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L^2-dissipativity of the linearized explicit finite-difference scheme with a kinetic regularization for 2D and 3D gas dynamics system of equations

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ABSTRACT

We study an explicit in time and symmetric in space finite-difference scheme with a kinetic regularization for the 2D and 3D gas dynamics system of equations linearized at a constant solution (with any velocity). We derive both necessary and sufficient conditions for L^2-dissipativity of the Cauchy problem for the scheme by the spectral method. The Courant number is uniformly bounded with respect to the Mach number in them.

1. Introduction

Among various numerical methods for solving gas dynamics systems of equations, see, in particular, [1,2] there are methods based on a preliminary regularization of equations, including a kinetic (or quasi-gasdynamic, QGD) regularization [3,4]. A variety of practical applications of this approach is also presented there.

In this paper, we study an explicit two-level in time and symmetric in space finite-difference scheme with such a regularization linearized at a constant solution (with arbitrary velocity). The problem of the stability analysis for schemes of this type has been known for many years. In the 2D and 3D cases and a uniform rectangular grid, we derive both necessary and sufficient conditions for the L^2-dissipativity of the solutions to the Cauchy problem for this scheme for the first time. The spectral method [5] is applied to this end. In these conditions, the Courant number is uniformly bounded with respect to the Mach number which is significant in computing super- and hypersonic flows. The similar results have previously been obtained in simpler 1D full and 2D and 3D barotropic cases [6,7].

Schemes related to other regularizations like [8] could be studied by this technique as well.

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2. L^2-dissipativity analysis

The gas dynamics system of equations with the QGD regularization consists of the following mass, momentum and total energy balance equations [4]

$$\partial_t\rho+\operatorname{div}\mathbf{j}=0,\ \ \partial_t(\rho\mathbf{u})+\operatorname{div}(\mathbf{j}\otimes\mathbf{u}-\Pi)+\nabla p=0,\ \ \partial_t E+\operatorname{div}\Big[(E+p)\frac{\mathbf{j}}{\rho}+\mathbf{q}-\Pi\mathbf{u}\Big]=0 \tag{1}$$

in $\mathbb{R}^n$, $n=2,3$, for $t\geqslant 0$. The sought functions are the gas density $\rho>0$, velocity $\mathbf{u}=(u_1,\dots,u_n)$ and the specific internal energy $\varepsilon>0$ depending on (x,t), where $x=(x_1,\dots,x_n)$. Moreover, $E=\frac{1}{2}\rho|\mathbf{u}|^2+\rho\varepsilon>0$ is the total energy and $p=(\gamma-1)\rho\varepsilon$ is the gas pressure, $\gamma>1$. The operators div and $\nabla=(\partial_1,\dots,\partial_n)$ are taken in x and $\partial_t=\partial/\partial t$, $\partial_i=\partial/\partial x_i$. The symbols $\otimes$ and $\cdot$ denote the tensor and inner products of vectors, and a tensor divergence is taken with respect to its first index.

The regularized mass flux $\mathbf{j}$, viscous stress tensor $\Pi=\Pi_{NS}+\Pi_\tau$ and heat flux $\mathbf{q}$ are as follows

$$\mathbf{j}=\rho\mathbf{u}-\mathbf{m},\quad \mathbf{m}=\tau\big[\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u})+\nabla p\big],\quad \widehat{\mathbf{m}}=\tau\big[\rho(\mathbf{u}\cdot\nabla)\mathbf{u}+\nabla p\big], \tag{2}$$

$$\Pi_{NS}=\mu\big(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\big)+\big(\lambda-\tfrac{2}{3}\mu\big)(\operatorname{div}\mathbf{u})\mathbb{I},\quad \Pi_\tau=\mathbf{u}\otimes\widehat{\mathbf{m}}+\tau(\mathbf{u}\cdot\nabla p+\gamma p\operatorname{div}\mathbf{u})\mathbb{I}, \tag{3}$$

$$-\mathbf{q}=\tilde{\varkappa}\nabla\varepsilon+\tau\rho\Big(\mathbf{u}\cdot\nabla\varepsilon-\frac{p}{\rho^2}\mathbf{u}\cdot\nabla\rho\Big)\mathbf{u}, \tag{4}$$

where Π_{NS} is the Navier–Stokes viscous stress tensor with $\nabla\mathbf{u}=\{\partial_i u_j\}_{i,j=1}^n$, $\mathbb{I}$ is the unit tensor, $\mathbf{m}$, $\widehat{\mathbf{m}}$ and Π_τ are regularizing momenta and tensor, $\mu>0$, $\lambda>0$ and $\tilde{\varkappa}>0$ are the artificial viscosity and (scaled) heat conductivity coefficients as well as $\tau>0$ is the relaxation parameter.

