Existence of Strong Solution for the Complexified Non-linear Poisson Boltzmann Equation

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Abstract

We prove the existence and uniqueness of the complexified Nonlinear Poisson-Boltzmann Equation (nPBE) in a bounded domain in $\mathbb{R}^3$. The nPBE is a model equation in nonlinear electrostatics. The standard convex optimization argument to the complexified nPBE no longer applies, but instead, a contraction mapping argument is developed. Furthermore, we show that uniqueness can be lost if the hypotheses given are not satisfied. The complexified nPBE is highly relevant to regularity analysis of the solution of the real nPBE with respect to the dielectric (diffusion) and Debye-Hückel coefficients. This approach is also well-suited to investigate the existence and uniqueness problem for a wide class of semi-linear elliptic Partial Differential Equations (PDEs).

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1 Introduction.

Linear elliptic partial differential equations have long been used to model problems in physics, engineering, biology, and chemistry [12]. In particular, simple linear elliptic equations are often used to model the potential field generated by molecular structures embedded in a solvent in thermal equilibrium. However, a more accurate representation of this is given by the non-linear Poisson Boltzmann Equation (nPBE). The nPBE is given by

$$-\nabla \cdot (\epsilon(x) \nabla u) + \kappa(x)^2 \sinh u = f, \quad x \in \Omega,$$

$$u = g, \quad x \in \partial \Omega,$$  \hspace{1cm} (1.1)

where $u$ is the nondimensionalized potential, $\epsilon$ is the dielectric, and $\kappa^2$ is the Debye-Hückel parameter [14]. The nPBE has found important applications in protein interactions and molecular dynamics [23, 20]. In fig. 1 an example of the electrostatic potential field is rendered from the solution of the nPBE by using the Adaptive Poisson Boltzmann Solver (APBS) [4] for E. Coli RHo Protein. (PDB: 1A63 [5]). However, the mathematical properties of the nPBE are less understood and significantly more complicated than the linear case.

In [14] Holst shows the existence and uniqueness of the solution in the appropriate functional spaces. This approach relies on the construction of a convex functional where the unique minimal energy state corresponds to the solution of the nPBE.

In this paper we are interested in determining the existence and uniqueness of the solution of the nPBE by extending the dielectric and Debye-Hückel parameters into the complex domain. The convexity theory developed in [14] is no longer valid for this case, thus motivating the construction of a novel theory to deal with the complex case. Our ultimate goal is to study analytic extension of the solution with respect to the complex parameters. This provides an approach to determine the regularity and sensitivity of the solution with respect to the dielectric and Debye-Hückel parameters. This has important connections to uncertainty quantification theory [11, 21, 3, 8, 10].

Here, we state a simplified version of our main statement; for more details, see theorems 3.3 and 3.4.

**Theorem 1.1.** Let $\Omega \subseteq \mathbb{R}^3$ be open, bounded, and convex with a smooth boundary. There exists $r = r(\epsilon, \kappa, \Omega) > 0$ such that whenever $(f, g) \in \overline{B}(0, r) \subseteq L^2(\Omega) \times H^{1/2} (\partial \Omega)$, where $\overline{B}(0, r)$ is a closed ball centered at the origin with radius $r > 0$ with respect to the product norm, there exists a solution $u \in H^2(\Omega)$ to eq. (1.1). With further technical hypotheses on the parameters (such as $\epsilon, \kappa^2, \Omega$), this solution is unique in a small ball in $H^2(\Omega)$. 
Most notably, our result is an analysis of a PDE with complex-valued functions. This renders a direct application of calculus of variation to our problem difficult, since \( \mathbb{C} \) is not ordered as in \( \mathbb{R} \). One could try to identify \( \mathbb{C} \) with \( \mathbb{R}^2 \) and apply the variational calculus to a system of two real-valued equations that is equivalent to eq. (1.1); however, the real and imaginary parts of \( \sinh z = \sinh(x + iy) = \sinh x \cos y + i \cosh x \sin y \) are not convex on \( \mathbb{R}^2 \) (in fact, infinitely oscillating in \( y \)), and therefore the method of variational calculus cannot be applied, at least directly. This difficulty does not arise when the given data (or the coefficient functions) are real-valued.

Broadly speaking, the smallness constant \( r > 0 \) in the main result is a reflection of our approach to the problem. Our approach is based on the topological fixed point argument. The desired fixed point arises as a consequence of a compact operator that we construct (see eq. (3.16)) where the compactness is contingent upon choosing \( r > 0 \) sufficiently small.

If the parameters are complex, then a solution to nPBE, even if it exists, is generally not globally unique in the solution space, in stark contrast to its real analogue; see proposition 4.1. We construct a specific example in Appendix B that illustrates the existence of multiple (smooth) solutions by posing the nPBE on a symmetric domain. Moreover, we prove that if the technical hypotheses of theorem 1.1 are not satisfied then multiple non-trivial solutions may exist for the homogeneous nPBE (see theorem 3.2 for more details).

This paper is organized as follows. In section 2, we introduce useful notations and fundamental mathematical background. In section 3, we state and prove the existence and uniqueness result. In appendix A, we give estimates for the various constants used in this paper. In appendix B, we discuss the failure of uniqueness of solution given a large inhomogeneous data.

2 Preliminaries.

2.1 Sobolev Spaces

The solution that we desire to obtain is a complex-valued function on \( \Omega \) with certain regularity and integrability, and so we briefly recall the necessary mathematical background. In this paper, a Banach space \( X \) is assumed to be over \( \mathbb{C} \) unless stated otherwise. As is usual, the integer-order Sobolev space is defined via
weak derivatives. For $k \in \mathbb{N} \cup \{0\}$ and $\Omega \subseteq \mathbb{R}^d$ open, bounded with a smooth boundary,

$$H^k(\Omega) = \{ u \in L^2(\Omega) : \|u\|_{H^k(\Omega)} < \infty \}$$

with $\|u\|_{H^k(\Omega)} := \left( \sum_{|\alpha| \leq k} \|\partial_\alpha u\|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}}$.

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

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

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

$$H^s(\Omega) = \{ u \in L^2(\Omega) : \|u\|_{H^s} < \infty \}$$

with $\|u\|_{H^s} := \left( \|u\|^2_{H^k} + [u]_{s'}^2 \right)^{\frac{1}{2}}$,

and $H^0(\Omega)$ to be the closure of $C_c^\infty(\Omega)$, the collection of smooth and compactly supported functions in $\Omega$, under $\|\cdot\|_{H^s}$. For a more thorough discussion on this material including the Sobolev spaces on the boundary $\partial \Omega$ and the negative-order Sobolev spaces, see [17, Chapter 3]. For a discussion regarding the structural difference between Banach spaces on $\mathbb{C}$ and $\mathbb{R}$, see [6, Chapter 11].

Now, we comment on the regularity of boundary data. Recall that $g : \partial \Omega \to \mathbb{C}$ and $w \in L^2(\Omega)$ such that $w = g$ in the trace sense. Since our proof heavily relies on the Elliptic Regularity Theorem, we assume that $w \in H^2(\Omega)$. To motivate this assumption, consider the linear elliptic PDE $Lu = f$ on $\Omega$ 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 $\Omega$ with $\tilde{u} = 0$ on $\partial \Omega$. If $f \in L^2(\Omega)$, we want $Lw \in L^2(\Omega)$ as well to ensure that $\tilde{u}$ has two more derivatives than $f - Lw$. Another application of the Elliptic Regularity Theorem yields $w \in H^2(\Omega)$, which in turn is guaranteed by assuming $g \in H^2(\partial \Omega)$ by the following lemma:

**Proposition 2.1.** [17 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

$$\Delta w = 0, \quad w = g, \quad x \in \partial \Omega,$$

and obtain an explicit form for $w$ as an integration against the Poisson kernel, and thereby establish a map $T^{-1}g := w$. 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 $\Omega$. In this paper, we are not concerned with this constant; henceforth, given $g \in H^{1/2}(\partial \Omega)$, we fix $w \in H^2(\Omega)$ and work entirely with functions defined on the domain, not the boundary.

