Higher-order discrete maximum principle for 1D diffusion-reaction problems

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Abstract

Sufficient conditions for the validity of the discrete maximum principle (DMP) for a 1D diffusion-reaction problem $-u''+\kappa^2 u = f$ with homogeneous Dirichlet boundary conditions discretized by the higher-order finite element method are presented. It is proved that the DMP is satisfied if the lengths h of all elements are shorter then one-third of the length of the entire domain and if $\kappa^2 h^2$ is small enough for all elements. In general, the bounds for $\kappa^2 h^2$ depend on the polynomial degree of the elements, on h, and on the size of the domain. The obtained conditions are simple and easy to verify. A technical assumption (nonnegativity of certain rational functions) was verified by computer for polynomial degrees up to 10. The paper contains an analysis of the discrete Green's function which can be of independent interest.

Key words: discrete maximum principle, discrete Green's function, diffusion-reaction problem, higher-order finite element method, *hp*-FEM, M-matrix
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1 Introduction

The standard (continuous) maximum principles for elliptic and parabolic problems, in particular, guarantee the nonnegativity of the solution provided that the data are nonnegative. This is especially important if naturally nonnegative quantities like temperature, concentration, density, etc. are modelled.

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There is a question if the discretization of these problems satisfies the discrete maximum principle (DMP) as well, or, equivalently, if the resulting discrete solution is guaranteed to be nonnegative provided the data are nonnegative.

Unfortunately, the standard methods, e.g., the finite element methods, do not satisfy the DMP in general. Therefore, additional conditions for the validity of the DMP are proposed and studied. Up to the author's knowledge the paper of Varga [14] from 1966 was the first paper about the DMP. Since then many other papers about the DMP for various problems and various discretizations were published [3–6,10,19].

Interestingly, the majority of the published works deal with the lowest-order approximations only. The results about the DMP for higher-order approximations are scarce, see [1,9,20] and the recent works of the author and his coauthors [15,17]. This paper extends the recent result [15] for the 1D Poisson problem to the 1D diffusion-reaction problem discretized by higher-order finite elements. In particular, this result is suitable for the *hp*-version of the finite element method (*hp*-FEM), see e.g. [16], because various polynomial degrees in different elements are allowed.

The generalization of the higher-order DMP from the Poisson problem to the diffusion-reaction problem is not straightforward. Many technical problems have to be overcome and new approaches introduced. For illustration let us mention that in contrast to the Poisson problem the bubble (interior) basis functions are not orthogonal to the vertex functions in the diffusion-reaction case, there is no explicit formula for the inverse of the stiffness matrix, the reaction coefficient κ^2 is a new free parameter, etc. Even for the lowest-order approximations, the DMPs for the diffusion-reaction problems were treated very recently [2,7].

The paper is organized as follows. Section 2 introduces the diffusion-reaction problem and briefly describes its discretization by the *hp*-FEM. In Section 3 the discrete maximum principle is defined and its relation to the discrete Green's function is explained. The usefull concept of discrete minimum energy extensions is introduced in Section 4 and it is used in Section 5 to define suitable basis functions for the higher-order finite element space. The splitting of the discrete Green's function to the vertex and bubble part is shown in Section 6 together with the proof of the nonnegativity of the vertex part. Section 7 analyzes the influence of the bubble part to the nonnegativity of the discrete Green's function in several steps. Sufficient conditions for the DMP are presented here. Section 8 comments the technical assumptions and their verification. The computer was used to verify nonnegativity of certain rational functions on an interval. The final conclusions are drawn in Section 9.

2 The problem and its discretization

Let us consider an open interval $\Omega \subset \mathbb{R}$, $\Omega = (a_\Omega, b_\Omega)$, and the 1D reaction-diffusion problem with the homogeneous Dirichlet boundary conditions

$$-u'' + \kappa^2 u = f \quad \text{in } \Omega, \qquad u(a_\Omega) = u(b_\Omega) = 0, \tag{1}$$

where the reaction coefficient $\kappa \geq 0$ is assumed to be constant. The standard maximum principle for this problem is equivalent to the so-called conservation of nonnegativity

$$f \geq 0 \quad \Rightarrow \quad u \geq 0.$$

In what follows, we will study an analogue of this implication for the discrete solution obtained by the hp-FEM.

Let $a_\Omega = x_0 < x_1 < \cdots < x_{M+1} = b_\Omega$ be a partition of the interval $\Omega = (a_\Omega, b_\Omega)$. Consider $M + 1 \geq 2$ finite elements $K_k = [x_{k-1}, x_k]$ with lengths $h_{K_k} = x_k - x_{k-1}$, $k = 1, 2, \ldots, M+1$. The set $\mathcal{T}_{hp} = \{K_k, k = 1, 2, \ldots, M+1\}$ is referred as the (finite element) mesh. Further, we consider an arbitrary distribution of polynomial degrees p_K assigned to the elements $K \in \mathcal{T}_{hp}$. The corresponding hp-FEM space V_{hp} is defined as follows

$$V_{hp} = \{v_{hp} \in H_0^1(\Omega) : v_{hp}|_K \in P^{p_K}(K),\ K \in \mathcal{T}_{hp}\}, \tag{2}$$

where $H_0^1(\Omega)$ is the standard Sobolev space of functions from $L^2(\Omega)$ with the generalized derivatives in $L^2(\Omega)$. The space $P^{p_K}(K)$ contains polynomials of degree at most p_K in the interval K. The hp-FEM solution $u_{hp} \in V_{hp}$ of problem (1) is defined by

$$a(u_{hp}, v_{hp}) = F(v_{hp}) \quad \forall v_{hp} \in V_{hp}, \tag{3}$$

where $a(u, v) = (u', v')_\Omega + \kappa^2 (u, v)_\Omega$, $F(v) = (f, v)_\Omega$, f is assumed in $L^2(\Omega)$, and $(u, v)_\Omega = \int_\Omega uv \,\mathrm{d}x$ denotes the $L^2(\Omega)$ inner product. Notice that there exists a unique solution $u_{hp} \in V_{hp}$ to problem (3).

3 Discrete maximum principle and the discrete Green's function

Definition 3.1 *Let V_{hp} given by* (2) *be the hp-FEM space based on the mesh $\mathcal{T}_{hp}$ and on the polynomial degrees p_K, $K \in \mathcal{T}_{hp}$. We say that approximate problem* (3) *satisfies the discrete maximum principle (DMP) if*

$$\max_{\overline{\Omega}} u_{hp} = \max_{\partial\Omega} u_{hp} = 0 \quad \textit{for all} \quad f \in L^2(\Omega),\ f \leq 0 \textit{ a.e. in } \Omega. \tag{4}$$

Notice that requirement (4) is equivalent to

$$u_{hp} \geq 0 \quad \text{for all} \quad f \in L^2(\Omega),\ f \geq 0 \text{ a.e. in } \Omega. \tag{5}$$

This DMP is also equivalent to the nonnegativity of the discrete Green's function G_{hp}, see Theorem 3.2 below.

Definition 3.2 *Let $y \in \Omega$ and let $G_{hp,y} \in V_{hp}$ be the unique solution of the problem*

$$a(w_{hp}, G_{hp,y}) = \delta_y(w_{hp}) = w_{hp}(y) \quad \forall w_{hp} \in V_{hp}. \tag{6}$$

The function $G_{hp}(x, y) = G_{hp,y}(x)$, $(x, y) \in \Omega^2$, is called the discrete Green's function (DGF).

A combination of (3) and (6) yields the discrete Kirchhoff-Helmholtz representation formula

$$u_{hp}(y) = \int_\Omega G_{hp}(x, y) f(x) \, \mathrm{d}x, \quad y \in \Omega. \tag{7}$$

Interestingly, the DGF can be explicitly expressed in terms of a basis of V_{hp}.

Theorem 3.1 *Let $\varphi_1, \varphi_2, \ldots, \varphi_N$ be a basis in V_{hp} and let $\mathbb{A} \in \mathbb{R}^{N \times N}$ be the stiffness matrix with entries $\mathbb{A}_{ij} = a(\varphi_i, \varphi_j)$, $i, j = 1, 2, \ldots, N$. Then*

$$G_{hp}(x, y) = \sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbb{A}^{-1})_{ij} \varphi_i(x) \varphi_j(y), \tag{8}$$

where $(\mathbb{A}^{-1})_{ij}$ are the entries of the inverse matrix to $\mathbb{A}$.

Proof. See [15]. □

Notice that Theorem 3.1 and the symmetry of the bilinear form $a(\cdot, \cdot)$ imply $G_{hp}(x, y) = G_{hp}(y, x)$. Consequently, $G_{hp,x} = G_{hp}(x, \cdot) \in V_{hp}$.

Theorem 3.2 *Problem (3) satisfies the DMP if and only if $G_{hp}(x, y) \geq 0$ for all $(x, y) \in \Omega^2$.*

Proof. Immediate consequence of (7). See [15]. □

Thus, our goal is to prove the nonnegativity of G_{hp} in Ω^2. To this end, we will use (8). First, in Section 5, a suitable basis of V_{hp} will be constructed. For this purpose we will utilize the concept of the discrete minimum energy extensions which will be described in Section 4. The analysis of the nonnegativity of G_{hp} will be postponed to the subsequent sections.

