^2 u}{\partial x^2} - \frac{2kuv}{\alpha + u}, \\ \frac{\partial v}{\partial t} &= D_v \frac{\partial^2 v}{\partial x^2} + \frac{kuv}{\alpha + u}, \end{aligned} \tag{1}$$

which was derived in [1] to model the acidic nitrate-ferroin reaction. Here α and k are positive constants, u and v represent the concentrations of the ferroin and acidic nitrate respectively, and D_u and D_v denote the constant diffusion rates of the ferroin and acidic nitrate respectively.

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J.H. Merkin and M.A. Sadiq in [4] studied (1) together with the initial and boundary conditions

$$\begin{aligned}
&u(x,0) = u_0, -\infty < x < \infty, \\
&v(x,0) = \begin{cases} v_0 g(x), & |x| < l, \\ 0, & |x| > l, \end{cases} \\
&u \to u_0, v \to 0 \text{ as } |x| \to \infty,\ t \geq 0,
\end{aligned} \tag{2}$$

where u_0 and v_0 are constants and $g(x)$ is a continuous and differentiable function on $-l < x < l$ with a maximum value of unity.

For convenience, we make a change of variables

$$\bar{u} = \frac{u}{u_0}, \bar{v} = \frac{v}{u_0}, \bar{t} = kt \text{ and } \bar{x} = \sqrt{\frac{k}{D_v}}x.$$

After dropping the bars, the initial and boundary value problem (1)-(2) becomes the dimensionless form

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \delta\frac{\partial^2 u}{\partial x^2} - \frac{2uv}{\beta + u}, \\
\frac{\partial v}{\partial t} &= \frac{\partial^2 v}{\partial x^2} + \frac{uv}{\beta + u},
\end{aligned} \tag{3}$$

together with the initial and boundary conditions

$$\begin{aligned}
&u(x,0) = 1, -\infty < x < \infty, \\
&v(x,0) = \begin{cases} v_0^* g(x), & |x| < l^*, \\ 0, & |x| > l^*, \end{cases} \\
&u \to 1, v \to 0 \text{ as } |x| \to \infty,\ t \geq 0,
\end{aligned} \tag{4}$$

where $\delta = D_u/D_v$, $\beta = \alpha/u_0$, $v_0^* = v_0/u_0$ and $l^* = \sqrt{kl^2/D_v}$.

By a travelling wave solution of (3), we mean a solution of the form

$$(u(x,t), v(x,t)) = (U(y), V(y)), \tag{5}$$

where $y = x - ct$, for some nonnegative functions U and V satisfying

$$U(-\infty) = 0, V(-\infty) = 1/2, U(+\infty) = 1, \text{ and } V(+\infty) = 0. \tag{6}$$

Here c denotes the wave speed. Substituting (5) into the system (3), we find that (U,V) solves the system

$$\begin{aligned} \delta U_{yy} + cU_y - \frac{2UV}{\beta + U} &= 0, \\ V_{yy} + cV_y + \frac{UV}{\beta + U} &= 0. \end{aligned} \tag{7}$$

J.H. Merkin and M.A. Sadiq in [4] established a necessary condition for the existence of nonnegative solutions of (6)–(7). Indeed they showed the following theorem.

Theorem 1 *There exists no nonnegative solutions of (6)–(7) if* $c < 2/\sqrt{\beta+1}$.

They also showed that the large time structure of the initial value problem (3)-(4) is a travelling wave with a constant speed. In addition, the asymptotic wave speed is exactly the minimum possible speed $2/\sqrt{\beta+1}$.

An important guestion in the study of (3) is the existence of a minimum speed travelling wave solution, the estimate of the minimum speed, as well as the range of c such that travelling wave solutions exist. For the case $\delta = 1$, it was proved in [4] that any nonnegative solution (U,V) of the problem (6)–(7) satisfies $U = 1 - 2V$. Thus the system (7) can be reduced to a single equation

$$V_{yy} + cV_y + (1 - 2V)V/(\beta + 1 - 2V).$$

Hence $A = 2V$ solves

$$\begin{aligned} &A_{yy} + cA_y + (1 - A)A/(\beta + 1 - A), \\ &A(-\infty) = 1, A(+\infty) = 0. \end{aligned}$$

Using the result in [5], we obtain the sufficient and necessary condition for the existence of nonnegative solutions of (6)–(7) in the following theorem.