### 2.2 Principal Eigenvalue of the Dirichlet Laplacian

Throughout this paper, we let $\Omega \subseteq \mathbb{R}^d$ be open, bounded, convex, and connected with a smooth boundary. Let $|\Omega|$ denote the Lebesgue measure of $\Omega$ and $d_\Omega := \sup_{x,y \in \Omega} |x - y|$, the diameter of $\Omega$. 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, where they are ordered such that

$$0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots$$

The principal eigenvalue is given by

$$\lambda_1 = \min_{u \in H^1_0(\Omega) \setminus \{0\}} \frac{\int_{|\Omega|} |\nabla u|^2}{\int_{|\Omega|} |u|^2}.$$

The variational formula above directly implies the Poincaré inequality given below:

$$\|u\|^2_{L^2(\Omega)} \leq \lambda_1^{-1}\|\nabla u\|^2_{L^2(\Omega)}, \quad \forall u \in H^1_0(\Omega). \quad (2.1)$$
Remark 2.1. If we further assume that $\Omega$ is convex, then $\lambda_1 \geq \frac{c}{\|u\|_{L^2}}$ by [24]. Conversely, it can be shown without convexity that $\lambda_1 \leq \frac{c}{\|u\|_{L^2}}$ for some constant $c = c(\Omega, d) > 0$, and therefore $\lambda_1$ is bounded above and below by $\frac{1}{\|u\|_{L^2}}$ up to a constant.

Now, we justify the last claim. By translation, assume $0 \in \Omega$. There exists $R > 0$ such that $B(0, R) \subseteq \Omega$. Denote $U = B(0, R)$ and $U' = B(0, \frac{R}{2})$. Let $c_1 > 0$ such that $R = c_1 d_0$. Construct a smooth function $v : [0, \infty) \to [0, 1]$ such that $v = 1$ on $[0, \frac{R}{2}]$, $v = 0$ on $[R, \infty)$, and $0 < v < 1$ on $(\frac{R}{2}, R)$ such that $\sup_{r \in [0, \infty)} |v'(r)| = \frac{c_2}{R}$ for some $c_2 > 0$. Define $u(x) = v(|x|)$. Then,

$$
\|u\|_{L^2}^2(\Omega) = \|u\|_{L^2(U)}^2 \geq |U|^{-1}\|u\|_{L^2(U)}^2 \geq |U|^{-1}|U'|^2 = 2^{-2d}|u| = \frac{2^{-2d}|S^{d-1}|R^d}{d},
$$

where $S^{d-1}$ is the unit sphere in $\mathbb{R}^d$. On the other hand,

$$
\int_{\Omega} |\nabla u|^2 = |S^{d-1}| \int_0^R |v'(r)|^2 r^{d-1} dr \leq \frac{c_2^2|S^{d-1}|}{d} R^{d-2},
$$

and hence

$$
\lambda_1 \leq \frac{\int_{\Omega} |\nabla u|^2}{\int_{\Omega} |u|^2} \leq 2^{2d} \left( \frac{c_2}{c_1} \right)^2 d^{-2}.
$$

3 Existence and uniqueness.

3.1 Sketch of Main Results and Assumptions

To show that a unique solution to eq. (1.1) exists we leverage the Schauder’s fixed point theorem. This method is developed by first rewriting eq. (1.1) as the functional equation

$$
F(u) = f
$$

with $u \in H^2(\Omega)$ and $f \in L^2(\Omega)$ and $F : H^2(\Omega) \to L^2(\Omega)$ a nonlinear map satisfying $F(0) = 0$. The map $F$ can be decomposed into its linear and nonlinear components. That is we can take $F(u) = Lu + N(u)$, where $L := DF(0)$ and $N(u) := F(u) - Lu$. Assuming that $L$ is invertible, then eq. (3.1) can be re-expressed as

$$
u = L^{-1}(f - N(u))
$$

with possible additional terms added to account for boundary conditions. So our solution $u$ should be a fixed point of the mapping $u \mapsto L^{-1}(f - N(u))$. The typical approach to finding a fixed point is to demonstrate the map is a contraction and apply the Banach Fixed Point Theorem to get a unique solution. However, since $N(u)$ can increase quadratically in norm as $u$ becomes larger in norm (in our case $\|N(u)\|$ can grow exponentially), it is not possible for us to have this map be a contraction on $H^2(\Omega)$. Instead, we restrict the norm of $u$ to a smaller space, add additional hypotheses to the parameters of eq. (1.1), and apply a corollary of Schauder’s fixed point theorem to get existence of a solution.

To apply this argument to eq. (1.1) we make the following assumptions on the parameters of the PDE:

**Hypothesis 1.** The domain $\Omega \subset \mathbb{R}^d$ is open, bounded, and convex with smooth (at least $C^2$) boundary.

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

$$
\text{Re} \left[ \sum_{i,j=1}^d \epsilon^{ij}(x) \xi_i \overline{\xi_j} \right] \geq \theta |\xi|^2
$$

for all $\xi \in \mathbb{C}^d$ and for a.e. $x \in \Omega$. 


Hypothesis 3. There exists $\mu \geq 0$ such that $\kappa^2 \in L^\infty(\Omega)$ satisfies

$$\text{Re} \left[ \kappa^2(x) \right] \geq -\mu \quad (3.3)$$

for a.e. $x \in \Omega$. Moreover, the parameters $\theta$ and $\mu$ characterized by eqs. (3.2) and (3.3), respectively, satisfy the inequality

$$\frac{\mu}{\theta} < \lambda_1, \quad (3.4)$$

where $\lambda_1$ is the principal eigenvalue of $-\Delta$ on $\Omega$.

Hypotheses 2 and 3 are sufficient to guarantee 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 2 and 3 no longer hold, then there may be a bifurcation of the unique solution. For the case where $\epsilon$ and $\kappa^2$ are scalar-valued and $f$ and $g$ set to zero functions, eq. (4.1) simplifies to

$$-\Delta u + (\eta - \lambda_1) \sinh(u) = 0 \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial \Omega, \quad (3.5)$$

where $\eta = \lambda_1 + \kappa^2/\epsilon \in \mathbb{R}$. The function $u \equiv 0$ is always a trivial solution for eq. (3.5). For eq. (3.5), hypotheses 2 and 3 are satisfied if and only if $\theta$ is greater than zero. The parameter $\eta$ 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 [11] can be used to show that the zero solution undergoes a bifurcation at $\eta = 0$:

**Theorem 3.1.** 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) $\dim N(D_x F(0, 0)) = \text{codim} R(D_x F(0, 0)) = 1$, 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

$$\{ (x(s), \eta(s)) \mid s \in (-\delta, \delta) \} \quad (3.6)$$

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

$$F(x(s), \eta(s)) = 0 \quad \text{for } s \in (-\delta, \delta). \quad (3.7)$$

Here $D_x$ and $D_\eta$ represent the Frechet 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 3.1 gives the existence of non-unique small solutions.

