Analytic regularity of strong solutions for the complexified stochastic nonlinear Poisson-Boltzmann Equation

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Abstract

The nonlinear Poisson-Boltzmann equation (nPBE) is a fundamental partial differential equation (PDE) in electrostatics, widely used in computational biology and chemistry to model potential fields in solvents or plasmas. In this paper, we consider the problem of quantifying the statistical uncertainty of the stochastic nPBE solution under random variations in its coefficients. We establish the existence and uniqueness of solutions of the complexified nPBE using a contraction mapping argument, as conventional convex optimization techniques for the real-valued nPBE do not naturally extend to the complex setting. Using the existence and uniqueness result, we demonstrate that the solutions admit analytic extensions over a well-defined region in the complex hyperplane The analyticity makes the computation for statistics of real-valued quantities of interest amenable to numerical techniques such as sparse grids. Sparse grids are applied to uniformly approximate analytic functions with algebraic to sub-exponential error with respect to the number of knots, thus allowing for efficient approximations of high-dimensional integrals. Our numerical experiments confirm the predicted error behavior.

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1. Introduction

Linear elliptic PDEs have long been fundamental in modeling problems in chemistry, physics, engineering and biology [31]. For example, the Poisson equation has been used extensively in electrical engineering to model potential fields in semi-conductors, leading to the capacitance extraction problem. However, as the physical scales are reduced, uncertainties in semi-conductor geometries introduce challenges such as impedance matching problems [21, 93]. Moreover, many of these classical paradigms assume that charge distributions in dielectrics exist in a vacuum, an assumption that does not hold for numerous important problems involving nonlinear electrostatics.

Nonlinear elliptic PDEs encompass a broad class of equations, including those arising in nonlinear electrostatics, where they play a crucial role in modeling potential fields generated by molecular interactions in solvents or plasmas. Unlike linear models, these interactions require a more accurate representation, leading to the nPBE, a well-established model in molecular dynamics (MD) simulations, chemical applications, protein interactions [39, 88, 76, 71]. As pointed out in [39], the nPBE has been investigated in biophysics [75, 78, 1, 11], surface science [49, 19], chemical physics [34, 54], polymer physics [69], plasma physics [91, 48], solid state physics [2, 55], condensed matter physics [24], many-body theory [18, 37], thermodynamics [38, 60], statistical mechanics [15, 59, 67], liquid state theory [41, 32, 63] , electrolyte solutions [9, 35], electrochemistry [82, 16, 87], soft matter [28, 27, 45, 79], physical chemistry [14, 3], biophysical chemistry [75, 29], biochemistry [12], medical physics [43], physiology [10, 44], molecular biology [86], colloids

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[19, 49, 92, 30, 47, 62], applied mathematics [20, 81, 61], materials science [25] and technology [65]. It has been particularly useful in modeling electrode-electrolyte interfaces [90, 89, 70], and many relevant software packages have been developed to facilitate its computational implementation [80, 50, 64, 8]. However, many of these applications involve shape and coefficient uncertainties. This motivates the extension of the nPBE to the probabilistic setting.

The stochastic nPBE is given by (see Section 2 for notations)

$$\begin{aligned} -\nabla \cdot (\epsilon(x,\omega_p)\nabla u(x,\omega_p)) + \kappa(x,\omega_p)^2 \sinh u(x,\omega_p) &= f(x,\omega_p), \quad x \in \Omega, \\ u(x,\omega_p) &= g(x,\omega_p), \quad x \in \partial\Omega, \end{aligned} \tag{1.1}$$

where u is the nondimensionalized potential, ϵ is the dielectric, κ is the Debye-Hückel parameter, and ω_p is a random element in the sample space $\Omega_{\mathbb{P}}$. In Figure 1, an example of the electrostatic potential field is rendered from the solution of the nPBE by using the Adaptive Poisson Boltzmann Solver (APBS) [8] for E. Coli RHo Protein. (PDB: 1A63 [13]). However, the mathematical properties of the nPBE are less understood and significantly more complicated than the linear case.

In practice, uncertainties in the dielectric properties and geometry introduce randomness into the potential field, and so the solutions to the nPBE are inherently stochastic. If these uncertainties are parameterized by N random variables, then the solutions are high-dimensional and in many cases computationally intractable. However, if the solutions exhibit sufficient complex analytic regularity with respect to these random variables, efficient numerical methods such as the stochastic collocation method with a sparse grid polynomial representation can be employed to achieve sub-exponential convergence with respect to the interpolation knots in the probabilistic domain [74, 73, 21, 23].

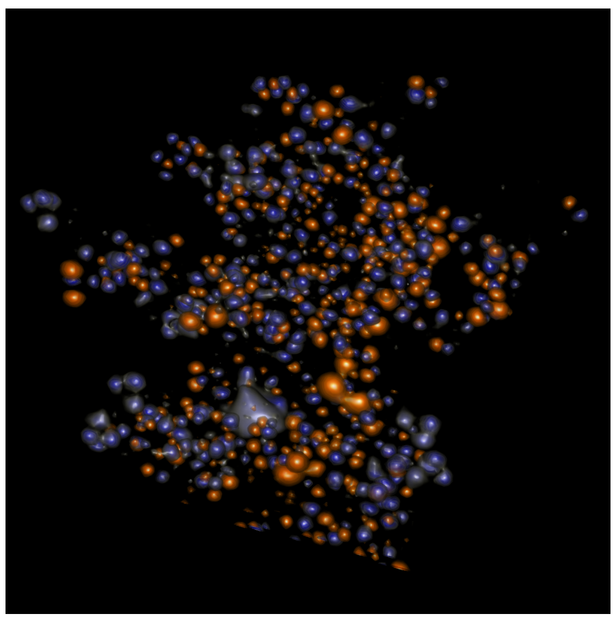

Figure 1: Electrostatic potential field obtained from the solution of the nPBE for the RNA binding domain of E. Coli RHO factor. The potential fields were created with the Adaptive Poisson Boltzmann Solver [8] rendered with VolRover [7, 6]. The positive and negative potential are rendered with blueish and orange/reddish colors respectively.

In [42], the authors investigated the application of stochastic collocation and stochastic Galerkin to the stochastic nPBE, formulating it as a semi-linear stochastic boundary value problem and proving the existence of a unique weak solution. This result extended the deterministic existence and uniqueness theory established in [46]. However showing analytic regularity results and convergence rates for the stochastic collocation method was not the main focus of [42, 46]. In our paper, the main contributions are:

- Theorem 3.1: The existence and uniqueness of H^2-solutions to the complexified nPBE are shown.
- Theorem 4.1: The analytic extension of the solutions of the nPBE exists with respect to the random variables that parametrize uncertainties.

A key consequence is that the stochastic nPBE can be solved with sub-exponential and algebraic convergence with respect to the dimensionality of the sparse grid. Numerical results in Section 6 are consistent with Theorem 4.1.

This paper is organized as follows. Section 2 introduces mathematical background. In Section 3, the existence and uniqueness results are proved. In Section 4, the strong solutions to the nPBE are shown to admit analytic extensions into a well defined region in $\mathbb{C}^N$. In Section 5, sparse grid tensor product polynomial approximations are discussed. The convergence rates predicted from the error bounds for sparse grids are consistent with the numerical experiments in Section 6. In Section 7, final remarks and future work are discussed. In Appendix A, analytic estimates for the various constants used in this paper are shown and in Appendix B, a discussion on the failure of uniqueness of solutions is given.

2. Problem Set-up

2.1. Fractional Sobolev spaces and spectral properties

Let $\Omega \subseteq \mathbb{R}^d$ be open, bounded, and convex with a sufficiently regular boundary (at least C^2). Let $|\Omega|$ denote the Lebesgue measure of Ω and $d_\Omega := \sup_{x,y\in\Omega}|x-y|$, the diameter of Ω. For $k \in \mathbb{N}\cup\{0\}$, define

$$H^k(\Omega) = \{u \in L^2(\Omega;\mathbb{C}) : \|u\|_{H^k(\Omega)} < \infty\} \quad \text{with } \|u\|_{H^k(\Omega)} := \Big(\sum_{|\alpha|\le k} \|\partial_\alpha u\|_{L^2}^2\Big)^{\frac{1}{2}}.$$

For $s' \in [0,1)$, recall the Gagliardo seminorm

$$[u]_{s'} := \Big(\int_\Omega\int_\Omega \frac{|u(x)-u(y)|^2}{|x-y|^{d+2s'}}dxdy\Big)^{\frac{1}{2}},$$

from which fractional Sobolev spaces are defined. Given $s \ge 0$, we have $s = k + s'$ for $k \in \mathbb{N}\cup\{0\}$ and $s' \in [0,1)$. Define

$$H^s(\Omega) = \{u \in L^2(\Omega;\mathbb{C}) : \|u\|_{H^s} < \infty\} \quad \text{with } \|u\|_{H^s} := \Big(\|u\|_{H^k}^2 + [u]_{s'}^2\Big)^{\frac{1}{2}},$$

and $H_0^s(\Omega)$ to be the closure of $C_c^\infty(\Omega)$, the collection of smooth and compactly supported functions in Ω, under $\|\cdot\|_{H^s}$. For a more thorough discussion on the Sobolev spaces on the boundary $\partial\Omega$, see [66, Chapter 3].

As for the regularity of boundary data, let $g : \partial\Omega \to \mathbb{C}$ and $w \in L^2(\Omega)$ such that $w = g$ in the trace sense. To invoke the elliptic regularity theorem, let $w \in H^2(\Omega)$. To motivate this assumption, consider the linear elliptic PDE $Lu = f$ on Ω with $u = g$ on $\partial\Omega$. Assuming that w exists, a formal calculation reveals that $\tilde{u} + w$ is the solution where $\tilde{u}$ satisfies $L\tilde{u} = f - Lw$ on Ω with $\tilde{u} = 0$ on $\partial\Omega$. If $f \in L^2(\Omega)$, we desire $Lw \in L^2(\Omega)$ to ensure that $\tilde{u}$ has two more derivatives than $f - Lw$. That $w \in H^2(\Omega)$ follows by assuming $g \in H^{\frac{3}{2}}(\partial\Omega)$.

Lemma 2.1. *[66, Theorem 3.37] Let $T : C^\infty(\overline{\Omega}) \to C^\infty(\partial\Omega)$ be given by $u \mapsto u|_{\partial\Omega}$. If $k \in \mathbb{N}$ and $\Omega \in C^{k-1,1}$, then T uniquely extends to a surjective bounded linear operator from $H^s(\Omega)$ to $H^{s-\frac{1}{2}}(\partial\Omega)$ for all $s \in (\frac{1}{2}, k]$. The trace map T has a right-continuous inverse.*

The map $g \mapsto w$ is not unique although one can uniquely solve the Laplace equation

$$\begin{aligned} \Delta w &= 0,\ x \in \Omega \\ w &= g,\ x \in \partial\Omega, \end{aligned} \tag{2.1}$$

and obtain an explicit form for w as an integral against the Poisson kernel. In this paper, we define $T^{-1}g := w$. It can be shown that $T^{-1} : H^{k-\frac{1}{2}}(\partial\Omega) \to H^k(\Omega)$ defines a bounded linear operator where the operator norm depends on $k \in \mathbb{N}$ and Ω.

To understand the dependence of solutions on randomness by leveraging the linear PDE theory, we apply the spectral properties of the Dirichlet Laplacian on Ω. Let $\{\lambda_i\}_{i=1}^\infty$ be the eigenvalues of the (negative)

Dirichlet Laplacian $-\Delta$, the Laplacian operator restricted to functions vanishing on the boundary defined via the Friedrich extension. The linear ordering $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$ holds and λ_1 is simple. The principal eigenvalue is given by

$$\lambda_1 = \min_{u \in H_0^1(\Omega)\setminus\{0\}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega |u|^2}.$$

The variational formula implies the Poincaré inequality

$$\|u\|_{L^2(\Omega)}^2 \leq \lambda_1^{-1} \|\nabla u\|_{L^2(\Omega)}^2, \quad \forall u \in H_0^1(\Omega),$$

where the sharp lower bound [77] is given by

$$\lambda_1 \geq \frac{\pi^2}{d_\Omega^2}. \tag{2.2}$$

2.2. Hypotheses

Suppose $(\Omega_{\mathbb{P}}, \mathcal{F}, \mathbb{P})$ denotes a complete probability space where $\Omega_{\mathbb{P}}$ is the set of outcomes, $\mathcal{F}$ is the sigma field, and $\mathbb{P}$ is the probability measure. The coefficients ϵ, κ, f, and g generally vary with $\omega_p \in \Omega$. In practical applications, these random inputs are typically expressed as functions of a random vector $\mathbf{Y}(\omega_p) = (Y_1(\omega_p), Y_2(\omega_p), \dots, Y_N(\omega_p))$, which takes values in a compact set $\Gamma \subset \mathbb{R}^N$ and follows some probability density function $\rho : \Gamma \to \mathbb{R}_{\geq 0}$. A common choice is $\Gamma \equiv [-1, 1]^N$ with ρ modeled as a truncated normal distribution, though other distributions may also be considered. Moreover, an unbounded Γ could be considered as in [4].

Under this framework, the stochastic nPBE can be formulated as a parameterized problem in $\mathbf{y} \in \Gamma \subset \mathbb{R}^N$ where $\mathbf{y}$ denotes a finite-dimensional realization of some random field. In numerous problems, randomness can be captured with a limited set of uncorrelated, and occasionally independent, random variables. This motivates the following hypothesis. A slight abuse of notation allows the same f in (2.3) to denote the dependence on $\omega_p \in \Omega_{\mathbb{P}}$ or $\mathbf{y} = \mathbf{Y}(\omega_p)$.

Hypothesis 1. ***(Finite dimensional noise)***
Let $N \in \mathbb{N}$. There exists a mean zero real-valued random vector $\mathbf{Y}(\omega_p) = (Y_1(\omega_p), Y_2(\omega_p), \dots, Y_N(\omega_p))$ such that the coefficient functions take the form

$$f(x, \omega_p) = f(x, \mathbf{Y}(\omega_p)) = f(x, y_1, \dots, y_N) \text{ on } \Omega \times \Gamma, \tag{2.3}$$

and similarly with $\epsilon(x, \omega_p)$, $\kappa(x, \omega_p)$, and $w(x, \omega_p)$. Further assume that $\mathbf{v} = \begin{pmatrix} \epsilon & \kappa^2 & f & w \end{pmatrix}^T$ is modeled as

$$\mathbf{v}(x, \omega_p) := \boldsymbol{\phi}_0(x) + \sum_{k=1}^N \alpha_k \boldsymbol{\phi}_k(x) Y_k(\omega_p) \tag{2.4}$$

where $\alpha_k \geq 0$ and $\boldsymbol{\phi}_k \in W^{1,\infty}(\Omega) \times L^\infty(\Omega) \times L^2(\Omega) \times H^2(\Omega)$ for $0 \leq k \leq N$. For $1 \leq k \leq N$, assume the normalization $\|\boldsymbol{\phi}_k\| \leq 1$ measured in the product norm. Denote $\boldsymbol{\phi}_k(x) = \begin{pmatrix} \epsilon_k(x) & K_k(x) & f_k(x) & w_k(x) \end{pmatrix}^T$.

Remark 2.1. A natural way this parametrization (2.4) may arise is through a truncated Karhunen-Loève (KL) expansion, where the dominant modes of variability are retained. For $1 \leq k \leq N$, $\boldsymbol{\phi}_k(x)$ may be given by the first N eigenfunctions of the covariance operator defined by $\mathbf{v}(x, \omega_p)$ where $\{\alpha_k\}$ is assumed to decrease monotonically. While KL expansion eigenfunctions are typically elements of $L^2(\Omega)$, under appropriate regularity conditions on the covariance function, they may extend to $L^\infty(\Omega)$ or spaces of even higher regularity (see [33]).

Let $\mathbf{z} \in \mathbb{C}^N$ denote the complexification of $\mathbf{y}$. We state hypotheses to show the well-posedness of (1.1) for any $\mathbf{z} \in \mathbb{C}^N$ and the regularity of $\mathbf{z} \mapsto u(\cdot, \mathbf{z})$. When it is understood that $\mathbf{z}$ is fixed, we suppress $\mathbf{z}$; for example, $f(x) = f(x, \mathbf{z})$.

Hypothesis 2. ***(Regularity)*** *There exists* $\Theta \subseteq \mathbb{C}^N$ *containing* Γ *to which the coefficient functions extend. More precisely,*

$$(\epsilon(\cdot,\mathbf{z}), \kappa(\cdot,\mathbf{z}), f(\cdot,\mathbf{z}), g(\cdot,\mathbf{z})) \in W^{1,\infty}(\Omega, \mathbb{C}^{d^2}) \times L^\infty(\Omega;\mathbb{C}) \times L^2(\Omega;\mathbb{C}) \times H^{3/2}(\partial\Omega;\mathbb{C}) \tag{2.5}$$

for all $\mathbf{z} \in \Theta$*, and the maps from* Θ *into the respective Banach spaces are analytic. Since the inverse trace operator is linear,* $\mathbf{z} \mapsto w(\cdot;\mathbf{z}) \in H^2(\Omega)$ *is also analytic.*

See (4.1) for an explicit description of Θ.