Theorem 2 *Let* $\delta = 1$. *The problem (6)–(7) possesses a nonnegative solution iff* $c \geq 2/\sqrt{\beta+1}$. *For a fixed c, this solution is unique up to translation.*

Modifying the method in [6] for a different system, we shall answer the question for the case $\delta \neq 1$. Our results are stated as follows.

Theorem 3 *Let* $0 < \delta < 1$. *There exists a number* $c_{min} > 0$ *such that (6)–(7) possesses a nonnegative solution iff* $c \geq c_{min}$. *For a fixed c, this solution is unique up to translation. Moreover,* $2/\sqrt{\beta+1} \leq c_{min} \leq (2/\sqrt{\beta})[(\sqrt{2}+1)/\sqrt{\delta + 2(\sqrt{2}+1)}]$.

From Theorem 2 and Theorem 3, we know that there exists a minimun speed travelling wave solution of (3) and the set of admissible wave speed is an interval $[c_{min}, \infty)$ if $\delta \leq 1$. Unfortunately, our result is incomplete for $\delta > 1$. Indeed, we can only give a sufficient condition for the existence of nonnegative solutions of (6)–(7) in this case.

Theorem 4 *Let $\delta > 1$. There exists a nonnegative solution of (6)–(7) if $c \geq 2/\sqrt{\beta}$. For a fixed c, this solution is unique up to translation.*

Combining Theorem 1 and Theorem 4, we get a upper bound and lower bound of the minimun speed. Whether the set of admissible wave speed is $[c_{min}, \infty)$ is still unknown.

The rest of this paper is organized as follows. Priminary results required for the study of existence of travelling waves are contained in Section 2. We prove the existence of travelling wave solutions in Section 3.

2 Preliminary

From now on, we always assume that $c > 2/\sqrt{\beta + 1}$. In [4], the following properties for travelling wave solutions were proved.

Proposition 5 *A nonnegative solution (U, V) of (6)–(7) has the following properties:*
(a) $U > 0$ and $V > 0$ on $(-\infty, \infty)$.
(b) $\delta U_y + 2V_y + c(U + 2V - 1) = 0$ on $(-\infty, \infty)$.
(c) $U_y > 0$ and $V_y < 0$ on $(-\infty, \infty)$.
(d) $c = 2\int_{-\infty}^{\infty} UV/(\beta + U)dy > 0$.

Putting $W = V_y$ and using Proposition 5(b), we may write (7) as the equivalent third-order system

$$\begin{aligned} U_y &= -\frac{1}{\delta}[2W + c(U + 2V - 1)], \\ V_y &= W, \\ W_y &= -cW - \frac{UV}{\beta + U}. \end{aligned} \tag{8}$$

Thus a nonnegative solution of (6)–(7) is a solution of (8) satisfying the conditions

$$\begin{aligned} (U, V, W) &\to (0, 1/2, 0), \text{ as } y \to -\infty, \\ (U, V, W) &\to (1, 0, 0), \text{ as } y \to +\infty. \end{aligned} \tag{9}$$

Note that the system (8) has just two equilibrium points $(1, 0, 0)$ and $(0, 1/2, 0)$. To see the behavior of the integral curves about the point $(1, 0, 0)$, we linearize the system (8). The eigenvalues and associated eigenvectors are

$$
\begin{aligned}
&\lambda_1 = -c/\delta, e_{\lambda_1} = (1,0,0)^T, \\
&\lambda_2 = -(c+\sqrt{c^2-4/(\beta+1})/2, e_{\lambda_2} = (-2(c+\lambda_2), c+\delta\lambda_2, \lambda_2(c+\delta\lambda_2))^T, \\
&\lambda_3 = -(c-\sqrt{c^2-4/(\beta+1})/2, e_{\lambda_3} = (-2(c+\lambda_3), c+\delta\lambda_3, \lambda_3(c+\delta\lambda_3))^T.
\end{aligned}
$$