**Theorem 3.2.** Let $c > 0$. Then there is $\eta^* < 0$ such that for any $\eta \in [\eta^*, 0)$ there is a non-trivial solution $u$ of eq. (3.5) 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

$$F(u, \eta) = -\Delta u + (\eta - \lambda_1) \sinh(u). \quad (3.8)$$

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 $\lambda_1$ is the principal eigenvalue of $-\Delta$. Let $\hat{v}_0$ be be the eigenfunction corresponding to $\lambda_1$. Then assumption (iv) states that $D^2_{x\eta} F(0, 0) \hat{v}_0 = \hat{v}_0 \notin R(D_u F(0, 0))$. This should hold since if $\hat{v}_0 \in R(D_u F(0, 0))$, then there is a generalized eigenfunction for $\lambda_1$ which contradicts
the simplicity of $\lambda_1$. Hence, we can apply theorem 3.1 to $F(u, \eta) = 0$ to get a nontrivial continuously differentiable curve
\[
\{(u(s), \eta(s)) \mid s \in (-\delta, \delta)\}. \tag{3.9}
\]
with $(u(0), \eta(0)) = (0, 0)$.

One can also compute derivatives of $\eta(s)$ (see [15, §1.6] for details) to get that $\eta'(0) = 0$ and $\eta''(0) < 0$. Thus it is possible to choose $\delta$ 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 eq. (3.5), given by $u = u(s(\eta))$ such that $\|u\|_{H^2} < c$.

\[\Box\]

Remark 3.1. There are two non-trivial solutions to eq. (3.5) for $\eta < 0$ sufficiently close to zero: one for $s > 0$ and one for $s < 0$. In fact, from the oddness of $\sinh(2\eta)$, one can undo the integration by parts, since $\epsilon \in (0, 1]$, so that $1$ and $3$. Moreover, this can also be true for the case of the non-homogeneous NPBE as demonstrated in appendix B.

### 3.2 Definitions

Before showing existence and uniqueness of solutions, we must first make precise how a function is a weak or strong solution of eq. (1.1).

**Definition 3.1.** A function $u \in H^1(\Omega)$ is a weak solution to eq. (1.1) if for all $\phi \in H^1_0(\Omega)$, we have
\[
\int_\Omega (\epsilon \nabla u) \cdot \nabla \phi + \int_\Omega \kappa^2 \sinh u \cdot \phi = \int_\Omega f \phi \tag{3.10}
\]
where the equality at the boundary is in the trace sense; if $w \in H^1(\Omega)$ whose trace is $g \in H^\frac{1}{2}(\partial\Omega)$, a weak solution $u$ satisfies $u - w \in H^1_0(\Omega)$. If a weak solution $u$ is twice weakly-differentiable and satisfies eq. (1.1) pointwise almost everywhere, then we say $u$ is a strong solution. We say $u \in H^1(\Omega)$ is a weak solution to the linearized Poisson-Boltzmann equation if it satisfies eq. (3.10) with $\sinh u$ replaced by $u$. We say that the nPBE equation is homogeneous if $(f, g) = (0, 0)$.

A weak solution that is in $H^2(\Omega)$ satisfies the strong form a.e. if one can *rewind* the integration by parts in the first term of eq. (3.10). This is possible since $\epsilon \in W^{1,\infty}(\Omega, \mathbb{C}^d)$. If $u \in H^2(\Omega)$ is a weak solution, then one can undo the integration by parts since $\epsilon \nabla u \in H^1(\Omega)$. Indeed for each $1 \leq i, k \leq d$,
\[
\|\partial_k \sum_{j=1}^d (\epsilon^{ij} \partial_j u)\|_{L^2} \leq C\|\epsilon\|_{W^{1,\infty}}\|u\|_{H^2}.
\]

Setting up the functional equation given in section 3.1 the non-linear operator $F : H^2(\Omega) \to L^2(\Omega)$ is given by
\[
F(u) = -\nabla \cdot (\epsilon \nabla u) + \kappa^2 \sinh(u) \tag{3.11}
\]
so that $u \in H^2(\Omega)$ is a strong solution to the eq. (1.1) if it satisfies
\[
F(u) = f, \quad x \in \Omega \\
u = g, \quad x \in \partial\Omega.
\]
The function $F$ can be broken up into its linear and non-linear components so that $F(u) = Lu + N(u)$ with
\[
Lu = -\nabla \cdot (\epsilon \nabla u) + \kappa^2 u \tag{3.11}
\]
\[
N(u) = \kappa^2 \sinh(u) = \kappa^2 \sum_{k=2}^\infty \nu_k u^k, \tag{3.12}
\]
where \( L \) is a linear uniformly elliptic second-order differential operator by hypothesis \( \frac{3}{2} \) and \( n_k = \frac{1}{(k!)^2} \) for odd \( k \) and \( n_k = 0 \) for even \( k \). Note that when \( d \leq 3 \), \( H^2(\Omega) \) is an algebra and so \( u^k \in H^2(\Omega) \) and \( N(u) \) is defined.

In order to determine if a strong solution to the NPBE exists, we also need control of certain fundamental constants of the operators and Sobolev spaces defined. To simplify the presentation and discussion in this section we define the relevant constants \( C_S(s) \), \( C_D \) and \( C_H \). Explicit estimates for these constants and their dependencies are derived in detail in Appendix A.

**Definition 3.2.** The Sobolev embedding for \( d = 3 \) and \( s > \frac{3}{2} \) gives that \( H^s(\Omega) \hookrightarrow L^\infty(\Omega) \) [17, Theorem 3.26]. The constant \( C_S = C_S(s, \Omega) > 0 \) is then defined as the norm of the inclusion operator from \( H^s(\Omega) \) into \( L^\infty(\Omega) \):

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

The linear operator \( L \) in eq. (3.11) takes functions in \( H^2(\Omega) \cap H^1_0(\Omega) \) to functions in \( L^2(\Omega) \). We shall denote \( C_D > 0 \) to be the norm of \( L \) with respect to these spaces:

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

By hypothesis 3, \( L \) is invertible and so \( L^{-1} : L^2(\Omega) \to H^2(\Omega) \cap H^1_0(\Omega) \) is defined. Define \( C_H > 0 \) to be the norm of \( L^{-1} \):

\[
C_H := \inf\{ C > 0 : \|u\|_{H^2(\Omega)} \leq C\|Lu\|_{L^2(\Omega)}, \forall u \in H^2(\Omega) \}.
\]

### 3.3 Main Results

In this section we present the main ideas of our paper. We employ a fix point argument to show the existence of the solution to the NPBE. This is based on producing a sequence of solutions of linear elliptic PDEs and showing that such sequence converges to the solution of the NPBE. We first state two useful lemmas that will be crucial to our mathematical argument.

**Lemma 3.1 (Lax-Milgram Theorem).** [12, Chapter 6] Given a complex Hilbert space \( \mathcal{H} \), let \( B : \mathcal{H} \times \mathcal{H} \to \mathbb{C} \) be a sesquilinear form that is bounded and coercive. By coercivity, suppose there exists \( \beta > 0 \) such that \( \text{Re}(B(u, u)) \geq \beta\|u\|^2 \) for all \( u \in \mathcal{H} \). Then, for every \( f \in \mathcal{H}' \), there exists a unique \( u \in \mathcal{H} \) such that \( B(u, \phi) = \langle f, \phi \rangle \) for all \( \phi \in \mathcal{H} \) where \( \langle \cdot, \cdot \rangle \) denotes the dual pairing. Moreover, we have \( \|u\| \leq \beta^{-1}\|f\|_{\mathcal{H}'} \).

For the readers’ convenience, we also state fixed point theorems that we need later.

**Lemma 3.2.** Let \( X \) be a Banach space over \( \mathbb{R} \) or \( \mathbb{C} \), and let \( A : X \to X \).

1. **(Banach’s Fixed Point Theorem)** If there exists \( \gamma \in (0, 1) \) such that \( \|A[u] - A[\bar{u}]\| \leq \gamma\|u - \bar{u}\| \) for all \( u, \bar{u} \in X \), then there exists a unique \( u_0 \in X \) such that \( A[u_0] = u_0 \).

2. **[15, Corollary 11.2]** Let \( K \subseteq X \) be closed and convex. If \( A : K \to K \) and \( \{A[u] : u \in K\} \) is precompact, then there exists \( u_0 \in K \) such that \( A[u_0] = u_0 \).

