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ZEROS OF A CROSS-PRODUCT OF THE COULOMB WAVE AND TRICOMI HYPERGEOMETRIC FUNCTIONS

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Dedicated to Prof. Péter T. Nagy on the occasion of his 70th birthday

Abstract. Motivated by a problem on conditions for the existence of clines in genetics, we show that the positive zeros of a cross-product of the regular Coulomb wave function and the Tricomi hypergeometric function are increasing with respect to one of the parameters. In particular, this implies that the eigenvalues of a certain boundary value problem are increasing with the dimension.

1. Introduction

In his study about the existence of clines in genetics, Nagylaki [5] considered a partial differential equation in space and time satisfied by the gene frequency in a monoecious population distributed continuously over an arbitrary habitat. He showed that this partial differential equation reduces to the simplest multidimensional generalization of the classical Fisher-Haldane cline model, and investigated the efficacy of migration and selection in maintaining genetic variability at equilibrium in this model by deducing conditions for the existence of clines in various circumstances. The boundary value problem considered by Nagylaki reads as follows

$$\Delta p+\lambda^2 g(r)p=0, \tag{1.1}$$

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where $p'(0)=0$ and $p(\infty)<\infty$, Δp is the n-dimensional Laplacian, r is the distance from the origin of an n-dimensional vector x, and

$$g(r)=\begin{cases} 1, & r\in[0,1],\\ -\alpha^2, & r>1.\end{cases}$$

Nagylaki [5] conjectured that for each fixed $\alpha>0$ the smallest positive eigenvalues of the above boundary value problem increase with the dimension. Motivated by Nagylaki's investigation, Ismail and Muldoon [4] considered the radial part of the boundary value problem (1.1), that is,

$$-\left(ry'(r)\right)'+\nu^2r^{-1}y(r)=\lambda^2rg(r)y(r), \tag{1.2}$$

where $p'(0)=0$, $p(\infty)<\infty$, $y(r)=r^{\nu}p(r)$ and $\nu=n/2-1$, and they showed that the positive eigenvalues of (1.2) are the positive zeros of fixed rank of the cross-product

$$J_{\nu+1}(r)K_{\nu}(\alpha r)-\alpha K_{\nu+1}(\alpha r)J_{\nu}(r),$$

where J_ν is the Bessel function of the first kind, while K_ν stands for the modified Bessel function of the second kind. Moreover, motivated by Askey's claim, Ismail and Muldoon [4] proved that the positive zeros of the cross-product

$$J_{\nu+\beta}(r)K_{\nu}(\alpha r)-\alpha^{\beta}K_{\nu+\beta}(\alpha r)J_{\nu}(r)$$

are increasing with respect to ν on $[-\beta/2,\infty)$, where $\beta\in(0,1]$. Thus, it is clear that Nagylaki's conjecture follows from the case $\beta=1$ of the above result. In [4], the authors actually stated more: they showed that the expression αr in the above affirmation can be changed to any strictly increasing differentiable function on $(0,\infty)$ and α^β can be replaced by an arbitrary positive constant. Motivated by the importance of the boundary value problem (1.1) and its radial part (1.2) in the existence of clines, and following the suggestion of Ismail, our aim is to show that Nagylaki's claim about the positive eigenvalues will be also true in a more general setting, we replace the Bessel function of the first kind by the regular Coulomb wave function, and the modified Bessel function of the second kind by the Tricomi hypergeometric function of the second kind. This is actually a generalization of the problem considered by Nagylaki. For more details on the special functions appearing in this paper we refer to [3, Chapter 6] and [6, Chapter 10].

2. The eigenvalue problem related to Coulomb and Tricomi functions

In order to extend Nagylaki's problem we consider the boundary value problem

$$\Delta p+\varphi_{\lambda}(r)r^{-2}p=0, \tag{2.1}$$

where $p'(0)=0$ and $p(\infty)<\infty$,

$$\varphi_{\lambda}(r)=L(L-1)+\lambda^2r^2g(r)-2\eta\lambda rh(r),$$

$L = (n-1)/2$, η is a real parameter, and

$$h(r) = \begin{cases} 1, & r \in [0,1], \\ \alpha, & r > 1. \end{cases}$$

It can be shown that the radial part of the above boundary value problem (2.1) is

$$r^2 y''(r) + \left(\lambda^2 r^2 g(r) - 2\eta\lambda r h(r) - L(L+1)\right) y(r) = 0, \tag{2.2}$$

where $p'(0) = 0$, $p(\infty) < \infty$ and $y(r) = r^L p(r)$. If we suppose that $r \in (0,1]$, then we obtain