Since all eignvalues are negative, it follows that the point $(1, 0, 0)$ is a stable node. By a similar way, since the eigenvalues and associated eigenvectors for the linearized system about the point $(0, 1/2, 0)$ are

$$
\begin{aligned}
&\lambda_1 = -c, e_{\lambda_1} = (0,1,-c)^T, \\
&\lambda_2 = -(c+\sqrt{c^2+4\delta/\beta})/(2\delta), e_{\lambda_2} = (2\beta(c+\lambda_2), -1/\lambda_2, -1))^T, \\
&\lambda_3 = -(c-\sqrt{c^2+4\delta/\beta})/(2\delta), e_{\lambda_3} = (2\beta(c+\lambda_3), -1/\lambda_3, -1))^T,
\end{aligned}
\tag{10}
$$

it follows that the point $(0, 1/2, 0)$ is a saddle point with a two-dimensional stable manifold and a one-dimensional unstable manifold. Therefore, a non-negative solution of (6)–(7), if it exists, must go out of the unstable manifold of the point $(0, 1/2, 0)$ and finally reaches the point $(1, 0, 0)$. In addition, this solution is unique up to translation for a fixed c.

Introducing new variables $\xi = 1 - 2V$, $y = z/c$, $R = U/c^2$ and using Propositiuon 5(b), the system (7) becomes

$$
\begin{aligned}
\xi_{zz} + \xi_z &= \frac{R(1-\xi)}{\beta + c^2 R}, \\
\delta R_z &= \frac{1}{c^2}(\xi_z + \xi) - R.
\end{aligned}
$$

Setting $\xi_z = P(\xi)$, we then consider the following initial value problem

$$
\begin{aligned}
&P'P + P = \frac{R(1-\xi)}{\beta + c^2 R}, \ \xi > 0, \\
&\delta R'P = \frac{1}{c^2}(P + \xi) - R, \ \xi > 0, \\
&R(0) = 0, \ P(0) = 0, \ P > 0, \ R > 0 \text{ for } \xi > 0.
\end{aligned}
\tag{11}
$$

Following the proof of Lemma 2.2 in [6] and using (10), we can easily prove the following theorem. We omit the proof here.

Lemma 6 *For any $c > 0$ and $\delta > 0$, the initial value problem (11) has an* *unique solution on* $[0,h]$ *for some* $h>0$. *In addition,*

$$P(\xi) = \lambda\xi + \mu\xi^2 + O(\xi^3),$$
$$R(\xi) = \beta\lambda(\lambda+1)\xi + \frac{\beta\lambda}{2\lambda\delta+1}(1-\delta)\mu\xi^2 + O(\xi^3),$$

as $\xi \to 0^+$, *where* $\lambda = [\sqrt{1+4\delta/(\beta c^2)}-1]/(2\delta)$ *is the unique positive root of the equation* $\delta\lambda^2+\lambda = 1/(\beta c^2)$ *and* $\mu = -[c^2\lambda^2(1+\lambda)^2+\lambda(1+\lambda)](2\delta\lambda+1)/[6\delta\lambda^2+(3\delta+2)\lambda+1]$.

Lemma 7 *For any* $c>0$ *and* $\delta>0$, *the solution* (P,R) *of (11) can be continued to* $[0,1)$ *and* $P(1-)$ *exists. In addition, there exists a nonnegative solution (unique up to translation) to (6)–(7) iff* $P(1-)=0$.

Proof. Note that R cannot hit zero before P does as long as (P,R) exists, since otherwise, there exists $\xi_1>0$ such that $P(\xi)>0$, $R(\xi)>0$, for all $0<\xi<\xi_1$ and $R(\xi_1)=0$. Then $R'(\xi_1) = (1+\xi_1/P(\xi_1))/(\delta c^2) > 0$, a contradition. We claim that $P>0$ and $R>0$ as long as (P,R) exists and $0<\xi<1$. For contradiction, we assume that $P>0$ in $(0,\xi_2)$ and $P(\xi_2-)=0$ for some $\xi_2\in(0,1)$. Then $(P'P)(\xi_2-)\le 0$. Hence, by (11), we get $R(\xi_2-)=0$ and so $R'(\xi_2-)\le 0$. On the other hand, $\delta(R'P)(\xi_2-) = \xi_2/c^2 > 0$, a contradiction. Since P and R remain positive and bounded as long as (P,R) exists and $0<\xi<1$, the solution (P,R) can be continued to $[0,1)$.