We now show that under hypotheses 1 to 3 there exists a unique solution to the linear PBE. Note that in the rest of the discussion in this section we assume that hypotheses 1 to 3 are always true.

**Lemma 3.3.** Let \( L \) be as in eq. (3.11) 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 \( u \in H^1(\Omega) \) such that \( u = g \) in the trace sense and

\[
\int_{\Omega} (\epsilon \nabla u) \cdot \nabla \phi + \kappa^2 u \phi = \int_{\Omega} f \phi,
\]

for all \( \phi \in H^1_0(\Omega) \).
Proof. Define a sesquilinear form \( B : H^1_0(\Omega) \times H^1_0(\Omega) \to \mathbb{C} \) given by
\[
B(u, \phi) = \int_{\Omega} (\varepsilon \nabla u) \cdot \nabla \phi + \kappa^2 u \phi,
\]
which defines a bounded operator. Additionally, \( B \) is coercive since
\[
\text{Re}[B(u, u)] = \int \text{Re}[(\varepsilon \nabla u) \cdot \nabla u] + \int \text{Re}(\kappa^2)|u|^2 \geq \theta \int |\nabla u|^2 - \mu \int |u|^2 \geq (\theta - \mu \lambda^{-1}) \int |\nabla u|^2,
\]
where the last inequality is by eq. (2.1). Hence, there exists a unique \( \tilde{u} \in H^1_0(\Omega) \) that satisfies
\[
B(\tilde{u}, \phi) = \int (f - Lw) \phi,
\]
for all \( \phi \in H^1_0(\Omega) \) by lemma 3.1. The proof is complete by taking \( u := \tilde{u} + w \). \( \square \)

A key ingredient in our approach is elliptic regularity. Let \( L \) be as in eq. (3.11) and consider solving \( Lu = f \in L^2(\Omega) \) with \( g = 0 \) on \( \partial \Omega \). From the standard elliptic theory (for instance, see [12, Section 6.3, Theorem 4]), there exists \( C_H > 0 \) as described in definition 3.2 such that \( \|u\|_{H^2} \leq C_H \|f\|_{L^2} \). For general boundary data, we have

Lemma 3.4. The unique weak solution of the linear PBE, \( u \in H^1(\Omega) \), satisfies
\[
\|u\|_{H^2} \leq C_H \|f\|_{L^2} + (C_H C_D + 1)\|w\|_{H^2}.
\]

Proof. As in the proof of lemma 3.3, absorb the boundary data into the inhomogeneous term by replacing \( f \) by \( f - Lw \) and considering the zero Dirichlet boundary condition. Then, an application of the Elliptic Regularity Theorem yields the estimate eq. (3.14). \( \square \)

To estimate the non-linear term in \( L^2(\Omega) \), we work with functions with sufficiently high Sobolev regularity.

Lemma 3.5. Let \( s > \frac{d}{2} \). Then for every \( u \in H^s(\Omega) \),
\[
\|N(u)\|_{L^2} \leq \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{d}{2}} \sum_{k=2}^\infty |n_k| (C_S(s)\|u\|_{H^s})^k.
\]

For \( N(u) \) for eq. (1.1), we have
\[
\|N(u)\|_{L^2} \leq \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{d}{2}} \left( \sinh(C_S(s)\|u\|_{H^s}) - C_S(s)\|u\|_{H^s} \right).
\]

Proof.
\[
\|N(u)\|_{L^2} \leq \|\kappa^2\|_{L^\infty} \sum_{k=2}^\infty |n_k|\|u\|_{L^2}^k \leq \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{d}{2}} \sum_{k=2}^\infty |n_k|\|u\|_{L^\infty}^k \leq \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{d}{2}} \sum_{k=2}^\infty |n_k| (C_S(s)\|u\|_{H^s})^k,
\]
where the inequalities are by the triangle inequality, the Hölder’s inequality, and the Sobolev inequality, respectively. \( \square \)

Remark 3.2. 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 [14, 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 \( H^1_0(\Omega) \). Such an approach does not apply in our setting where complex-valued functions are studied.

For \( d = 3 \), we have the embedding \( H^2(\Omega) \to L^\infty(\Omega) \), but such embedding for \( H^1(\Omega) \) does not hold. For \( d \geq 3 \), 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 \( \zeta \in C^\infty_c(B(0, R)) \) is a smooth non-negative function such that \( \zeta = 1 \) on \( B(0, \frac{R}{2}) \). If \( N(u) \in L^2(\Omega) \), then \( \sinh(u(\cdot)) \in L^2(\Omega) \). Since \( \sinh u \geq \frac{u^N}{N!} \) for every odd \( N \geq 1 \), we have \( u^N \in L^2(\Omega) \). However, this is false due to the blow-up of \( u \) at the origin.
To prove the existence of a solution, define a non-linear operator \( A : C_c^\infty(\Omega) \to H^2(\Omega) \) where for every \( u \in C_c^\infty(\Omega), A(u) \) satisfies

\[
L(A(u)) = f - N(u), \quad x \in \Omega \\
A(u) = g, \quad x \in \partial \Omega.
\]

Denoting \( K : L^2(\Omega) \to H_0^1(\Omega) \cap H^2(\Omega) \) to be the inverse of \( L \) stated in lemma 3.4, we conclude

\[
A(u) = K(f - N(u) - Lw) + w.
\]

Equivalently, the operator \( A \) defines an iteration map on some Banach space where each iterate is a unique solution to the linear PBE. More precisely, let \( u_0 \in H^2(\Omega) \) be the solution for the linearized nPBE; by lemma 3.3, there exists a unique weak solution \( u_0 \in H^1(\Omega) \) and by lemma 3.4, \( u_0 \in H^2(\Omega) \). By the Sobolev embedding theorem, \( H^2(\Omega) \hookrightarrow C^{0, 1/2}(\Omega) \), and therefore \( N(u_0) \in L^2(\Omega) \). Then, consider

\[
Lu_k + N(u_{k-1}) = f, \quad k \geq 1, \\
\left. u_k \right|_{\partial \Omega} = g,
\]

or equivalently, \( u_k = A(u_{k-1}) \).

There are three possible outcomes. Firstly, the sequence is divergent, a dead end. Secondly, the sequence is convergent to a function that does not solve eq. (1.1) in any meaningful way; see [7]. In contrast to the first two situations, we show that \( \{u_k\} \) converges to a solution of eq. (1.1). We show that \( A \) uniquely extends to a compact operator on fractional Sobolev spaces. In the rest of this section, we assume \( d = 3 \).

**Proposition 3.1.** \( A : L^\infty(\Omega) \to H^2(\Omega) \) is 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 \( u_n \xrightarrow{n \to \infty} u \) in \( L^\infty(\Omega) \) where \( u_n, u \in L^\infty(\Omega) \). There exists \( N \in \mathbb{N} \) such that if \( n \geq N \), then \( \|u_n\|_{L^\infty} \leq 2\|u\|_{L^\infty} \). Then,

\[
\|A(u_n) - A(u)\|_{H^2} = \|K(N(u_n) - N(u))\|_{H^2} \leq C_H \|N(u_n) - N(u)\|_{L^2} \\
\leq C_H \|k^2\|_{L^\infty} \sum_{k=2}^{\infty} |n_k| \|u_n^k - u^k\|_{L^2} \\
\leq C_H \|k^2\|_{L^\infty} \|u_n - u\|_{L^\infty} \sum_{k=2}^{\infty} |n_k| \sum_{j=0}^{k-1} \|u_n^{k-1-j} u^j\|_{L^2} \\
\leq C_H \|k^2\|_{L^\infty} |\Omega|^{1/2} \|u_n - u\|_{L^\infty} \sum_{k=2}^{\infty} |n_k| \sum_{j=0}^{k-1} \|u_n\|_{L^\infty}^{k-1-j} \|u\|_{L^\infty}^j \\
\leq C_H \|k^2\|_{L^\infty} |\Omega|^{1/2} \|u_n - u\|_{L^\infty} \sum_{k=2}^{\infty} |n_k| \|u\|_{L^\infty}^{k-1} (2^k - 1).
\]

The proof is done if \( u = 0 \), so assume \( u \neq 0 \) and let \( R > 4\|u\|_{L^\infty} \). If we show that the series in eq. (3.18) 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 with eq. (3.18), 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 \( A \)
Theorem 3.4. \( u \) is smoothing, \( u \) is continuous.