Hypothesis 3. ***(Uniform ellipticity)*** *The function* $\epsilon(\cdot,\mathbf{z}) \in W^{1,\infty}(\Omega,\mathbb{C}^{d^2})$ *, where* $\epsilon^{ij} = \overline{\epsilon^{ji}}$ *for* $1 \le i,j \le d$*, satisfies the following uniform ellipticity condition: there exists* $\theta > 0$ *such that*

$$\mathrm{Re}\left[\sum_{i,j=1}^{d} \epsilon^{ij}(x,\mathbf{z})\xi_i\overline{\xi_j}\right] \ge \theta|\xi|^2 \tag{2.6}$$

for all $\xi \in \mathbb{C}^d$*, a.e.* $x \in \Omega$*, and* $\mathbf{z} \in \Theta$*.*

Hypothesis 4. ***(Coercivity)*** *There exists* $\mu \ge 0$ *such that* $\kappa(\cdot,\mathbf{z}) \in L^\infty(\Omega;\mathbb{C})$ *satisfies*

$$\mathrm{Re}\left[\kappa^2(\mathrm{x},\mathbf{z})\right] \ge -\mu \tag{2.7}$$

for a.e. $x \in \Omega$ *and* $\mathbf{z} \in \Theta$*. Moreover, the parameters* θ *and* μ *characterized by Equations* (2.6) *and* (2.7)*, respectively, satisfy the inequality*

$$\frac{\mu}{\theta} < \lambda_1. \tag{2.8}$$

Remark 2.2. Hypotheses 3 and 4 are sufficient to show the existence of a unique strong solution within a small ball in $H^2(\Omega)$, and omitting these hypotheses may result in non-uniqueness. If the parameters are allowed to continuously vary until Hypotheses 3 and 4 no longer hold, then there may be a bifurcation of the unique small solution. See Appendix B for details.

Remark 2.3. Stochastic collocation and sparse grids are a popular approach to computing the statistics of a Quantity of Interest (QoI) of partial differential equations due to the sub-exponential convergence rates with respect to the number of interpolation knots. To obtain reliable sub-exponential convergence rates with uniformly bounded coefficients, a sufficient condition is to show that the solution of the PDE can be analytically extended in the complex hyperplane $\mathbb{C}^N$ [74] with respect to random variables $Y_1,\dots,Y_N$. As a first step, we need to show that the solution of the complexified nPBE exists and is unique in an appropriate space. This is a non-trivial task. The convex optimization framework used in [46, 42] for the real-valued nPBE does not extend directly. Their arguments rely on variational principles that hinge on the convexity of the functional $u \mapsto \int_\Omega \cosh(u(x))dx$. Although one could formally interpret a complex-valued PDE as a system of two coupled real-valued PDEs, this does not circumvent the core issue: the function $\cosh(z)$ is not convex in $\mathbb{C}$. Using the identity $\cosh(x+iy) = \cosh x \cos y + i \sinh x \sin y$ for $x, y \in \mathbb{R}$, the imaginary component y induces oscillations in both the real and imaginary parts of $\cosh(z)$. Henceforth, assume that all functions are complex-valued unless specified otherwise.

2.3. Definitions

Definition 2.1. A function $u(\cdot,\omega_p) \in H^1(\Omega)$ is a *weak solution* to (1.1) if for all $\phi \in H_0^1(\Omega)$, we have

$$\begin{aligned}\int_\Omega (\epsilon(x,\omega_p)\nabla u(x,\omega_p)) \cdot \overline{\nabla\phi(x)}dx + \int_\Omega (\kappa(x,\omega_p)^2 \sinh u(x,\omega_p))\overline{\phi(x)}dx &= \int_\Omega f(x,\omega_p)\overline{\phi(x)}dx \\ u(\cdot,\omega_p)|_{\partial\Omega} &= g(\cdot,\omega_p),\end{aligned} \tag{2.9}$$

almost surely (a.s.), where the equality at the boundary is in the trace sense; if $w(\cdot,\omega_p) \in H^1(\Omega)$ whose trace is $g(\cdot,\omega_p) \in H^{\frac{1}{2}}(\partial\Omega)$ a.s., a weak solution u satisfies $u - w \in H_0^1(\Omega)$. If a weak solution u is twice weakly-differentiable and satisfies (1.1) pointwise a.e. in $x \in \Omega$, then we say u is a *strong solution.*

We omit statements a.e. or a.s. unless more detail is needed. A weak solution that is in $H^2(\Omega)$ satisfies the strong form, if one can undo the integration by parts in the first term of (2.9), and this motivates us to find a H^2-solution. This is possible since $\epsilon \in W^{1,\infty}(\Omega, \mathbb{C}^{d^2})$ and $\epsilon\nabla u \in H^1(\Omega)$. Indeed for each $1 \le i, k \le d$,

$$\|\partial_k \sum_{j=1}^{d} (\epsilon^{ij}\partial_j u)\|_{L^2} \le C\|\epsilon\|_{W^{1,\infty}}\|u\|_{H^2}.$$

We reformulate (1.1) into a functional form and realize the H^2-solution as its fixed point. Define $F : H^2(\Omega) \to L^2(\Omega)$ as

$$\begin{aligned} F(u) &= -\nabla \cdot (\epsilon\nabla u) + \kappa^2 \sinh(u) \\ Lu &= -\nabla \cdot (\epsilon\nabla u) + \kappa^2 u \\ N(u) &= \kappa^2(\sinh(u) - u) = \kappa^2 \sum_{k=2}^{\infty} n_k u^k, \end{aligned} \tag{2.10}$$

where L is a uniformly elliptic second-order differential operator by Hypothesis 3. Here, $n_k = \frac{1}{k!}$ for odd $k \ge 3$ and $n_k = 0$ for even k. Our contraction mapping argument extends beyond the sinh nonlinearity, making it applicable to a variety of choices for $\{n_k\}_{k\ge2}$. Note that when $d \le 3$, $H^2(\Omega)$ is a Banach algebra and so $u^k \in H^2(\Omega)$ and $N(u)$ is well-defined. To simplify the presentation, the relevant operator norms are defined. Explicit estimates for these constants and their dependencies are derived in detail in Appendix A.

Definition 2.2. The Sobolev embedding for $s > \frac{d}{2}$ gives that $H^s(\Omega) \hookrightarrow L^\infty(\Omega)$ [66, Theorem 3.26]. The constant $C_S = C_S(s, \Omega, d) > 0$ is then defined as the norm of the inclusion operator from $H^s(\Omega)$ into $L^\infty(\Omega)$:

$$C_S := \inf\{C > 0 : \|u\|_{L^\infty(\Omega)} \le C\|u\|_{H^s(\Omega)},\ \forall u \in H^s(\Omega)\}.$$

The linear operator L in (2.10) takes functions in $H^2(\Omega) \cap H_0^1(\Omega)$ to functions in $L^2(\Omega)$. Let $C_D > 0$ be the norm of L with respect to these spaces:

$$C_D := \inf\{C > 0 : \|Lu\|_{L^2(\Omega)} \le C\|u\|_{H^2(\Omega)},\ \forall u \in H^2(\Omega)\}.$$

By Hypothesis 4, L is invertible, and so $L^{-1} : L^2(\Omega) \to H^2(\Omega) \cap H_0^1(\Omega)$ is defined. Let $C_H > 0$ be the norm of L^{-1}:

$$C_H := \inf\{C > 0 : \|L^{-1}u\|_{H^2(\Omega)} \le C\|u\|_{L^2(\Omega)},\ \forall u \in L^2(\Omega)\}.$$

3. Existence and uniqueness

To understand the regularity properties of $\mathbf{z} \mapsto u(\cdot, \mathbf{z})$, we need to show the well-posedness of the complexified nPBE. The linear PDE theory with our hypotheses is used to control a possible exponential growth of $N(u)$.

Lemma 3.1. *Let L be as in (2.10) and let $f \in L^2(\Omega)$. Fix $w \in H^2(\Omega)$ whose trace is $g \in H^{\frac{3}{2}}(\partial\Omega)$. Then, there exists a unique $v \in H^1(\Omega)$ such that $v = g$ in the trace sense and*

$$\int_\Omega (\epsilon\nabla v) \cdot \overline{\nabla\phi} + (\kappa^2 v)\overline{\phi} = \int_\Omega f\overline{\phi},$$

for all $\phi \in H_0^1(\Omega)$.

Consider solving $Lu = f \in L^2(\Omega)$ with $g = 0$ on $\partial\Omega$. From the standard elliptic theory (for instance, see [31, Section 6.3, Theorem 4]), there exists $C_H > 0$ as defined in Definition 2.2 such that $\|u\|_{H^2} \le C_H\|f\|_{L^2}$. General boundary data can be absorbed into the homogeneous term by replacing f by $f - Lw$ and considering the zero Dirichlet boundary condition, which yields an estimate in H^2.

Lemma 3.2. *The unique weak solution of the linear PBE, $u \in H^1(\Omega)$, satisfies*

$$\|u\|_{H^2} \le C_H \|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2}. \tag{3.1}$$

The nonlinear term is handled iteratively where, at each iteration, the regularity gain coming from the elliptic regularity theory is used to estimate the nonlinear term in $L^2(\Omega)$.

Lemma 3.3. *Let $s > \frac{d}{2}$. Then for every $v \in H^s(\Omega)$,*

$$\|N(v)\|_{L^2} \le \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| (C_S \|v\|_{H^s})^k, \tag{3.2}$$

where C_S is defined in Definition 2.2. For $N(v)$ for (1.1), we have

$$\|N(v)\|_{L^2} \le \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \Big(\sinh(C_S \|v\|_{H^s}) - C_S \|v\|_{H^s} \Big).$$

Proof.

$$\|N(v)\|_{L^2} \le \|\kappa\|_{L^\infty}^2 \sum_{k=2}^{\infty} |n_k| \|v^k\|_{L^2} \le \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| \|v\|_{L^\infty}^k \le \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| (C_S \|v\|_{H^s})^k,$$

estimated by the triangle inequality, the Hölder's inequality, and the Sobolev embedding, respectively. ☐

To motivate the fixed point argument, we define an iterated map given by a nonlinear operator $A : C_c^\infty(\Omega) \to H^2(\Omega)$ where $A(v)$ is implicitly defined by

$$\begin{aligned} L(A(v)) &= f - N(v),\ x \in \Omega \\ A(v) &= g,\ x \in \partial\Omega, \end{aligned} \tag{3.3}$$

and study its operator-theoretic properties. Denoting $K : L^2(\Omega) \to H_0^1(\Omega) \cap H^2(\Omega)$ to be the inverse of L under the zero Dirichlet boundary condition, it can be verified that

$$A(v) = K(f - N(v) - Lw) + w.$$

Consider $u_k = A(u_{k-1})$ for $k \ge 1$, and let $u_0 \in H^2(\Omega)$ be the unique solution to the linear PBE (see Lemmas 3.1 and 3.2). By the Sobolev embedding theorem, note that $H^2(\Omega) \hookrightarrow C^{0,\frac{1}{2}}(\overline{\Omega})$, and therefore $N(u_0) \in L^2(\Omega)$. This ensures $f - N(u_0) \in L^2$ in (3.3), and thus u_1 and all higher iterates are well-defined. By definition of $A(v)$, it follows that

$$\begin{aligned} Lu_k + N(u_{k-1}) &= f,\ k \ge 1, \\ u_k &= g. \end{aligned} \tag{3.4}$$

Remark 3.1. By working in Sobolev algebras, we bypass the problem of whether $N(u) \in L^2(\Omega)$ or not, for $u \in L^\infty(\Omega)$. Note that Holst [46, Chapter 2] bypasses this issue as well, not by working with more regular functions as we do, but by constructing a conditional action functional on $H_0^1(\Omega)$. For $d = 3$, the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ holds, but an analogous embedding for $H^1(\Omega)$ does not hold. For $d \ge 3$, it is straightforward to construct an example of $u \in H^1(\Omega)$ such that $N(u) = \kappa^2(\sinh u - u) \notin L^2(\Omega)$. For simplicity, take $\Omega = \mathbb{R}^d$ and $\kappa = 1$. For $R > 0$, define $u(x) = |x|^{-\alpha}\zeta(x)$ where $\alpha = \frac{d}{2} - 1 - \epsilon$ with $\epsilon \ll 1$ and $\zeta \in C_c^\infty(B(0,R))$ is a smooth non-negative function such that $\zeta = 1$ on $\overline{B(0, \frac{R}{2})}$. If $N(u) \in L^2(\Omega)$, then $\sinh(u(\cdot)) \in L^2(\Omega)$. Since $\sinh u \ge \frac{u^N}{N!}$ for every odd $N \ge 1$, we have $u^N \in L^2(\Omega)$. However, this is false due to the blow-up of u at the origin.

It may be that the sequence is convergent to a function that does not solve (1.1) in any meaningful way; for example, see [17]. By showing that A uniquely extends to a compact operator on fractional Sobolev spaces, it is shown that $\{u_k\}$ converges to a solution of (1.1). In the rest of this section, assume $d = 3$ unless specified otherwise.

Lemma 3.4. *$A : L^\infty(\Omega) \to H^2(\Omega)$ is locally Lipschitz continuous. Consequently, A is continuous on $H^s(\Omega)$ for every $s \in (\frac{3}{2}, 2]$. Furthermore, A is compact on $H^s(\Omega)$ for every $s \in (\frac{3}{2}, 2)$.*

Proof. Let $u, v \in L^\infty(\Omega)$ with $\|u\|_{L^\infty}, \|v\|_{L^\infty(\Omega)} \leq M$. Then by the Mean Value Theorem,

$$\begin{aligned}
\|A(u) - A(v)\|_{H^2} &= \|K(N(u) - N(v))\|_{H^2} \leq C_H \|N(u) - N(v)\|_{L^2} \\
&\leq C_H \|u - v\|_{L^\infty} \int_0^1 \|N'((1-t)u + tv)\|_{L^2} dt \\
&\leq C_H \|\kappa\|_{L^\infty}^2 \|u - v\|_{L^\infty} \int_0^1 \sum_{k\geq 2} k|n_k| \|(1-t)u + tv\|_{L^{2(k-1)}}^{k-1} dt \\
&\leq \left\{ C_H \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k\geq 2} k|n_k| 2^{k-2} (\|u\|_{L^\infty}^{k-1} + \|v\|_{L^\infty}^{k-1}) \right\} \|u - v\|_{L^\infty}.
\end{aligned} \tag{3.5}$$

If we show that the series in (3.5) converges, then the proof is complete. By the Cauchy integral formula, we obtain an upper bound on $|n_k|$

$$|n_k| \leq \frac{\max_{|z|=R} |N(z)|}{R^k},$$

and combining this bound for $R = 4M$ with (3.5), the infinite sum is a convergent geometric series, and therefore the desired continuity has been shown.

The rest follows from the Sobolev embedding and the Rellich-Kondrachov compactness theorem. Indeed, the continuity of A on $H^s(\Omega)$ follows by considering the embedding $H^s(\Omega) \hookrightarrow L^\infty(\Omega)$. Compactness of A on $H^s(\Omega)$ is immediate once we show A sends a bounded subset of $H^s(\Omega)$ into a bounded subset of $H^2(\Omega)$. For $\|u\|_{H^s} \leq M$,

$$\begin{aligned}
\|A(u)\|_{H^2} &= \|K(f - N(u) - Lw) + w\|_{H^2} \\
&\leq C_H \|f - N(u) - Lw\|_{L^2} + \|w\|_{H^2} \\
&\leq C_H \|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2} + C_H \|N(u)\|_{L^2} \\
&\leq C_H \|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2} + C_H \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^\infty |n_k| (C_S M)^k,
\end{aligned} \tag{3.6}$$

where (3.6) follows from (3.2). ∎

We apply the a priori estimates above to obtain a strong solution to (1.1). A general result is given, followed by a concrete application to the complexified nPBE corresponding to $N(u) = \kappa^2(\sinh u - u)$ in Corollary 3.1.

Theorem 3.1. *Suppose $z \mapsto N(z)$ is analytic in $z \in \mathbb{C}$ and has the form (2.10). Further assume*

$$C_H \|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2} + C_H \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^\infty |n_k| (C_S M)^k \leq M \tag{3.7}$$

$$C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^\infty k|n_k| (C_S M)^{k-1} < 1, \tag{3.8}$$

for some $s \in (\frac{3}{2}, 2)$, $M > 0$. Then there exists a unique strong solution $u \in H^2(\Omega)$ to (1.1) with $\|u\|_{H^2} \leq M$.

Proof. Let $\|v\|_{H^s} \leq M$. Then, (3.7) yields $\|A(v)\|_{H^s} \leq M$ by a similar argument to (3.6). By Schauder's fixed point theorem ([36, Corollary 11.2]) on $\overline{B_{H^s}(0, M)}$, a closed convex subset of $H^s(\Omega)$ on which A is continuous and compact by Lemma 3.4, there exists $u \in \overline{B_{H^s}(0, M)}$ such that $A(u) = u$. Since A is smoothing (elliptic regularity), $u \in H^2(\Omega)$. By (3.7) and the last inequality of (3.6), we have $\|u\|_{H^2} = \|A(u)\|_{H^2} \leq M$.