By Lemma 6, $R'(0) = \beta\lambda(\lambda+1) > 0$. Thus, by continuity, $R'>0$ near $\xi=0$. Set $\phi(\xi) = (P+\xi)/c^2 - R$. Then $\phi = \delta R'P > 0$ near $\xi=0$ and $\phi' + 1/(\delta P)\phi = R(1-\xi)/[c^2P(\beta+c^2R)] > 0$ on $(0,1)$. So we can easily deduce that $\phi>0$ on $(0,1)$. Hence $R'>0$ on $[0,1)$. Since $(P+\xi)' = P'+1 = R(1-\xi)/[P(\beta+c^2R)] > 0$, for all $0<\xi<1$, the function $P+\xi$ is increasing on $(0,1)$. Hence $\lim_{\xi\to 1^-}(P+\xi)$ exists snd so $P(1-)$ exists. Now, there are two cases: $P(1-)=0$ or $P(1-)>0$.

Suppose $P(1-)=0$. To show the existence of nonnegative solutions to (6)–(7), it suffices to show that $R(1-)=1/c^2$ (i.e. $U\to 1$ and $V\to 0$ as $\xi\to 1-$). Since $P+\xi$ is increasing on $(0,1)$, we have $P(\xi)+\xi < P(1-)+1 = 1$ on $[0,1)$ and so $P(\xi) < 1-\xi$ on $[0,1)$. Therefore,

$$R(1-) = \int_0^1 \frac{1}{\delta P}[\frac{(P+\xi)}{c^2} - R]d\xi \ge \frac{1}{\delta c^2}\int_0^1 \frac{1-c^2R}{1-\xi} - 1d\xi. \qquad (12)$$

Since $\phi(1-)\ge 0$, it follows that $R(1-)\le 1/c^2$. Together with the fact that R is increasing on $[0,1)$, we get

$$R(\xi) < R(1-) \le 1/c^2 \quad \forall \xi\in[0,1). \qquad (13)$$

Combinining (12) and (13), we can deduce that $R(1-) = 1/c^2$. Transfering back to the original variables, we get a nonnegative solution to (6)–(7).

Suppose $P(1-) > 0$. Then the solution (P, R) can be continued beyond $\xi = 1$. Since $V < 0$ when $\xi > 1$, we conclude that there exists no nonnegative solutions to (6)–(7). $\square$

Lemma 8 *(i) For* $0 < \delta < 1$, $R > \xi/c^2$, *for all* $\xi \in (0, 1)$.
(ii) For $\delta > 1$, $R < \xi/c^2$, *for all* $\xi \in (0, 1)$.

Proof. Since the proofs of (i) and (ii) are similar, we shall only prove (i). Suppose $0 < \delta < 1$. By Lemma 6, we get

$$R - \frac{\xi}{c^2} = [\beta\lambda(\lambda + 1) - \frac{1}{c^2}]\xi + O(\xi^2) = \beta(1 - \delta)\lambda^2\xi + O(\xi^2) > 0,$$

if $\xi > 0$ is sufficiently small. In addition, for all $0 < \xi < 1$, we have

$$\begin{aligned}
\delta(R - \frac{\xi}{c^2})'P &= \delta R'P - \frac{\delta}{c^2}P \\
&= \frac{1}{c^2}(P + \xi) - R - \frac{\delta}{c^2}P \\
&= \frac{1 - \delta}{c^2}P + \frac{\xi}{c^2} - R \\
&> -(R - \frac{\xi}{c^2}).
\end{aligned}$$

Therefore we can easily deduce that $R - \xi/c^2 > 0$ for all $\xi \in (0, 1)$. $\square$

3 The existence of travelling wave solutions

For the case $0 < \delta < 1$, we shall give a sufficient condition for the existence of travelling solutions in the following lemma.

Lemma 9 *Let* $0 < \delta < 1$. *There exists a nonnegative solution to (6)–(7) if* $c > (2/\sqrt{\beta})[(\sqrt{2} + 1)/\sqrt{\delta + 2(\sqrt{2} + 1)}]$.