$$r^2 y''(r) + \left(\lambda^2 r^2 - 2\eta\lambda r - L(L+1)\right) y(r) = 0.$$

By using the change of variable $u = \lambda r$ (and taking $y(r) = z(u)$), this equation becomes the Coulomb wave equation

$$u^2 z''(u) + \left(u^2 - 2\eta u - L(L+1)\right) z(u) = 0.$$

Moreover, when $r > 1$, (2.2) becomes

$$r^2 y''(r) - \left(\alpha^2\lambda^2 r^2 + 2\eta\alpha\lambda r - L(L+1)\right) y(r) = 0,$$

which after the change of variable $v = \alpha\lambda r$ (and taking $y(r) = q(v)$) becomes a transformation of the Kummer confluent hypergeometric differential equation

$$v^2 q''(v) - \left(v^2 + 2\eta v + L(L+1)\right) q(v) = 0.$$

Thus, when $r \in (0,1]$ the differential equation (2.2) has as a particular solution the regular Coulomb wave function

$$y(r) = F_L(\eta, u),$$

while for $r > 1$ the equation (2.2) has the particular solution a transformation of the Tricomi hypergeometric function

$$y(r) = v^{L+1} e^{-v} \psi(L + \eta + 1, 2L + 2, 2v).$$

When $\eta = 0$ the above particular solutions reduce to

$$y(r) = \sqrt{\frac{\pi}{2u}} J_{L+\frac{1}{2}}(u) \quad \text{and} \quad y(r) = 2^{-L} \sqrt{\frac{2v}{\pi}} K_{L+\frac{1}{2}}(v),$$

which show that the boundary value problem (2.1) is a natural extension of (1.1), while (2.2) is a natural extension of (1.2).

Now, we are ready to state the main result of this paper.

Theorem 1. **a.** *The boundary value problem* (2.2) *has for its eigenvalues the zeros of the cross-product of the regular Coulomb wave and Tricomi hypergeometric functions*

$$F_L'(\eta, r) Q_L(\eta, \alpha r) - \alpha Q_L'(\eta, \alpha r) F_L(\eta, r)$$

and corresponding eigenfunctions

$$r \mapsto \Theta_L(\eta, r) = \begin{cases} Q_L(\eta, \alpha\lambda) \cdot F_L(\eta, \lambda r), & r \in (0,1], \\ F_L(\eta, \lambda) \cdot Q_L(\eta, \alpha\lambda r), & r > 1, \end{cases}$$

where

$$Q_L(\eta,r)=r^{L+1}e^{-r}\psi(L+\eta+1,2L+2,2r).$$

b. *For fixed* $\alpha>0$, $\eta\in\mathbb{R}$ *such that* $L+\eta>0$, *and* $L>-3/2$, $L\neq-1$ *if* $\eta\neq0$ *and* $L>-3/2$ *if* $\eta=0$, *the equation*

$$F_L'(\eta,r)/F_L(\eta,r)=\alpha Q_L'(\eta,\alpha r)/Q_L(\eta,\alpha r) \tag{2.3}$$

has infinitely many positive roots, which we denote in increasing order by $\lambda_{L,\eta,\alpha,n}$, $n\in\mathbb{N}$. *These zeros satisfy*

$$x_{L,\eta,n-1}<\lambda_{L,\eta,\alpha,n}<x_{L,\eta,n},$$

$n\in\{2,3,\dots\}$, *where* $x_{L,\eta,n}$ *is the nth positive zero of the Coulomb wave function* $\rho\mapsto F_L(\eta,\rho)$. *Moreover, if* $\alpha>0$, $\eta\in\mathbb{R}$ *and* $L>-1/2$, *then we have* $\lambda_{L,\eta,\alpha,1}<x_{L,\eta,1}$.

c. *For fixed* $\alpha>0$, $\eta\geq0$ *and* $n\in\mathbb{N}$ *the zeros* $\lambda_{L,\eta,\alpha,n}$ *increase with* L *on* $[0,\infty)$.

We note that since the boundary value problem (2.1) is an extension of (1.1), while (2.2) is an extension of (1.2), if we take $\eta=0$ in the above theorem, we obtain some of the main results of [4] for the case $\beta=1$.