Following the steps leading to (3.5), we obtain

$$\|A(u)-A(v)\|_{H^s} \le \left(C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} k|n_k| (C_S M)^{k-1} \right) \|u-v\|_{H^s}, \tag{3.9}$$

where the strict contraction of A on $\overline{B_{H^s}(0,M)}$ follows from (3.8) and the Banach fixed point theorem. □

Corollary 3.1. *There exists $M>0$ satisfying (3.7), (3.8) if and only if $y_0 < y_0^*$ where*

$$\begin{aligned} y_0 &= C_H\|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2}, \\ y_0^* &= C_S^{-1}\left((1 + C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{1/2}) \cosh^{-1}\left(1 + \frac{1}{C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{1/2}}\right) - \sqrt{1 + 2C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{1/2}} \right). \end{aligned} \tag{3.10}$$

If $y_0 < y_0^*$, then $M(y_0) > 0$ can be taken to be the smallest root of

$$y_0 + C_H \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} (\sinh C_S M - C_S M) = M. \tag{3.11}$$

Proof. Let $F(M,y) = y + C_H \|\kappa\|_{L^\infty}^2 |\Omega|^{\frac{1}{2}} (\sinh C_S M - C_S M)$. It is a calculus exercise to check that $y_0^* > 0$ is uniquely determined by the curve $y = F(M, y_0^*)$ tangentially intersecting the identity line $y = M$ at (see Figure 2)

$$M = M_0 := C_S^{-1} \cosh^{-1}\left(1 + \frac{1}{C_H C_S \|\kappa\|_{L^\infty}^2 |\Omega|^{1/2}}\right). \tag{3.12}$$

By standard algebra, (3.7) is equivalent to $F(M, y_0) \le M$, where the existence of $M > 0$ satisfying the inequality holds if and only if $y_0 \le y_0^*$. Additionally, (3.8) is equivalent to $M < M_0$, which cannot hold if $y_0 \ge y_0^*$. □

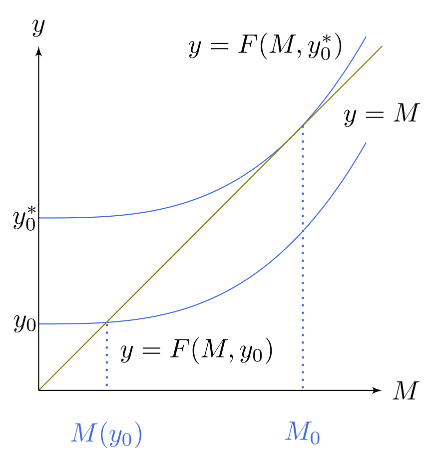

Figure 2: The sufficient and necessary condition for existence and uniqueness illustrated by $y_0 < y_0^*$ in Corollary 3.1.

By the restrictive hypotheses (3.7) and (3.8), our fixed point approach works for small data where the given parameters need to be small measured in various norms. For the complexified nPBE, however, this restriction is necessary if we wish to preserve uniqueness of solution; see Proposition B.1. On the other hand, our approach establishes existence and uniqueness for a wide class of analytic nonlinearities that may grow super-linearly.

Remark 3.2. Although the condition $y_0 < y_0^*$ depends on a delicate interplay between the loads and material properties of nPBE, it is insightful to examine the linear Poisson equation as a limiting case as $\kappa \to 0$ in $L^\infty(\Omega)$. The Poisson equation admits unique solutions for any arbitrary large data $(f, g) \in L^2(\Omega) \times H^{\frac{3}{2}}(\partial\Omega)$, or equivalently in our notation, $y_0^* = \infty$. As the nonlinear parameter κ vanishes, y_0^* tends to infinity, thus recovering the linear case. Indeed, (3.10) yields the asymptotics

$$y_0^*(\|\kappa\|_\infty) = C_S^{-1}\left(\ln\left(\frac{2}{C_H C_S |\Omega|^{1/2}\|\kappa\|_{L^\infty}^2}\right) - 1\right) + O_\epsilon(\|\kappa\|_{L^\infty}^{2-\epsilon}) \text{ as } \|\kappa\|_\infty \to 0, \tag{3.13}$$

for any $0 < \epsilon \ll 1$, and the upper bound $C_H = O(1)$ is by (A.7), (A.21). Hence the argument of $\ln(\cdot)$ tends to zero as $\|\kappa\|_{L^\infty} \to 0$, and our small data analysis of the complexified nPBE recovers the large data well-posedness theory of the Poisson equation at the rate logarithmic in $\|\kappa\|_{L^\infty}$.

By inductive arguments using Lemma 3.4 and Theorem 3.1, the local Lipschitz continuity of A on general Sobolev spaces can be shown with more restrictive hypotheses. Denote $A \lesssim B$ whenever there exists an implicit constant $C > 0$ dependent only on the given parameters such that $A \leq CB$.

Corollary 3.2. *Let $s > \frac{d}{2}$ and $\sigma \leq s \leq \sigma + 2$ for $\sigma \in \mathbb{N} \cup \{0\}$, and assume $\epsilon \in C^{\sigma+1}(\overline{\Omega}), \kappa \in H^s(\Omega)$ and $\partial\Omega$ is $C^{\sigma+2}$. For any given $f \in H^\sigma(\Omega), g \in H^{\sigma+\frac{3}{2}}(\partial\Omega)$, it follows that $A : H^s(\Omega) \to H^{\sigma+2}(\Omega)$ is locally Lipschitz continuous. Hence for $s > \frac{d}{2}$ and $\sigma \leq s < \sigma + 2$, there exists a unique fixed point for A in $B_{H^s(\Omega)}(0, R) \subseteq H^s(\Omega)$ for some $R > 0$, if the smallness hypotheses analogous to Equations* (3.8) *and* (3.9) *are assumed.*

Proof. By the Elliptic Regularity Theorem and the Mean Value Theorem,

$$\begin{aligned}\|A(u) - A(v)\|_{H^{\sigma+2}} &= \|K(N(u) - N(v))\|_{H^{\sigma+2}} \lesssim \|N(u) - N(v)\|_{H^\sigma} \\ &\lesssim \|\kappa\|_{H^s}^2 \|u - v\|_{H^s} \int_0^1 \|N'((1-t)u + tv)\|_{H^s} dt.\end{aligned} \tag{3.14}$$

The rest is analogous to the proofs of Lemma 3.4 and theorem 3.1 using the Sobolev algebra property and the fixed point argument. ☐

4. Analytic Regularity

In this section, the complex analytic regularity of the unique solution obtained in Theorem 3.1 is shown. Understanding the analyticity of the solution is crucial for approximating quantities of interest under random input perturbations, which allows for algebraic to sub-exponential convergence of the surrogate model to the exact solution with respect to the sparse grid approximation as shown in [4, Lemma 4.4]. The solution's analytic extension into the complex plane, particularly within a Bernstein ellipse, facilitates the use of techniques like Chebyshev polynomial expansions to enhance approximation accuracy. More precisely, it is shown that the solution extends analytically on stochastic domains that obey the inclusion $\Gamma \subseteq \mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N} \subseteq \Theta$ (see Figure 3). We also show that the norm of the analytic extension is uniformly bounded on Θ.

The Bernstein ellipse $\mathcal{E}_{\hat{\sigma}} \subseteq \mathbb{C}$ is given by

$$\mathcal{E}_{\hat{\sigma}} = \left\{ z \in \mathbb{C} : \operatorname{Re} z = \frac{e^{\sigma'} + e^{-\sigma'}}{2}\cos(\theta), \operatorname{Im} z = \frac{e^{\sigma'} - e^{-\sigma'}}{2}\sin(\theta), \theta \in [0, 2\pi), 0 \leq \sigma' \leq \hat{\sigma} \right\},$$

and for N dimensions, the polyellipse $\mathcal{E}_{\hat{\sigma}_1,\hat{\sigma}_2,\ldots,\hat{\sigma}_N} := \prod_{k=1}^N \mathcal{E}_{\hat{\sigma}_k} \subset \mathbb{C}^N$ is defined as a direct product of one-dimensional Bernstein ellipses. For $\beta > 0$, we consider

$$\Theta_\beta = \{\mathbf{z} = \mathbf{y} + \tilde{\mathbf{y}} \in \mathbb{C}^N : \mathbf{y} \in \Gamma \equiv [-1, 1]^N,\ \tilde{\mathbf{y}} \in \mathbb{C}^N,\ \sum_{k=1}^N \alpha_k |\tilde{y}_k| \leq \beta\} \tag{4.1}$$

and give quantitative bounds on β that is applied in Section 5 to derive error convergence rate. For more details on the construction of Θ_β and the embedding $\mathcal{E}_{\hat{\sigma}_1,\hat{\sigma}_2,\ldots,\hat{\sigma}_N} \subseteq \Theta_\beta$, see [21]. The domain of $\mathbf{v}(x, \mathbf{y}) := \boldsymbol{\phi}_0(x) + \sum_{k=1}^N \alpha_k \boldsymbol{\phi}_k(x) y_k$ is extended to the complex plane by replacing $\mathbf{y}$ with $\mathbf{z}$.

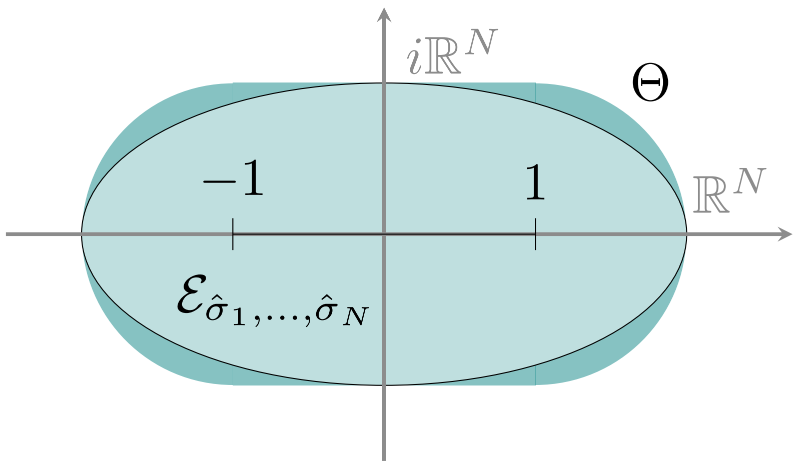

Figure 3: Cartoon example of embedding of the Bernstein polyellipse $\mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N}$ in $\Theta \subseteq \mathbb{C}^N$. Note that this cartoon is a one dimensional representation of the Bernstein ellipse embedded in Θ.

For convenience, absorb the boundary data and consider

$$\begin{aligned} -\nabla_x \cdot (\epsilon(x,\mathbf{z})\nabla_x \tilde{u}(x,\mathbf{z})) + \kappa(x,\mathbf{z})^2 \sinh\left(\tilde{u}(x,\mathbf{z}) + w(x,\mathbf{z})\right) &= f(x,\mathbf{z}) + \nabla_x \cdot (\epsilon(x,\mathbf{z})\nabla_x w(x,\mathbf{z})), \quad x \in \Omega, \\ \tilde{u}(x,\mathbf{z}) &= 0, \quad x \in \partial\Omega, \end{aligned} \tag{4.2}$$

where $\mathbf{z} \in \Theta$ and $u = \tilde{u} + w$ is the solution to (1.1). In Theorem 4.1, let $\epsilon(\mathbf{z}) := \epsilon(\cdot,\mathbf{z}) \in W^{1,\infty}(\Omega;\mathbb{C})$ be a scalar field satisfying $\mathrm{Re}(\epsilon(x,\mathbf{z})) \geq \theta > 0$ for a.e. x as Hypothesis 3. This simplification that the dielectric coefficient is scalar-valued is justified by the isotropic nature of the medium at the macroscopic scale and the mean-field assumptions inherent to the nPBE. This approach effectively averages out molecular-scale anisotropies, allowing for a tractable and physically relevant description of electrostatic interactions in the system.

To show the desired analyticity in Theorem 4.1 on some non-vanishing stochastic region in the complex hyperplane, a technical lemma is needed.

Lemma 4.1. *Let $|\Omega| \geq \delta_\Omega d_\Omega^3$ for some $\delta_\Omega \in (0,1)$. Denote $\tilde{\alpha} = \sum_{k=1}^{N} \alpha_k$ and*

$$\begin{aligned} C_0 &= \frac{\left(1 + \frac{\theta^2}{4\mu^2}\right)^{\frac{3}{2}}}{\theta}\left(1 + \frac{2}{\pi^2} + \frac{2\cdot 3^{1/2}}{\pi}\right),\ l_0 = \log\left(\frac{2^{-\frac{1}{2}}\theta}{eC_0}\right), \\ A &= \frac{C_0}{\theta}\left(\|f_0\|_{L^2} + \tilde{\alpha}\right) + \left\{\frac{C_0}{\theta}\left(18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha}\right) + 1\right\}(\|w_0\|_{H^2} + \tilde{\alpha}), \\ A' &= \frac{20C_0}{\theta} + \frac{19C_0}{\theta}(\|w_0\|_{H^2} + \tilde{\alpha}) + \frac{C_0}{\theta}(18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha}) + 1. \end{aligned}$$

Given $\mathbf{v}(x,\mathbf{z}) = \boldsymbol{\phi}_0(x) + \sum_{k=1}^{N} \alpha_k \boldsymbol{\phi}_k(x) z_k$*, assume the quantitative bounds:*

$$d_\Omega^2 < \min\left(\frac{\pi^2\theta}{2(18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha})},\ \frac{\pi^2\theta}{2\mu},\ \frac{\theta}{\|K_0\|_{L^\infty}+\tilde{\alpha}},\ \frac{\theta^2}{(\|\epsilon_0\|_{W^{1,\infty}}+\tilde{\alpha})^2}\right) \tag{4.3}$$

$$d_\Omega^{\frac{3}{2}} > \frac{A}{2^{-\frac{3}{2}}\delta_\Omega^{\frac{1}{2}}\left(-\log(\|K_0\|_{L^\infty}+\tilde{\alpha}) + l_0\right)} \tag{4.4}$$

$$0 < \beta \le \beta_0 := \min\Bigg(\frac{\pi^2\theta - 2d_\Omega^2(18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha})}{38 d_\Omega^2},\ \frac{\theta - d_\Omega^2(\|K_0\|_{L^\infty}+\tilde{\alpha})}{d_\Omega^2},$$
$$\frac{\theta - d_\Omega(\|\epsilon_0\|_{W^{1,\infty}}+\tilde{\alpha})}{d_\Omega},\ \frac{\|K_0\|_{L^\infty}+\tilde{\alpha}}{2},\ \frac{d_\Omega^{\frac{3}{2}}\left\{2^{-\frac{3}{2}}\delta_\Omega^{\frac{1}{2}}(-\log(\|K_0\|_{L^\infty}+\tilde{\alpha})+l_0)\right\} - A}{A' + \frac{2^{-\frac{3}{2}}\delta_\Omega^{\frac{1}{2}} d_\Omega^{\frac{3}{2}}}{\|K_0\|_{L^\infty}+\tilde{\alpha}}}\Bigg). \tag{4.5}$$

Then for all $\mathbf{z} \in \Theta_\beta$ *and* $y_0^*(\mathbf{z})$ *defined as* (3.10),

$$\|\kappa(\mathbf{z})\|_{L^\infty}^2 \le \frac{\pi^2\theta}{d_\Omega^2} - \frac{1}{C_H}, \tag{4.6}$$

$$C_H\|f(\mathbf{z})\|_{L^2} + (C_H C_D + 1)\|w(\mathbf{z})\|_{H^2} < y_0^*(\mathbf{z}). \tag{4.7}$$

Proof. By Definition 2.2 and (A.1),

$$C_H \ge C_D^{-1} \ge \frac{1}{18\|\epsilon\|_{W^{1,\infty}} + \|\kappa\|_{L^\infty}^2}.$$

Since $\|\epsilon(z)\|_{W^{1,\infty}} \le \|\epsilon_0\|_{W^{1,\infty}} + \sum_{k=1}^{N}\alpha_k|z_k| \le \|\epsilon_0\|_{W^{1,\infty}} + \tilde{\alpha} + \beta$, and likewise for κ^2,

$$\begin{aligned}\frac{\pi^2\theta}{d_\Omega^2} - \frac{1}{C_H} &\ge \frac{\pi^2\theta}{d_\Omega^2} - (18\|\epsilon\|_{W^{1,\infty}} + \|\kappa^2\|_{L^\infty}) \\ &\ge \frac{\pi^2\theta}{d_\Omega^2} - (18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha} + 19\beta) \\ &\ge 18\|\epsilon_0\|_{W^{1,\infty}} + \|K_0\|_{L^\infty} + 19\tilde{\alpha} + 19\beta,\end{aligned} \tag{4.8}$$

where (4.8) is by the first bound of (4.5). Then (4.6) follows from (4.8). Now we show $C_H \le \frac{C_0}{\theta}$. By $d_\Omega^2 < \frac{\pi^2\theta}{2\mu}$ in (4.4), the second and third bounds in (4.5), and (A.7), we have

$$C_H \le \frac{\lambda_1^{-1}\langle\lambda_1^{\frac{1}{3}}\rangle^3}{\theta}\left(1 + \frac{2}{\theta\lambda_1}\left(\|\kappa^2\|_{L^\infty} + (3\lambda_1)^{\frac{1}{2}}\|\epsilon\|_{W^{1,\infty}}\right)\right) \le \frac{C_0}{\theta}, \tag{4.9}$$

where $C_0 = 100$ suffices. Hence if β is sufficiently small, say by taking $\|K_0\|_{L^\infty} + \tilde{\alpha}$ small in (4.5), then

$$C_H\|f(\mathbf{z})\|_{L^2} + (C_H C_D + 1)\|w(\mathbf{z})\|_{H^2} \le A + A'\beta. \tag{4.10}$$

To estimate the lower bound of $y_0^*(\mathbf{z})$, note that $C_S \le 2^{\frac{3}{2}}\delta_\Omega^{-\frac{1}{2}} d_\Omega^{-\frac{3}{2}}$ by $|\Omega| \ge \delta_\Omega d_\Omega^3$ and Lemma A.5. By an argument similar to (3.13), we have

$$\begin{aligned} y_0^*(\mathbf{z}) &> C_S^{-1}\left(\log\left(\frac{2}{C_H C_S|\Omega|^{\frac{1}{2}}\|\kappa^2\|_{L^\infty}}\right) - 1\right) \\ &\ge 2^{-\frac{3}{2}}\delta_\Omega^{\frac{1}{2}} d_\Omega^{\frac{3}{2}}\left(-\log\left(\|K_0\|_{L^\infty} + \tilde{\alpha} + \beta\right) + l_0\right) \\ &\ge 2^{-\frac{3}{2}}\delta_\Omega^{\frac{1}{2}} d_\Omega^{\frac{3}{2}}\left(-\log\left(\|K_0\|_{L^\infty} + \tilde{\alpha}\right) - \frac{\beta}{\|K_0\|_{L^\infty}+\tilde{\alpha}} + l_0\right).\end{aligned} \tag{4.11}$$

The condition that the upper bound in (4.10) is less than or equal to the lower bound in (4.11) is equivalent to (4.4) and the last bound of (4.5), and this shows (4.7). □

Remark 4.1. We remark that the conditions (4.3) and (4.4), which impose upper and lower bounds on d_Ω, are feasible, provided that the random inputs are sufficiently small, in their respective norms, with small variations $\tilde{\alpha}$. With these technical conditions, d_Ω is not arbitrarily small.