Proof. By lemma 6, we know that $P(\xi) < \lambda\xi$ and $R(\xi) < \beta\lambda(\lambda + 1)\xi$ if ξ is sufficiently small. Thus, Setting $B = \sup\{\eta \in (0, 1) \mid P(\xi) < \lambda\xi \text{ and } R(\xi) < \beta\lambda(\lambda + 1)\xi, \forall\xi \in (0, \eta)\}$, we obtain $B > 0$. We will show that $B = 1$. For contradiction, we assume that $0 < B < 1$. Then either $P(B) = \lambda B$ or $R(B) = \beta\lambda(\lambda + 1)B$. Since

$$\begin{aligned}\delta P[R-\beta\lambda(\lambda+1)\xi]' &= \delta R'P - \delta\beta\lambda(\lambda+1)P\\ &= \frac{1}{c^2}(P+\xi) - R - \delta\beta\lambda(\lambda+1)P\\ &= \beta(\delta\lambda^2+\lambda)(P+\xi) - R - \delta\beta\lambda(\lambda+1)P\\ &= [\beta(1-\delta)\lambda](P-\lambda\xi) - [R-\beta\lambda(\lambda+1)\xi]\\ &\le -[R-\beta\lambda(\lambda+1)\xi],\ \forall\xi\in(0,B],\end{aligned}$$

and

$$\begin{aligned}(P-\lambda\xi)'P &= P'P-\lambda P\\ &= \frac{R(1-\xi)}{\beta+c^2R} - (\lambda+1)P\\ &= -(\lambda+1)(P-\lambda\xi) + \frac{R(1-\xi)}{\beta+c^2R} - \lambda(\lambda+1)\xi\\ &< -(\lambda+1)(P-\lambda\xi),\ \forall\xi\in(0,B],\end{aligned}$$

we can easily obtain that $P(\xi) < \lambda\xi$ and $R(\xi) < \beta\lambda(\lambda+1)\xi$ on $(0,B]$. In particular, $P(B) < \lambda B$ and $R(B) < \beta\lambda(\lambda+1)B$, a contradiction. Hence $P(\xi) < \lambda\xi$ and $R(\xi) < \beta\lambda(\lambda+1)\xi$ on $(0,1)$.

Now suppose $c > (2/\sqrt{\beta})[(\sqrt{2}+1)/\sqrt{\delta+2(\sqrt{2}+1)}]$. Then we have $\lambda(\lambda+1) < 1/4$. Thus if we choose $\hat{k}$ such that $\lambda(\lambda+1) < \hat{k} < 1/4$ then

$$P'P+P < \frac{\beta\lambda(\lambda+1)\xi(1-\xi)}{\beta+c^2R} < \lambda(\lambda+1)\xi(1-\xi) < \hat{k}\xi(1-\xi), 0<\xi<1.$$

Let $Q(\xi)$ be the unique solution of

$$\begin{aligned}&QQ'+Q=\hat{k}\xi(1-\xi),\\ &Q(0)=0,\ Q>0 \text{ on } (0,1).\end{aligned}$$

Then $Q(\xi) = \gamma\xi + O(\xi^2)$, as $\xi\to 0+$, where γ is the unique positive root of $\gamma^2+\gamma=\hat{k}$. It is easy to see that $\gamma>\lambda$. Thus $P<Q$ near $\xi=0$. Hence it follows from comparison principle that $P\le Q$ on $[0,1)$. Using Lemma 2.1 of [6], we have $Q(1-)=0$. Hence we conclude that $P(1-)=0$. By Lemma 7, there exists a nonnegative solution to (6)–(7). □

Proof of Theorem 3. By using continuous dependence, we can see that the set of admissible speed is closed. For each $i=1,2$, let (P_i,R_i) be the solution of (11) on $[0,1)$ with $c=c_i$, where $c_1>c_2>0$. To show the existence of c_{min}, it suffices to show that $P_1(1-)=0$ if $P_2(1-)=0$.