Then, there exists a strong solution \( u \in H^s(\Omega) \) into a bounded subset of \( H^s(\Omega) \). For \( \|u\|_{H^s} \leq M \),

\[
\|A(u)\|_{H^2} = \|K(f - N(u) - Lu) + w\|_{H^2} \leq C_H \|f - N(u) - Lu\|_{L^2} + \|w\|_{H^2}
\]

\[
\leq C_H \|f\|_{L^2} + (C_HC_D + 1)\|w\|_{H^2} + C_H \|N(u)\|_{L^2}
\]

\[
\leq C_H \|f\|_{L^2} + (C_HC_D + 1)\|w\|_{H^2} + C_H \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| (C_SM)^k,
\]

where eq. (3.19) follows from eq. (3.15).

\[
\begin{aligned}
\text{Figure 2: The tangency condition of eq. (3.23) where } y_0 &= C_H \|f\|_{L^2} + (C_HC_D + 1)\|w\|_{H^2} \text{ and } F \text{ is the LHS of eq. (3.23).}
\end{aligned}
\]

Now we apply the a priori estimate above to obtain a strong solution to eq. (1.1).

Theorem 3.3. Let \( s \in \left(\frac{3}{2}, 2\right) \) and \( M > 0 \) satisfy

\[
C_H \|f\|_{L^2} + (C_HC_D + 1)\|w\|_{H^2} + C_H \|\kappa^2\|_{L^\infty} |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| (C_SM)^k \leq M.
\]

Then, there exists a strong solution \( u \in H^2(\Omega) \) to eq. (1.1) with \( \|u\|_{H^s} \leq M \).

Proof. Let \( \|u\|_{H^s} \leq M \). Then, a similar argument to eq. (3.19) yields \( \|A(u)\|_{H^s} \leq M \). By Schauder’s fixed point theorem (lemma 3.2 on \( B_{H^s}(0, M) \), a closed convex subset of \( H^s(\Omega) \) on which \( A \) is continuous and compact by proposition 3.1, we obtain \( u \in B_{H^s}(0, M) \) such that \( A(u) = u \). Since \( A \) is smoothing, \( u \in H^2(\Omega) \).

Since the existence result above is a consequence of the Schauder fixed point theorem, no uniqueness is guaranteed. However, a more restrictive assumption on the parameters yields uniqueness.

Theorem 3.4. Let \( s \in \left(\frac{3}{2}, 2\right) \) and \( M > 0 \) satisfy eq. (3.20). Further assume

\[
C_HC_S(\|\kappa^2\|_{L^\infty} |\Omega|^{\frac{1}{2}} \sum_{k=2}^{\infty} |n_k| (C_SM)^k)^{-1} < 1.
\]

Then, there exists a strong solution \( u \in H^2(\Omega) \) to eq. (1.1) that is unique in \( B_{H^s}(0, M) \subseteq H^s(\Omega) \).
Proof. We invoke the Banach fixed point theorem by showing that $A$ defines a strict contraction on $B_{H^s}(0, M)$. Following the steps leading to eq. (3.18), we obtain
\[
\|A(u) - A(v)\|_{H^s} \leq \left( C_H C_S \|\kappa^2\|_{L^\infty} [\Omega]^{\frac{1}{2}} \sum_{k=2}^{\infty} k|n_k|(C_SM)^{k-1}\right) \|u - v\|_{H^s},
\] (3.22)
and recall that the infinite series is $\cosh(C_SM) - 1$ in eq. (3.22). \qed

Remark 3.3. When $N(u) = \sinh u$, there exists $M > 0$ that satisfies eq. (3.20) if and only if
\[
C_H \|f\|_{L^2} + (C_HC_D + 1) \|w\|_{H^2} + C_H \|\kappa^2\|_{L^\infty} [\Omega]^{\frac{1}{2}} (\sinh C_SM_0 - C_SM_0) \leq M_0
\] (3.23)
where $M_0 = C_S^{-1} \cosh^{-1}(1 + \frac{1}{C_H \|\kappa^2\|_{L^\infty} [\Omega]^{\frac{1}{2}}})$, which is independent of $\|f\|_{L^2}, \|w\|_{H^2}$. Moreover, the condition in eq. (3.21) is equivalent to $M < M_0$. The case when the equality of eq. (3.23) holds is illustrated in fig. 2. The equality occurs precisely when the LHS of eq. (3.23), as a function of $M$, is tangent to the identity.

Remark 3.4. As can be shown in eqs. (3.20) and (3.21), our fixed point approach works for small data where the given parameters must be small measured in various norms. For 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 nonlinearities that are complex-analytic in $u$. For instance, nonlinearities of the form $e^u, \cosh u$ fall under this category.

4 Discussion.

In this paper, we have studied the existence and uniqueness theory of the complexified nPBE equation. The biggest difference between our model and the real-valued nPBE equation stems from the non-convexity of the nonlinearity on $\mathbb{C}$, which makes it difficult to directly apply variational calculus to our model. In fact, for the real-valued nPBE, we have

Proposition 4.1. [14] Theorem 2.14] Let $\Omega \subseteq \mathbb{R}^3$ be open and bounded with a Lipschitz boundary. Let $\epsilon = \text{diag}(\hat{\epsilon}(x))$ where $\epsilon \in L^\infty(\Omega, \mathbb{R})$ with $\epsilon_1 \leq \hat{\epsilon}(x) \leq \epsilon_2$ for $0 < \epsilon_1 \leq \epsilon_2$ for all $x \in \Omega$, and let $\kappa \in L^\infty(\Omega, \mathbb{R})$. For every $f \in L^2(\Omega, \mathbb{R})$ and real-valued $g \in H^\frac{1}{2}(\partial\Omega)$, there exists a unique weak solution to eq. (1.1) in $H^1(\Omega)$.

A good control of nPBE with complex-valued coefficients has consequences in uncertainty quantification. In particular, it is shown that the solution to the nPBE is analytic in a well-defined region with respect to a collection of stochastic parameters, then the regularity of the solution can be precisely determined. This is important for computing the statistics of a linear bounded Quantity of Interest of the solution $u$ with respect to high dimensional stochastic parameters [22, 11, 9]. If the sequence of approximate solutions $\{u_n\}$, given by eq. (3.17), is also complex-analytic with respect to the stochastic parameters, then the solution $u$ will also be complex-analytic in the same region. Since $u_n$ is the solution of a linear elliptic PDE, there already exist detailed studies of the analytic properties of $u_n$ with respect to stochastic diffusion coefficients and random domains [11, 9, 22].