One can linearize system (1)–(4) at a constant solution $(\rho,\mathbf{u},\varepsilon)(x,t)\equiv(\rho_*,\mathbf{u}_*,\varepsilon_*)$, where $\rho_*>0$, $\mathbf{u}_*=(u_{*1},\dots,u_{*n})$, $\varepsilon_*>0$ [9]. Let $\tau=\tau_*>0$ and

$$c_*=\sqrt{\gamma(\gamma-1)\varepsilon_*},\ \ \mu_*=\widehat{\alpha}_s\tau_*\rho_*c_*^2,\ \ \lambda_*=\widehat{\alpha}_{1s}\tau_*\rho_*c_*^2,\ \widehat{\alpha}_s\geqslant 0,\ \widehat{\alpha}_{1s}\geqslant 0,\ \ \tilde{\varkappa}_*=\widehat{\alpha}_P\tau_*\rho_*c_*^2,\ \ \widehat{\alpha}_P\geqslant 0$$

(see [3,4]), where c_* is the background sound velocity, $\alpha_s=\gamma\widehat{\alpha}_s$ and $\frac{1}{\widehat{\alpha}_P}$ are the Schmidt and Prandtl numbers. Substituting the solution in the form $(\rho,\mathbf{u},\varepsilon)=(\rho_*+\rho_*\tilde{\rho},\mathbf{u}_*+\frac{c_*}{\sqrt{\gamma}}\tilde{\mathbf{u}},\varepsilon_*+\sqrt{\gamma-1}\varepsilon_*\tilde{\varepsilon})$ into Eqs. (1)–(4), where $\mathbf{z}=(\tilde{\rho},\tilde{\mathbf{u}},\tilde{\varepsilon})^T$ is the vector of dimensionless small perturbations, and omitting the 2nd order terms with respect to $\mathbf{z}$, one can derive the linearized QGD system of equations

$$\partial_t\mathbf{z}+c_*B^{(i)}\partial_i\mathbf{z}-\tau_*c_*^2\big(A^{(ii)}\partial_i^2\mathbf{z}+(1-\delta^{(ij)})\hat{A}^{(ij)}\partial_i\partial_j\mathbf{z}\big)=0 \tag{5}$$

in $\mathbb{R}^n$ for $t\geqslant 0$, where $A^{(ii)}$, $\hat{A}^{(ij)}$ and $B^{(i)}$ are matrices of viscous and convective terms of the order $n+2$. Hereafter the summation over the repeated indexes i and j (and only over them) is assumed from 1 to n. Also $\delta^{(ij)}$ is the Kronecker symbol. Let $\mathbf{e}_0,\dots,\mathbf{e}_{n+1}$ be the column vectors of the standard coordinate basis in $\mathbb{R}^{n+2}$ and $E^{(k,l)}:=\mathbf{e}_k\mathbf{e}_l^T+\mathbf{e}_l\mathbf{e}_k^T$, then

$$B^{(k)}=M_kI_{n+2}+\frac{1}{\sqrt{\gamma}}E^{(0,k)}+\frac{1}{\sqrt{\gamma_*}}E^{(k,n+1)},$$

$$A^{(kk)}=D_\gamma+M_k^2I_{n+2}+\frac{2}{\sqrt{\gamma}}M_kE^{(0,k)}+\frac{2}{\sqrt{\gamma_*}}M_kE^{(k,n+1)}+(\widehat{a}_0+1)\mathbf{e}_k\mathbf{e}_k^T+\frac{1}{\sqrt{\gamma\gamma_*}}E^{(0,n+1)},$$

$$D_\gamma:=\operatorname{diag}\Big\{\frac{1}{\gamma},\widehat{\alpha}_s,\dots,\widehat{\alpha}_s,\widehat{\alpha}_P+\frac{1}{\gamma_*}\Big\},\ \ \widehat{a}_0=\frac{1}{3}\widehat{\alpha}_s+\widehat{\alpha}_{1s},$$

$$\hat{A}^{(kl)}=M_kM_lI_{n+2}+\frac{1}{\sqrt{\gamma}}\big(M_kE^{(0,l)}+M_lE^{(0,k)}\big)+\frac{1}{\sqrt{\gamma_*}}\big(M_kE^{(l,n+1)}+M_lE^{(k,n+1)}\big)+\frac{\widehat{a}_0+1}{2}E^{(k,l)}$$

for all k and l from 1 to n. Hereafter $\gamma_*=\frac{\gamma}{\gamma-1}$, $M_k=\frac{u_{*k}}{c_*}$, I_l is the lth order unit matrix and $\operatorname{diag}\{a_1,\dots,a_l\}$ is the diagonal matrix with the listed diagonal elements. Clearly $B^{(k)}$, $A^{(kk)}$ and $\hat{A}^{(kl)}$ are symmetric matrices, and $\hat{A}^{(kl)}=\hat{A}^{(lk)}$.

The equalities $(E^{(k,l)})^2 = \mathbf{e}_k\mathbf{e}_k^T + \mathbf{e}_l\mathbf{e}_l^T$ $(k \neq l)$, $E^{(0,k)}E^{(k,n+1)} = \mathbf{e}_0\mathbf{e}_{n+1}^T$, $E^{(k,n+1)}E^{(0,k)} = \mathbf{e}_{n+1}\mathbf{e}_0^T$ $(1 \leqslant k \leqslant n)$ and $\frac{1}{\gamma} + \frac{1}{\gamma_*} = 1$ allow one to check the important formula

$$A^{(kk)} = (B^{(k)})^2 + \operatorname{diag}\{0, \widehat{\alpha}_s, \dots, \widehat{\alpha}_s, \widehat{\alpha}_P\} + \widehat{a}_0\mathbf{e}_k\mathbf{e}_k^T, \quad 1 \leqslant k \leqslant n. \tag{6}$$