Now, we suppose $P_2(1-)=0$. Let λ_i be the positive root of $\delta\lambda^2+\lambda=1/(\beta c_i^2)$ for each $i=1,2$. Then $\lambda_1<\lambda_2$. Hence, by Lemma 6, $P_1(\xi)<P_2(\xi)$ and

$R_1(\xi) < R_2(\xi)$ for sufficiently small ξ. Set $U_i = c_i^2 R_i$, for each $i = 1, 2$. Then, by Lemma 6, we have

$$\begin{aligned} U_1 - U_2 &= c_1^2 R_1 - c_2^2 R_2 \\ &= [c_1^2 \beta\lambda_1(\lambda_1+1) - c_2^2\beta\lambda_2(\lambda_2+1)]\xi + O(\xi^2) \\ &= \frac{(1-\delta)(\lambda_1-\lambda_2)}{(\delta\lambda_1+1)(\delta\lambda_2+1)}\xi + O(\xi^2) < 0, \end{aligned}$$

if ξ is sufficiently small. We claim that $P_1 < P_2$ on $(0,1)$. For contradiction, we suppose $\eta^* = \sup\{\eta > 0 \mid P_1 < P_2 \text{ in } (0,\eta)\} < 1$. So $P_1(\eta^*) = P_2(\eta^*) > 0$. Now, we claim that $R_1 < R_2$ in $(0,\eta^*]$. For contradiction, we suppose there exists $\xi^* \in (0,\eta^*]$ such that $R_1(\xi^*) = R_2(\xi^*)$. Then $U_1 > U_2$ at $\xi = \xi^*$. Recall that $U_1 < U_2$ if ξ is small. Hence, there exists $\xi_* \in (0,\xi^*)$ such that $U_1 = U_2$ and $(U_1 - U_2)' \geq 0$ at $\xi = \xi_*$. On the other hand, at $\xi = \xi_*$,

$$\begin{aligned} \delta(U_1 - U_2)' &= (\frac{\xi_*}{P_1} - \frac{U_1}{P_1}) - (\frac{\xi_*}{P_2} - \frac{U_2}{P_2}) \\ &= \xi_*(\frac{1}{P_1} - \frac{1}{P_2}) - U_1(\frac{1}{P_1} - \frac{1}{P_2}) \\ &= (\xi_* - U_1)(\frac{1}{P_1} - \frac{1}{P_2}) \\ &= (\xi_* - c_1^2 R_1(\xi_*))(\frac{1}{P_1} - \frac{1}{P_2}). \end{aligned}$$

Hence it follows from Lemma 8(i) that $\delta(U_1 - U_2)' < 0$, a contradiction. For $0 < \xi \leq \eta^*$,

$$\begin{aligned} \frac{1}{2}(P_1^2 - P_2^2)' &= P_1P_1' - P_2P_2' \\ &= -P_1 + \frac{R_1(1-\xi)}{\beta + c_1^2 R_1} + P_2 - \frac{R_2(1-\xi)}{\beta + c_2^2 R_2} \\ &= -(P_1 - P_2) + \frac{(1-\xi)[\beta(R_1 - R_2) + (c_1^2 - c_2^2)R_1R_2]}{(\beta + c_1^2 R_1)(\beta + c_2^2 R_2)} \\ &< -(P_1 - P_2) \\ &= -\frac{P_1^2 - P_2^2}{P_1 + P_2}. \end{aligned}$$

Since $P_1 < P_2$ for small ξ, we conclude that $P_1 < P_2$ on $(0,\eta^*]$. In particular, $P_1(\eta^*) < P_2(\eta^*)$, a contradiction. Thus $P_1(1-) \leq P_2(1-) = 0$. Hence $P_1(1-) = 0$.

Finally, by applying Theorem 1 and Lemma 9, we can get the estimate of c_{min}. □

Proof of Theorem 4. By Lemma 8,

$$PP' + P < \xi(1-\xi)/(\beta c^2) \leq \hat{k}\xi(1-\xi),$$

if we choose $\hat{k}$ such that $1/(\beta c^2) \leq \hat{k} \leq 1/4$. Arguing as the proof of Lemma 9, we get the proof. $\square$

Acknowledgements

This work was partially supported by National Science Council of the Republic of China under the contract NSC 96-2115-M-004-002. The author thanks professor Je-Chiang Tsai for many helpful comments.

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