We remark that our work has a room for improvements. In the Debye-Hückel model, a collection of macromolecules such as proteins is located in the region $\Omega_1 \subseteq \mathbb{R}^3$, surrounded by the ion-exclusion layer $\Omega_2$, which in turn is surrounded by the solvent of positive and negative charges in $\Omega_3$. Altogether, let $\Omega := \bigcup_{i=1}^3 \Omega_i$. In an equilibrium, a well-defined potential function of the system gives rise to a well-defined dielectric constant $\epsilon(x)$. Conversely, we wish to study the properties of solution given a dielectric constant. According to the Debye-Hückel model,
\[
\epsilon(x) = \begin{cases} 
\epsilon_1 > 0, & x \in \Omega_1 \\
\epsilon_2 > 0, & x \in \Omega_2 \cup \Omega_3.
\end{cases}
\] (4.1)
We remark that our analysis assumes that $\epsilon$ is Lipschitz-continuous, and therefore does not cover the case eq. (4.1). The Lipschitz-continuity assumption plays a crucial role in obtaining the elliptic regularity results such as lemma [A.6] and lemma [A.7]. For now, we leave this interesting question open.
Appendices

A Estimates for the Constants.

In theorems 3.3 and 3.4 the existence and uniqueness of solutions of eq. (1.1) depend in part on the values of the constants $C_S(8)$, $C_H$, and $C_D$ described in definition 3.2. 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 1 to 3 are still assumed to hold throughout appendix A.

A.1 Estimates for $C_D$

Lemma A.1. Let $L$ be as in eq. (3.11). Then

$$C_D \leq 2d^2 \| \kappa \|_{W^{1,\infty}} + \| \kappa \|_{L^\infty}.$$  \hspace{1cm} (A.1)

Proof. Since

$$\| \kappa^2 u \|_{L^2} \leq \| \kappa^2 \|_{L^\infty} \| u \|_{L^2} \leq \| \kappa^2 \|_{L^\infty} \| u \|_{H^2},$$

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

$$\| \nabla \cdot (\kappa \nabla u) \|_{L^2} \leq \sum_{i,j} \| \partial_i (\kappa^{ij} \partial_j u) \|_{L^2} \leq \sum_{i,j} \| \partial_i \kappa^{ij} \partial_j u \|_{L^2} + \| \kappa^{ij} \partial_j u \|_{L^2}$$

$$\leq \sum_{i,j} (\| \partial_i \kappa^{ij} \|_{L^\infty} + \| \kappa^{ij} \|_{L^\infty}) \| u \|_{H^2} \leq 2d^2 \| \kappa \|_{W^{1,\infty}} \| u \|_{H^2},$$

and hence eq. (A.1). \qed

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

In this subsection, we are interested in obtaining an upper bound of the operator norm of $H^2(\Omega) \rightarrow L^\infty(\Omega)$ 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 $\Omega$ can be extended to $\mathbb{R}^d$ via an extension operator. Composing these two, one obtains a Sobolev inequality on $\Omega$. See [12 Chapter 5] for an exposition of this material. To apply the estimates obtained in [19], 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 $u \in W^{1,q}(\Omega)$ and $u_\Omega := |\Omega|^{-1} \int_\Omega u$,

$$\| u \|_{L^q(\Omega)} \leq C_{p,q} \| u \|_{W^{1,p}(\Omega)}, \quad \| u - u_\Omega \|_{L^q(\Omega)} \leq D_{p,q} \| \nabla u \|_{L^p(\Omega)}.$$  \hspace{1cm} (A.2)

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

Lemma A.2. [19] Theorem 2.1] For $\Omega \subseteq \mathbb{R}^d$, if $D_{p,q} > 0$ is given as eq. (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. [19] Theorem 3.2] Let $p \in (2,6]$ and $u \in H^1(\Omega)$ where we further suppose that $\Omega$ is convex. Then, we have $\| u - u_\Omega \|_{L^p(\Omega)} \leq D_{2,p} \| \nabla u \|_{L^2(\Omega)}$ with

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

Hence

$$C_{2,p} = 2^{\frac{1}{p}} \max(|\Omega|^{\frac{1}{p}} - \frac{1}{p}, D_{2,p}).$$
Lemma A.4. [19, Theorem 3.4] For $p > 3$ and $u \in W^{1,p}(\Omega)$, we have $\|u - u_\Omega\|_{L^\infty} \leq D_{p,\infty}\|\nabla u\|_{L^p}$ with
\[
D_{p,\infty} = \frac{d^3}{3|\Omega|} \left\| |x|^{-2} \right\|_{L^{p'}(V)} ,
\] (A.4)
where $\Omega_\varepsilon := \{x - y : y \in \Omega\}$ and $V = \bigcup_{x \in \Omega} \bar{B}(x)$. 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.

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 $u \in W^{1,p}(\Omega)$
\[
\|u\|_{L^q(\Omega)} \leq C_{p,q}\|u\|_{W^{1,p}(\Omega)}.
\]
If we further assume that $|\Omega| = C d_\Omega^3$ for some $C > 0$, then there exists $d_0 > 0$ such that for every $d_\Omega \leq d_0$,
\[
|\Omega|^{-\frac{1}{2}} \leq C_S(2) \leq 2^{\frac{1}{p}} |\Omega|^{-\frac{1}{2}}.
\]

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
\[
\|u\|_{W^{1,p}}^p = \|u\|^p_{L^p} + \sum_{i=1}^d \|\partial_i u\|^p
\]
\[
\leq C_{2,p}\|u\|^p_{H^1} + C_{2,p}^2 \sum_{i=1}^d \|\partial_i u\|^p_{H^1} \leq C_{2,p}\|u\|^p_{H^1} + C_{2,p} \left( \sum_{i=1}^d \|\partial_i u\|^2_{H^1} \right)^{p/2}
\]
\[
\leq C_{2,p}\|u\|^p_{H^1} + C_{2,p}^2 \|u\|^p_{H^2} \leq 2C_{2,p}\|u\|^p_{H^2},
\]
and from the second embedding,
\[
\|u\|_{L^\infty} \leq C_{p,\infty}\|u\|_{W^{1,p}}.
\]
Combining the two, we obtain the upper bound. For the lower bound, consider a family of constant functions defined on $\Omega$. Then
\[
\|c\|_{L^\infty} = \|c\|_{L^\infty} = |\Omega|^{-\frac{1}{2}} \leq C_S(2).
\]
Now we assume $|\Omega| = C d_\Omega^3$ for some $C > 0$ and give a sharp bound for $C_S(2)$ for $d_\Omega$ 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 $D_{2,p} = C(p)d_\Omega^{\frac{1}{p}-\frac{1}{2}}$ by eq. (A.3) and $|\Omega|^{\frac{1}{2}} = (Cd_\Omega^3)^{\frac{1}{2}-\frac{1}{2}}$, we have
\[
C_{2,p} = 2^{\frac{1}{p}} |\Omega|^{\frac{1}{2}-\frac{1}{2}} ,
\]
(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 $d_\Omega = \sup_{x \in \Omega} |x|$. Then, $V \subseteq B(0,d_\Omega)$ and
\[
\|\|x|^{-2}\|_{L^{p'}(V)} \leq \|\|x|^{-2}\|_{L^{p'}(B(0,d_\Omega))} = 4\pi \int_0^{d_\Omega} r^{-2p'+2}dr = \frac{4\pi}{2p'+3} d_\Omega^{-2p'+3},
\]
and thus $D_{p,\infty} = C'(p)d_\Omega^{-\frac{2}{p'}+1}$ by eq. (A.4), and we have
\[
C_{p,\infty} = 2^{1 - \frac{1}{p}} |\Omega|^{-\frac{1}{2}},
\]
(A.6)
for all $d_\Omega \leq d'_0(p)$ for some $d'_0(p) > 0$. Combining eq. (A.5) and eq. (A.6), we have
\[
|\Omega|^{\frac{1}{2}} \leq C_S(2) \leq 2^{\frac{1}{p}} |\Omega|^{-\frac{1}{2}},
\]
for all $d_\Omega$ sufficiently small. \hfill $\square$
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 $\epsilon$ 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