4 Discrete minimum energy extensions

Let us consider a splitting of the space V_{hp} into a direct sum of two nontrivial subspaces $V_{hp} = V_{hp}^{*} \oplus V_{hp}^{\#}$. The discrete minimum energy extension $\psi^{\mathrm{me}} \in V_{hp}$ of a function $\psi^{*} \in V_{hp}^{*}$ with respect to $V_{hp}^{\#}$ is uniquely defined as

$$\psi^{\mathrm{me}} = \psi^{*} - \psi^{\#},$$

where $\psi^{\#} \in V_{hp}^{\#}$ is the elliptic projection of ψ^{*} into $V_{hp}^{\#}$, i.e.,

$$0 = a(\psi^{\mathrm{me}}, v^{\#}) = a(\psi^{*} - \psi^{\#}, v^{\#}) \quad \text{for all } v^{\#} \in V_{hp}^{\#}. \tag{9}$$

Due to the symmetry of $a(\cdot,\cdot)$ and due to (9) we have

$$a(\psi^{\mathrm{me}}, \psi^{\mathrm{me}}) = a(\psi^{\mathrm{me}}, \psi^{*}) = a(\psi^{*}, \psi^{*}) - a(\psi^{\#}, \psi^{*}) = a(\psi^{*}, \psi^{*}) - a(\psi^{\#}, \psi^{\#}).$$

Hence, $\|\psi^{\mathrm{me}}\|^2 + \|\psi^{\#}\|^2 = \|\psi^{*}\|^2$, where $\|v\|^2 = a(v,v)$. Consequently,

$$\|\psi^{\mathrm{me}}\| \le \|\psi^{*}\| \quad \text{and} \quad \|\psi^{\#}\| \le \|\psi^{*}\|. \tag{10}$$

Now, let us compute the discrete minimum energy extensions of basis functions from V_{hp}^{*}. Let $\mathcal{B}^{*} = \{\varphi_1^{*}, \varphi_2^{*}, \ldots, \varphi_{N^{*}}^{*}\}$ be a basis in V_{hp}^{*} and let $\mathcal{B}^{\#} = \{\varphi_1^{\#}, \varphi_2^{\#}, \ldots, \varphi_{N^{\#}}^{\#}\}$ be a basis in $V_{hp}^{\#}$. The stiffness matrix $\overline{\mathbb{A}}$ corresponding to the basis $\mathcal{B}^{*} \cup \mathcal{B}^{\#}$ of V_{hp} has the following 2-by-2 block structure

$$\overline{\mathbb{A}} = \begin{pmatrix} \overline{A} & \overline{B} \\ \overline{B}^T & \overline{D} \end{pmatrix},$$

where $\overline{A}_{ij} = a(\varphi_i^{*}, \varphi_j^{*})$, $i,j = 1,2,\ldots,N^{*}$, $\overline{B}_{ij} = a(\varphi_i^{*}, \varphi_j^{\#})$, $i = 1,2,\ldots,N^{*}$, $j = 1,2,\ldots,N^{\#}$, and $\overline{D}_{ij} = a(\varphi_i^{\#}, \varphi_j^{\#})$, $i,j = 1,2,\ldots,N^{\#}$.

The discrete minimum energy extensions $\varphi_i^{\mathrm{me}} \in V_{hp}$ of $\varphi_i^{*} \in V_{hp}^{*}$ with respect to $V_{hp}^{\#}$ can be computed as

$$\varphi_i^{\mathrm{me}} = \varphi_i^{*} - \sum_{j=1}^{N^{\#}} \overline{C}_{ij} \varphi_j^{\#}, \quad i = 1,2,\ldots,N^{*}. \tag{11}$$

The requirement (9) uniquely determines coefficients $\overline{C}_{ij}$ as follows

$$0 = a(\varphi_i^{*}, \varphi_k^{\#}) - \sum_{j=1}^{N^{\#}} \overline{C}_{ij} a(\varphi_j^{\#}, \varphi_k^{\#}) \quad \forall i = 1,2,\ldots,N^{*}, \; k = 1,2,\ldots,N^{\#}. \tag{12}$$

This can be formulated in a matrix form as $0 = \overline{A} - \overline{C}\,\overline{D}$, where the matrix $\overline{C} \in \mathbb{R}^{N^* \times N^\#}$ consists of entries $\overline{C}_{ij}$. Hence,

$$\overline{C} = \overline{B}\,\overline{D}^{-1} \tag{13}$$

The discrete minimum energy extensions $\varphi_i^{\mathrm{me}} \in V_{hp}$ can be used as an alternative basis $\mathcal{B}^{\mathrm{me}} = \{\varphi_1^{\mathrm{me}}, \varphi_2^{\mathrm{me}}, \ldots, \varphi_{N^*}^{\mathrm{me}}\}$ in V_{hp}^*. It can be easily verified that the corresponding stiffness matrix $\overline{S} \in \mathbb{R}^{N^* \times N^*}$ with entries $\overline{S}_{ij} = a(\varphi_i^{\mathrm{me}}, \varphi_j^{\mathrm{me}})$, $i, j = 1, 2, \ldots, N^*$ is just the Schur complement

$$\overline{S} = \overline{A} - \overline{B}\,\overline{D}^{-1}\overline{B}^T. \tag{14}$$

Finally, the well known formula for the inversion of a 2-by-2 block matrix implies that the upper-left block of $\overline{\mathbb{A}}^{-1}$ is equal to the inverse of the Schur complement, i.e.,

$$(\overline{\mathbb{A}}^{-1})_{ij} = (\overline{S}^{-1})_{ij} \quad \forall i, j = 1, 2, \ldots, N^*. \tag{15}$$

5 Construction of the hp-FEM bases

As usual, we construct the finite element basis functions on elements $K_k \in \mathcal{T}_{hp}$ as images of the shape functions defined on the reference element $K_{\mathrm{ref}} = [-1, 1]$ under the reference maps

$$\chi_{K_k}(\xi) = \frac{h_{K_k}}{2}\xi + \frac{x_k + x_{k-1}}{2}, \quad \xi \in K_{\mathrm{ref}},\ k = 1, 2, \ldots, M + 1. \tag{16}$$

The hp-FEM shape functions comprise two vertex functions

$$\ell_0(\xi) = (1 - \xi)/2, \qquad \ell_1(\xi) = (1 + \xi)/2, \qquad \xi \in K_{\mathrm{ref}},$$

and $p - 1$ bubble functions ℓ_i^p, $i = 2, \ldots, p$, for each polynomial degree p. For the analysis of the DMP it is convenient to construct the bubble functions as the generalized eigenfunctions of the discrete Laplacian [18]. Hence, for given $p \geq 2$ we define $\ell_i^p \in \mathbb{P}_0^p(K_{\mathrm{ref}})$ by requirement

$$\left((\ell_i^p)', v'\right)_{K_{\mathrm{ref}}} = \lambda_i^p (\ell_i^p, v)_{K_{\mathrm{ref}}} \quad \forall v \in \mathbb{P}_0^p(K_{\mathrm{ref}}),$$

where $\mathbb{P}_0^p(K_{\mathrm{ref}})$ stands for the space of polynomials of degree at most p which vanishes at the endpoints of the interval K_{ref}. For each polynomial degree $p \geq 2$ there exists $p - 1$ distinct positive eigenvalues $\lambda_2^p < \lambda_3^p < \cdots < \lambda_p^p$. The corresponding eigenfunctions ℓ_i^p, $i = 2, \ldots, p$, are orthogonal in both $H_0^1(K_{\mathrm{ref}})$-

and $L^2(K_{\mathrm{ref}})$-inner products and they are normalized such that

$$\big((\ell_i^p)', (\ell_i^p)'\big)_{K_{\mathrm{ref}}} = 1/2 \quad \text{and} \quad (\ell_i^p, \ell_i^p)_{K_{\mathrm{ref}}} = 1/(2\lambda_i^p), \quad i = 2, 3, \dots, p. \tag{17}$$

Finally, since each polynomial ℓ_i^p has roots ± 1, we can factor out these root factors and define the corresponding kernels $\mathcal{K}_i^p$ as follows

$$\ell_i^p(\xi) = \ell_0(\xi)\ell_1(\xi)\mathcal{K}_i^p(\xi), \quad i = 2, \dots, p, \ p \geq 2. \tag{18}$$

To define the basis of V_{hp} we transform the shape functions from the reference element K_{ref} to the physical elements $K \in \mathcal{T}_{hp}$ using the reference mapping (16). The standard piecewise linear vertex functions φ_k are constructed for $k = 1, 2, \dots, M$ as follows

$$\varphi_k(x) = \begin{cases} \ell_1\big(\chi_{K_k}^{-1}(x)\big), & \text{for } x \in K_k, \\ \ell_0\big(\chi_{K_{k+1}}^{-1}(x)\big), & \text{for } x \in K_{k+1}, \\ 0 & \text{otherwise.} \end{cases}$$

The $N - M$ bubble functions $\varphi_{M+1}, \dots, \varphi_N$, where $N = -1 + \sum_{K \in \mathcal{T}_{hp}} p_K$ is the dimension of V_{hp}, are defined in a similar way. The $p_K - 1$ bubble functions $\varphi_2^{b,K}, \varphi_3^{b,K}, \dots, \varphi_{p_K}^{b,K}$ in an element K are constructed as

$$\varphi_i^{b,K}(x) = \begin{cases} \ell_i^{p_K}(\chi_K^{-1}(x)), & \text{for } x \in K, \\ 0 & \text{otherwise,} \end{cases} \qquad i = 2, 3, \dots, p_K. \tag{19}$$

As usual, we assemble the stiffness matrix $\mathbb{A} \in \mathbb{R}^{N \times N}$, $\mathbb{A}_{ij} = a(\varphi_i, \varphi_j)$, $i, j = 1, 2, \dots, N$, from the local stiffness matrices $\mathbb{A}^K \in \mathbb{R}^{(p_K+1)\times(p_K+1)}$, $K \in \mathcal{T}_{hp}$. The entries of $\mathbb{A}^K$ can be computed as follows

$$\mathbb{A}_{ij}^K = \frac{2}{h_K}(\ell_{i-1}', \ell_{j-1}')_{K_{\mathrm{ref}}} + \frac{h_K}{2}\kappa^2(\ell_{i-1}, \ell_{j-1})_{K_{\mathrm{ref}}}, \quad i, j = 1, \dots, p_K + 1,$$

where $\ell_i = \ell_i^{p_K}$ for $i = 2, 3, \dots, p_K$.