The solution to a system like (5) under the initial condition $\mathbf{z}|_{t=0} = \mathbf{z}_0$ satisfies the uniform in t bound [9]

$$\sup_{t\geqslant 0} \|\mathbf{z}(\cdot, t)\|_{L^2(\mathbb{R}^n)} \leqslant \|\mathbf{z}_0\|_{L^2(\mathbb{R}^n)} \quad \forall\, \mathbf{z}_0 \in L^2(\mathbb{R}^n). \tag{7}$$

Let ω_{kh} and $\bar{\omega}^{\Delta t}$ be meshes in x_k and t with the nodes lh_k, $l \in \mathbb{Z}$, and $t_m = m\Delta t$, $m \geqslant 0$, and steps $h_k > 0$ and $\Delta t > 0$, $1 \leqslant k \leqslant n$. Define the finite-difference operators

$$\mathring{\delta}_k v_l = \frac{v_{l+1} - v_{l-1}}{2h_k}, \quad (\delta_k^*\delta_k v)_l = \frac{v_{l+1} - 2v_l + v_{l-1}}{h_k^2}, \quad \delta_t v = \frac{v^+ - v}{\Delta t}, \quad v^{+,m} = v^{m+1}.$$

Let $\omega_\mathbf{h} := \omega_{1h} \times \dots \times \omega_{nh}$, $\mathbf{h} = (h_1, \dots, h_n)$, $h_{\min} := \min_{1\leqslant k\leqslant n} h_k$ and $h_V = (h_1 \dots h_n)^{1/n}$.

We approximate system (5) using the defined finite-difference operators and get an explicit two-level in t and three-point in each direction $x_1, \dots, x_n$ finite-difference scheme

$$\delta_t\mathbf{y} + c_* B^{(i)}\mathring{\delta}_i\mathbf{y} - \tau_* c_*^2\big(A^{(ii)}\delta_i^*\delta_i\mathbf{y} + (1 - \delta^{(ij)})\hat{A}^{(ij)}\mathring{\delta}_i\mathring{\delta}_j\mathbf{y}\big) = 0 \tag{8}$$

on $\omega_\mathbf{h} \times \bar{\omega}^{\Delta t}$. Similar schemes arise also after the linearization of schemes for the original equations (1)–(4) including those from [3,4].

Let H be a Hilbert space of vector-functions $\mathbf{v}\colon \omega_\mathbf{h} \to \mathbb{C}^{n+2}$ that are square summable over $\omega_\mathbf{h}$ and be endowed with the inner product

$$(\mathbf{v}, \mathbf{y})_H = h_1 \dots h_n \sum_{\mathbf{k}\in\mathbb{Z}^n} (\mathbf{v}_\mathbf{k}, \mathbf{y}_\mathbf{k})_{\mathbb{C}^{n+2}}, \quad \mathbf{k} = (k_1, \dots, k_n).$$

The question is about conditions related to validity of the mesh counterpart of bound (7):

$$\sup_{m\geqslant 0} \|\mathbf{y}^m\|_H \leqslant \|\mathbf{y}^0\|_H \quad \forall\, \mathbf{y}^0 \in H. \tag{9}$$

Recall that this bound is equivalent to both the bound $\|\mathcal{A}\|_{\mathcal{L}[H]} \leqslant 1$ for the transition operator

$$\mathcal{A} = I - \Delta t\big[c_* B^{(i)}\mathring{\delta}_i - \tau_* c_*^2\big(A^{(ii)}\delta_i^*\delta_i + (1 - \delta^{(ij)})\hat{A}^{(ij)}\mathring{\delta}_i\mathring{\delta}_j\big)\big]$$

and H–dissipativity of the scheme: $\|\mathbf{y}^m\|_H \leqslant \|\mathbf{y}^{m-1}\|_H \leqslant \dots \leqslant \|\mathbf{y}^0\|_H$ for any $\mathbf{y}^0 \in H$, $m \geqslant 1$.

Let Δt and τ_* be given by the formulas

$$\Delta t \equiv \frac{\beta h_{\min}}{(M+1)c_*} = \frac{\tilde{\beta} h_{\min}}{c_*}, \quad \tau_* \equiv \frac{\alpha h_\tau}{c_*} = \frac{\widehat{\alpha} h_\tau}{(M+1)c_*} = \frac{\alpha_{h_\tau} h_{\min}}{c_*} = \frac{\widehat{\alpha}_{h_\tau} h_{\min}}{(M+1)c_*} \tag{10}$$

with the parameters $\beta > 0$ (the Courant number) and $\alpha > 0$; $M = |\mathbf{u}_*|/c_*$ is the background Mach number. Also $h_\tau = h_\tau(\mathbf{h}) > 0$ (in particular, $h_\tau = h_{\min}$ or h_V) whereas $\tilde{\beta}$, $\widehat{\alpha}$, α_{h_τ} and $\widehat{\alpha}_{h_\tau}$ are defined for convenience (here $\alpha_{h_\tau} = \alpha$ and $\widehat{\alpha}_{h_\tau} = \widehat{\alpha}$ if $h_\tau = h_{\min}$). Below we derive conditions on $\tilde{\beta}$ depending on α_{h_τ}, or β depending on $\widehat{\alpha}_{h_\tau}$, related to the validity of bound (9).