Theorem 4.1. *Assuming the hypotheses of Lemma 4.1, the solution map $\Theta_\beta \to H^2(\Omega)$ given by $\mathbf{z} \mapsto u(\mathbf{z})$ is complex-analytic for any $0 < \beta \le \beta_0$. If $\kappa(\mathbf{z})$ is non-vanishing on Θ_β, then*

$$\|u(\mathbf{z})\|_{H^2} < |\Omega|^{\frac{1}{2}} \cosh^{-1}\left(1 + \frac{18 \max_{\mathbf{z}\in\partial\Theta_\beta} \|\epsilon(\mathbf{z})\|_{W^{1,\infty}} + \max_{\mathbf{z}\in\partial\Theta_\beta} \|\kappa^2(\mathbf{z})\|_{L^\infty}}{\min_{\mathbf{z}\in\partial\Theta_\beta} \|\kappa^2(\mathbf{z})\|_{L^\infty}}\right). \tag{4.12}$$

Proof. A strategy of the proof is given. Since β is fixed, let $\Theta = \Theta_\beta$. By the Hartog's Theorem [57, Chap 1], any separately holomorphic functions are continuous on Θ, and therefore analytic by the Osgood's Lemma [40, Chap 1]. Let $\mathbf{z} = (z_n; z_n') \in \Theta$ where $z_n \in \mathbb{C}$ is the n^{th} coordinate of $\mathbf{z}$ and $z_n' \in \mathbb{C}^{N-1}$ is the rest of the coordinates. Let $s := \Re z_n,\ \omega := \Im z_n$. Based on the proof of [23, Lemma 8], we justify the existence of the partial derivatives of the solution $(\partial_s u, \partial_\omega u)$, after which, $u(z)$ is shown to satisfy the Cauchy-Riemann equation in z_n by taking the complex derivatives of (4.2). The non-vanishing assumption of κ emphasizes that our model is nonlinear.

By (4.7), the nPBE (4.2) admits a solution $\tilde{u} : \Theta \to H_0^1(\Omega) \cap H^2(\Omega)$ unique in $\{\phi \in H^2(\Omega) : \|\phi + w\|_{H^2} < M_0\}$ by Corollary 3.1. Let ζ_1, ζ_2 be the formal derivatives $\partial_s \tilde{u}_R, \partial_s \tilde{u}_I$, respectively. Taking the formal partial derivatives of (4.2) in s, the vector equation that consists of the real and imaginary parts is given by

$$-\nabla \cdot \left(\begin{pmatrix} \epsilon_R & -\epsilon_I \\ \epsilon_I & \epsilon_R \end{pmatrix} \nabla \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} \right) + \mathbf{V} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \tag{4.13}$$

where $u = \tilde{u} + w$ and

$$\mathbf{V}(\mathbf{z}) = \begin{pmatrix} \cosh(u_R)\cos(u_I) & -\sinh(u_R)\sin(u_I) \\ \sinh(u_R)\sin(u_I) & \cosh(u_R)\cos(u_I) \end{pmatrix} \begin{pmatrix} \kappa_R^2 - \kappa_I^2 & -2\kappa_R\kappa_I \\ 2\kappa_R\kappa_I & \kappa_R^2 - \kappa_I^2 \end{pmatrix},$$
$$\begin{pmatrix} f_1(\mathbf{z}) \\ f_2(\mathbf{z}) \end{pmatrix} = \nabla \cdot \left(\begin{pmatrix} \partial_s\epsilon_R & -\partial_s\epsilon_I \\ \partial_s\epsilon_I & \partial_s\epsilon_R \end{pmatrix} \nabla \begin{pmatrix} u_R \\ u_I \end{pmatrix} \right) + \nabla \cdot \left(\begin{pmatrix} \epsilon_R & -\epsilon_I \\ \epsilon_I & \epsilon_R \end{pmatrix} \nabla \begin{pmatrix} \partial_s w_R \\ \partial_s w_I \end{pmatrix} \right) + \mathbf{V} \begin{pmatrix} \partial_s w_R \\ \partial_s w_I \end{pmatrix} + \begin{pmatrix} \partial_s f_1 \\ \partial_s f_2 \end{pmatrix}.$$

By Hypothesis 2, it can be shown that $f_1(\mathbf{z}), f_2(\mathbf{z}) \in L^2(\Omega; \mathbb{R})$. Considering $L^2(\Omega; \mathbb{C}), H_0^1(\Omega; \mathbb{C})$ as product spaces of two function spaces over $\mathbb{R}$, the product $\mathscr{H} = H_0^1(\Omega; \mathbb{R})^{\otimes 2} \times H_0^1(\Omega; \mathbb{R})^{\otimes 2}$ defines a Hilbert space under

$$\langle \phi, \psi \rangle = \left\langle \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \right\rangle = \int_\Omega (\nabla\phi_1 \cdot \nabla\psi_1 + \nabla\phi_2 \cdot \nabla\psi_2)\, dx.$$

Let $B : \mathscr{H} \times \mathscr{H} \to \mathbb{R}$ be the bilinear form corresponding to (4.13). Consider $B = B_1 + B_2$ defined by

$$B_1(\phi, \psi) = \int_\Omega \left(\begin{pmatrix} \epsilon_R & -\epsilon_I \\ \epsilon_I & \epsilon_R \end{pmatrix} \begin{pmatrix} \nabla\phi_1 \\ \nabla\phi_2 \end{pmatrix} \right) \cdot \begin{pmatrix} \nabla\psi_1 \\ \nabla\psi_2 \end{pmatrix} dx$$
$$B_2(\phi, \psi) = \int_\Omega \left(\mathbf{V} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \right) \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} dx.$$

By the uniform ellipticity condition Hypothesis 3, we have

$$\begin{aligned} |B_1(\phi, \psi)| &\le \|\epsilon(\mathbf{z})\|_{L^\infty} \|\phi\|_{\mathscr{H}} \|\psi\|_{\mathscr{H}}, \\ B_1(\phi, \phi) &\ge \theta \|\phi\|_{\mathscr{H}}^2, \end{aligned} \tag{4.14}$$

and hence B_1 is coercive. The boundedness of B_2 follows immediately from the Minkowski inequality

$$|B_2(\phi, \psi)| \le \left(2\lambda_1^{-1} \cosh(2\|u_R(\mathbf{z})\|_{L^\infty}) \|\kappa(\mathbf{z})\|_{L^\infty}^2\right) \|\phi\|_{\mathscr{H}} \|\psi\|_{\mathscr{H}}.$$

Let $r(x,\mathbf{z}) := \sqrt{\cosh^2(u_R(x,\mathbf{z}))|\kappa(x,\mathbf{z})|^4 - (2\kappa_R(x,\mathbf{z})\kappa_I(x,\mathbf{z}))^2}$. Combining the lower bound

$$\begin{aligned} B_2(\phi,\phi) &= \int_\Omega (\cosh(u_R)\cos(u_I)(\kappa_R^2 - \kappa_I^2) - 2\sinh(u_R)\sin(u_I)\kappa_R\kappa_I)(\phi_1^2 + \phi_2^2) \\ &\geq -\int_\Omega r(x,\mathbf{z})(\phi_1^2 + \phi_2^2) \geq -\|r(\cdot,\mathbf{z})\|_\infty \lambda_1^{-1}\|\phi\|_{\mathscr{H}}^2, \end{aligned}$$

with the coercivity estimate (4.14) of B_1, we have

$$B(\phi,\phi) \geq \left(\theta - \|r(\cdot,\mathbf{z})\|_\infty \lambda_1^{-1}\right)\|\phi\|_{\mathscr{H}}^2. \tag{4.15}$$

By the Sobolev Embedding Theorem and Theorem 3.1, we obtain

$$\begin{aligned} r(x,\mathbf{z}) &\leq \cosh(|u(x,\mathbf{z})|)|\kappa(\mathbf{z})|^2 \leq \cosh(C_S(2)\|u\|_{H^2})|\kappa(\mathbf{z})|^2 < \cosh(C_S M_0)|\kappa(\mathbf{z})|^2 \\ &\leq \|\kappa(\mathbf{z})\|_{L^\infty}^2 + \frac{1}{C_H C_S |\Omega|^{\frac{1}{2}}}, \end{aligned}$$

where the last inequality is by (3.12). It follows from Lemma A.5 that $C_S|\Omega|^{\frac{1}{2}} \geq 1$. By (4.6) and (2.2),

$$r(x,\mathbf{z}) < \|\kappa(\mathbf{z})\|_{L^\infty}^2 + \frac{1}{C_H} \leq \frac{\pi^2\theta}{d_\Omega^2} \leq \lambda_1\theta,$$

and hence the coercivity of B from (4.15). By the Lax-Milgram Theorem, (4.13) is well-posed in $\mathscr{H}$ and by the elliptic regularity theory, it follows that $\begin{pmatrix}\zeta_1(\mathbf{z})\\ \zeta_2(\mathbf{z})\end{pmatrix} \in \mathscr{H} \cap (H^2(\Omega;\mathbb{R}) \times H^2(\Omega;\mathbb{R}))$. Adopting the argument in [23, Lemma 8] where (4.2) is considered in its weak form, it can be shown that $\partial_s\tilde{u}_R(\mathbf{z}), \partial_s\tilde{u}_I(\mathbf{z})$ exist for every $z \in \Theta$ and

$$\zeta_1(\mathbf{z}) = \partial_s\tilde{u}_R(\mathbf{z}),\ \zeta_2(\mathbf{z}) = \partial_s\tilde{u}_I(\mathbf{z}).$$

Taking the formal derivative of (4.2) in the imaginary variable yields an analogous conclusion for $\partial_\omega\tilde{u}$.

Let $P(x,\mathbf{z}) = \partial_s\tilde{u}_R(\mathbf{z}) - \partial_\omega\tilde{u}_I(\mathbf{z})$ and $Q(x,\mathbf{z}) = \partial_\omega\tilde{u}_R(\mathbf{z}) + \partial_s\tilde{u}_I(\mathbf{z})$. By taking the partial derivatives of (4.2) and using the Cauchy-Riemann equations satisfied by the coefficient functions given by the hypotheses, one can argue as (22) of [21] that P, Q satisfy

$$-\nabla\cdot\left(\begin{pmatrix}\epsilon_R & -\epsilon_I\\ \epsilon_I & \epsilon_R\end{pmatrix}\nabla\begin{pmatrix}P\\ Q\end{pmatrix}\right) + \mathbf{V}\begin{pmatrix}P\\ Q\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix} \text{ in } \Omega\times\Theta,$$

under the zero Dirichlet boundary condition. By the Lax-Milgram Theorem, the Cauchy-Riemann equation $P(z_n; z_n') = Q(z_n; z_n') = 0$ holds for all

$$z_n \in \Theta(z_n') := \{\zeta \in \mathbb{C} : (\zeta; z_n') \in \Theta\},$$

for each z_n'. Then $\tilde{u} : \Theta \to H_0^1(\Omega) \cap H^2(\Omega)$ defines a complex-analytic map as outlined in the beginning of our proof, and so does $u = \tilde{u} + w$ define a $H^2(\Omega)$-valued analytic map. Indeed the analytic extension of g implies that of $w = T^{-1}g$.

From Corollary 3.1, $\|u(\mathbf{z})\|_{H^2} < M_0$ where $M_0 > 0$ is given by (3.12). By (A.1) and Lemma A.5, we have

$$\|u(\mathbf{z})\|_{H^2} < M_0 \leq |\Omega|^{\frac{1}{2}}\cosh^{-1}\left(1 + \frac{18\|\epsilon(\mathbf{z})\|_{W^{1,\infty}} + \|\kappa^2(\mathbf{z})\|_{L^\infty}}{\|\kappa^2(\mathbf{z})\|_{L^\infty}}\right),$$

and (4.12) follows from the maximum modulus principle. □

Suppose that the QoI function $Q : H^2(\Omega) \to \mathbb{R}$ extends analytically to the Bernstein polyellipse, i.e, $\mathbf{z} \mapsto Q(u(\cdot,\mathbf{z})) \in \mathbb{C}$ is analytic. In the following section, we apply Theorem 4.1 to obtain well-defined error bounds for a QoI of the solution of the nPBE. This is achieved by using a sparse grid stochastic collocation method.

5. Tensor sparse grid polynomial approximation

Consider the problem of approximating a function $\nu : \Gamma \to W$ on the domain Γ and Banach space W. The goal is to efficiently approximate such a function using tensor product polynomials. The accuracy of the polynomial representation depends on the existence of an analytic extension of ν onto the complex domain $\Theta \subset \mathbb{C}^N$. In this section, we briefly discuss sparse grids, which have become a popular method for approximating functions with complex analytic extensions. A more detailed exposition can be found in [4, 74, 21, 23].

Let $\mathcal{P}_p(\tilde{\Gamma}) := \text{span}(y^k,\, k = 0, \ldots, p)$ where $\tilde{\Gamma} \equiv [-1, 1]$. Consider a univariate function $\nu : \tilde{\Gamma} \to W$ and the univariate Lagrange interpolant $\mathcal{I}_p^{m(i)} : C^0(\tilde{\Gamma}) \to \mathcal{P}_{m(i)-1}(\tilde{\Gamma})$ such that

$$\mathcal{I}_p^{m(i)}(\nu(y)) := \sum_{k=1}^{m(i)} \nu(\cdot, y_k) l_k^p(y),$$

where $i \geq 0$ is the level of approximation and $m(i) \in \mathbb{N}_0$ is the number of evaluation points at level $i \in \mathbb{N}_0$. Let $m(0) = 0$, $m(1) = 1$, and $m(i) \leq m(i+1)$ if $i \geq 1$. By convention, for $m(0) = 0$, let $\mathcal{P}_{-1} = \emptyset$. Furthermore, the Lagrange polynomials l_k^p form a basis for $\mathcal{P}_p(\tilde{\Gamma})$.

The Lagrange interpolant can be easily extended to N dimensions by taking tensor products. Let $\mathcal{P}_{\mathbf{p}}(\Gamma) = \bigotimes_{n=1}^N \mathcal{P}_{p_n}(\Gamma_n)$ be an index of polynomial degree along each dimension of Γ. The interpolant $\mathcal{I}_{\mathbf{p}} : C^0(\Gamma) \to \mathcal{P}_{\mathbf{p}}(\Gamma)$ can be constructed as $\mathcal{I}^{\mathbf{p}} := \mathcal{I}_{p_1}^{m(i)} \otimes \mathcal{I}_{p_2}^{m(i)} \otimes \cdots \otimes \mathcal{I}_{p_N}^{m(i)}$. Thus for any function $\nu : \Gamma \to W$, we have

$$\mathcal{I}^{\mathbf{p}}(\nu(\mathbf{y})) = \sum_{k \in \mathcal{K}} \nu(\cdot, \mathbf{y}_k) l_k^{\mathbf{p}}(\mathbf{y}),$$

where $\mathcal{K}$ is an appropriate index set and $l_k^{\mathbf{p}}(\mathbf{y})$ are tensors of univariate Lagrange polynomials. However, the dimensionality of $\mathcal{P}_p$ and the index set $\mathcal{K}$ increases as $\prod_{n=1}^N (p_n + 1)$ with N. This polynomial representation suffers from the curse of dimensionality and becomes intractable for even a moderate amount of dimensions [52]. In contrast, if sufficient regularity of $\nu(\mathbf{y})$ exists with respect to $\mathbf{y} \in \Gamma$ the, dimensionality of the polynomial approximation can be significantly reduced by restricting the degree of the tensor product polynomial along each dimension.

Consider the difference operator along the n^{th} dimension of Γ

$$\Delta_{p,n}^{m(i)} := \mathcal{I}_p^{m(i)} - \mathcal{I}_p^{m(i-1)}.$$

Let $\mathbf{i} = (i_1, \ldots, i_N) \in \mathbb{N}_+^N$ be a multi-index, w be the level of approximation of the sparse grid, and $g : \mathbb{N}_+^N \to \mathbb{N}$ be a restriction function that acts on $\mathbf{i}$; in this section, we adopt the notation $g(\mathbf{i})$ from [21]. The sparse grid approximation of ν is constructed as

$$\mathcal{S}_w^{m,g}[\nu] = \sum_{\mathbf{i} \in \mathbb{N}_+^N : g(\mathbf{i}) \leq w} \bigotimes_{n=1}^N \Delta_n^{m(i_n)}(\nu(\mathbf{y})).$$

By choosing the function $m(i)$ and g appropriately the dimensionality of the sparse grid can be controlled. The Smolyak sparse grid [74] can be built with the following formulas:

$$m(i) = \begin{cases} 1, & \text{for } i = 1 \\ 2^{i-1} + 1, & \text{for } i > 1 \end{cases} \quad \text{and} \quad g(\mathbf{i}) = \sum_{n=1}^N (i_n - 1),$$

where

$$f(p) = \begin{cases} 0, \; p = 0 \\ 1, \; p = 1 \\ \lceil \log_2(p) \rceil, \; p \geq 2. \end{cases}$$

The second step is to choose the location of the knots $\mathbf{y}_k$. For the domain Γ, a good choice is the Clenshaw-Curtis (CC) abscissa [72]. This consists of the extrema of Chebyshev polynomials:

$$y_j^n = -\cos\left(\frac{\pi(j-1)}{m(i)-1}\right).$$

Remark 5.1. Note that isotropic sparse grids can be extended to anisotropic setting. By adapting the function g to the contribution of each dimension to the function $\nu(\mathbf{y})$, higher convergence rates can be achieved [73].