Due to the existence of the vertex and bubble functions, the matrices $\mathbb{A}$ and $\mathbb{A}^K$ have a natural 2-by-2 block structure

$$\mathbb{A} = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix}, \quad \text{and} \quad \mathbb{A}^K = \begin{pmatrix} A^K & B^K \\ (B^K)^T & D^K \end{pmatrix},$$

where $A \in \mathbb{R}^{M \times M}$, $B \in \mathbb{R}^{M \times (N-M)}$, and $D \in \mathbb{R}^{(N-M)\times(N-M)}$, $A^K \in \mathbb{R}^{2\times 2}$, $B^K \in \mathbb{R}^{2\times(p_K-1)}$, and $D^K \in \mathbb{R}^{(p_K-1)\times(p_K-1)}$. The entries of the local stiffness matrix $\mathbb{A}^K$ can be easily computed. If the length of the element K is denoted by h then

$$hA^K = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \frac{\kappa^2 h^2}{6} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \tag{20}$$

The entries of B^K depend on the polynomial degree p_K in a nontrivial way. There are no explicit formulas for them, but they can be computed easily as follows

$$hB_{ij}^K = \kappa^2 h^2 \overline{B}_{ij}^{p_K}, \quad \text{where} \quad \overline{B}_{ij}^{p_K} = \frac{1}{2}(\ell_{i-1}, \ell_{j+1}^{p_K})_{K_{\mathrm{ref}}}, \tag{21}$$

$i = 1, 2,\ j = 1, \ldots, p_K - 1$. Notice that the values $\overline{B}_{ij}^{p_K}$ are independent from h and κ^2. The final block D^K is diagonal with entries

$$hD_{ii}^K = 2\Big((\ell_{i+1}^{p_K})', (\ell_{i+1}^{p_K})'\Big)_{K_{\mathrm{ref}}} + \kappa^2 h^2 \frac{1}{2}(\ell_{i+1}^{p_K}, \ell_{i+1}^{p_K})_{K_{\mathrm{ref}}} = 1 + \kappa^2 h^2 \mu_i^{p_K}, \tag{22}$$

where $\mu_i^{p_K} = 1/(4\lambda_{i+1}^{p_K})$ is independent form h and κ^2, see (17), and $i = 1, 2, \ldots, p_K - 1$.

We remark that it is convenient to multiply the formulas for A^K, B^K, and D^K by h because then the entries of matrices hA^K, hB^K, and hD^K are functions of a single parameter $\zeta = \kappa^2 h^2$.

To prove the DMP it is convenient to introduce the discrete minimum energy extensions $\psi_1, \psi_2, \ldots, \psi_M$ of the vertex functions $\varphi_1, \varphi_2, \ldots, \varphi_M$ with respect to the space of all bubbles $V_{hp}^b = \mathrm{span}\{\varphi_i^{b,K},\ i = 2, 3, \ldots, p_K,\ K \in \mathcal{T}_{hp}\}$.

In analogy with (12) we express

$$\psi_i = \varphi_i - \sum_{\substack{K \in \mathcal{T}_{hp} \\ K \subset \operatorname{supp} \varphi_i}} \sum_{j=1}^{p_K - 1} C_{\iota_K(i),j}^K \varphi_{j+1}^{b,K}, \quad i = 1, 2, \ldots, M. \tag{23}$$

where $\iota_K(i)$ is the standard connectivity mapping, see, e.g., [16]. In our case $\iota_K(i) = 1$ if ψ_i corresponds to the left endpoint of K and $\iota_K(i) = 2$ if ψ_i corresponds to the right endpoint of K. The matrix C^K of coefficients $C_{\iota_K(i),j}^K$ is given by (13) as $C^K = B^K (D^K)^{-1}$ and hence, putting $\zeta = \kappa^2 h_K^2$, the entries of C^K can be expressed by (21) and (22) as

$$C_{mj}^K = \zeta \overline{B}_{mj}^{p_K} (1 + \zeta \mu_j^{p_K})^{-1}, \quad m = 1, 2,\ j = 1, \ldots, p_K. \tag{24}$$

Thus, if the vertex functions ψ_i is supported in an element $K \in \mathcal{T}_{hp}$ then we can transform it to the reference element K_{ref} as follows

$$\overline{\psi}_{m-1}(\xi) = \psi_i(\chi_K(\xi)) = \ell_{m-1}(\xi) - \sum_{j=1}^{p_K - 1} C_{mj}^K \ell_{j+1}^{p_K}(\xi) = \ell_{m-1}(\xi) \Psi_{m-1}^{p_K}(\zeta, \xi), \tag{25}$$

where $m = \iota_K(i) \in \{1, 2\}$, $\xi \in K_{\mathrm{ref}}$, $\zeta = \kappa^2 h_K^2$, and by (18) and (24) we obtain

$$\Psi_{m-1}^{p_K}(\zeta, \xi) = 1 - \ell_{2-m}(\xi)\zeta \sum_{j=1}^{p_K-1} \overline{B}_{mj}^{p_K}(1 + \zeta\mu_j^{p_K})^{-1}\mathcal{K}_{j+1}^{p_K}(\xi). \tag{26}$$

Notice that $\Psi_0^p(\zeta, \xi) = \Psi_1^p(\zeta, -\xi)$ for $\zeta \geq 0$ and $\xi \in K_{\mathrm{ref}}$, because each generalized eigenfunction $\ell_j^p(\xi)$ is either odd or even.

Further, by (9) the discrete minimum energy extensions $\psi_1, \psi_2, \ldots, \psi_M$ are orthogonal to all bubbles $\varphi_i^{b,K}$, $i = 2, 3, \ldots, p_K$, $K \in \mathcal{T}_{hp}$, where the orthogonality is understood in the energy inner product $a(\cdot, \cdot)$. Hence, by (14) the stiffness matrix $\mathbb{S} \in \mathbb{R}^{N\times N}$ formed from the discrete minimum energy extensions $\psi_1, \psi_2, \ldots, \psi_M$ and from the eigenfunctions $\varphi_i^{b,K}$, $i = 2, 3, \ldots, p_K$, $K \in \mathcal{T}_{hp}$, has the following structure

$$\mathbb{S} = \begin{pmatrix} S & 0 \\ 0 & D \end{pmatrix}, \tag{27}$$

where $S = A - BD^{-1}B^T$ stands for the Schur complement and D is diagonal.

6 Nonnegativity of the discrete Green's function

The DGF corresponding to problem (3) can be expressed by (8) using the discrete minimum energy extensions ψ_i, $i = 1, 2, \ldots, M$, see (23), and the bubble functions $\varphi_i^{b,K}$, $i = 2, 3, \ldots, p_K$, $K \in \mathcal{T}_{hp}$, see (19). Thanks to the structure of the stiffness matrix $\mathbb{S}$, see (27), we can express the DGF as a sum of the vertex and bubble parts

$$G_{hp}(x, y) = G_{hp}^v(x, y) + G_{hp}^b(x, y), \quad (x, y) \in \Omega^2, \tag{28}$$

where

$$G_{hp}^v(x, y) = \sum_{i=1}^{M}\sum_{j=1}^{M} S_{ij}^{-1}\psi_i(x)\psi_j(y), \quad (x, y) \in \Omega^2, \tag{29}$$

$$G_{hp}^b(x, y) = \sum_{K\in\mathcal{T}_{hp}} \sum_{i=1}^{p_K-1} (D_{ii}^K)^{-1}\varphi_{i+1}^{b,K}(x)\varphi_{i+1}^{b,K}(y), \quad (x, y) \in \Omega^2, \tag{30}$$

and the entries D_{ii}^K are given by (22).

The following theorem introduces three sufficient conditions for the nonnegativity of the DGF G_{hp}.

Theorem 6.1 *Let ψ_i, $i = 1, 2, \ldots, M$, $S \in \mathbb{R}^{M\times M}$, and G_{hp} be given by* (23), (27), *and* (28)–(30), *respectively. If*

(a) $\psi_i(x) \geq 0$ *for all* $i = 1, 2, \ldots, M$ *and* $x \in \Omega$,
(b) $S_{ij} \leq 0$ *for all* $i \neq j$, $i, j = 1, 2, \ldots, M$,
(c) $G^v_{hp} + G^b_{hp} \geq 0$ *in* K^2 *for all* $K \in \mathcal{T}_{hp}$,

then $G_{hp}(x, y) \geq 0$ *for all* $(x, y) \in \Omega^2$.