Proof of Theorem 1. **a.** Subject to the stated boundary condition the differential equation in (2.2) has solution

$$y(r)=\begin{cases}A\cdot F_L(\eta,\lambda r), & r\in(0,1],\\ B\cdot Q_L(\eta,\alpha\lambda r), & r>1.\end{cases}$$

Since y and y' are to be continuous at $r=1$ we must have

$$A\cdot F_L(\eta,\lambda)=B\cdot Q_L(\eta,\alpha\lambda)$$

and

$$A\cdot\lambda F_L'(\eta,\lambda)=B\cdot\alpha\lambda Q_L'(\eta,\alpha\lambda),$$

and there will be a notrivial solution of this system if and only if

$$F_L'(\eta,\lambda)Q_L(\eta,\alpha\lambda)=\alpha Q_L'(\eta,\alpha\lambda)F_L(\eta,\lambda).$$

Hence we may take $A=Q_L(\eta,\alpha\lambda)$ and $B=F_L(\eta,\lambda)$. Thus, indeed the boundary value problem (2.2) has for its eigenvalues the zeros of the cross-product of the regular Coulomb wave and Tricomi hypergeometric functions, that is,

$$F_L'(\eta,r)Q_L(\eta,\alpha r)-\alpha Q_L'(\eta,\alpha r)F_L(\eta,r),$$

and corresponding eigenfunctions $r\mapsto\Theta_L(\eta,r)$.

b. The equation (2.3) is equivalent to

$$\frac{F_L'(\eta,r)}{F_L(\eta,r)}-\frac{L+1}{r}=\alpha+\frac{2\alpha\,\psi'(L+\eta+1,2l+2,2\alpha r)}{\psi(L+\eta+1,2L+2,2\alpha r)}. \tag{2.4}$$

Now, we shall use the Mittag-Leffler expansion of regular Coulomb wave function (obtained from its infinite product representation, see [1, 7, 8] for more details). Namely, since for $L > -3/2$, $L \neq -1$ if $\eta \neq 0$ and $L > -3/2$ if $\eta = 0$ we have [1, Lemma 1]

$$\frac{F_L'(\eta, r)}{F_L(\eta, r)} - \frac{L+1}{r} = \frac{\eta}{L+1} - \sum_{n\geq 1} \left(\frac{r}{x_{L,\eta,n}(x_{L,\eta,n} - r)} + \frac{r}{y_{L,\eta,n}(y_{L,\eta,n} - r)} \right),$$

the left-hand side of the equation (2.4) is decreasing on $(0, x_{L,\eta,1})$ and also on each interval $(x_{L,\eta,n}, x_{L,\eta,n+1})$, $n \in \mathbb{N}$. Here $y_{L,\eta,n}$ stands for the nth negative zero of the regular Coulomb wave function $r \mapsto F_L(\eta, r)$. When $r \searrow 0$ the left-hand side of (2.4) tends to $\eta/(L+1)$, when $r \nearrow x_{L,\eta,n}$, $n \in \mathbb{N}$ it tends to $-\infty$ and when $r \searrow x_{L,\eta,n}$, $n \in \mathbb{N}$ it tends to $+\infty$. On the other hand, according to [2, Remark 3] we know that for $a > 1$ and $c \in \mathbb{R}$ the function $r \mapsto \psi'(a, c, r)/\psi(a, c, r)$ is increasing on $(0, \infty)$. Note that this monotonicity result is in fact equivalent to a Turán-type inequality for Tricomi hypergeometric functions. Moreover, by using the recurrence relation

$$\psi'(a, c, r) = -a\psi(a+1, c+1, r),$$

the fact that $\psi(a, c, r)$ is positive for $a, c, r \in \mathbb{R}$, and the asymptotic expansion

$$\psi(a, c, r) = r^{-a}(1 + \mathcal{O}(r^{-1})) \quad \text{as} \quad r \to \infty,$$

it follows that $r \mapsto \psi'(a, c, r)/\psi(a, c, r)$ maps $(0, \infty)$ into $(-\infty, 0)$. Thus, the right-hand side of (2.4) is increasing on $(0, \infty)$ for $\alpha > 0$ and $L + \eta > 0$ and maps the interval $(0, \infty)$ into $(-\infty, \alpha)$. These show that the equation (2.4) has infinitely many positive roots, and starting from the second positive root they are certainly located between the positive zeros of the regular Coulomb wave function. Now, by using the asymptotic relation

$$\psi(a, c, r) \sim \Gamma(c-1)r^{1-c}/\Gamma(a) \quad \text{as} \quad r \to 0 \quad \text{and} \quad c > 1,$$

it follows that $\psi'(a, c, r)/\psi(a, c, r) \sim (1-c)/r$ as $r \to 0$ and $c > 1$, and thus the right-hand side of (2.4) tends to $-\infty$ as $r \to 0$ and $L > -1/2$. This shows that if $\alpha > 0$, $\eta \in \mathbb{R}$ and $L > -1/2$, then we have $\lambda_{L,\eta,\alpha,1} < x_{L,\eta,1}$.