Following [5–7], we take particular solutions to scheme (8) in the form $\mathbf{y}_\mathbf{k}^m(\boldsymbol{\xi}) = e^{\mathbf{i}\mathbf{k}\cdot\boldsymbol{\xi}}\mathbf{w}^m(\boldsymbol{\xi})$, where $\mathbf{k} \in \mathbb{Z}^n$, $m \geqslant 0$, $\mathbf{i}$ is the imaginary unit and $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)^T \in [0, 2\pi]^n$ is a parameter. Substituting them into (8) and using formulas (10) lead to the explicit formula $\mathbf{w}^+ = G_\mathbf{s}\mathbf{w}$ on $\bar{\omega}^{\Delta t}$, with the matrices

$$G_\mathbf{s} = I_{n+2} - \tilde{\beta} F_\mathbf{s}, \;\; F_\mathbf{s} = 4\alpha_{h_\tau} A_\mathbf{s} + 2\mathbf{i} B_\mathbf{s}, \;\; B_\mathbf{s} = d_i s_i B^{(i)}, \;\; A_\mathbf{s} = d_i^2 A^{(ii)} + (1 - \delta^{(ij)}) d_i d_j s_i s_j \hat{A}^{(ij)},$$

where $G_{\mathbf{s}}$ is the symbol of the operator $\mathcal{A}$, $\mathbf{s} = (s_1, \dots, s_n)$ and

$$\sigma_k = \sin^2 \tfrac{\xi_k}{2} \in [0,1], \quad d_k = r_k\sqrt{\sigma_k}, \quad r_k = \frac{h_{\min}}{h_k} \leqslant 1, \quad s_k = (-1)^{l_k}\sqrt{1-\sigma_k} \in [-1,1], \quad 1 \leqslant k \leqslant n,$$

with $l_k = 0$ for $0 \leqslant \xi_k \leqslant \pi$ or $l_k = 1$ for $\pi < \xi_k \leqslant 2\pi$.

Define a column vector $\mathbf{M} = (M_1, \dots, M_n)^T$ (then $|\mathbf{M}| = M$ is the background Mach number) and a row vector $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_n)$ with $\zeta_k = d_k s_k$, $1 \leqslant k \leqslant n$, and set $d = (d_1^2 + \cdots + d_n^2)^{1/2}$.

Lemma 1. *1. The matrices $B_{\mathbf{s}}$ and $A_{\mathbf{s}}$ can be written in the 3 × 3-block form*

$$B_{\mathbf{s}} = \begin{pmatrix} \boldsymbol{\zeta}\mathbf{M} & \frac{1}{\sqrt{\gamma}}\boldsymbol{\zeta} & 0 \\ \frac{1}{\sqrt{\gamma}}\boldsymbol{\zeta}^T & (\boldsymbol{\zeta}\mathbf{M})I_n & \frac{1}{\sqrt{\gamma_*}}\boldsymbol{\zeta}^T \\ 0 & \frac{1}{\sqrt{\gamma_*}}\boldsymbol{\zeta} & \boldsymbol{\zeta}\mathbf{M} \end{pmatrix}, \quad A_{\mathbf{s}} = \begin{pmatrix} a_{\mathbf{M}} + \frac{1}{\gamma}d^2 & \frac{2}{\sqrt{\gamma}}\mathbf{p} & \frac{1}{\sqrt{\gamma\gamma_*}}d^2 \\ \frac{2}{\sqrt{\gamma}}\mathbf{p}^T & a_{\mathbf{M}}I_n + C_0 & \frac{2}{\sqrt{\gamma_*}}\mathbf{p}^T \\ \frac{1}{\sqrt{\gamma\gamma_*}}d^2 & \frac{2}{\sqrt{\gamma_*}}\mathbf{p} & a_{\mathbf{M}} + \big(\widehat{\alpha}_P + \frac{1}{\gamma_*}\big)d^2 \end{pmatrix},$$

where

$$a_{\mathbf{M}} = (\boldsymbol{\zeta}\mathbf{M})^2 + \mathbf{M}^TQ\mathbf{M} = \mathbf{p}\mathbf{M}, \;\; \mathbf{p} = (\boldsymbol{\zeta}\mathbf{M})\boldsymbol{\zeta} + \mathbf{M}^TQ, \;\; C_0 = \widehat{\alpha}_s d^2 I_n + \big(\widehat{a}_0 + 1\big)\big(\boldsymbol{\zeta}^T\boldsymbol{\zeta} + Q\big)$$

and $Q = \operatorname{diag}\{q_1, \dots, q_n\}$ with $q_k := d_k^2\sigma_k = r_k^2\sigma_k^2$, $1 \leqslant k \leqslant n$.

2. The following matrix inequality holds: $B_{\mathbf{s}}^2 \leqslant A_{\mathbf{s}}$ for any $\mathbf{s} \in S := [-1,1]^n$.