Proof. By the theory of M-matrices, see, e.g., [13], if all offdiagonal entries of S are nonpositive and if S is symmetric and positive definite then S^{-1} consists of nonnegative entries, i.e, $(S^{-1})_{ij} \geq 0$ for all $i, j = 1, 2, \ldots, M$. Hence, this fact together with (a) imply the nonnegativity of the vertex part G^v_{hp} in Ω^2, see (29). Since the support of any bubble function consists of a single element, we find that

$$G^b_{hp}(x, y) = 0 \quad \text{for } (x, y) \in K \times K^*,\ K \neq K^*,\ K, K^* \in \mathcal{T}_{hp}.$$

This together with (c) proves the nonnegativity of $G_{hp} = G^v_{hp} + G^b_{hp}$ in the entire square Ω^2. $\square$

6.1 Nonnegativity of the vertex DGF

We present two lemmas which show the validity of conditions (a) and (b) from Theorem 6.1 provided that the products $\kappa^2 h_K^2$ are bounded from above by values α^{p_K} and β^{p_K} for all elements $K \in \mathcal{T}_{hp}$. The bounds α^{p_K} and β^{p_K} are given by

$$\alpha^p = \sup\{\overline{\zeta} : \Psi^p_1(\zeta, \xi) \geq 0 \text{ for all } \xi \in K_{\text{ref}} \text{ and all } 0 \leq \zeta \leq \overline{\zeta}\}, \tag{31}$$
$$\beta^p = \sup\{\overline{\zeta} : q^p(\zeta) \leq 0 \text{ for all } 0 \leq \zeta \leq \overline{\zeta}\}, \tag{32}$$

where

$$q^p(\zeta) = -1 + \zeta/6 - \zeta^2 \sum_{i=1}^{p-1} \overline{B}^p_{1i} \overline{B}^p_{2i} (1 + \zeta \mu^p_i)^{-1}. \tag{33}$$

Notice that $q^p(\kappa^2 h^2) = h S^K_{12}$, where and $S^K = A^K - B^K (D^K)^{-1} (B^K)^T \in \mathbb{R}^{2\times 2}$, see (20)–(22). Further notice that both α^p and β^p are positive due to the continuity of Ψ^p_1 and q^p and due to the fact that $\Psi_1(0, \xi) = 1$ and $q^p(0) = -1$.

Lemma 6.1 *Let* h_K *and* p_K *stand for the length and polynomial degree of the element* $K \in \mathcal{T}_{hp}$. *Further, let* ψ_i, $i = 1, 2, \ldots, M$, *be given by* (23). *If*

$$\kappa^2 h_K^2 \leq \alpha^{p_K} \quad \textit{for all } K \in \mathcal{T}_{hp}$$

then $\psi_i(x) \geq 0$ *for all* $x \in \Omega$, *i.e., condition* (a) *from Theorem 6.1 is satisfied.*

Proof. Let the vertex function ψ_i corresponds to a nodal point x_i, $i = 1, 2, \ldots, M$. The nonnegativity of ψ_i in $K_i = [x_{i-1}, x_i]$ follows immediately from (25) and (26) with $m = 1$ and then from (31). The nonnegativity of ψ_i in $K_{i+1} = [x_i, x_{i+1}]$ follows symmetrically, because $\Psi_0^p(\zeta, \xi) = \Psi_1^p(\zeta, -\xi)$. □

Lemma 6.2 *Let h_K and p_K denote the length and the polynomial degree of the element $K \in \mathcal{T}_{hp}$. Further, let S be given by (27). If*

$$\kappa^2 h_K^2 \leq \beta^{p_K} \quad \textit{for all } K \in \mathcal{T}_{hp}$$

then $S_{ij} \leq 0$ for all $i \neq j$, $i, j = 1, 2, \ldots, M$, i.e., condition (b) *from Theorem 6.1 is satisfied.*

Proof. Clearly, the matrix S is tridiagonal, hence, the only nonzero off-diagonal entries are

$$S_{k,k-1} = S_{k-1,k} = a_K(\psi_{k-1}, \psi_k) = S_{12}^K, \quad k = 2, 3, \ldots, M,$$

where ψ_{k-1} and ψ_k are the vertex functions corresponding to the endpoints of $K \in \mathcal{T}_{hp}$, S is given by (27), and $S^K = A^K - B^K(D^K)^{-1}(B^K)^T$ is the local Schur complement. The nonpositivity of the entry S_{12}^K follows immediately from (33) and (32). □

We remark that β^p can be computed as the smallest positive root of the polynomial $q^p(\zeta)\prod_{i=1}^{p-1}(1 + \zeta\mu_i^p)$. Similarly, the computation of the values α^p requires root finding of certain polynomials. The conclusions from Theorem 6.1 and Lemmas 6.1 and 6.2 are summarized in the following corollary.

Corollary 6.1 *Let $\mathcal{T}_{hp}$ be a finite element mesh and let h_K and p_K denote the length and the polynomial degree of the element $K \in \mathcal{T}_{hp}$. If*

$$\kappa^2 h_K^2 \leq \min\{\alpha^{p_K}, \beta^{p_K}\} \quad \textit{for all } K \in \mathcal{T}_{hp}$$

then $G_{hp}^v(x, y) \geq 0$ for all $(x, y) \in \Omega^2$.

7 The bubble part of the DGF

In this section we study the validity of condition (c) from Theorem 6.1. The bubble part G_{hp}^b defined by (30) is not nonnegative, in general. For $p = 3$, $p = 5$, and $p \geq 7$, there always are regions, where G_{hp}^b is negative. In these regions, the negative bubble part G_{hp}^b has to be compensated by the positive vertex part G_{hp}^v in order to obtain the nonnegativity of $G_{hp} = G_{hp}^v + G_{hp}^b$ and consequently the DMP. Fortunately, condition (c) can be investigated for each element $K \in \mathcal{T}_{hp}$ independently.

Therefore, throughout this section, we consider an arbitrary but fixed element $K = [x_{k-1}, x_k]$ in $\mathcal{T}_{hp}$. The length and the polynomial degree of this K are denoted by h and p.

For this K we will define two auxiliary DGFs $\widetilde{G}_{hp}$ and $\widehat{G}_{hp}$, see Figure 1 for an illustration. We will show that $\widehat{G}_{hp} \leq \widetilde{G}_{hp} \leq G_{hp}$ in K^2. The nonnegativity of the second auxiliary DGF $\widehat{G}_{hp}$ is investigated below in Section 7.4.

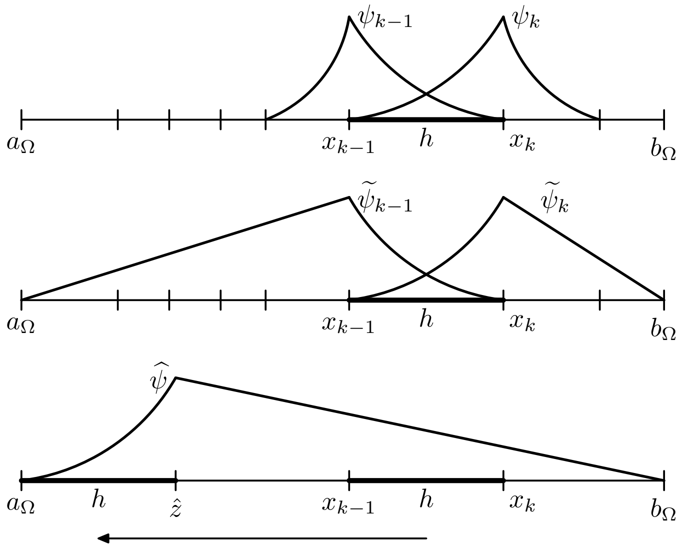

Fig. 1. An illustration of the basis functions used for the construction of G^v_{hp} (top), $\widetilde{G}^v_{hp}$ (middle), and $\widehat{G}^v_{hp}$ (bottom) corresponding to the element $K = [x_{k-1}, x_k]$ of the length h.

7.1 The first auxiliary DGF

An element $K \in \mathcal{T}_{hp}$ is called interior if it is not adjacent to the boundary of Ω, i.e., if $K \subset \Omega$. We define the first auxiliary DGF $\widetilde{G}_{hp}$ for interior elements only. Thus, let $K = [x_{k-1}, x_k]$ be an interior element. We consider a partition $a_\Omega < x_{k-1} < x_k < b_\Omega$ which defines a mesh $\widetilde{\mathcal{T}}_{hp}$ consisting of three elements. The polynomial degree assigned to the element $K = [x_{k-1}, x_k] \in \widetilde{\mathcal{T}}_{hp}$ is p while the degree of the other two elements in $\widetilde{\mathcal{T}}_{hp}$ is set to 1. These polynomial degrees and the mesh $\widetilde{\mathcal{T}}_{hp}$ lead to an hp-FEM space $\widetilde{V}_{hp}$ defined in analogy with (2). In $\widetilde{V}_{hp}$ we consider two piecewise linear vertex functions $\widetilde{\varphi}_{k-1}$ and $\widetilde{\varphi}_k$ and $p-1$ bubble functions $\varphi_2^{b,K}, \varphi_3^{b,K}, \dots, \varphi_p^{b,K}$, see (19). Notice that these bubble functions (generalized eigenfunctions of the Laplacian) coincide with the bubbles defined on the original mesh $\mathcal{T}_{hp}$.

Further, we consider the discrete minimum energy extensions $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$ of $\widetilde{\varphi}_{k-1}$ and $\widetilde{\varphi}_k$ with respect to the space $V_{hp}^{b,K} = \operatorname{span}\{\varphi_2^{b,K}, \varphi_3^{b,K}, \dots, \varphi_p^{b,K}\}$. Hence, $\widetilde{\psi}_{k-1}$ is linear in $[a_\Omega, x_{k-1}]$, $\widetilde{\psi}_{k-1} = \psi_{k-1}$ in $K = [x_{k-1}, x_k]$, and $\widetilde{\psi}_{k-1} = 0$ in $[x_k, b_\Omega]$. Similarly, $\widetilde{\psi}_k = 0$ in $[a_\Omega, x_{k-1}]$, $\widetilde{\psi}_k = \psi_k$ in $K = [x_{k-1}, x_k]$, and $\widetilde{\psi}_k$ is linear in $[x_k, b_\Omega]$. See the middle panel of Figure 1.