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

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

**Lemma A.6.** Let $L$ be as in eq. (3.11). Furthermore, suppose $\epsilon^{ij} = \epsilon(x)\delta_{ij}$ where $\delta_{ij}$ is the Kronecker delta function and $\epsilon \in W^{1,\infty}(\Omega)$ such that $\text{Re}(\epsilon(x)) \geq \theta > 0$ for all $x \in \Omega$. Then

$$C_H \leq \frac{\lambda_1^{-1} (\lambda_1^2)^{\frac{3}{4}}}{\theta} \left( 1 + \frac{\|\kappa^2\|_{L^\infty(\Omega)} + d^2 \max_{1 \leq i \leq d} \|\partial_i \epsilon\|_{L^\infty(\Omega)} \lambda_1^{\frac{3}{2}}}{\theta \lambda_1 - \mu} \right). \quad (A.7)$$

**Proof.** Given $F \in L^2(\Omega)$ and a unique weak solution $u \in H^1_0(\Omega)$ of the Laplace equation $-\Delta u = F$ in $\Omega$, 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 $F \in C^\infty_c(\Omega)$. By an integration-by-parts argument, it can be shown that $u \in C^2_c(\Omega)$. Hence, we extend $u$ to a function in $C^2_c(\mathbb{R}^d)$, which we continue to call $u$, by defining $u(x) = 0$ for $x \in \mathbb{R}^d \setminus \text{supp}(u)$. Then,

$$\|u\|_{H^2(\Omega)}^2 \leq \|\hat{u}\|_{H^2(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} \langle \xi \rangle^4 |\hat{u}(\xi)|^2 d\xi$$

$$= \int_{|\xi| \leq c} \langle \xi \rangle^4 |\hat{u}(\xi)|^2 d\xi + \int_{|\xi| \geq c} \langle \xi \rangle^4 |\hat{u}(\xi)|^2 d\xi =: I + II$$

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

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

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

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

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 $c = \lambda_1^{\frac{1}{2}}$, we fix that value of $c$ to obtain

$$\|u\|_{H^2(\Omega)} \leq C_1 \|F\|_{L^2(\Omega)} \quad \text{where} \quad C_1 := \lambda_1^{-1} (\lambda_1^2)^{\frac{3}{4}}. \quad (A.8)$$

Now we assume $u \in H^1_0(\Omega)$ is the unique weak solution of

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

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

$$-\Delta u = \epsilon(x)^{-1} (F + \nabla \epsilon \cdot \nabla u).$$
Noting that $|\epsilon(x)| \geq |\text{Re}(\epsilon(x))| \geq \text{Re}(\epsilon(x)) \geq \theta$, an immediate application of eq. (A.8) yields

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

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

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

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

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

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

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

Another application of the Poincaré inequality to eq. (A.11) yields $(\theta - \mu \lambda_1^{-1}) \int_{\Omega} |\nabla u|^2 \leq \theta \int_{\Omega} |\nabla u|^2 + \int_{\Omega} \text{Re}(\kappa^2)|u|^2$, which gives

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

Hence,

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

(13)

On the other hand, the Cauchy-Schwarz inequality yields

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

(14)

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

$$\|u\|_{H^2(\Omega)} \leq \lambda_1^{-1}(\lambda_1^{\frac{1}{2}})^2(1 + \lambda_1^{\frac{1}{2}})^{\frac{1}{2}} \left(1 + \frac{\|\kappa^2\|_{L^\infty(\Omega)} + d^{\frac{1}{2}} \max_{1 \leq i \leq d} \|\partial_i \epsilon\|_{L^\infty(\Omega)} \lambda_1^{\frac{1}{2}}}{\theta \lambda_1 - \mu}\right)\|f\|_{L^2(\Omega)}.$$  \hfill \Box

In general when $\epsilon$ is a tensor, a direct application of Fourier transform seems infeasible. Instead, we closely follow the argument of [12] 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 eq. (3.11). Then

$$C_H \leq N(\Omega)\left(\frac{1 + \lambda_1}{\theta \lambda_1 - \mu}\right)^{\frac{1}{2}} + d C_0,$$  \hfill (A.15)

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

**Remark A.1.** For every $\Omega$ such that $\lambda_1 \sim d_\Omega^2$, the RHS of eqs. (A.7) and (A.15) converge to $\frac{C(\Omega)}{\theta}$ as $d_\Omega \to 0$.

**Remark A.2.** Since the estimate of eq. (A.15) depends on the number of finitely many open balls covering $\Omega$, the geometry of $\partial \Omega$ plays a big role in the computation of $N(\Omega)$. This will be pursued in future research.
Recalling the following variant of Cauchy-Schwarz inequality

\begin{align*}
\text{applied to the test function } \phi &= -D_k^{-h}\zeta^2 D_k^h u,
\end{align*}

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

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

\[
\text{Re} \int_\Omega \zeta^2 \epsilon^{ij,h} D_k^h \partial_j u D_k^h \partial_i u \geq \theta \int_\Omega \zeta^2 |D_k^h \nabla u|^2.
\]

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

\[
R \leq \left| \int \zeta \partial_i \zeta \epsilon^{ij,h} D_k^h \partial_j u D_k^h \partial_i u \right| + \int \zeta \partial_i \zeta D_k^h \epsilon^{ij} \partial_j u D_k^h \partial_i u + \int \zeta \partial_i \zeta D_k^h \epsilon^{ij} \partial_j u D_k^h \partial_i u
\]

\[
\leq 2 \|
\nabla \zeta \|_{L^\infty(\Omega)} \| \epsilon \|_{W^{1,\infty}(\Omega)} \left( \int \zeta |D_k^h \nabla u|^2 |D_k^h u| + \int \zeta |\nabla u|^2 |D_k^h u| \right) + \| \epsilon \|_{W^{1,\infty}(\Omega)} \int \zeta |\partial_j u|^2 |D_k^h \partial_i u|.
\]

Recalling the following variant of Cauchy-Schwarz inequality

\[
ab \leq \frac{a^2}{2\delta} + \frac{\delta b^2}{2},
\]

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

\[
\| D_k^h \phi \|_{L^2(V)} \leq \| \partial_k \phi \|_{L^2(\Omega)} \quad \forall \phi \in H^1(\Omega), \ V \in \Omega,
\]

eq. \( \text{(A.17)} \) is bounded above by

\[
\leq C_1 \delta \int \zeta^2 |D_k^h \nabla u|^2 + C_2 \int |\nabla u|^2
\]

where

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

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

\[
\text{Re} \int_\Omega (\epsilon \nabla u) \cdot \nabla u \geq \frac{\theta}{2} \int_\Omega \zeta^2 |D_k^h \nabla u|^2 - C_2 \int_\Omega |\nabla u|^2.
\]

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

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

Proof. Let \( V \in W \subseteq \Omega \). Let \( \zeta \in C_0^\infty(\Omega) \) such that \( 0 \leq \zeta \leq 1 \) and \( \zeta = 1 \) on \( V \), and \( \text{supp}(\zeta) \subseteq W \). Set \( F = f - \kappa^2 u \in L^2(\Omega) \). Consider the weak form of

\begin{align*}
- \nab \cdot (\epsilon \nab u) + \kappa^2 u &= f \quad \text{in } \Omega
\end{align*}

\[(A.16)\]
where the first term is estimated above as in eq. (A.13).

\[
\int_\Omega |\phi|^2 \leq \int_\Omega |\partial_k (\zeta^2 D_k^h u)|^2 \\
\leq 2 \int_\Omega |2\zeta \partial_k \zeta D_k^h u|^2 + 2 \int_\Omega \zeta^2 |D_k^h \partial_k u|^2 \\
\leq 8 \|\nabla \zeta\|_{L^\infty(\Omega)}^2 \int_\Omega |\nabla u|^2 + 2 \int_\Omega \zeta^2 |D_k^h \nabla u|^2,
\]