Proof. 1. The matrix $B_{\mathbf{s}}$ satisfies the formulas

$$B_{\mathbf{s}} = \zeta_i B^{(i)} = \zeta_i M_i I_{n+2} + \frac{1}{\sqrt{\gamma}}\zeta_i E^{(0,i)} + \frac{1}{\sqrt{\gamma_*}}\zeta_i E^{(i,n+1)}$$
$$= (\boldsymbol{\zeta}\mathbf{M})I_{n+2} + \begin{pmatrix} 0 & \frac{1}{\sqrt{\gamma}}\boldsymbol{\zeta} & 0 \\ \frac{1}{\sqrt{\gamma}}\boldsymbol{\zeta}^T & O_n & \mathbf{0}^T \\ 0 & \mathbf{0} & 0 \end{pmatrix} + \begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & O_n & \frac{1}{\sqrt{\gamma_*}}\boldsymbol{\zeta}^T \\ 0 & \frac{1}{\sqrt{\gamma_*}}\boldsymbol{\zeta} & 0 \end{pmatrix},$$

where $\mathbf{0}$ and O_n are zero row vector and matrix of the nth order.

We write down the formula $A_{\mathbf{s}} = d_i^2 A^{(ii)} - \zeta_i^2 \hat{A}^{(ii)} + \zeta_i\zeta_j\hat{A}^{(ij)}$, and since $d_i^2 = q_i + \zeta_i^2$, we further obtain

$$d_i^2A^{(ii)} - \zeta_i^2\hat{A}^{(ii)} = d^2D_\gamma + q_iM_i^2I_{n+2} + \frac{2}{\sqrt{\gamma}}q_iM_iE^{(0,i)} + \frac{2}{\sqrt{\gamma_*}}q_iM_iE^{(i,n+1)}$$
$$+ \big(\widehat{a}_0 + 1\big)q_i\mathbf{e}_i\mathbf{e}_i^T + d^2\frac{1}{\sqrt{\gamma\gamma_*}}E^{(0,n+1)} = d^2D_\gamma + \mathbf{M}^TQ\mathbf{M}I_{n+2} + \frac{2}{\sqrt{\gamma}}\begin{pmatrix} 0 & \mathbf{M}^TQ & 0 \\ Q\mathbf{M} & O_n & \mathbf{0}^T \\ 0 & \mathbf{0} & 0 \end{pmatrix}$$
$$+ \frac{2}{\sqrt{\gamma_*}}\begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & O_n & Q\mathbf{M} \\ 0 & \mathbf{M}^TQ & 0 \end{pmatrix} + \big(\widehat{a}_0 + 1\big)\begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & Q & \mathbf{0}^T \\ 0 & \mathbf{0} & 0 \end{pmatrix} + \frac{d^2}{\sqrt{\gamma\gamma_*}}\begin{pmatrix} 1 & \mathbf{0} & 1 \\ \mathbf{0}^T & O_n & \mathbf{0}^T \\ 1 & \mathbf{0} & 1 \end{pmatrix},$$

$$\zeta_i\zeta_j\hat{A}^{(ij)} = \zeta_iM_i\zeta_jM_jI_{n+2} + \frac{1}{\sqrt{\gamma}}\big(\zeta_iM_i\zeta_jE^{(0,j)} + \zeta_jM_j\zeta_iE^{(0,i)}\big)$$
$$+ \frac{1}{\sqrt{\gamma_*}}\big(\zeta_iM_i\zeta_jE^{(j,n+1)} + \zeta_jM_j\zeta_iE^{(i,n+1)}\big) + \frac{1}{2}(\widehat{a}_0 + 1)\zeta_i\zeta_jE^{(i,j)} = (\boldsymbol{\zeta}\mathbf{M})^2I_{n+2}$$
$$+ \frac{2}{\sqrt{\gamma}}\boldsymbol{\zeta}\mathbf{M}\begin{pmatrix} 0 & \boldsymbol{\zeta} & 0 \\ \boldsymbol{\zeta}^T & O_n & \mathbf{0}^T \\ 0 & \mathbf{0} & 0 \end{pmatrix} + \frac{2}{\sqrt{\gamma_*}}\boldsymbol{\zeta}\mathbf{M}\begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & O_n & \boldsymbol{\zeta}^T \\ 0 & \boldsymbol{\zeta} & 0 \end{pmatrix} + \big(\widehat{a}_0 + 1\big)\begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & \boldsymbol{\zeta}^T\boldsymbol{\zeta} & \mathbf{0}^T \\ 0 & \mathbf{0} & 0 \end{pmatrix}.$$

The specified form of matrices $B_{\mathbf{s}}$ and $A_{\mathbf{s}}$ follows from the presented formulas.

2. For the matrix $\tilde{A}_{\mathbf{s}} := \zeta_i^2 A^{(ii)} + (1-\delta^{(ij)})\zeta_i\zeta_j \hat{A}^{(ij)}$, from the same formulas it follows that

$$\tilde{A}_{\mathbf{s}} - B_{\mathbf{s}}^2 = \begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0}^T & \widehat{\alpha}_s|\boldsymbol{\zeta}|^2 I_n + \widehat{a}_0\boldsymbol{\zeta}^T\boldsymbol{\zeta} & \mathbf{0}^T \\ 0 & \mathbf{0} & \widehat{\alpha}_P|\boldsymbol{\zeta}|^2 \end{pmatrix} \geqslant 0$$

since $\boldsymbol{\zeta}^T\boldsymbol{\zeta} \geqslant 0$. Since also $A^{(ii)} \geqslant 0$, see (6), we derive $A_{\mathbf{s}} = q_i A^{(ii)} + \tilde{A}_{\mathbf{s}} \geqslant \tilde{A}_{\mathbf{s}} \geqslant B_{\mathbf{s}}^2$. □

Denote by $\lambda_{\max}(A)$ the maximal eigenvalue of a Hermitian matrix A.