We construct a stiffness matrix $\widetilde{A} \in \mathbb{R}^{2\times 2}$ from $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$ as follows

$$\widetilde{A}_{ij} = a(\widetilde{\psi}_{k-2+i}, \widetilde{\psi}_{k-2+j}), \quad i,j = 1,2. \tag{34}$$

In agreement with (28)–(30), we define the first auxiliary DGF

$$\widetilde{G}_{hp}(x,y) = \widetilde{G}^v_{hp}(x,y) + \widetilde{G}^b_{hp}(x,y), \quad (x,y) \in \Omega^2, \tag{35}$$

where

$$\widetilde{G}^v_{hp}(x,y) = \sum_{i=1}^{2}\sum_{j=1}^{2} \widetilde{A}^{-1}_{ij} \widetilde{\psi}_{k-2+i}(x)\widetilde{\psi}_{k-2+j}(y), \quad (x,y) \in \Omega^2 \tag{36}$$

and $\widetilde{G}^b_{hp}(x,y) = G^b_{hp}(x,y)$, see (30).

The main result about $\widetilde{G}_{hp}(x,y)$ is formulated in the following lemma.

Lemma 7.1 *Let condition* (b) *from Theorem 6.1 be satisfied. For an interior element $K \in \mathcal{T}_{hp}$, $K = [x_{k-1}, x_k] \subset \Omega$, $k = 2,3,\dots,M$, consider the first auxiliary DGF $\widetilde{G}_{hp}$ defined by* (35)–(36) *and the DGF G_{hp} given by* (28)–(30). *Then*

$$G_{hp}(x,y) \ge \widetilde{G}_{hp}(x,y) \quad \textit{for all } (x,y) \in K^2.$$

Proof. Clearly, it suffices to prove $G^v_{hp}(x,y) \ge \widetilde{G}^v_{hp}(x,y)$ for all $(x,y) \in K^2$. Let $K \in \mathcal{T}_{hp}$, $K = [x_{k-1}, x_k] \subset \Omega$, be an arbitrary but fixed interior element. First, we consider the original vertex functions $\psi_1, \psi_2, \dots, \psi_M$. Let ψ^{me}_{k-1} and ψ^{me}_k be the discrete minimum energy extensions of ψ_{k-1} and ψ_k with respect to $V^{v\#}_{hp} = \mathrm{span}\{\psi_1, \dots, \psi_{k-2}, \psi_{k+1}, \dots, \psi_M\}$. Definition (11) yields $\psi^{\mathrm{me}}_{k-1}(x) = \psi_{k-1}(x)$ and $\psi^{\mathrm{me}}_k(x) = \psi_k(x)$ for all $x \in K$, because $\psi_j(x) = 0$ for all $x \in K$ and all $\psi_j \in V^{v\#}_{hp}$. Using the definition of $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$, we summarize

$$\psi_{k-1} = \widetilde{\psi}_{k-1} = \psi^{\mathrm{me}}_{k-1} \quad \text{and} \quad \psi_k = \widetilde{\psi}_k = \psi^{\mathrm{me}}_k \quad \text{in } K. \tag{37}$$

The stiffness matrix $S^{\mathrm{me}} \in \mathbb{R}^{2\times 2}$ corresponding to the basis functions ψ^{me}_{k-1} and ψ^{me}_k can be computed as a suitable Schur complement, cf. (15).

Now, let us concentrate on $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$. We remark that the discrete minimum energy extensions $\widetilde{\psi}^{\mathrm{me}}_{k-1}$ and $\widetilde{\psi}^{\mathrm{me}}_k$ of $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$ with respect to $V^{v\#}_{hp}$ are equal to the already defined discrete minimum energy extensions ψ^{me}_{k-1} and ψ^{me}_k, respectively. Indeed, see (9), if $0 = a(\psi^{\mathrm{me}}_k, v^\#) = a(\widetilde{\psi}^{\mathrm{me}}_k, v^\#)$ for all $v^\# \in V^{v\#}_{hp}$ then $0 = a(\psi^{\mathrm{me}}_k - \widetilde{\psi}^{\mathrm{me}}_k, v^\#)$ for all $v^\# \in V^{v\#}_{hp}$ and since $\psi^{\mathrm{me}}_k - \widetilde{\psi}^{\mathrm{me}}_k \in V^{v\#}_{hp}$ then $\psi^{\mathrm{me}}_k = \widetilde{\psi}^{\mathrm{me}}_k$. The same steps can be repeated to show that $\psi^{\mathrm{me}}_{k-1} = \widetilde{\psi}^{\mathrm{me}}_{k-1}$.

From (37) we conclude that

$$\widetilde{A}_{12} = a_K(\widetilde{\psi}_{k-1}, \widetilde{\psi}_k) = a_K(\psi^{\mathrm{me}}_{k-1}, \psi^{\mathrm{me}}_k) = S^{\mathrm{me}}_{12}.$$

Similarly, from (10) we infer the inequalities

$$
\begin{aligned}
\widetilde{A}_{11} &= a(\widetilde{\psi}_{k-1}, \widetilde{\psi}_{k-1}) \geq a(\widetilde{\psi}^{\mathrm{me}}_{k-1}, \widetilde{\psi}^{\mathrm{me}}_{k-1}) = a(\psi^{\mathrm{me}}_{k-1}, \psi^{\mathrm{me}}_{k-1}) = S^{\mathrm{me}}_{11},\\
\widetilde{A}_{22} &= a(\widetilde{\psi}_{k}, \widetilde{\psi}_{k}) \geq a(\widetilde{\psi}^{\mathrm{me}}_{k}, \widetilde{\psi}^{\mathrm{me}}_{k}) = a(\psi^{\mathrm{me}}_{k}, \psi^{\mathrm{me}}_{k}) = S^{\mathrm{me}}_{22}.
\end{aligned}
$$

Hence, all entries of $\widetilde{A}$ are greater or equal to the corresponding entries of S^{me} and we write $\widetilde{A} \geq S^{\mathrm{me}}$. Condition (b) from Theorem 6.1 implies that both $\widetilde{A}$ and S^{me} are M-matrices. In particular, they have the nonnegative inverse and therefore $(S^{\mathrm{me}})^{-1} \geq \widetilde{A}^{-1}$. By this fact and by (29), (15), (37), we conclude

$$
\begin{aligned}
G^{v}_{hp}(x,y) = \sum_{i=1}^{M}\sum_{j=1}^{M}(S^{-1})_{ij}\psi_i(x)\psi_j(y) &= \sum_{i=1}^{2}\sum_{j=1}^{2}(S^{\mathrm{me}})^{-1}_{ij}\psi^{\mathrm{me}}_{k-2+i}(x)\psi^{\mathrm{me}}_{k-2+j}(y)\\
&\geq \sum_{i=1}^{2}\sum_{j=1}^{2}(\widetilde{A}^{-1})_{ij}\widetilde{\psi}_{k-2+i}(x)\widetilde{\psi}_{k-2+j}(y) = \widetilde{G}^{v}_{hp}(x,y)
\end{aligned}
$$

for all $(x,y) \in K^2$. $\square$

7.2 Analysis of the first auxiliary DGF

Let us analyze the auxiliary DGF $\widetilde{G}_{hp}$ in more detail. For arbitrary element $K \in \mathcal{T}_{hp}$, $K = [x_{k-1}, x_k]$, with the polynomial degree p and with the length h we introduce a parameter $t \in [0,1]$ such that

$$
\begin{aligned}
x_{k-1} &= (1-t)a_\Omega + t(b_\Omega - h),\\
x_k &= (1-t)(a_\Omega + h) + t b_\Omega.
\end{aligned}
\tag{38}
$$

Clearly, the parameter t determines the position of K in $\Omega = (a_\Omega, b_\Omega)$. In addition, we define an auxiliary parameter $\theta \in (0,\infty]$ as

$$
\theta = \frac{h}{|\Omega| - h},
\tag{39}
$$

where $|\Omega| = b_\Omega - a_\Omega$ stands for the length of Ω.

Here, we restrict ourselves to the interior elements only, i.e., we assume $t \in (0,1)$. To express the stiffness matrix $\widetilde{A} \in \mathbb{R}^{2\times 2}$ assembled from $\widetilde{\psi}_{k-1}$ and $\widetilde{\psi}_k$ we introduce functions

$$
r^p(\zeta) = hS^K_{11} = hS^K_{22} = 1 + \zeta/3 - \zeta^2 \sum_{i=1}^{p-1}\left(\overline{B}^p_{1i}\right)^2 (1+\zeta\mu^p_i)^{-1},
\tag{40}
$$

where $\zeta = \kappa^2 h^2$, $S^K = A^K - B^K(D^K)^{-1}(B^K)^T$, cf. (27), and matrices A^K, B^K, D^K are given by (20)–(22). We remark that $\left(\overline{B}^p_{1i}\right)^2 = \left(\overline{B}^p_{2i}\right)^2$, because the generalized eigenfunctions of the Laplacian are either odd or even. Further we stress that $r^p(\zeta) = r^p(\kappa^2 h^2) = a_K(\psi_{k-1}, \psi_{k-1}) = a_K(\psi_k, \psi_k) > 0$ for $h > 0$.