We are now interested in obtaining bounds for the error of the sparse grid i.e. $\|\nu - \mathcal{S}^{m,g}_{v}[\nu]\|_{L^{\infty}(\Gamma)}$. This bound can be shown to be controlled by i) the number of dimensions N, ii) the number of knots η in the sparse grid, but most importantly iii) the size of the region of complex region of the analytic extension of $\nu(\mathbf{y})$ onto $\mathbb{C}^N$.

It is known that if a one dimensional function $v : \tilde{\Gamma} \rightarrow W$ can be analytically extended onto the Bernstein ellipse $\mathcal{E}_{\hat{\sigma}_n}$ then the error of the Lagrange interpolation of u will decay exponentially with respect to the degree of the polynomial and the rate of decay we will controlled by the size of the parameter $\hat{\sigma}_n > 0$ [5, 23]. This result has been extended to sparse grid polynomials in [74, 73] on suitable Banach spaces where the convergence rate was shown to be algebraic or sub-exponential.

We set $\hat{\sigma} \equiv \min_{n=1,\ldots,N} \hat{\sigma}_n$, i.e. the decay is controlled by the Bernstein ellipse with the smallest size. This setting corresponds to an isotropic sparse grid. For simplicity, we restrict our attention to the statistics of the QoI, therefore suppose that $W = \mathbb{R}$ and let

$$\tilde{M}(\nu) := \sup_{\mathbf{z} \in \mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N}} \|\nu(\mathbf{z})\|_W.$$

In addition, let $\sigma = \hat{\sigma}/2$, $\mu_1 = \frac{\sigma}{1+\log(2N)}$, $\mu_2(N) = \frac{\log(2)}{N(1+\log(2N))}$, $\tilde{C}_2(\sigma) = 1 + \frac{1}{\log 2}\sqrt{\frac{\pi}{2\sigma}}$, $\delta^*(\sigma) = \frac{e\log(2)-1}{\tilde{C}_2(\sigma)}$, $C_1(\sigma, \delta, \tilde{M}(\nu)) = \frac{4C\tilde{C}_2(\sigma)a(\delta,\sigma)}{e\delta\sigma}$, $C := \frac{4}{e^{2\sigma}-1}$,

$$a(\delta, \sigma) := \exp\left(\delta\sigma\left\{\frac{1}{\sigma\log^2(2)} + \frac{1}{\log(2)\sqrt{2\sigma}} + 2\left(1 + \frac{1}{\log(2)}\sqrt{\frac{\pi}{2\sigma}}\right)\right\}\right),$$

$\mu_3 = \frac{\sigma\delta^*\tilde{C}_2(\sigma)}{1+2\log(2N)}$, and

$$\mathcal{Q}(\sigma, \delta^*(\sigma), N, \tilde{M}(\nu)) = \frac{C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu))}{\exp(\sigma\delta^*(\sigma)\tilde{C}_2(\sigma))} \frac{\max\{1, C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu))\}^N}{|1 - C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu))|}.$$

The following result is obtained [74, 23, 22]:

Theorem 5.1. *Suppose that $\nu \in C^0(\Gamma; \mathbb{R})$ admits an analytic extension on $\mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N}$ and is absolutely bounded by $\tilde{M}(\nu)$. Let $\mathcal{S}^{m,g}_{w}[\nu]$ be the sparse grid approximation of the function ν with Clenshaw-Curtis abcissas. If $w > N/\log 2$, then*

$$\|\nu - \mathcal{S}^{m,g}_{w}[\nu]\|_{L^{\infty}(\Gamma)} \leq \mathcal{Q}(\sigma, \delta^*(\sigma), N, \tilde{M}(\nu))\eta^{\mu_3(\sigma,\delta^*(\sigma),N)} \exp\left(-\frac{N\sigma}{2^{1/N}}\eta^{\mu_2(N)}\right), \tag{5.1}$$

Furthermore, if $w \leq N/\log 2$, then the following algebraic convergence bound holds:

$$\|\nu - \mathcal{S}^{m,g}_{w}[\nu]\|_{L^{\infty}(\Gamma)} \leq \frac{C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu)) \max\{1, C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu))\}^N}{|1 - C_1(\sigma, \delta^*(\sigma), \tilde{M}(\nu))|}\eta^{-\mu_1}. \tag{5.2}$$

Proof. Theorem 3.10 and 3.11 in [74]. □

Note that in many practical cases, not all dimensions of Γ are equally important. In these cases, the dimensionality of the sparse grid can be significantly reduced by exploiting the size of each Bernstein ellipse. By adapting the restriction function g to the $\hat{\sigma}_n$ along each dimension, an anisotropic sparse grid is produced with higher convergence rates with respect to the number of knots η [73].

Remark 5.2. From Theorem 5.1, a priori error bounds for applying a Smolyak sparse grid on the QoI of the solution of the nPBE are obtained. In particular, from Theorem 4.1, the coefficient $\tilde{M}(\nu)$ where $\nu := Q(u)$ will be uniformly bounded and controlled by the bound on $\|u(\mathbf{z})\|_{H^2} < M_0$ on the Bernstein polyellipse $\mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N}$, which is properly embedded in Θ_β. The size of the parameter σ from the polyellipse $\mathcal{E}_{\hat{\sigma}_1,\ldots,\hat{\sigma}_N}$ controls the decay of the error with respect to the number of collocation points of the sparse grid.

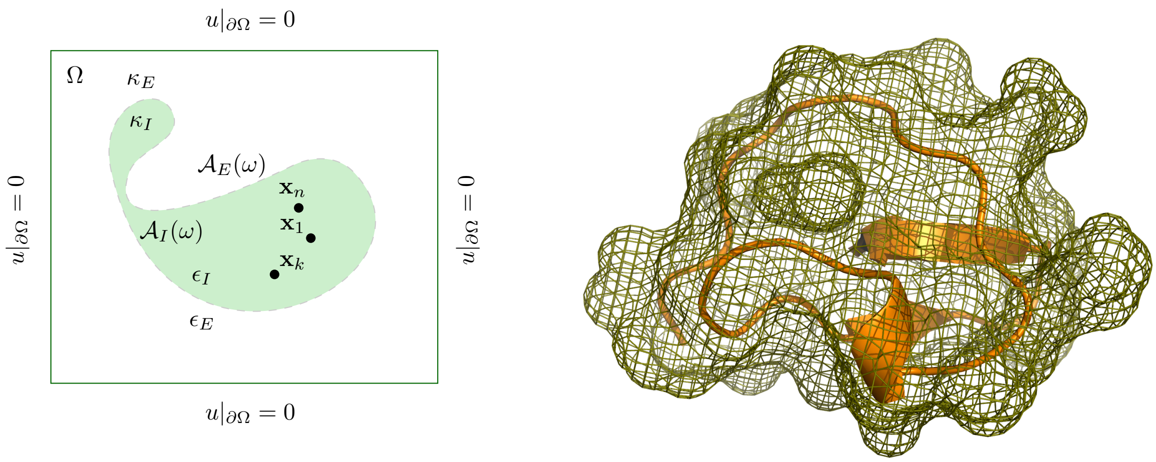

Figure 4: Cartoon example of a protein embedded in a solvent. On the right side the surface of the CMTI molecule is rendered using Pymol with the cartoon representation of CMTI embedded inside.

6. Numerical Results

We validate the complex analyticity of the NPBE. This will be achieved by applying a series of numerical experiments that show that we achieve algebraic and sub-exponential convergence rates with respect to the number of knots of the sparse grid. This would be consistent with Theorem 5.1. We test our stochastic solver on the Cucurbita Maxima Trypsin Inhibitor I (CMTI-I) [56] and compute the potential fields inside a pre-defined volume. This molecule consists of 268 atoms immersed in a solvent.

The domain Ω is split into an internal component $\mathcal{A}_I$, which consists of the CMTI molecule and $\mathcal{A}_E$ is the external domain, which corresponds to the solvent. The point charges $\mathcal{C} := \{\mathbf{x}_1, \dots \mathbf{x}_n\}$ correspond to the center of each atom in CMTI. However, in practice,, the nPBE numerical solver replaces these point charges with functions in $L^2(\Omega)$. The dielectric constant is assigned as $\epsilon_I = 1$ within the molecule and $\epsilon_E = 1$ in the surrounding solvent, both being dimensionless quantities. The Debye-Hückel parameter κ is separated into internal and external regions where $\kappa_I = 0.1$ Å^{-1} and $\kappa_E = 0$. Note that Å corresponds to the unit of length of one angstrom. The molecule is enclosed in the region Ω and the Dirichlet boundary condition on $\partial\Omega$ is set to zero. The temperature of the solvent is set to 310 Kelvin. In Figure 4 a cartoon example of the CMTI molecule enclosed in the region Ω is shown. On the right-hand side of Figure 4 the surface of CMTI molecule is rendered using Pymol [83, 84, 85]. The embedded cartoon representation of the molecule is contained in the surface.

The potential field is calculated using the Adaptive Poisson-Boltzmann Solver (APBS) [8, 51]. APBS solves the nPBE by using a finite difference scheme. The grid size is set to the maximum resolution, which corresponds to 609^3. The size of the domain Ω is set to $\mathcal{D}$ of size $40 \times 40 \times 40$ Å^3, or $50 \times 50 \times 50$ Å^3.

Let $u(x, Y_1, \dots, Y_N)$ denote the solution of nPBE with respect to the random variables $Y_1, \dots, Y_N$. The quantity of interest (QoI) is defined as

$$Q(u) := \int_\Omega u(x, Y_1, \dots, Y_N) dx.$$

To evaluate the uncertainty, the mean error $|\mathbb{E}[Q(u)] - \mathbb{E}[\mathcal{S}_w^{m,g}[Q(u)]]|$ and the variance error $|Var[Q(u)] - Var[\mathcal{S}_w^{m,g}[Q(u)]]|$ are calculated using a sparse grid approach. Furthermore, the relative mean and variance errors are computed as

$$\frac{|\mathbb{E}[Q] - \mathbb{E}[\mathcal{S}_w^{m,g}[Q]]|}{|\mathbb{E}[Q]|} \quad \text{and} \quad \frac{|Var[Q] - Var[\mathcal{S}_w^{m,g}[Q]]|}{|Var[Q]|}.$$

Next, the CMTI-I molecule undergoes random shifts and rotations within the domain Ω using a stochastic model. Due to the zero Dirichlet boundary conditions, the solution does not simply translate or rotate with

N		$S_w^{m,g}$	Stochastic operator on $\mathcal{C}$	Ω
2	$\beta = 2$	$w = 0,\dots,6$	$\mathbf{x} \to \mathbf{Q}_1(\beta, Y_1)\mathbf{Q}_2(\beta, Y_2)\mathbf{x}$	$40 \times 40 \times 40$ Å^3
3	$\alpha = 5$	$w = 0,\dots,5$	$\mathbf{x} \to \mathbf{T}(Y_1, Y_2, Y_3)\mathbf{x}$	$50 \times 50 \times 50$ Å^3
5	$\alpha = 4$, $\beta = 8$	$w = 0,\dots,5$	$\mathbf{x} \to \mathbf{Q}_1(\beta, Y_1)\mathbf{Q}_2(\beta, Y_2)\mathbf{T}(\alpha, Y_3, Y_4, Y_5)\mathbf{x}$	$40 \times 40 \times 40$ Å^3

Table 1: Rotation and translation stochastic perturbation test of the CMTI molecule in the domain Ω.

the molecule but instead varies in a non-linear manner with the atomic displacements defined by $\mathcal{C}$. For each interpolation knot in the stochastic domain Γ the molecular domain Ω is discretized and the corresponding potential field is recalculated using APBS. Define the translation operator $\mathbf{T}$ on any element $\mathbf{x} \in \mathcal{C}$ as

$$\mathbf{x} \to \mathbf{T}(Z_1, Z_2, Z_3)\mathbf{x} := \mathbf{x} + \alpha(Z_1\mathbf{e}_1 + Z_2\mathbf{e}_2 + Z_3\mathbf{e}_3),$$

where $\alpha \geq 0$, $\mathbf{e}_1 = [1,0,0]^T$, $\mathbf{e}_2 = [0,1,0]^T$, and $\mathbf{e}_3 = [0,0,1]^T$. The random variables Z_i, for $i = 1, \dots 3$, are iid uniform on $[-\sqrt{3}, \sqrt{3}]$. Similarly, form the rotation operators on any element $\mathbf{x} \in \mathcal{C}$ as

$$\mathbf{x} \to \mathbf{Q}_1(\beta, Z_1)\mathbf{Q}_2(\beta, Z_2)\mathbf{x},$$

where $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are the rotation matrices:

$$\mathbf{Q}_1(\beta, Z_1) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(Z_1/\beta) & -\sin(Z_1/\beta) \\ 0 & \sin(Z_1/\beta) & \cos(Z_1/\beta) \end{bmatrix}, \mathbf{Q}_2(\beta, Z_2) = \begin{bmatrix} \cos(Y_2/\beta) & 0 & -\sin(Z_2/\beta) \\ 0 & 1 & 0 \\ \sin(Z_2/\beta) & 0 & \cos(Z_2/\beta) \end{bmatrix}$$

and the coefficient $\beta > 0$ throttles the scale of the rotation angle.

Suppose that $Y_1, \dots, Y_5$ are iid random variables uniformly distributed and takes values on $[-\sqrt{3}, \sqrt{3}]$. We now perform 3 tests of dimensions $N = 2, 3, 5$: i) For $N = 2$ we perform a stochastic rotation of the molecule. ii) For $N = 3$ a translation test is performed; and iii) For $N = 5$ a combination of rotation and translation tests is performed. In Table 1 the numerical test parameters are given. We control the size of the perturbation with the parameters α and β.

In Figure 5 the convergence rates for the mean and variance of the tests in Table 1 are shown. Relative and absolute values are plotted with respect to the number of interpolation knots in the sparse grid $\mathcal{S}^{m,g}$. For $\mathbb{E}[Q]$ and $Var[Q]$ we assume that the sparse grid interpolation for the maximum level is the actual value. Note that we did not plot all the sparse grid levels. This is due to the limitation of the accuracy of the solver, and thus we plot until saturation is reached.

Observe that the mean convergence rates for $N = 2, 3, 5$ are at least sub-exponential. This is consistent with our result for complex analyticity and Theorem 5.1. However, the sub-exponential rate in Figure 4 is clearly faster than the algebraic bound predicted by Theorem 5.1 i.e. when $w > N/log(2)$. From Theorem 5.1 for $N = 3$, sub-exponential rate is predicted when $w > N/log(2) = 4.32$ and for $N = 5$ this is achieved when $w > 7.2$.

In Figure 4 the variance error plot shows sub-exponential convergence for $N = 2$. For $N = 3$ and $N = 5$ the convergence rate reduces to algebraic. This is consistent with Theorem 5.1 as algebraic convergence rates are predicted for these two cases.

7. Conclusion

We established the existence and uniqueness of solutions to the complexified nonlinear Poisson-Boltzmann equation (nPBE) and proved that these solutions admit complex analytic extensions with respect to stochastic variables. A key challenge was the non-convexity of the nonlinearity in $\mathbb{C}$, which precludes variational methods; instead, we employed a contraction mapping approach. Crucially, the exponentially-growing nonlinearity necessitates smallness conditions on the data to ensure well-posedness—without these, uniqueness may fail.

Beyond the theoretical contributions, our numerical results validated the predicted convergence rates of the sparse grid stochastic collocation method using Clenshaw-Curtis abscissas. Specifically, we observed algebraic to sub-exponential convergence, consistent with the analyticity properties established in our analysis.

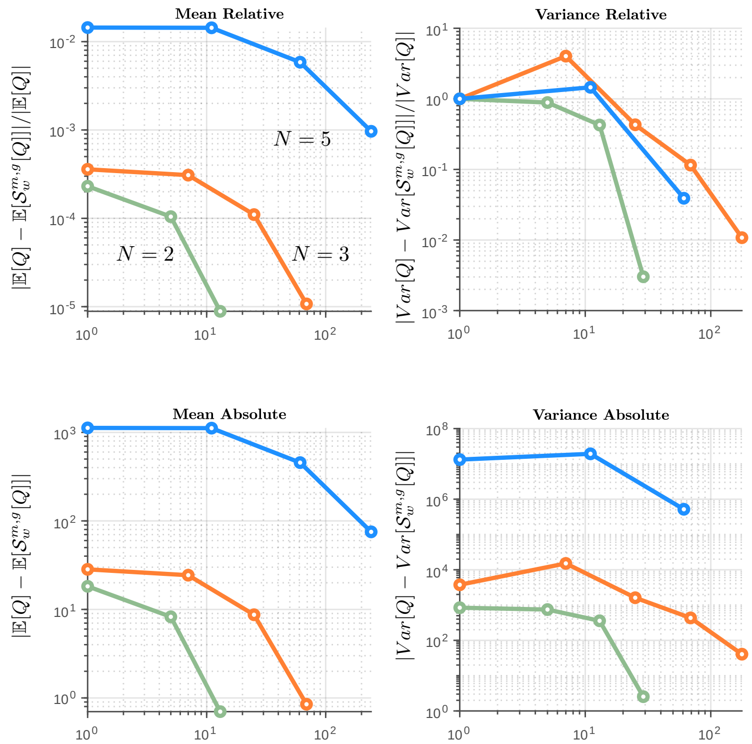

Figure 5: Convergence graphs of the relative and absolute error for the stochastic experiments from Table 1. For all 3 tests ($N = 2, 3, 5$) the convergence rates for the mean are sub-exponential. For $N = 2$ the convergence rate is also sub-exponential for the variance error. As the stochastic N increases the rate reduces to algebraic. This is consistent with Theorem 5.1

This highlights the practical advantage of using sparse grids in uncertainty quantification, enabling efficient approximation of moderately high-dimensional stochastic solutions.