Theorem 1. *Let $\mathcal{H} = [L^2(S)]^K$ with $K = n+2$. Then the following equalities hold*

$$\|\mathcal{A}\|_{\mathcal{L}[H]} = \|G.\|_{\mathcal{L}[\mathcal{H}]} \equiv \sup_{\|\mathbf{w}\|_{\mathcal{H}}=1} \|G_{\mathbf{s}}\mathbf{w}(\mathbf{s})\|_{\mathcal{H}} = \max_{\mathbf{s}\in S} \|G_{\mathbf{s}}\|_{\mathcal{L}[\mathbb{C}^K]} = \max_{\mathbf{s}\in S} \lambda_{\max}^{1/2}(G_{\mathbf{s}}^* G_{\mathbf{s}}).$$

The first equality follows from the isomorphism of the complex Hilbert spaces $(\ell^2)^K$ and $\mathcal{H}$ established by means of the complex Fourier series, and the last one (without $\max_{\mathbf{s}\in S}$) is well known. The inequality $\|G.\|_{\mathcal{L}[\mathcal{H}]} \leqslant \max_{\mathbf{s}\in S} \|G_{\mathbf{s}}\|_{\mathcal{L}[\mathbb{C}^K]}$ is obvious whereas the opposite inequality $\max_{\mathbf{s}\in S} \lambda_{\max}(G_{\mathbf{s}}^* G_{\mathbf{s}}) = \lambda_{\max}(G_{\mathbf{s}_0}^* G_{\mathbf{s}_0}) \leqslant \|G.\|_{\mathcal{L}[\mathcal{H}]}^2$, $\mathbf{s}_0 \in S$, is proved by contradiction (taking the function $\mathbf{w}(\mathbf{s}) = \mathbf{w}_0 \neq 0$ for $|\mathbf{s}-\mathbf{s}_0| \leqslant \delta$ or $\mathbf{w}(\mathbf{s}) = 0$ otherwise, where $G_{\mathbf{s}_0}^* G_{\mathbf{s}_0}\mathbf{w}_0 = \lambda_{\max}(G_{\mathbf{s}_0}^* G_{\mathbf{s}_0})\mathbf{w}_0$, for sufficiently small $\delta > 0$, and using the continuity of $G_{\mathbf{s}}^* G_{\mathbf{s}}$ in $\mathbf{s}$).

One can generalize Theorem 1 for any $\mathcal{A} \in \mathcal{L}[H]$ with the continuous symbol $G(\boldsymbol{\xi})$ and $K \geqslant 1$.

Now we give necessary conditions and sufficient conditions for bound (9) to hold [7].

Theorem 2. *Let $[A_{\mathbf{s}}, B_{\mathbf{s}}] := A_{\mathbf{s}}B_{\mathbf{s}} - B_{\mathbf{s}}A_{\mathbf{s}}$. The validity of the following matrix inequalities*

$$\tilde{\beta}\big(2\alpha_{h_\tau} A_{\mathbf{s}}^2 + \tfrac{1}{2\alpha_{h_\tau}} B_{\mathbf{s}}^2 + \mathbf{i}[A_{\mathbf{s}}, B_{\mathbf{s}}]\big) \leqslant A_{\mathbf{s}} \quad \forall \mathbf{s} \in S, \tag{11}$$

$$2\alpha_{h_\tau} r_k^2 \tilde{\beta} A^{(kk)} \leqslant I_{n+2}, \quad \tfrac{\tilde{\beta}}{2\alpha_{h_\tau}} (B^{(k)})^2 \leqslant A^{(kk)} \quad \forall 1 \leqslant k \leqslant n, \tag{12}$$

$$\tilde{\beta}\big[2\alpha_{h_\tau}(1+\varepsilon) A_{\mathbf{s}}^2 + \tfrac{1}{2\alpha_{h_\tau}}\big(1+\varepsilon^{-1}\big) B_{\mathbf{s}}^2\big] \leqslant A_{\mathbf{s}} \quad \forall \mathbf{s} \in S, \ \textit{for some } \varepsilon > 0 \tag{13}$$

respectively is necessary and sufficient, or necessary, or sufficient for bound (9) to hold.

For $\max_{\mathbf{s}\in S} \lambda_{\max}(A_{\mathbf{s}}) \leqslant \bar{\lambda}$, bound (9) holds under the validity of the number inequality

$$\tilde{\beta}\big[(2\alpha_{h_\tau}\bar{\lambda})^{1/2} + (2\alpha_{h_\tau})^{-1/2}\big]^2 \leqslant 1. \tag{14}$$

Condition (11) follows from Theorem 1, and (14) follows from (13) using the above inequality $B_{\mathbf{s}}^2 \leqslant A_{\mathbf{s}}$. The derivation of conditions (12) and (13) from (11) is similar to [7].