Using (33), (40), and the parameters t and θ, we can express $\widetilde{A}$ as

$$h\widetilde{A} = \begin{pmatrix} r^p(\kappa^2h^2) + \dfrac{\theta}{t} + \dfrac{\kappa^2h^2}{3}\dfrac{t}{\theta} & q^p(\kappa^2h^2) \\ q^p(\kappa^2h^2) & r^p(\kappa^2h^2) + \dfrac{\theta}{1-t} + \dfrac{\kappa^2h^2}{3}\dfrac{1-t}{\theta} \end{pmatrix}.$$

Our goal is to study the limit of $h\widetilde{A}$ for $t \to 0$. The entry $(h\widetilde{A})^{-1}_{11} \to 0$ for $t \to 0$ and, therefore, we concentrate on

$$s(t,\theta,\zeta) = (h\widetilde{A})^{-1}_{22} = \left(r^p(\zeta) + \frac{\theta}{1-t} + \frac{\zeta}{3}\frac{1-t}{\theta} - \frac{(q^p)^2(\zeta)}{r^p(\zeta) + \dfrac{\theta}{t} + \dfrac{\zeta}{3}\dfrac{t}{\theta}} \right)^{-1}, \tag{41}$$

which is well defined for $t \in (0,1)$, $\theta \in (0,\infty)$, and $\zeta = \kappa^2h^2 \in [0,\infty)$. For $t = 0$ we define $s(t,\theta,\zeta)$ by the following limit

$$s(0,\theta,\zeta) = \lim_{t\to 0_+} s(t,\theta,\zeta) = \left(r^p(\zeta) + \theta + \frac{\zeta}{3\theta} \right)^{-1}. \tag{42}$$

Lemma 7.2 *If $s(t,\theta,\zeta)$ is defined by (41) and (42) then*

$$s(0,\theta,\zeta) \le s(t,\theta,\zeta) \quad \textit{for all } \theta \in (0,1/2],\ t \in [0,1/2],\ \zeta \in [0,\infty). \tag{43}$$

Proof. For $t > 0$ the inequality (43) is equivalent to

$$s^*(t,\theta,\zeta) = \frac{[s(t,\theta,\zeta)]^{-1} - [s(0,\theta,\zeta)]^{-1}}{t} = \frac{\theta}{1-t} - \frac{\zeta}{3\theta} - \frac{(q^p)^2(\zeta)}{r^p(\zeta)t + \theta + \dfrac{\zeta}{3}\dfrac{t^2}{\theta}} \le 0. \tag{44}$$

Clearly, since $r^p(\zeta) > 0$, the function $s^*(t,\theta,\zeta)$ is increasing in the variable t. Hence,

$$s^*(t,\theta,\zeta) \le s^*(1/2,\theta,\zeta) = 2\theta - \frac{\zeta}{3\theta} - \frac{(q^p)^2(\zeta)}{\dfrac{1}{2}r^p(\zeta) + \theta + \dfrac{\zeta}{12\theta}}. \tag{45}$$

Differentiating $s^*(1/2,\theta,\zeta)$ with respect to θ and using the fact that $\det(hS^K) = (r^p)^2(\zeta) - (q^p)^2(\zeta) > 0$, we find out that $s^*(1/2,\theta,\zeta)$ is increasing in θ. Thus,

$$s^*(1/2,\theta,\zeta) \le s^*(1/2,1/2,\zeta) = 1 - \frac{2}{3}\zeta - \frac{2(q^p)^2(\zeta)}{r^p(\zeta) + 1 + \dfrac{\zeta}{3}}. \tag{46}$$

Similarly, it can be verified that $s^*(1/2, 1/2, \zeta)$ is decreasing in ζ and, therefore,

$$s^*(1/2, 1/2, \zeta) \le s^*(1/2, 1/2, 0) = 0, \tag{47}$$

because $r^p(0) = 1$ and $q^p(0) = -1$. The combination of (44)–(47) finishes the proof. $\square$

7.3 The second auxiliary DGF

In general, there are two second auxiliary DGF. The fist one is adjacent to the left endpoint a_Ω and the second one is adjacent to the right endpoint b_Ω. For an interior element $K = [x_{k-1}, x_k] \in \mathcal{T}_{hp}$ we consider the parameter t given by (38). If $t \le 1/2$ we define the second auxiliary DGF $\widehat{G}_{hp}$ as a limit of the first auxiliary DGF $\widetilde{G}_{hp}$ for $t \to 0_+$. If $t > 1/2$ then $\widehat{G}_{hp}$ is a limit of $\widetilde{G}_{hp}$ for $t \to 1_-$. However, the situation is symmetric and we can without loss of generality concentrate on the fist case only.

If h and p stand for the length and polynomial degree of K then we set $\hat{z} = a_\Omega + h$ and consider two-element-mesh $\widehat{\mathcal{T}}_{hp}$ consisting of elements $\widehat{K} = [a_\Omega, \hat{z}]$ and $[\hat{z}, b_\Omega]$ with polynomial degrees p and 1, respectively. The hp-FEM basis on $\widehat{\mathcal{T}}_{hp}$ comprises one piecewise linear vertex function $\widehat{\varphi}$ and $p-1$ bubble functions $\widehat{\varphi}_2^{b,\widehat{K}}, \widehat{\varphi}_3^{b,\widehat{K}}, \dots, \widehat{\varphi}_p^{b,\widehat{K}}$ supported in $\widehat{K}$.

As before, we define $\widehat{\psi}$ as the discrete minimum energy extension of the vertex function $\widehat{\varphi}$ with respect to the space of the bubbles $V_{hp}^{b,\widehat{K}} = \mathrm{span}\{\widehat{\varphi}_2^{b,\widehat{K}}, \widehat{\varphi}_3^{b,\widehat{K}}, \dots, \widehat{\varphi}_p^{b,\widehat{K}}\}$, see the bottom panel of Figure 1. Notice that $\widehat{\psi}$ is a linear function in $[\hat{z}, b_\Omega]$ and that $\widehat{\psi}$ restricted to $\widehat{K}$ is just the shifted function $\widetilde{\psi}_k = \psi_k$ restricted to K, i.e.,

$$\widehat{\psi}(x - x_{k-1} + a_\Omega) = \widetilde{\psi}_k(x) = \psi_k(x) \quad \text{for all } x \in K. \tag{48}$$

Furthermore, we can easily compute $a\left(\widehat{\psi}, \widehat{\psi}\right) = [hs(0, \theta, \kappa^2 h^2)]^{-1}$. Hence, in agreement with (28)–(30) we define

$$\widehat{G}_{hp}(x, y) = \widehat{G}_{hp}^v(x, y) + \widehat{G}_{hp}^b(x, y), \quad (x, y) \in \Omega^2, \tag{49}$$

$$\widehat{G}_{hp}^v(x, y) = hs(0, \theta, \kappa^2 h^2)\widehat{\psi}(x)\widehat{\psi}(y), \quad (x, y) \in \Omega^2, \tag{50}$$

$$\widehat{G}_{hp}^b(x, y) = \sum_{i=1}^{p-1} (D_{ii}^{\widehat{K}})^{-1} \widehat{\varphi}_{i+1}^{b,\widehat{K}}(x) \widehat{\varphi}_{i+1}^{b,\widehat{K}}(y), \quad (x, y) \in \Omega^2. \tag{51}$$

We recall that the entries $D_{ii}^{\widehat{K}} = D_{ii}^K$ are given by (22).

For completeness, we also introduce the auxiliary DGFs for the elements adjacent to the boundary of Ω. For $K = [a_\Omega, x_1] \in \mathcal{T}_{hp}$ we define

$$\widetilde{G}_{hp}(x, y) = \widehat{G}_{hp}(x, y) \quad \text{for all } (x, y) \in \Omega^2, \tag{52}$$

where $\widehat{G}_{hp}(x, y)$ is given by (49)–(51) with $\widehat{K} = K$. For $K = [x_M, b_\Omega] \in \mathcal{T}_{hp}$ we define $\widehat{G}_{hp}(x, y) = \widetilde{G}_{hp}(x, y)$ symmetrically. The relation of the first and of the second auxiliary DGF explains the following lemma.

Lemma 7.3 *Let conditions* (a) *and* (b) *from Theorem 6.1 be satisfied. Further, let $K \in \mathcal{T}_{hp}$ be such that $t \le 1/2$, see* (38)*, and let $\theta \le 1/2$, see* (39)*. If $\widehat{G}_{hp}(x, y)$ and $\widetilde{G}_{hp}(x, y)$ are given by* (49)–(51) *and* (35)–(36) *with* (52) *then*

$$\widehat{G}_{hp}(\hat{x}, \hat{y}) \le \widetilde{G}_{hp}(x, y) \quad \textit{for all } (x, y) \in K^2,$$

where $\hat{x} = x - x_{k-1} + a_\Omega$ and $\hat{y} = y - x_{k-1} + a_\Omega$.

Proof. First, if $K = [a_\Omega, x_1]$ then there is nothing to prove due to (52). The element K is not adjacent to the right endpoint due to the assumptions $t \le 1/2$ and $\theta \le 1/2$. Thus, it remains to consider the interior elements $K \in \mathcal{T}_{hp}$.