Future work will extend this framework to nPBE models with discontinuous dielectric interfaces, which better capture molecular electrostatics. Developing a functional-analytic approach for these cases will be key to bridging mathematical theory with practical applications.

Appendices

A. Estimates for the Constants.

In Theorem 3.1, the existence and uniqueness of solutions of (1.1) depend in part on the values of the constants $C_S(s)$, C_H, and C_D described in Definition 2.2. Thus having explicit estimates for these constants is important in determining the parameter values for which there are solutions. In this section, we demonstrate bounds for these constants. Hypotheses 3 and 4 are still assumed to hold throughout Appendix A.

A.1. Estimates for C_D

Lemma A.1. *Let L be as in Equation (2.10). Then*

$$C_D \le 2d^2\|\epsilon\|_{W^{1,\infty}} + \|\kappa\|_{L^\infty}^2. \tag{A.1}$$

Proof. Since

$$\|\kappa^2 v\|_{L^2} \le \|\kappa\|_{L^\infty}^2 \|v\|_{L^2} \le \|\kappa\|_{L^\infty}^2 \|v\|_{H^2},$$

it suffices to estimate $\|\nabla \cdot (\epsilon \nabla v)\|_{L^2}$. By the triangle inequality,

$$\|\nabla \cdot (\epsilon \nabla v)\|_{L^2} = \|\sum_{i,j} \partial_i(\epsilon^{ij}\partial_j v)\|_{L^2} \leq \sum_{i,j} \|\partial_i(\epsilon^{ij}\partial_j v)\|_{L^2} \leq \sum_{i,j} \|\partial_i \epsilon^{ij} \partial_j v\|_{L^2} + \|\epsilon^{ij}\partial_{ij} v\|_{L^2}$$
$$\leq \sum_{i,j} (\|\partial_i \epsilon^{ij}\|_{L^\infty} + \|\epsilon^{ij}\|_{L^\infty})\|v\|_{H^2} \leq 2d^2 \|\epsilon\|_{W^{1,\infty}} \|v\|_{H^2},$$

and hence (A.1).

□

A.2. Estimates for $C_S(2)$.

In this subsection, we are interested in obtaining an upper bound of the operator norm of $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ where $\Omega \subseteq \mathbb{R}^3$. To obtain this Sobolev inequality constant, a standard trick is to obtain the desired constant for the full domain $\mathbb{R}^d$. Any reasonably regular function defined on Ω can be extended to $\mathbb{R}^d$ via an extension operator. Composing these two, one obtains a Sobolev inequality on Ω. See [31, Chapter 5] for an exposition of this material. To apply the estimates obtained in [68], we lay out the following notation. For $1 \leq p < q \leq \infty$, let $C_{p,q}, D_{p,q} > 0$ such that for every $v \in W^{1,p}(\Omega)$ and $v_\Omega := |\Omega|^{-1} \int_\Omega v$,

$$\|v\|_{L^q(\Omega)} \leq C_{p,q} \|v\|_{W^{1,p}(\Omega)}, \ \|v - v_\Omega\|_{L^q(\Omega)} \leq D_{p,q} \|\nabla v\|_{L^p(\Omega)}. \tag{A.2}$$

To estimate $C_{2,p}$ and $C_{p,\infty}$, we cite

Lemma A.2. *[68, Theorem 2.1] For $\Omega \subseteq \mathbb{R}^d$, if $D_{p,q} > 0$ is given as* (A.2)*, then*

$$C_{p,q} = 2^{1-\frac{1}{p}} \max(|\Omega|^{\frac{1}{q}-\frac{1}{p}}, D_{p,q}).$$

The estimation for the Sobolev embedding constant, therefore, reduces to computing $D_{p,q}$, which is summarized in the following two lemmas:

Lemma A.3. *[68, Theorem 3.2] Let $p \in (2, 6]$ and $v \in H^1(\Omega)$ where we further suppose that Ω is convex. Then, we have $\|v - v_\Omega\|_{L^p(\Omega)} \leq D_{2,p} \|\nabla v\|_{L^2(\Omega)}$ with*

$$D_{2,p} = \frac{d_\Omega^{1+\frac{3(p+2)}{2p}} \pi^{\frac{3(p+2)}{4p}}}{3|\Omega|} \frac{\Gamma(\frac{3(p-2)}{4p})}{\Gamma(\frac{3(p+2)}{4p})} \sqrt{\frac{\Gamma(\frac{3}{p})}{\Gamma(\frac{3(p-1)}{p})}} \left(\frac{4}{\sqrt{\pi}}\right)^{\frac{p-2}{2p}}. \tag{A.3}$$

Hence

$$C_{2,p} = 2^{\frac{1}{2}} \max(|\Omega|^{\frac{1}{p}-\frac{1}{2}}, D_{2,p}).$$

Lemma A.4. *[68, Theorem 3.4] For $p > 3$ and $v \in W^{1,p}(\Omega)$, we have $\|v - v_\Omega\|_{L^\infty} \leq D_{p,\infty} \|\nabla v\|_{L^p}$ with*

$$D_{p,\infty} = \frac{d_\Omega^3}{3|\Omega|} \left|\left||x|^{-2}\right|\right|_{L^{p'}(V)}, \tag{A.4}$$

where $\Omega_x := \{x - y : y \in \Omega\}$ and $V = \bigcup_{x \in \Omega} \Omega_x$.[1] *Hence*

$$C_{p,\infty} = 2^{1-\frac{1}{p}} \max(|\Omega|^{-\frac{1}{p}}, D_{p,\infty}).$$

Our proof for the existence of solution depends on the size of the Sobolev inequality constant.

[1] $p' := \frac{p}{p-1}$ denotes the Hölder conjugate of p.

Lemma A.5. *For every $p \in (3,6)$ and $\Omega \subseteq \mathbb{R}^3$ bounded and convex, we have*

$$|\Omega|^{-\frac{1}{2}} \leq C_S(2) \leq 2^{\frac{1}{p}} C_{2,p} C_{p,\infty},$$

where for $1 \leq p < q \leq \infty$, denote $C_{p,q} > 0$ by a constant such that for every $u \in W^{1,p}(\Omega)$

$$\|v\|_{L^q(\Omega)} \leq C_{p,q} \|v\|_{W^{1,p}(\Omega)}.$$

If we further assume that $|\Omega| = C d_\Omega^3$ for some $C > 0$, then there exists $d_0 > 0$ such that for every $d_\Omega \leq d_0$,

$$|\Omega|^{-\frac{1}{2}} \leq C_S(2) \leq 2^{\frac{3}{2}} |\Omega|^{-\frac{1}{2}}.$$

Proof. Consider the embedding $H^2(\Omega) \hookrightarrow W^{1,p}(\Omega) \hookrightarrow L^\infty(\Omega)$, which is continuous when $p \in (3,6)$. From the first embedding, we obtain

$$\begin{aligned}
\|v\|_{W^{1,p}}^p &= \|v\|_{L^p}^p + \sum_{i=1}^d \|\partial_i v\|^p \\
&\leq C_{2,p}^p \|v\|_{H^1}^p + C_{2,p}^p \sum_{i=1}^d \|\partial_i v\|_{H^1}^p \leq C_{2,p}^p \|v\|_{H^1}^p + C_{2,p}^p \Big(\sum_{i=1}^d \|\partial_i v\|_{H^1}^2 \Big)^{p/2} \\
&\leq C_{2,p}^p \|v\|_{H^1}^p + C_{2,p}^p \|v\|_{H^2}^p \leq 2 C_{2,p}^p \|v\|_{H^2}^p,
\end{aligned}$$

and from the second embedding,

$$\|v\|_{L^\infty} \leq C_{p,\infty} \|v\|_{W^{1,p}}.$$

Combining the two, we obtain the upper bound. For the lower bound, consider a family of constant functions defined on Ω. Then

$$\frac{\|c\|_{L^\infty}}{\|c\|_{H^2}} = \frac{\|c\|_{L^\infty}}{\|c\|_{L^2}} = |\Omega|^{-\frac{1}{2}} \leq C_S(2).$$

Now we assume $|\Omega| = C d_\Omega^3$ for some $C > 0$ and give a sharp bound for $C_S(2)$ for d_Ω sufficiently small. Note that this hypothesis includes domains such as a ball $B(0,R) \subseteq \mathbb{R}^3$ or a cube $[-R,R]^3$ for $R > 0$.

Since $D_{2,p} = C(p) d_\Omega^{\frac{3}{p} - \frac{1}{2}}$ by Equation (A.3) and $|\Omega|^{\frac{1}{p} - \frac{1}{2}} = (C d_\Omega^3)^{\frac{1}{p} - \frac{1}{2}}$, we have

$$C_{2,p} = 2^{\frac{1}{2}} |\Omega|^{\frac{1}{p} - \frac{1}{2}}, \tag{A.5}$$

for all $d_\Omega \leq d_0(p)$ for some $d_0(p) > 0$. On the other hand, we may translate the domain and assume $\frac{d_\Omega}{2} = \sup_{x \in \Omega} |x|$. Then, $V \subseteq B(0, d_\Omega)$ and

$$\big|\big| |x|^{-2} \big|\big|_{L^{p'}(V)}^{p'} \leq \big|\big| |x|^{-2} \big|\big|_{L^{p'}(B(0,d_\Omega))}^{p'} = 4\pi \int_0^{d_\Omega} r^{-2p'+2} dr = \frac{4\pi}{-2p'+3} d_\Omega^{-2p'+3},$$

and thus $D_{p,\infty} = C'(p) d_\Omega^{-\frac{3}{p}+1}$ by Equation (A.4), and we have

$$C_{p,\infty} = 2^{1-\frac{1}{p}} |\Omega|^{-\frac{1}{p}}, \tag{A.6}$$

for all $d_\Omega \leq d_0'(p)$ for some $d_0'(p) > 0$. Combining Equation (A.5) and Equation (A.6), we have

$$|\Omega|^{-\frac{1}{2}} \leq C_S(2) \leq 2^{\frac{3}{2}} |\Omega|^{-\frac{1}{2}},$$

for all d_Ω sufficiently small. □

A.3. Estimates for C_H.

To do a numerical simulation, it is of interest to obtain an estimate for the elliptic regularity constant $C_H > 0$. In applications, the tensor ϵ is usually assumed to be a scalar-valued function, in which case, an estimate for C_H can be obtained by the Fourier transform:

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} f(x)e^{-ix\cdot\xi}d\xi \quad \text{and} \quad f(x) = (2\pi)^{-d}\int_{\mathbb{R}^d} \hat{f}(\xi)e^{ix\cdot\xi}d\xi.$$

For any $s \in \mathbb{R}$, define

$$H^s(\mathbb{R}^d) = \{f \in \mathscr{S}' : \langle\xi\rangle^s \hat{f} \in L^2(\mathbb{R}^d)\},$$

where $\langle\xi\rangle \coloneqq (1 + |\xi|^2)^{\frac{1}{2}}$ and $\mathscr{S}'$ is the space of tempered distributions.

Lemma A.6. *Let L be as in Equation (2.10). Furthermore, suppose $\epsilon^{ij} = \epsilon(x)\delta_{ij}$ where δ_{ij} is the Kronecker delta function and $\epsilon \in W^{1,\infty}(\Omega)$ such that $\mathrm{Re}(\epsilon(x)) \geq \theta > 0$ for all $x \in \Omega$. Then*

$$C_H \leq \frac{\lambda_1^{-1}\langle\lambda_1^{\frac{1}{3}}\rangle^3}{\theta}\left(1 + \frac{\|\kappa^2\|_{L^\infty(\Omega)} + d^{\frac{1}{2}}\max_{1\leq i\leq d}\|\partial_i\epsilon\|_{L^\infty(\Omega)}\lambda_1^{\frac{1}{2}}}{\theta\lambda_1 - \mu}\right). \tag{A.7}$$

Proof. Given $F \in L^2(\Omega)$ and a unique weak solution $u \in H_0^1(\Omega)$ of the Laplace equation $-\Delta u = F$ in Ω, we find $C_1 > 0$ such that $\|u\|_{H^2(\Omega)} \leq C_1\|F\|_{L^2(\Omega)}$. We use this energy estimate to handle the more complicated case.

By the density argument, it suffices to assume $F \in C_c^\infty(\Omega)$. By an integration-by-parts argument, it can be shown that $u \in C_c^2(\Omega)$. Hence, we extend u to a function in $C_c^2(\mathbb{R}^d)$, which we continue to call u, by defining $u(x) = 0$ for $x \in \mathbb{R}^d \setminus \mathrm{supp}(u)$. Then,

$$\begin{aligned}\|u\|_{H^2(\Omega)}^2 \leq \|u\|_{H^2(\mathbb{R}^d)}^2 &= \int_{\mathbb{R}^d}\langle\xi\rangle^4|\hat{u}(\xi)|^2d\xi \\ &= \int_{|\xi|\geq c}\langle\xi\rangle^4|\hat{u}(\xi)|^2d\xi + \int_{|\xi|<c}\langle\xi\rangle^4|\hat{u}(\xi)|^2d\xi \eqqcolon I + II\end{aligned}$$

for some $c > 0$ to be fixed later. For the high frequencies,

$$I = \int_{|\xi|\geq c}\langle\xi\rangle^4|\hat{u}(\xi)|^2d\xi = \int_{|\xi|\geq c}\frac{\langle\xi\rangle^4}{|\xi|^4}|\widehat{\Delta u}|^2d\xi = \int_{|\xi|\geq c}\frac{\langle\xi\rangle^4}{|\xi|^4}|\hat{F}(\xi)|^2d\xi \leq \frac{\langle c\rangle^4}{|c|^4}\|F\|_{L^2(\Omega)}^2.$$

Combining the Poincaré inequality and the weak form of the Laplace equation, we have

$$\|u\|_{L^2(\Omega)}^2 \leq \lambda_1^{-1}\|\nabla u\|_{L^2(\Omega)}^2 \leq \lambda_1^{-1}\|F\|_{L^2(\Omega)}\|u\|_{L^2(\Omega)},$$

and therefore, for the low frequencies,

$$II \leq \langle c\rangle^4\|u\|_{L^2(\Omega)}^2 \leq \langle c\rangle^4\lambda_1^{-2}\|F\|_{L^2(\Omega)}^2.$$

Combining I and II,

$$\|u\|_{H^2(\Omega)} \leq \langle c\rangle^2(|c|^{-4} + \lambda_1^{-2})^{\frac{1}{2}}\|F\|_{L^2(\Omega)}.$$

Noting that $c \mapsto \langle c\rangle^2(|c|^{-4} + \lambda_1^{-2})^{\frac{1}{2}}$ has a global minimum at $c = \lambda_1^{\frac{1}{3}}$, we fix that value of c to obtain

$$\|u\|_{H^2(\Omega)} \leq C_1\|F\|_{L^2(\Omega)} \quad \text{where} \quad C_1 \coloneqq \lambda_1^{-1}\langle\lambda_1^{\frac{1}{3}}\rangle^3. \tag{A.8}$$

Now we assume $u \in H_0^1(\Omega)$ is the unique weak solution of

$$-\nabla\cdot(\epsilon\nabla u) + \kappa^2 u = f \quad \text{in } \Omega. \tag{A.9}$$

Setting $F \coloneqq f - \kappa^2 u \in L^2(\Omega)$, the product rule applied to Equation (A.9) yields

$$-\Delta u = \epsilon(x)^{-1}(F + \nabla\epsilon\cdot\nabla u).$$

Noting that $|\epsilon(x)| \geq |\operatorname{Re}(\epsilon(x))| \geq \operatorname{Re}(\epsilon(x)) \geq \theta$, an immediate application of Equation (A.8) yields

$$\|u\|_{H^2(\Omega)} \leq \frac{C_1}{\theta}(\|F\|_{L^2(\Omega)} + \|\nabla\epsilon \cdot \nabla u\|_{L^2(\Omega)}). \tag{A.10}$$

Taking the real part of the weak form of Equation (A.9), we have

$$\int_\Omega \operatorname{Re}(\epsilon(x))|\nabla u|^2 + \int_\Omega \operatorname{Re}(\kappa^2)|u|^2 = \operatorname{Re}\int_\Omega f\overline{u}.$$

Recalling that $\operatorname{Re}(\kappa^2(x)) \geq -\mu$ for all $x \in \Omega$ and the uniform ellipticity,

$$\theta\int_\Omega |\nabla u|^2 + \int_\Omega \operatorname{Re}(\kappa^2)|u|^2 \leq \|f\|_{L^2(\Omega)}\|u\|_{L^2(\Omega)}. \tag{A.11}$$

The Poincaré inequality yields $(\theta\lambda_1 - \mu)\|u\|^2_{L^2(\Omega)} \leq \theta\int_\Omega |\nabla u|^2 + \int_\Omega \operatorname{Re}(\kappa^2)|u|^2$, which gives

$$\|u\|_{L^2(\Omega)} \leq \frac{\|f\|_{L^2(\Omega)}}{\theta\lambda_1 - \mu}.$$

Another application of the Poincaré inequality to Equation (A.11) yields

$$(\theta - \mu\lambda_1^{-1})\int_\Omega |\nabla u|^2 \leq \theta\int_\Omega |\nabla u|^2 + \int_\Omega \operatorname{Re}(\kappa^2)|u|^2,$$

which gives

$$\|\nabla u\|_{L^2(\Omega)} \leq \lambda_1^{\frac{1}{2}}\frac{\|f\|_{L^2(\Omega)}}{\theta\lambda_1 - \mu}. \tag{A.12}$$

Hence,

$$\|F\|_{L^2(\Omega)} \leq \Big(1 + \frac{\|\kappa^2\|_{L^\infty(\Omega)}}{\theta\lambda_1 - \mu}\Big)\|f\|_{L^2(\Omega)}. \tag{A.13}$$

On the other hand, the Cauchy-Schwarz inequality yields

$$\|\nabla\epsilon \cdot \nabla u\|_{L^2(\Omega)} \leq \sqrt{d}\max_{1\leq i\leq d}\|\partial_i\epsilon\|_{L^\infty(\Omega)}\|\nabla u\|_{L^2(\Omega)} \leq \sqrt{d}\max_{1\leq i\leq d}\|\partial_i\epsilon\|_{L^\infty(\Omega)}\lambda_1^{\frac{1}{2}}\frac{\|f\|_{L^2(\Omega)}}{\theta\lambda_1 - \mu}. \tag{A.14}$$

By Equations (A.8), (A.10), (A.13) and (A.14),

$$\|u\|_{H^2(\Omega)} \leq \frac{\lambda_1^{-1}\langle\lambda_1^{\frac{1}{3}}\rangle^2(1 + \lambda_1^{\frac{2}{3}})^{\frac{1}{2}}}{\theta}\Big(1 + \frac{\|\kappa^2\|_{L^\infty(\Omega)} + d^{\frac{1}{2}}\max_{1\leq i\leq d}\|\partial_i\epsilon\|_{L^\infty(\Omega)}\lambda_1^{\frac{1}{2}}}{\theta\lambda_1 - \mu}\Big)\|f\|_{L^2(\Omega)}.$$

□

In general when ϵ is a tensor, a direct application of Fourier transform seems infeasible. Instead, we closely follow the argument of [31, Section 6.3, Theorem 4] to obtain an estimate on C_H. An emphasis here is that we keep track of the implicit constants.