Next we derive from condition (12) a specific necessary condition.

Theorem 3. *For bound (9) to hold, the following condition is necessary:*

$$\beta \leqslant \beta_{nec}(\widehat{\alpha}_{h_\tau}) := \min\Big\{2\widehat{\alpha}_{h_\tau}, \frac{1}{2\widehat{\alpha}_{h_\tau}} \min_{1\leqslant k\leqslant n} \frac{h_k^2}{h_{\min}^2} \frac{(M+1)^2}{M_k^2 + \underset{\sim}{\lambda}[M_k]}\Big\} = \beta_{nec}(\widehat{\alpha} r_{h_\tau}), \tag{15}$$

where $r_{h_\tau} = h_\tau / h_{\min}$ and $M_k^2 + \underset{\sim}{\lambda}[M_k] \leqslant \lambda_{\max}(A^{(kk)})$ with

$$\underset{\sim}{\lambda}[M_k] := \max\Bigg\{ \frac{\widehat{\alpha}_P + 1}{2} + \sqrt{\Big(\frac{\widehat{\alpha}_P - 1}{2}\Big)^2 + \frac{1}{\gamma_*}\widehat{\alpha}_P}, \ \frac{1}{2}\Big(\widetilde{a}_0 + 1 + \frac{1}{\gamma}\Big) + \sqrt{\frac{1}{4}\Big(\widetilde{a}_0 + \frac{1}{\gamma_*}\Big)^2 + \frac{4}{\gamma} M_k^2},$$
$$\frac{1}{2}\Big(\widetilde{a}_0 + \widehat{\alpha}_P + 1 + \frac{1}{\gamma_*}\Big) + \sqrt{\frac{1}{4}\Big(\widetilde{a}_0 - \widehat{\alpha}_P + \frac{1}{\gamma}\Big)^2 + \frac{4}{\gamma_*} M_k^2} \Bigg\} \geqslant \max\Big\{\widetilde{a}_0 + 1, \widehat{\alpha}_P + \frac{1}{\gamma_*}\Big\}$$

and $\widetilde{a}_0 = \widehat{\alpha}_s + \widehat{a}_0 = \frac{4}{3}\widehat{\alpha}_s + \widehat{\alpha}_{1s}$.

If $h_1 = \cdots = h_n = h_\tau = h$, then $r_{h_\tau} = 1$ and $\beta_{nec}(\widehat{\alpha})$ is independent of h and takes the form

$$\beta_{nec}(\widehat{\alpha}) = \min\Big\{2\widehat{\alpha},\ \frac{(M+1)^2}{2\widehat{\alpha}\big(M_{\max}^2 + \tilde{\lambda}[M_{\max}]\big)}\Big\} \ \text{ with } \ M_{\max} := \max_{1\leqslant k\leqslant n} |M_k|.$$

Proof. Similarly to [7], since $A^{(kk)} \geqslant 0$, the first inequality (12) is equivalent to the following one

$$\tilde{\beta} \leqslant \frac{h_k^2}{h_{\min}^2}\frac{1}{2\alpha_{h_\tau}\lambda_{\max}(A^{(kk)})}.$$

Due to (6) we have $(B^{(k)})^2 \leqslant A^{(kk)}$, and the second inequality (12) is valid under $\tilde{\beta} \leqslant 2\alpha_{h_\tau}$. On the other hand, $(B^{(k)})^2_{11} = A^{(kk)}_{11} > 0$, thus the second inequality (12) implies the inequality $\tilde{\beta} \leqslant 2\alpha_{h_\tau}$ and finally is equivalent to it (as in [6,7]). The presented lower bound for $\lambda_{\max}(A^{(kk)})$ follows from the Cauchy theorem on separation of eigenvalues of a symmetric matrix and considering the 2nd order main minors of $A^{(kk)}$ (it coincides with the bound given in the 1D case in [6]). The transition from $\tilde{\beta}$ and α_{h_τ} to β and $\widehat{\alpha}_{h_\tau}$ leads to condition (15). $\square$

The sufficient condition (14) can be rewritten in the form

$$\beta \leqslant \beta_{\text{suf}}(\widehat{\alpha}_{h_\tau}) := 1\Big/\Big(\sqrt{2\widehat{\alpha}_{h_\tau}}\frac{\bar{\lambda}^{1/2}}{M+1} + \frac{1}{\sqrt{2\widehat{\alpha}_{h_\tau}}}\Big)^2, \tag{16}$$

cp. [10]. The maximum of the right-hand side is achieved for $\widehat{\alpha}_{h_\tau} = \widehat{\alpha}_{h_\tau *} := (M+1)/(2\bar{\lambda}^{1/2})$ and equals $\widehat{\alpha}_{h_\tau *}/2$. Note that both $\beta_{\text{nec}}(\widehat{\alpha}_{h_\tau}) \to 0$ and $\beta_{\text{suf}}(\widehat{\alpha}_{h_\tau}) \to 0$ as $\widehat{\alpha}_{h_\tau} \to +0$ or $\widehat{\alpha}_{h_\tau} \to +\infty$.