The bubble functions $\widehat{\varphi}_2^{b,\widehat{K}}, \widehat{\varphi}_3^{b,\widehat{K}}, \dots, \widehat{\varphi}_p^{b,\widehat{K}}$ in $\widehat{K}$ are just shifted bubble functions $\varphi_2^{b,K}, \varphi_3^{b,K}, \dots \varphi_p^{b,K}$ from K, see (48). Therefore,

$$\widehat{G}^b_{hp}(\hat{x}, \hat{y}) = \widetilde{G}^b_{hp}(x, y) \quad \text{for all } (x, y) \in K^2,$$

where $\hat{x} = x - x_{k-1} + a_\Omega$ and $\hat{y} = y - x_{k-1} + a_\Omega$. By (48)–(51), Lemma 7.2, the facts that $\widetilde{A}^{-1} \ge 0$, see (34), $\widetilde{\psi}_{k-1} \ge 0$ and $\widetilde{\psi}_k \ge 0$ in K, and by (36) we obtain

$$\begin{aligned}\widehat{G}^v_{hp}(\hat{x}, \hat{y}) = hs(0, \theta, \kappa^2 h^2)\widehat{\psi}(\hat{x})\widehat{\psi}(\hat{y}) &\le hs(t, \theta, \kappa^2 h^2)\widetilde{\psi}_k(x)\widetilde{\psi}_k(y) \\ &\le \sum_{i=1}^{2}\sum_{j=1}^{2} \widetilde{A}^{-1}_{ij}\widetilde{\psi}_{k-2+i}(x)\widetilde{\psi}_{k-2+j}(y) = \widetilde{G}^v_{hp}(x, y)\end{aligned}$$

for all $(x, y) \in K^2$ with $\hat{x} = x - x_{k-1} + a_\Omega$ and $\hat{y} = y - x_{k-1} + a_\Omega$. □

Corollary 7.1 *Let G_{hp} be given by* (28)–(30)*. Further, let $\widehat{G}_{hp}$ given by* (49)–(52) *be the second auxiliary DGF corresponding to an element $K \in \mathcal{T}_{hp}$ and let $\theta \le 1/2$, see* (39)*. If*

$$\widehat{G}_{hp}(\hat{x}, \hat{y}) \ge 0 \quad \textit{for all } (\hat{x}, \hat{y}) \in \hat{K}^2 \tag{53}$$

then

$$G_{hp}(x, y) \ge 0 \quad \textit{for all } (x, y) \in K^2,$$

i.e., the condition (c) from Theorem 6.1 is satisfied.

Proof. Let $K \in \mathcal{T}_{hp}$ be arbitrary. If $t \le 1/2$, see (38), then assumption (53) and Lemmas 7.3 and 7.1 imply

$$0 \le \widehat{G}_{hp}(\hat{x}, \hat{y}) \le \widetilde{G}_{hp}(x, y) \le G_{hp}(x, y) \quad \forall (x, y) \in K^2,$$

where $\hat{x} = x - x_{k-1} + a_\Omega$ and $\hat{y} = y - x_{k-1} + a_\Omega$. The same conclusion is valid also for $t > 1/2$ due to the symmetry. $\square$

7.4 Nonnegativity of the second auxiliary DGF

Finally, we will seek conditions for nonnegativity of $\widehat{G}_{hp}(\hat{x}, \hat{y})$ in $\widehat{K}^2$. It is convenient to transform $\widehat{G}_{hp}$ from $\widehat{K}^2 = [a_\Omega, \hat{z}]$ to $K^2_{\mathrm{ref}} = [-1,1]^2$ using $\hat{x} = \chi_{\widehat{K}}(\xi)$ and $\hat{y} = \chi_{\widehat{K}}(\eta)$, where the reference map $\chi_{\widehat{K}}$ is given by (16). From (25) we have

$$\widehat{\psi}|_{\widehat{K}}(\chi_{\widehat{K}}(\xi)) = \overline{\psi}_1(\xi) = \ell_1(\xi)\Psi_1^p(\zeta, \xi), \tag{54}$$

where $\zeta = \kappa^2 h^2$, h is the length of K, p is the polynomial degree of K, and Ψ_1^p is given by (26).

With the help of (49)–(51), (54), and (42), the transformed DGF $\widehat{G}_{hp}$ can be expressed as follows

$$\begin{aligned} G_{hp}^{\mathrm{ref}}(\xi, \eta) = \widehat{G}_{hp}(\chi_{\widehat{K}}(\xi), \chi_{\widehat{K}}(\eta)) = hs(0, \theta, \kappa^2 h^2)\widehat{\psi}(\chi_{\widehat{K}}(\xi))\widehat{\psi}(\chi_{\widehat{K}}(\eta)) \\ + h\sum_{i=1}^{p-1}(hD_{ii}^K)^{-1}\ell_{i+1}^p(\xi)\ell_{i+1}^p(\eta) = h\ell_1(\xi)\ell_1(\eta)\omega^p(\theta, \kappa^2 h^2, \xi, \eta), \end{aligned} \tag{55}$$

where, see (18), (22), and (25),

$$\omega^p(\theta, \zeta, \xi, \eta) = s(0, \theta, \zeta)\Psi_1^p(\zeta, \xi)\Psi_1^p(\zeta, \eta) + \ell_0(\xi)\ell_0(\eta)\mathrm{Ker}^{b,p}(\zeta, \xi, \eta), \tag{56}$$

$$\mathrm{Ker}^{b,p}(\zeta, \xi, \eta) = \sum_{i=1}^{p-1}(1 + \zeta\mu_i^p)^{-1}\mathcal{K}_{i+1}^p(\xi)\mathcal{K}_{j+1}^p(\eta), \tag{57}$$

and $\zeta = \kappa^2 h^2$. Finally, we define

$$\widehat{\omega}^p(\theta, \zeta) = \min_{(\xi,\eta)\in K^2_{\mathrm{ref}}} \omega^p(\theta, \zeta, \xi, \eta). \tag{58}$$

The motivation for this definition is clear. The second auxiliary DGF $\widehat{G}_{hp}(\hat{x}, \hat{y})$ is nonnegative in $\widehat{K}$ if and only if $\widehat{\omega}^p(\theta, \zeta) \geq 0$.

To analyze the nonnegativity of $\widehat{\omega}^p(\theta, \zeta)$, we set

$$\sigma^p(\theta) = \sup\{\bar{\zeta} : \widehat{\omega}^p(\theta, \zeta) \geq 0 \quad \text{for all } 0 \leq \zeta \leq \bar{\zeta}\}, \text{ where } \theta \in (0, 1/2].$$

By this definition, we immediately conclude that $\widehat{G}_{hp}$ is nonnegative provided $0 < \theta \leq 1/2$ and $0 \leq \zeta \leq \sigma^p(\theta)$.

For given p and θ we can approximately compute the value of $\sigma^p(\theta)$ by halving intervals. The results of these computations for $p = 3, 4, \ldots, 10$ are presented

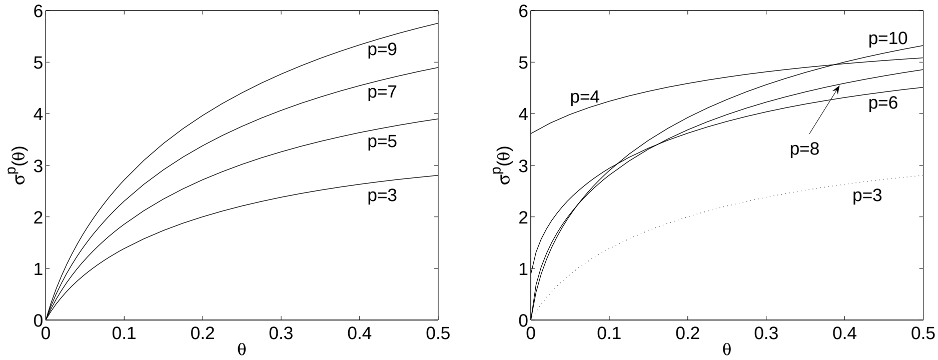

Fig. 2. The graphs of $\sigma^p(\theta)$ for $p = 3, 5, 7, 9$ (left) and for $p = 4, 6, 8, 10$ (right). The dotted line in the right panel shows $\sigma^3(\theta)$ to indicate that $\sigma^3(\theta) \leq \sigma^p(\theta)$ for all $p = 3, 4, \dots, 10$, $\theta \in (0, 1/2]$.

Table 1
The critical values α^p, β^p, γ^p, and δ^p.

p	α^p	β^p	γ^p	δ^p
1	∞	6	0	∞
2	20/3	∞	0	∞
3	38.61	25.89	5.608	0
4	18.91	∞	2.936	3.614
5	49.44	59.82	7.799	0
6	37.56	∞	7.247	0.887
7	72.82	107.81	9.791	0
8	62.62	∞	9.709	0
9	104.09	169.85	11.510	0
10	94.10	∞	10.644	0

in Figure 2. This figure suggests that functions $\sigma^p(\theta)$ are concave and that they can be estimated from below by a line

$$\gamma^p \theta + \delta^p \leq \sigma^p(\theta) \quad \text{for } p = 3, 4, \dots, 10 \text{ and } \theta \in (0, 1/2]. \tag{59}$$

The constants γ^p and δ^p are defined as

$$\delta^p = \sup\{0\} \cup \{\overline{\zeta} : \mathrm{Ker}^{b,p}(\zeta, \xi, \eta) \geq 0 \text{ for all } 0 \leq \zeta \leq \overline{\zeta}\}, \tag{60}$$

$$\gamma^p = \begin{cases} 2\Big(\sigma^p(1/2) - \delta^p\Big) & \text{for } \delta^p < \infty, \\ 0 & \text{for } \delta^p = \infty. \end{cases} \tag{61}$$

The computed values of γ^p and δ^p are presented in Table 1 for $p = 1, 2, \dots, 10$. We remark that $\sigma^p(\theta) \to \delta^p$ for $\theta \to 0$.

The nonnegativity result for the second auxiliary DGF $\widehat{G}_{hp}$ is based on the following assumption.

$$\text{In case } \delta^p < \infty \text{ assume } \gamma^p \geq 3/2 \text{ and } \widehat{\omega}^p(\theta, \gamma^p\theta + \delta^p) \geq 0 \text{ for all } \theta \in (0, 1/2]. \tag{62}$$

This assumption is verified in Section 8 for p up to 10.