Lemma A.7. *Let L be as given in Equation* (2.10)*. Then*

$$C_H \leq N(\Omega)\Big(\Big(\frac{1 + \lambda_1}{\theta\lambda_1 - \mu}\Big)^2 + dC_0\Big)^{\frac{1}{2}}, \tag{A.15}$$

where $N(\Omega) \in \mathbb{N}$ and C_0 is defined in Equation (A.21)*.*

Remark A.1. Since $\lambda_1 \geq \frac{\pi^2}{d_\Omega^2}$ for convex Ω, the RHS of Equations (A.7) and (A.15) converges to $\frac{C(\Omega)}{\theta}$ as $d_\Omega \to 0$.

Remark A.2. Since the estimate of Equation (A.15) depends on the number of finitely many open balls covering Ω, the geometry of $\partial\Omega$ plays a big role in the computation of $N(\Omega)$. This will be pursued in future research.

Proof. Let $V \Subset W \Subset \Omega$. Let $\zeta \in C_c^\infty(\Omega)$ such that $0 \le \zeta \le 1$ and $\zeta = 1$ on V, and $\mathrm{supp}(\zeta) \subseteq W$. Set $F = f - \kappa^2 u \in L^2(\Omega)$. Consider the weak form of

$$-\nabla \cdot (\epsilon \nabla u) + \kappa^2 u = f \quad \text{in } \Omega \tag{A.16}$$

applied to the test function $\phi = -D_k^{-h}\zeta^2 D_k^h u$, where

$$D_k^h u(x) = \frac{u(x + he_k) - u(x)}{h}$$

and $\{e_k\}_{k=1}^d$ forms the standard basis of $\mathbb{R}^d$. Using integration by parts and the product rule of discrete derivatives,

$$\begin{aligned}
\int_\Omega \epsilon^{ij}\partial_j u \overline{\partial_i \phi} &= \int_\Omega D_k^h(\epsilon^{ij}\partial_j u)\overline{\partial_i(\zeta^2 D_k^h u)} \\
&= \int_\Omega (\epsilon^{ij,h} D_k^h \partial_j u + D_k^h \epsilon^{ij}\partial_j u)(\overline{2\zeta\partial_i\zeta D_k^h u} + \overline{\zeta^2 D_k^h \partial_i u}) \\
&= \int_\Omega \zeta^2 \epsilon^{ij,h} D_k^h \partial_j u \overline{D_k^h \partial_i u} + R,
\end{aligned}$$

where $\epsilon^{ij,h}(x) := \epsilon^{ij}(x + he_k)$. By uniform ellipticity,

$$\mathrm{Re}\int_\Omega \zeta^2 \epsilon^{ij,h} D_k^h \partial_j u \overline{D_k^h \partial_i u} \ge \theta \int_\Omega \zeta^2 |D_k^h \nabla u|^2.$$

The other three products are estimated above by the Cauchy-Schwarz inequality:

$$\begin{aligned}
R &\le \left|\int_\Omega 2\zeta\partial_i\zeta\epsilon^{ij,h} D_k^h \partial_j u \overline{D_k^h u}\right| + \left|\int_\Omega 2\zeta\partial_i\zeta D_k^h \epsilon^{ij}\partial_j u \overline{D_k^h u}\right| + \left|\int_\Omega D_k^h \epsilon^{ij}\zeta^2 \partial_j u \overline{D_k^h \partial_i u}\right| \\
&\le 2\|\nabla\zeta\|_{L^\infty(\Omega)}\|\epsilon\|_{W^{1,\infty}(\Omega)}\Big(\int_\Omega \zeta|D_k^h \nabla u||D_k^h u| + \int_\Omega \zeta|\nabla u||D_k^h u|\Big) + \|\epsilon\|_{W^{1,\infty}(\Omega)}\int_\Omega \zeta|\partial_j u||D_k^h \partial_i u|.
\end{aligned} \tag{A.17}$$

Recalling the following variant of Cauchy-Schwarz inequality

$$ab \le \frac{a^2}{2\delta} + \frac{\delta b^2}{2},$$

for $a, b \ge 0$ and $\delta > 0$ and the following control of discrete derivatives with respect to the continuous derivatives for sufficiently small $|h| > 0$,

$$\|D_k^h \phi\|_{L^2(V)} \le \|\partial_k \phi\|_{L^2(\Omega)},\ \forall \phi \in H^1(\Omega),\ V \Subset \Omega, \tag{A.18}$$

Equation (A.17) is bounded above by

$$\le C_1\delta \int_\Omega \zeta^2 |D_k^h \nabla u|^2 + C_2 \int_\Omega |\nabla u|^2$$

where

$$C_1 := \|\epsilon\|_{W^{1,\infty}(\Omega)}\Big(\|\nabla\zeta\|_{L^\infty(\Omega)} + \frac{1}{2}\Big) \quad \text{and} \quad C_2 := \|\epsilon\|_{W^{1,\infty}(\Omega)}\Big(2\|\nabla\zeta\|_{L^\infty(\Omega)} + \frac{1 + 2\|\nabla\zeta\|_{L^\infty(\Omega)}}{2\delta}\Big).$$

Choosing $\delta = \frac{\theta}{2C_1}$, we use the triangle inequality to obtain

$$\mathrm{Re}\int_\Omega (\epsilon\nabla u) \cdot \overline{\nabla u} \ge \frac{\theta}{2}\int_\Omega \zeta^2 |D_k^h \nabla u|^2 - C_2 \int_\Omega |\nabla u|^2. \tag{A.19}$$

On the other hand, we estimate the right-hand side of the weak form:

$$\left|\int_\Omega F\overline{\phi}\right| \leq \frac{1}{2\delta}\int_\Omega |F|^2 + \frac{\delta}{2}\int_\Omega |\phi|^2,$$

where the first term is estimated above as in Equation (A.13).

$$\begin{aligned}\int_\Omega |\phi|^2 &\leq \int_\Omega |\partial_k(\zeta^2 D_k^h u)|^2\\ &\leq 2\int_\Omega |2\zeta\partial_k\zeta D_k^h u|^2 + 2\int_\Omega \zeta^2 |D_k^h\partial_k u|^2\\ &\leq 8\|\nabla\zeta\|^2_{L^\infty(\Omega)}\int_\Omega |\nabla u|^2 + 2\int_\Omega \zeta^2|D_k^h\nabla u|^2,\end{aligned}$$

where the last inequality is by Equation (A.18). Let $\delta = \frac{\theta}{4}$. Then,

$$\left|\int_\Omega F\overline{\phi}\right| \leq \frac{2}{\theta}\Big(1+\frac{\|\kappa^2\|_{L^\infty(\Omega)}}{\theta\lambda_1-\mu}\Big)^2\int_\Omega |f|^2 + \theta\|\nabla\zeta\|^2_{L^\infty(\Omega)}\int_\Omega|\nabla u|^2 + \frac{\theta}{4}\int_\Omega \zeta^2|D_k^h\nabla u|^2. \tag{A.20}$$

Combining Equation (A.20) and Equation (A.19),

$$\frac{\theta}{4}\int_V |D_k^h\nabla u|^2 \leq \frac{\theta}{4}\int_\Omega \zeta^2|D_k^h\nabla u|^2 \leq \frac{2}{\theta}\Big(1+\frac{\|\kappa^2\|_{L^\infty(\Omega)}}{\theta\lambda_1-\mu}\Big)^2\int_\Omega |f|^2 + (C_2+\theta\|\nabla\zeta\|^2_{L^\infty(\Omega)})\int_\Omega |\nabla u|^2,$$

and by Equation (A.12),

$$\begin{aligned}\int_V |D_k^h\nabla u|^2 &\leq C_0\int_\Omega |f|^2,\\ C_0 &= \frac{4}{\theta}\bigg(\frac{2}{\theta}\Big(1+\frac{\|\kappa^2\|_{L^\infty(\Omega)}}{\theta\lambda_1-\mu}\Big)^2 + \frac{\lambda_1(C_2+\theta\|\nabla\zeta\|^2_{L^\infty(\Omega)})}{(\theta\lambda_1-\mu)^2}\bigg).\end{aligned} \tag{A.21}$$

By [31, Section 5.8.2, Theorem 3], this shows $\partial_k\nabla u \in L^2(V,\mathbb{C}^d)$ for all $1\leq k\leq d$ with the same bound on the L^2-norm. Hence,

$$\sum_{1\leq i,j\leq d}\|\partial_{ij}u\|^2_{L^2(V)} \leq dC_0\int_\Omega |f|^2. \tag{A.22}$$

By the Lax-Milgram Theorem, we have

$$\|u\|_{H^1(\Omega)} \leq \frac{1+\lambda_1}{\theta\lambda_1-\mu}\|f\|_{L^2(\Omega)}. \tag{A.23}$$

Combining Equation (A.22) with Equation (A.23), we obtain

$$\|u\|_{H^2(V)} \leq \Big(\Big(\frac{1+\lambda_1}{\theta\lambda_1-\mu}\Big)^2 + dC_0\Big)^{\frac{1}{2}}\|f\|_{L^2(\Omega)}. \tag{A.24}$$

Since Ω is bounded, $\{x\in\Omega : \inf_{y\in\partial\Omega}|x-y|\geq\delta\}$ can be covered by finitely many open sets for every $\delta>0$. Given any point $y\in\partial\Omega$, there exists a diffeomorphism that takes a small neighborhood of y (in $\overline{\Omega}$) into a neighborhood in the half-plane $\mathbb{R}^d_+ := \mathbb{R}^{d-1}\times[0,\infty)$ where y is identified with $0\in\mathbb{R}^d_+$. Via this diffeomorphism, one can show that the H^2-norm of u in the neighborhood of y obeys an estimate similar to Equation (A.24). Hence, there exists $N = N(\Omega)\in\mathbb{N}$ such that

$$\|u\|_{H^2(\Omega)} \leq N(\Omega)\Big(\Big(\frac{1+\lambda_1}{\theta\lambda_1-\mu}\Big)^2 + dC_0\Big)^{\frac{1}{2}}\|f\|_{L^2(\Omega)}.$$

□

B. Failure of Uniqueness

In this appendix, we demonstrate that the assumptions made in proving the existence of unique solutions were reasonable. In particular, if Hypotheses 3 and 4 or the smallness assumptions on $(f, g) \in L^2(\Omega) \times H^{3/2}(\Omega)$ are violated, then there can be multiple small solutions of the nPBE. Two approaches are given: abstract dynamical systems approach and an explicit construction involving ODEs.

Let us first examine what can happen if we allow Hypotheses 3 and 4 to be violated. For the case where ϵ and κ^2 are scalars (κ may be complex) and f and g are set to zero functions, (1.1) simplifies to

$$\begin{aligned} -\Delta u + (\eta - \lambda_1)\sinh(u) &= 0 \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{B.1}$$

where $\eta = \lambda_1 + \kappa^2/\epsilon \in \mathbb{R}$. The function $u \equiv 0$ is always a trivial solution for the above PDE. Recall $\lambda_1 > \frac{\mu}{\theta}$. For (B.1), if Hypotheses 3 and 4 are satisfied, then

$$\eta \geq \lambda_1 - \frac{\mu}{\epsilon} \geq \lambda_1 - \frac{\mu}{\theta} > 0.$$

The parameter η is the smallest eigenvalue of the $-\Delta + (\eta - \lambda_1)$, so this linear operator is non-invertible when $\eta = 0$. The following result proved by Crandall and Rabinowitz in [26] can be used to show that the zero solution undergoes a bifurcation at $\eta = 0$:

Theorem B.1. *Let X and Y be Banach spaces and assume*

(i) $F \in C^2(X \times \mathbb{R}, Y)$,

(ii) $F(0, \eta) = 0$ *for all* $\eta \in \mathbb{R}$,

(iii) $\dim N(D_x F(0,0)) = \operatorname{codim} R(D_x F(0,0)) = 1$, *and*

(iv) $D^2_{x\eta} F(0,0)\hat{v}_0 \notin R(D_x F(0,0))$ *where* $\hat{v}_0 \neq 0$ *is in* $N(D_x F(0,0))$.

Then there is a nontrivial continuously differentiable curve

$$\{(x(s), \eta(s)) \mid s \in (-\delta, \delta)\} \tag{B.2}$$

such that $(x(0), \eta(0)) = (0, 0)$, $x'(0) = \hat{v}_0$ *and*

$$F(x(s), \eta(s)) = 0 \quad \text{for} \quad s \in (-\delta, \delta). \tag{B.3}$$

Here D_x and D_η represent the Fréchet derivatives of F with respect to the X and $\mathbb{R}$ components, respectively. Note that $D_\eta F(x, \eta) \in \mathcal{L}(\mathbb{R}, Y)$, the set of linear operators from $\mathbb{R}$ into Y. An element $A \in \mathcal{L}(\mathbb{R}, Y)$ can be uniquely associated with an element $y \in Y$ by setting $y \in A(1)$. Thus $D^2_{x\eta} F(x, \eta)$ can be associated with an element of $\mathcal{L}(X, Y)$, which is how the map $D^2_{x\eta} F(0,0)$ is being viewed in Item (iv). Applying Theorem B.1 gives the existence of non-unique small solutions.

Theorem B.2. *Let $c > 0$. Then there is $\eta^* < 0$ such that for any $\eta \in [\eta^*, 0)$ there is a non-trivial solution u of* (B.1) *such that $\|u\|_{H^2} < c$.*

Proof. Define $F : H^2(\Omega) \cap H^1_0(\Omega) \times \mathbb{R} \to L^2(\Omega)$ as

$$F(u, \eta) = -\Delta u + (\eta - \lambda_1)\sinh(u). \tag{B.4}$$

Assumptions (i) and (ii) are clearly satisfied. Note that $D_u F(0,0) = -\Delta - \lambda_1$. Thus assumption (iii) follows from the Fredholm properties of $-\Delta$ and from the fact that λ_1 is the principal eigenvalue of $-\Delta$. Let $\hat{v}_0$ be be the eigenfunction corresponding to λ_1. Then assumption (iv) states that $D^2_{u\eta} F(0,0)\hat{v}_0 = \hat{v}_0 \notin R(D_u F(0,0))$. This should hold since if $\hat{v}_0 \in R(D_u F(0,0))$, then there is a generalized eigenfunction for λ_1 which contradicts the simplicity of λ_1. Hence, we can apply Theorem B.1 to $F(u, \eta) = 0$ to get a nontrivial continuously differentiable curve

$$\{(u(s), \eta(s)) \mid s \in (-\delta, \delta)\}. \tag{B.5}$$

with $(u(0), \eta(0)) = (0, 0)$.