To apply condition (16), we also need to bound $\lambda_{\max}(A_{\mathbf{s}})$ from above. Let $\mathbf{r} = (r_1, \ldots, r_n)$.

Theorem 4. *For $n = 2, 3$, the following bounds hold*

$$\max_{\mathbf{s}\in S}\lambda_{\max}(A_{\mathbf{s}}) \leqslant \bar{\lambda} := \max\big\{\widehat{\alpha}_s|\mathbf{r}|^2 + c_n\big(\widehat{a}_0+1\big), |\mathbf{r}|^2\bar{\lambda}(\widehat{\alpha}_P,\gamma)\big\} + c_n r_i^2 M_i^2 + 2\big(\delta^{(ii)}r_i^4\big)^{1/2}M$$
$$\leqslant \max\big\{\widehat{\alpha}_s n + c_n\big(\widehat{a}_0+1\big), n\bar{\lambda}(\widehat{\alpha}_P,\gamma)\big\} + c_n M^2 + 2\sqrt{n}M$$

with $c_2 = 1$, $c_3 = \frac{9}{8}$ and $\bar{\lambda}(\widehat{\alpha}_P,\gamma) := \frac{\widehat{\alpha}_P+1}{2} + \sqrt{\big(\frac{\widehat{\alpha}_P+1}{2}\big)^2 - \frac{\widehat{\alpha}_P}{\gamma}}$.

If $h_1 = \cdots = h_n$, then the second inequality turns into equality.

Proof. We apply the decomposition $A_{\mathbf{s}} = A_{\mathbf{s}0} + a_{\mathbf{M}}I_{n+2} + 2A_{\mathbf{M}1}$, where

$$A_{\mathbf{s}0} := A_{\mathbf{s}}|_{\mathbf{M}=0} = \begin{pmatrix} \frac{1}{\gamma}d^2 & \mathbf{0} & \frac{1}{\sqrt{\gamma\gamma_*}}d^2 \\ \mathbf{0}^T & C_0 & \mathbf{0}^T \\ \frac{1}{\sqrt{\gamma\gamma_*}}d^2 & \mathbf{0} & \big(\widehat{\alpha}_P + \frac{1}{\gamma_*}\big)d^2 \end{pmatrix}, \quad A_{\mathbf{M}1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{\gamma}}\mathbf{p} & 0 \\ \frac{1}{\sqrt{\gamma}}\mathbf{p}^T & O_n & \frac{1}{\sqrt{\gamma_*}}\mathbf{p}^T \\ 0 & \frac{1}{\sqrt{\gamma_*}}\mathbf{p} & 0 \end{pmatrix}.$$

Due to the classical Rayleigh formula for $\lambda_{\max}(A)$ the inequality $\lambda_{\max}(A_{\mathbf{s}}) \leqslant \lambda_{\max}(A_{\mathbf{s}0}) + a_{\mathbf{M}} + 2\lambda_{\max}(A_{\mathbf{M}1})$ is valid. Moreover, due to [7] the following estimates hold

$$\lambda_{\max}(\boldsymbol{\zeta}\boldsymbol{\zeta}^T + Q) \leqslant c_n, \quad a_{\mathbf{M}} \leqslant c_n r_i^2 M_i^2, \quad |\mathbf{p}|^2 \leqslant \delta^{(ii)} r_i^4 M^2. \tag{17}$$

We have $\operatorname{Sp} A_{\mathbf{s}0} = \operatorname{Sp} C_0 \cup \operatorname{Sp} C_1$, where the 2nd order matrix C_1 is obtained from $A_{\mathbf{s}0}$ by deleting all rows and columns except the first and last ones. It is straightforward to calculate that $\lambda_{\max}(C_1) = d^2\bar{\lambda}(\widehat{\alpha}_P,\gamma)$ (using $\frac{1}{\gamma} + \frac{1}{\gamma_*} = 1$). Since also $d^2 \leqslant |\mathbf{r}|^2$, we derive

$$\lambda_{\max}(A_{\mathbf{s}0}) \leqslant \max\big\{\widehat{\alpha}_s d^2 + \big(\widehat{a}_0+1\big)\lambda_{\max}(\boldsymbol{\zeta}\boldsymbol{\zeta}^T + Q), d^2\bar{\lambda}(\widehat{\alpha}_P,\gamma)\big\} \leqslant$$
$$\leqslant \max\big\{\widehat{\alpha}_s|\mathbf{r}|^2 + c_n\big(\widehat{a}_0+1\big), |\mathbf{r}|^2\bar{\lambda}(\widehat{\alpha}_P,\gamma)\big\}.$$

The eigenvalue problem for $A_{\mathbf{M}1}$ is solved easily, and $\operatorname{Sp} A_{\mathbf{M}1} = \{0, \pm|\mathbf{p}|\}$ (using $\frac{1}{\gamma} + \frac{1}{\gamma_*} = 1$ once again) thus $\lambda_{\max}(A_{\mathbf{M}1}) = |\mathbf{p}|$. Now from (17) we obtain the result. $\square$

Importantly, both $\beta_{\text{nec}}(\widehat{\alpha}_{h_\tau})$ and $\beta_{\text{suf}}(\widehat{\alpha}_{h_\tau})$ are uniformly bounded in M.

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