Lemma 7.4 *Let $K \in \mathcal{T}_{hp}$, let $\widehat{G}_{hp}$ be defined by* (49)–(52)*, let h and p be the length and the polynomial degree of K, let $\theta = h/(|\Omega| - h)$, let $\zeta = \kappa^2 h^2$, and let γ^p and δ^p be given by* (61) *and* (60)*. In case $\delta^p < \infty$ assume $\theta \leq 1/2$. If the inequality $\zeta \leq \gamma^p\theta + \delta^p$, the condition* (a) *from Theorem 6.1, and the assumption* (62) *are satisfied then $\widehat{G}_{hp}(\hat{x}, \hat{y}) \geq 0$ for all $(\hat{x}, \hat{y}) \in \widehat{K}$.*

Proof. Due to (55)–(58) it suffices to prove the nonnegativity of $\widehat{\omega}^p(\theta, \zeta)$. Since $0 \leq \delta^p \leq \gamma^p\theta + \delta^p$, we can split the proof into three cases.

(i) If $\zeta \in (\delta^p, \gamma^p\theta + \delta^p]$ then $\delta^p < \infty$ and we set $\theta^* = (\zeta - \delta^p)/\gamma^p$. Clearly, $\zeta = \gamma^p\theta^* + \delta^p$ and $0 < \theta^* \leq \theta \leq 1/2$. Furthermore, $\zeta - 3\theta^*\theta \geq \zeta - 3\theta^*/2 = (\gamma^p - 3/2)\theta^* + \delta^p \geq 0$, where we use assumption $\gamma^p \geq 3/2$. From these inequalities and from (42) we infer

$$0 \leq \frac{1}{3\theta^*\theta}(\theta - \theta^*)(\zeta - 3\theta^*\theta) = \theta^* - \theta + \left(\frac{1}{3\theta^*} - \frac{1}{3\theta}\right)\zeta = [s(0, \theta^*, \zeta)]^{-1} - [s(0, \theta, \zeta)]^{-1}.$$

Hence, $s(0, \theta, \zeta) \geq s(0, \theta^*, \zeta) = s(0, \theta^*, \gamma^p\theta^* + \delta^p)$ and consequently $\omega^p(\theta, \zeta, \xi, \eta) \geq \omega^p(\theta^*, \gamma^p\theta^* + \delta^p, \xi, \eta) \geq \widehat{\omega}^p(\theta^*, \gamma^p\theta^* + \delta^p) \geq 0$ for all $(\xi, \eta) \in K_{\mathrm{ref}}^2$, where we use assumption (62).

(ii) If $\zeta \in (0, \delta^p]$ then condition (a) from Theorem 6.1 guarantees $\Psi_1^p(\zeta, \xi) \geq 0$. From definition (60) we obtain $\mathrm{Ker}^{b,p}(\zeta, \xi, \eta) \geq 0$ for all $(\xi, \eta) \in K_{\mathrm{ref}}^2$. Since $s(0, \theta, \zeta) \geq 0$ by (42), we conclude that $\widehat{\omega}^p(\theta, \zeta) \geq 0$, see (56)–(58).

(iii) If $\zeta = 0$ then we consider a sequence ζ_i, $i = 1, 2, \ldots$, such that $\zeta_i \to 0$ for $i \to \infty$ and $0 < \zeta_i \leq \gamma^p\theta + \delta^p$. For each ζ_i we may use either (i) or (ii) to conclude that $\omega^p(\theta, \zeta_i, \xi, \eta) \geq 0$ for all $(\xi, \eta) \in K_{\mathrm{ref}}^2$. Since $\omega^p(\theta, \zeta, \xi, \eta)$ is a continuous function for $\theta > 0$, $\zeta \geq 0$, and $(\xi, \eta) \in K_{\mathrm{ref}}^2$, we conclude that $\omega^p(\theta, \zeta_i, \xi, \eta) \to \omega^p(\theta, 0, \xi, \eta) \geq 0$ as $i \to \infty$ for all $(\xi, \eta) \in K_{\mathrm{ref}}^2$. □

The following theorem concludes our analysis and summarizes the sufficient conditions for the DMP.

Theorem 7.1 *Let us consider the hp-FEM problem* (3) *discretized on a mesh $\mathcal{T}_{hp}$. Denote by h_K and p_K the lengths and the polynomial degrees of elements $K \in \mathcal{T}_{hp}$. Further, consider $\theta^K = h_K/(|\Omega| - h_K)$ and constants α^p, β^p, γ^p, and δ^p introduced in* (31), (32), (61)*, and* (60)*, respectively. Let assumption* (62) *be satisfied for all $p \in \{p_K : K \in \mathcal{T}_{hp}\}$. In case $\delta^{p_K} < \infty$ assume*

$$h_K \leq |\Omega|/3. \tag{63}$$

If

$$\kappa^2 h_K^2 \le \min\left\{\alpha^{p_K}, \beta^{p_K}, \gamma^{p_K}\theta^K + \delta^{p_K}\right\} \quad \textit{for all } K \in \mathcal{T}_{hp} \tag{64}$$

then the approximate problem (3) *satisfies the DMP.*

Proof. First notice that (63) is equivalent to $\theta^K \le 1/2$. The DMP then follows from Theorems 6.1 and 3.2. The assumptions (a) and (b) of Theorem 6.1 are guaranteed by Lemmas 6.1 and 6.2 and hypothesis (64). The assumption (c) of Theorem 6.1 follows from (63)–(64), Lemma 7.4 and Corollary 7.1. □

8 Verification of assumptions

The computation of sharp lower estimates of constants α^p, β^p, γ^p, and δ^p is not very demanding. For $p = 1$ and $p = 2$ we can easily compute even the exact values. The results up to $p = 10$ are presented in Table 1. First, we observe the two exceptional cases $p = 1$ and $p = 2$. In these cases assumption (62) does not apply. We also verified that $\gamma^p \ge 3/2$ for $p = 3, 4, \dots, 10$. A closer look shows that $\gamma^p\theta + \delta^p \le \min\{\alpha^p, \beta^p\}$ for $p = 3, 4, \dots, 10$. Hence, condition (64) can be replaced for $p_K = 3, 4, \dots, 10$ by simpler condition

$$\kappa^2 h_K^2 \le \gamma^{p_K}\theta^K + \delta^{p_K} \quad \text{for all } K \in \mathcal{T}_{hp}. \tag{65}$$

The crucial assumption (62) can be reformulated as nonnegativity of a polynomial in variables θ, ξ, η in a domain $(0, 1/2] \times K_{\mathrm{ref}} \times K_{\mathrm{ref}}$. Indeed, $\omega^p(\theta, \zeta, \xi, \eta)$ is a rational function with a positive denominator. The nonnegativity of a polynomial on an interval can be further reformulated as nonnegativity of a polynomial on entire $\mathbb{R}$. The verification of nonnegativity of a polynomial is connected with the 17th Hilbert problem [12]. There exist (NP-hard) algorithms for verification of nonnegativity of a polynomials, see e.g. [11]. These algorithms, however, are difficult to implement and lead to reasonale solution for small number of variables and for small polynomial degrees, only.

Another possibility is the usage of interval arithmetic. The idea is to compute an interval $R = f(I)$ containing all possible outputs of a function f on an interval I. If R is nonnegative (contains nonnegative numbers only) then nonnegativity of f in I is verified. If not, we split I into two (or more) subintervals and repeat the process for all these subintervals. If this algorithm terminates after a finite number of steps, the nonnegativity of f in I is verified.

Assumption (62) was verified by this algorithm for $p = 3, 4, \dots, 10$. The `matlab` codes can be downloaded from `http://www.math.cas.cz/vejchod/DMPabs.html`. These codes utilize the interval arithmetic package `intlab` [8], where the interval operations provide guaranteed results even in the floating-point arithmetic.

9 Conclusions

The DMP for the diffusion-reaction problem discretized by hp-FEM, see (3), is essentially satisfied if the hp-mesh $\mathcal{T}_{hp}$ satisfies conditions (63)–(64) from Theorem 7.1. The other assumptions of this theorem are technical and were verified by computer for polynomial degrees up to 10.

The presented analysis applies to all polynomial degrees $p \geq 1$, but it is mainly relevant for $p \geq 3$. The cases $p = 1$ and $p = 2$ are exceptional, because the bubble part of the DGF is zero (for $p = 1$) or trivially nonnegative (for $p = 2$). Hence, the difficult analysis from Section 7 including assumption (62) is not needed for $p = 1$ and $p = 2$. In case $p = 1$ we can even show that the obtained condition is also necessary, i.e. in case of linear FEM with $M \geq 2$, the DMP for problem (3) is satisfied if and only if $\kappa^2 h_K^2 \leq 6$ for all $K \in \mathcal{T}_{hp}$.

Finally, let us notice that $\sigma^3(\theta) \leq \sigma^p(\theta)$ for all $p = 3, 4, \ldots, 10$, see Figure 2. This (or more precisely the values of γ^p and δ^p in Table 1) implies that condition (64) in Theorem 7.1 or its simplified version (65) is the most strict for $p = 3$. This observation is in agreement with the previous results for the Poisson problem, see [15]. The growing trend of values $\sigma^p(\theta)$ for increasing p observed in Figure 2 allows us to conclude this paper by the following conjecture.

Conjecture 9.1 *Let us consider a finite element mesh $\mathcal{T}_{hp}$ with an arbitrary distribution of polynomial degrees. Denote by h_K the length of the element K and set $\theta^K = h_K/(|\Omega| - h_K)$. If*

$$\kappa^2 h_K^2/\gamma^3 \leq \theta^K \leq 1/2 \quad \text{for all } K \in \mathcal{T}_{hp},$$

where $\gamma^3 \approx 5.608797$, then the approximate problem (3) satisfies the DMP.

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