c. We shall follow the approach considered in [4], namely, the Sturmian-type arguments and the approach of the Hellman-Feynman theorem of quantum chemistry. Since $r \mapsto \Theta_L(\eta, r)$ are eigenfunctions of the boundary value problem (2.2), we have

$$-\Theta_L''(\eta, r)\Theta_L(\eta, r) + 2\eta\lambda\frac{1}{r}h(r)\Theta_L^2(\eta, r) + L(L+1)\frac{1}{r^2}\Theta_L^2(\eta, r) = \lambda^2 g(r)\Theta_L^2(\eta, r).$$

Integrating from zero to infinity we get

$$\int_0^\infty \left(\lambda^2 g(r) - 2\eta\lambda\frac{1}{r}h(r)\right)\Theta_L^2(\eta, r)dr$$
$$= L(L+1)\int_0^\infty \frac{1}{r^2}\Theta_L^2(\eta, r)dr + \int_0^\infty \left(\Theta_L'(\eta, r)\right)^2 dr,$$

where we used integration by parts in the last integral. Since the right-hand side of the above relation is positive for $L \geq 0$, it follows that

$$\lambda^2 \int_0^\infty g(r)\Theta_L^2(\eta,r)dr \geq \lambda \int_0^\infty 2\eta\frac{1}{r}h(r)\Theta_L^2(\eta,r)dr. \tag{2.5}$$

Now, writing λ_L instead of $\lambda_{L,\eta,\alpha,n}$, multiplying the equations

$$-\Theta_L''(\eta,r) + 2\eta\lambda_L\frac{1}{r}h(r)\Theta_L(\eta,r) + L(L+1)\frac{1}{r^2}\Theta_L(\eta,r) = \lambda_L^2 g(r)\Theta_L(\eta,r),$$

$$-\Theta_M''(\eta,r)+2\eta\lambda_M\frac{1}{r}h(r)\Theta_M(\eta,r)+M(M+1)\frac{1}{r^2}\Theta_M(\eta,r) = \lambda_M^2 g(r)\Theta_M(\eta,r)$$

by $\Theta_M(\eta,r)$, $\Theta_L(\eta,r)$ respectively, subtracting and integrating between 0 and ∞ we get

$$\begin{aligned}&\left(\Theta_M'(\eta,r)\Theta_L(\eta,r) - \Theta_L'(\eta,r)\Theta_M(\eta,r)\right)\Big|_0^\infty \\ &+ (\lambda_L - \lambda_M)\int_0^\infty 2\eta\frac{1}{r}h(r)\Theta_L(\eta,r)\Theta_M(\eta,r)dr \\ &+ [L(L+1) - M(M+1))]\int_0^\infty \frac{1}{r^2}\Theta_L(\eta,r)\Theta_M(\eta,r)dr \\ &= (\lambda_L^2 - \lambda_M^2)\int_0^\infty g(r)\Theta_L(\eta,r)\Theta_M(\eta,r)dr.\end{aligned}$$

Note that the integrated term vanishes at 0 and ∞ for $L, M > 0$, and consequently dividing both parts of the above equation by $L-M$ and taking the limit $M \to L$ we obtain

$$\begin{aligned}\frac{d\lambda_L}{dL}\int_0^\infty 2\eta\frac{1}{r}h(r)\Theta_L^2(\eta,r)dr + (2L+1)\int_0^\infty \frac{1}{r^2}\Theta_L^2(\eta,r)dr \\ = \frac{d\lambda_L^2}{dL}\int_0^\infty g(r)\Theta_L^2(\eta,r)dr\end{aligned}$$

or equivalently

$$\begin{aligned}\frac{d\lambda_L}{dL}\int_0^\infty 2\eta\frac{1}{r}h(r)\Theta_L^2(\eta,r)dr + (2L+1)\int_0^\infty \frac{1}{r^2}\Theta_L^2(\eta,r)dr \\ = 2\lambda_L\frac{d\lambda_L}{dL}\int_0^\infty g(r)\Theta_L^2(\eta,r)dr.\end{aligned}$$

This implies that

$$\begin{aligned}\frac{d\lambda_L}{dL}\left(2\lambda_L\int_0^\infty g(r)\Theta_L^2(\eta,r)dr - \int_0^\infty 2\eta\frac{1}{r}h(r)\Theta_L^2(\eta,r)dr\right) \\ = (2L+1)\int_0^\infty \frac{1}{r^2}\Theta_L^2(\eta,r)dr > 0,\end{aligned}$$

which in view of (2.5) and the fact that λ_L is positive according to part **b**, yields $d\lambda_L/dL > 0$, so for fixed $\alpha > 0$ and $\eta \geq 0$ the zero λ_L is increasing with respect to L on $[0,\infty)$. □

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