One can also compute derivatives of $\eta(s)$ (see [53, §1.6] for details) to get that $\eta'(0) = 0$ and $\eta''(0) < 0$. Thus it is possible to choose δ small enough so that $\eta(s)$ is strictly decreasing on $s \in [0, \delta)$. Given $c > 0$, we can find $s^* > 0$ small enough to get $\|u(s)\|_{H^2} \leq c$ for all $s \in (0, s^*]$ by the continuity of the curve. Since $s \mapsto \eta(s)$ is strictly decreasing on $(0, s^*]$, we can invert this mapping to get $\eta \mapsto s(\eta)$ for $\eta \in [\eta^*, 0)$ where $\eta^* = \eta(s^*)$. Therefore, for each $\eta \in [\eta^*, 0)$ we have a solution of (B.1), given by $u = u(s(\eta))$ such that $\|u\|_{H^2} < c$. ☐

Remark B.1. There are two non-trivial solutions to (B.1) for $\eta < 0$ sufficiently close to zero: one for $s > 0$ and one for $s < 0$. In fact, from the oddness of $\sinh(u)$, if u is a solution of (B.1) then so is $-u$.

Comparing Theorem B.2 with Theorem 3.1 shows that uniqueness cannot be guaranteed without Hypotheses 3 and 4.

Alternatively, uniqueness of solutions may be lost if (f, g) becomes too large in norm. We explicitly construct multiple solutions to nPBE with large data. By construction, this family of nPBEs fails to satisfy the invertibility condition given in Hypothesis 4 and/or the smallness assumption on $(f, g) \in L^2(\Omega) \times H^{\frac{3}{2}}(\partial\Omega)$. In particular, this example is consistent with the well-known uniqueness result of [58].

We wish to obtain a radial solution $u(x) = u(|x|) = y(r)$, where $r = |x| \geq 0$, to (1.1) where $\epsilon = 1$ for simplicity and $\kappa = i\tilde{\kappa} \in i\mathbb{R}$ on domain $\Omega = B(0, R) \subseteq \mathbb{R}^d$ for $R > 0, d \geq 1$. Let f, g be constants given by $f(x) = \lambda \in \mathbb{R}$, $g(x) = \sinh^{-1}(\frac{\lambda}{\tilde{\kappa}^2})$. In the polar coordinate, our example reduces to the ODE

$$\begin{aligned} ry'' + (d-1)y' + \tilde{\kappa}^2 r \sinh y = r\lambda, \ r \in (0, R) \\ y(R) = \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right), \end{aligned} \tag{B.6}$$

where it is clear that the constant function $r \mapsto \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right)$ is a trivial solution. Since (B.6) is symmetric under $r \mapsto -r$, we may consider $\lambda \geq 0$. It is also clear that $(f, g) \in L^2(\Omega) \times H^{\frac{3}{2}}(\partial\Omega)$ can be taken as large as possible (in norm) by taking λ arbitrarily large. Furthermore, we note that Hypothesis 4 is violated when $R \gg 1$ depending on $\tilde{\kappa}$. To elaborate, fix $\tilde{\kappa} > 0$. If Hypothesis 4 holds, then $\tilde{\kappa}^2 \leq \mu < \lambda_1 = \frac{C_B}{R^2}$. Hence if $R \geq \frac{\sqrt{C_B}}{\tilde{\kappa}}$, then Hypothesis 4 cannot hold.

Proposition B.1. *Let $d \geq 1, \tilde{\kappa} > 0, \lambda \geq 0$. Then, there exists a non-trivial solution to* (B.6) *for some $R > 0$.*

Reducing (B.6) into a first-order ODE by introducing $w = y'$, we obtain

$$\begin{pmatrix} y \\ w \end{pmatrix}' = F(r, y, w) := \begin{pmatrix} w \\ -\tilde{\kappa}^2 \sinh y - (d-1)\frac{w}{r} + \lambda \end{pmatrix}. \tag{B.7}$$

For $d = 1$, (B.7) admits an autonomous Hamiltonian vector field where the Hamiltonian is given by

$$H(y, w) = \frac{w^2}{2} + \tilde{\kappa}^2(\cosh y - 1) - \lambda y.$$

Since the level sets of H are a collection of closed one-dimensional curves, all solutions are global and periodic. The inner curves have lower values of H than the outer curves. Indeed, the global minimum of H occurs at $P = (\sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right), 0)$ where $H(P) \leq 0$ with the equality if and only if $\lambda = 0$. Hence for each initial datum $\begin{pmatrix} c \\ 0 \end{pmatrix}$, there exists a unique solution y to (B.6) where $y(R) = 0$ for infinitely many $R > 0$. We include a phase portrait where the solutions lie on the curves of constant Hamiltonian.

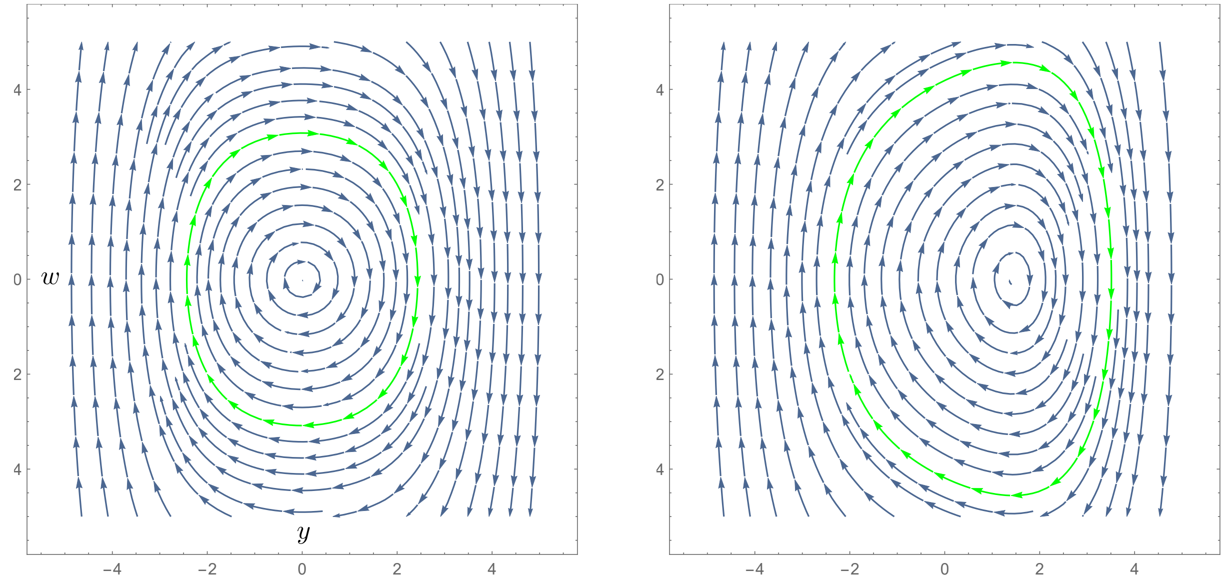

Figure 6: Vector fields of Equation (B.7) with $d = 1, \tilde{\kappa} = 1$ with the left plot portraying $\lambda = 0$, and the right $\lambda = 2$.

For $d \geq 2$, the vector field corresponding to (B.7) is non-autonomous, and F in (B.7) is not well-defined at $r = 0$ where our initial data are given. We regularize the ODE so that the regularized vector field is continuous (in r) near $r = 0$, and show that the limiting solution satisfies (B.6). We solve an ODE that is slightly more general than (B.6). The notations of Proposition B.1 are adopted.

Lemma B.1. *For every $A \geq 0$ and $c > \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right)$, there exist $R > 0$ and $y \in C^\infty_{\mathrm{loc}}((0,\infty);\mathbb{R})$ such that y satisfies*

$$\begin{gathered} r y'' + A y' + \tilde{\kappa}^2 r \sinh y = r\lambda, \ r \in (0,\infty), \\ \lim_{r\to 0+} y(r) = c, \ \lim_{r\to 0+} y'(r) = 0, \ y(R) = \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right). \end{gathered} \tag{B.8}$$

Proof of Proposition B.1. Set $A = d - 1$ in Lemma B.1. □

Proof of Lemma B.1. The $A = 0$ case is equal to that when $d = 1$, and therefore assume $A > 0$. For $\epsilon > 0$, consider the perturbed ODE:

$$\begin{gathered} (r+\epsilon) y_\epsilon'' + A y_\epsilon' + \tilde{\kappa}^2 (r+\epsilon) \sinh y_\epsilon = (r+\epsilon)\lambda, \ r \in [-\frac{\epsilon}{2}, \infty), \\ y_\epsilon(0) = c, \ y_\epsilon'(0) = 0, \end{gathered} \tag{B.9}$$

which, after setting $w_\epsilon = y_\epsilon'$, reduces to

$$\begin{pmatrix} y_\epsilon \\ w_\epsilon \end{pmatrix}' = F_\epsilon(r, y_\epsilon, w_\epsilon) := \begin{pmatrix} w_\epsilon \\ -\tilde{\kappa}^2 \sinh y_\epsilon - \frac{A w_\epsilon}{r+\epsilon} - \lambda \end{pmatrix}.$$

Since F_ϵ is smooth in r near $r = 0$ and locally Lipschitz in (y, w), there exists $T_\epsilon \in (0, \frac{\epsilon}{2})$ and $y_\epsilon \in C([-T_\epsilon, T_\epsilon];\mathbb{R}) \cap C^\infty_{\mathrm{loc}}((-T_\epsilon, T_\epsilon);\mathbb{R})$ such that y_ϵ is a unique solution to (B.9). In the maximal interval of existence, $\begin{pmatrix} y_\epsilon \\ w_\epsilon \end{pmatrix}$ satisfies

$$\frac{d}{dr} H(y_\epsilon(r), w_\epsilon(r)) = w_\epsilon(r)(y_\epsilon''(r) + \tilde{\kappa}^2 \sinh y_\epsilon(r) - \lambda) = -\frac{A w_\epsilon(r)^2}{r+\epsilon} \leq 0, \tag{B.10}$$

for $r \geq -\frac{\epsilon}{2}$, and therefore the forward orbit of $\begin{pmatrix} y_\epsilon \\ w_\epsilon \end{pmatrix}$ is bounded in the compact subset $\{(y,w) \in \mathbb{R}^2 : H(y,w) \leq H(c,0)\}$ on which F_ϵ is Lipschitz. Hence, $\begin{pmatrix} y_\epsilon \\ w_\epsilon \end{pmatrix}$ can be uniquely extended globally in forward time, obeying the estimate

$$H(y_\epsilon(r), w_\epsilon(r)) \leq H(c,0),\ r \geq 0. \tag{B.11}$$

This global bound on $|y_\epsilon| + |w_\epsilon|$ yields an existence of a limit function, since for $r_1, r_2 \geq 0$,

$$|y_\epsilon(r_2) - y_\epsilon(r_1)| = \left| \int_{r_1}^{r_2} w_\epsilon(\rho) d\rho \right| \leq C|r_2 - r_1|,$$

where $C > 0$ is independent of $\epsilon > 0$. The Arzelà-Ascoli Theorem implies that there exists a subsequence $\epsilon_k > 0$ that tends to zero (from the right) and $y \in C_{\text{loc}}([0,\infty);\mathbb{R})$ such that $y_{\epsilon_k} \xrightarrow[k\to 0]{} y$ in the topology of uniform convergence on compact subsets; in particular, $y(0) = c$.

Let $T > 0$. Since $\{w_{\epsilon_k}\}$ is uniformly bounded in $L^2((0,T);\mathbb{R})$ due to (B.11), there exists a subsequence of $\{\epsilon_k\}$ and $w \in L^2((0,T);\mathbb{R})$ such that, possibly after relabelling the subsequence, $w_{\epsilon_k} \rightharpoonup w$ in $L^2((0,T);\mathbb{R})$. This weak convergence of derivatives and the uniform convergence $y_{\epsilon_k} \to y$ on $[0,T]$ implies that w is the weak derivative of y. Furthermore, we have

$$((r+\epsilon_k)y'_{\epsilon_k})'(r) = (1-A)y'_{\epsilon_k} - \tilde{\kappa}^2(r+\epsilon_k)\sinh y_{\epsilon_k}(r) + (r+\epsilon_k)\lambda$$

from (B.9) where the right-hand side is uniformly bounded in $L^2((0,T);\mathbb{R})$. Another application of the Arzelà-Ascoli Theorem implies that there exists $Y \in C([0,T];\mathbb{R})$ such that $(\cdot + \epsilon_k)y'_{\epsilon_k} \xrightarrow[k\to\infty]{} Y$ in $C([0,T];\mathbb{R})$, possibly after relabelling the subsequence, and follows $y'_{\epsilon_k} \xrightarrow[k\to\infty]{} \frac{Y}{r}$ in $C([\delta,T];\mathbb{R})$ for every $\delta > 0$, and therefore we identify $w(r)$ with a continuous function $\frac{Y(r)}{r}$ on $(0,T)$; indeed, $w = y'$ classically on $(0,T)$. Yet another application of (B.11) and the triangle inequality $|w(r)| \leq |w(r) - y'_{\epsilon_k}(r)| + |y'_{\epsilon_k}(r)|$ yields the bound $|w(r)| \leq M$ for some $M > 0$ on $(0,T)$.

Since y_{ϵ_k} is a classical solution to (B.9), it is also a weak solution. Writing (B.9) in the weak form, integrating by parts, and taking $k \to \infty$, we obtain $ry'' + Ay' + \tilde{\kappa}^2 r \sinh y = r\lambda$ on $(0,T)$ in the weak sense where the distributional derivative y'' can be identified with a continuous function on $(0,T)$ using the equation above. Using (B.9) and the uniform convergence of y_{ϵ_k} and its derivative as $k \to \infty$, we conclude $(r+\epsilon_k)y''_{\epsilon_k} \xrightarrow[k\to\infty]{} -(Ay' + \tilde{\kappa}^2 r \sinh y) + r\lambda = ry''$ uniformly on $[\delta, T]$, and therefore $y''_{\epsilon_k} \xrightarrow[k\to\infty]{} y''$ in $C([\delta,T];\mathbb{R})$ for every $\delta > 0$. We have shown that $y^{(j)}_{\epsilon_k} \xrightarrow[k\to\infty]{} y^{(j)}$ uniformly on compact subsets of $(0,T)$ for $j = 0,1,2$. Taking $k \to \infty$ from (B.9), we conclude that y satisfies the desired ODE pointwise on $(0,T)$. Since the vector field F is smooth on $(0,T) \times \mathbb{R}^2$ where $T > 0$ was arbitrary, we conclude $y \in C^\infty_{\text{loc}}((0,\infty);\mathbb{R}))$.

Since y'' is continuous on $(0,T)$ and $y'_{\epsilon_k} \rightharpoonup y'$ in $L^2((0,T);\mathbb{R})$ as $k \to \infty$, for every $\phi \in C^\infty_c((0,T);\mathbb{R})$,

$$\int_0^T y''_{\epsilon_k}\phi = -\int_0^T y'_{\epsilon_k}\phi' \xrightarrow[k\to\infty]{} -\int_0^T y'\phi' = \int_0^T y''\phi.$$

Therefore, $\{y''_{\epsilon_k}\}$ is uniformly bounded in $L^2((0,T);\mathbb{R})$, and another application of the Arzelà-Ascoli Theorem shows that there exists a convergent subsequence of $\{y'_{\epsilon_k}\}$ in $C([0,T];\mathbb{R})$. Since we showed $y'_{\epsilon_k} \xrightarrow[k\to\infty]{C([\delta,T];\mathbb{R})} y'$ for every $\delta > 0$, we conclude that δ could be taken to be zero. In particular, $y'(0) = \lim_{k\to\infty} y'_{\epsilon_k}(0) = 0$.

From the phase portrait analysis, the solution $(y(r), w(r))$ exhibits an oscillatory behavior in $\mathbb{R}^2$ around $P = (\sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right), 0)$. Note that P is a stable center of the asymptotic limit (in t) of (B.7), which is Hamiltonian and autonomous. Moreover, the orbits are contained within a compact subset by (B.10). Hence, there exists $R > 0$ such that $y(R) = \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right)$. □

Remark B.2. For $d = 3$, (B.6) with $\tilde{\kappa} = 1,\ \lambda = 0$ can be understood as a nonlinear zeroth-order spherical Bessel equation. To be more precise, a (linear) zeroth-order spherical Bessel ODE is given by

$$rj_0'' + 2j_0' + rj_0 = 0,$$

where the solution non-singular at the origin is given by $j_0(r) = \frac{\sin r}{r}$. We give plots comparing the linear and nonlinear solutions for $d = 3$. Note the existence of roots of the nonlinear solutions, verifying $y(R) = 0$ for some $R > 0$.

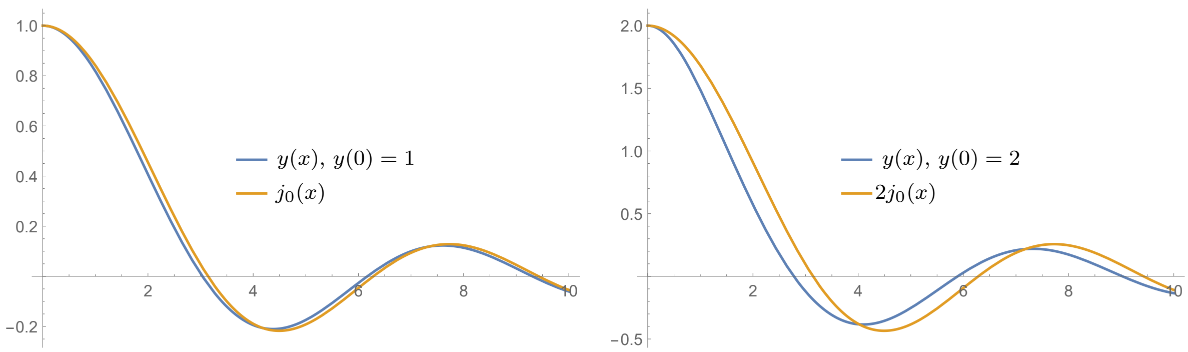

Figure 7: Comparison of solutions to Equation (B.6) and its corresponding linearization.

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