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

\[
\left|\int_\Omega F d\bar{\delta}\right| \leq \frac{2}{\theta} \left(1 + \frac{\|\nabla \zeta\|_{L^\infty(\Omega)}^2}{\theta \lambda_1 - \mu}\right)^2 \int_\Omega |f|^2 + \theta \|\nabla \zeta\|_{L^\infty(\Omega)} \int_\Omega |\nabla u|^2 + \frac{\theta}{4} \int_\Omega \zeta^2 |D_k^h \nabla u|^2.
\]  

(A.20)

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

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

and by eq. (A.12),

\[
\int_V |D_k^h \nabla u|^2 \leq C_0 \int_\Omega |f|^2,
\]

where

\[
C_0 = \frac{4}{\theta} \left(1 + \frac{\|\nabla \zeta\|_{L^\infty(\Omega)}^2}{\theta \lambda_1 - \mu}\right)^2 + \lambda_1 \frac{C_2 + \theta \|\nabla \zeta\|_{L^\infty(\Omega)}}{(\theta \lambda_1 - \mu)^2}.
\]  

(A.21)

By [12] 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,

\[
\sum_{1 \leq i, j \leq d} \|\partial_{ij} u\|_{L^2(V)}^2 \leq d C_0 \int_\Omega |f|^2.
\]

(A.22)

Recall that the linear theory (lemma 3.1 and eq. (3.13)) yields

\[
\|u\|_{H^1(\Omega)} \leq \frac{1 + \lambda_1}{\theta \lambda_1 - \mu} \|f\|_{L^2(\Omega)}.
\]

(A.23)

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

\[
\|u\|_{H^2(V)} \leq \left(\frac{1 + \lambda_1}{\theta \lambda_1 - \mu}\right)^2 + d C_0 \right)^{\frac{1}{2}} \|f\|_{L^2(\Omega)}.
\]

(A.24)

Since \(\Omega\) 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 \(\mathbb{R}^d_+ := \mathbb{R}^d_+ \times [0, \infty)\) 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 eq. (A.24). Hence, there exists \(N = N(\Omega) \in \mathbb{N}\) such that

\[
\|u\|_{H^2(\Omega)} \leq N(\Omega) \left(\frac{1 + \lambda_1}{\theta \lambda_1 - \mu}\right)^2 + d C_0 \right)^{\frac{1}{2}} \|f\|_{L^2(\Omega)}.
\]

(B) Failure of Uniqueness

Most notably, our result has a smallness assumption on data \((f, g)\) and further restrictions on the given parameters; see hypotheses \([1]\) to \([3]\) in section \(3\) and theorems \(3.3\) and \(3.4\) When eq. (1.1) is complexified, it
is not obvious whether or not these sufficient conditions are in fact necessary. We construct an example of nPBE that admits multiple solutions. By construction, this family of nPBEs fails to satisfy the invertibility condition given in hypothesis 3 and/or the smallness assumption on $(f, g) \in L^2(\Omega) \times H^2(\partial \Omega)$. In particular, this example is consistent with the well-known uniqueness result of [16].

We wish to obtain a radial solution $u(x) = u(|x|) = y(r)$, where $r = |x| \geq 0$, to eq. (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 $R > 0$, $d \geq 1$ and $f(x) = \lambda \in \mathbb{R}$, $g(x) = \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right)$. In the polar coordinate, our example reduces to an ODE

$$ry'' + (d - 1)y' + \tilde{\kappa}^2 r \sinh y = r\lambda, \quad r \in (0, R)$$

$$y(R) = \sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right).$$

(B.1)

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

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

Reducing eq. (B.1) into a first-order ODE by introducing $w = y'$, we obtain

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

(B.2)

For $d = 1$, eq. (B.2) 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 $P = \left(\sinh^{-1}\left(\frac{\lambda}{\tilde{\kappa}^2}\right), 0\right)$ 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 eq. (B.1) 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 3: Vector fields of eq. (B.2) 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 eq. (B.2) is non-autonomous, and $F$ in eq. (B.2) 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 eq. (B.1). We solve an ODE that is slightly more general than eq. (B.1). We use the notations of proposition B.1.

Lemma B.1. For every $A \geq 0$ and $c \in \mathbb{R}$, there exists $R > C_{\tilde{\kappa}}$ and $y \in C^\infty_{\text{loc}}((0, \infty); \mathbb{R})$ such that $y$ satisfies

$$ry'' + Ay' + \tilde{\kappa}^2 r \sinh y = r\lambda, \quad r \in (0, \infty),$$

$$\lim_{r \to 0^+} y(r) = c, \quad \lim_{r \to 0^+} y'(0+) = 0, \quad y(R) = \sinh^{-1}(\frac{\lambda}{\tilde{\kappa}^2}).$$

(B.3)

Proof of proposition B.1. Set $A = d - 1$. □

Proof of lemma B.1. The $A = 0$ case is equal to that when $d = 1$, and therefore assume $A > 0$. Moreover, assume $c \neq \sinh^{-1}(\frac{\lambda}{\tilde{\kappa}^2})$ since it yields a trivial solution. For $\epsilon > 0$, consider the perturbed ODE:

$$(r + \epsilon) y'' + Ay' + \tilde{\kappa}^2(r + \epsilon) \sinh y = (r + \epsilon)\lambda, \quad r \in [-\epsilon, \infty),$$

$$y(0) = c, \quad y'(0) = 0,$$

(B.4)

which, after setting $w_{\epsilon} = y'_\epsilon$, reduces to

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

Since $F_{\epsilon}$ is smooth in $r$ near $r = 0$ and locally Lipschitz in $(y, w)$, there exists $T_{\epsilon} \in (0, \frac{\epsilon}{2})$ and $y_{\epsilon} \in C([-T_{\epsilon}, T_{\epsilon}; \mathbb{R}) \cap C^\infty_{\text{loc}}([-T_{\epsilon}, T_{\epsilon}); \mathbb{R})$ such that $y_{\epsilon}$ is a unique solution to eq. (B.4). In the maximal interval of existence, $\left(\begin{array}{c} y_{\epsilon} \\ w_{\epsilon} \end{array}\right)$ satisfies

$$\frac{d}{dr} H(y_{\epsilon}(r), w_{\epsilon}(r)) = w_{\epsilon}(r)(y''_{\epsilon}(r) + \tilde{\kappa}^2 \sinh y_{\epsilon}(r) - \lambda) = -\frac{Aw_{\epsilon}(r)^2}{r + \epsilon} \leq 0, \quad r \geq -\frac{\epsilon}{2}$$
and therefore the forward orbit of \( \left( \frac{y_e}{w_e} \right) \) is bounded in the compact subset \( \{(y, w) \in \mathbb{R}^2 : H(y, w) \leq H(c, 0)\} \) on which \( F_e \) is Lipschitz. Hence, \( \left( \frac{y_e}{w_e} \right) \) can be uniquely extended globally in forward time, obeying the estimate

\[
H(y_e(r), w_e(r)) \leq H(c, 0), \quad r \geq 0.
\]

(B.5)

This global bound on \( |y_e| + |w_e| \) yields an existence of a limit function, since for \( r_1, r_2 \geq 0 \),

\[
|y_e(r_2) - y_e(r_1)| = \left| \int_{r_1}^{r_2} w_e(\rho)d\rho \right| \leq C|r_2 - r_1|,
\]

where \( C > 0 \) is independent of \( \epsilon > 0 \). An immediate application of Arzelà-Ascoli Theorem implies that there exists a subsequence \( \epsilon_k \) that tends to zero (from the right) and \( y \in C_{loc}(0, \infty; \mathbb{R}) \) 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 eq. (B.5), there exists a subsequence of \( \{\epsilon_k\} \) and \( w \in L^2((0, T); \mathbb{R}) \) such that, possibly after relabelling the subsequence, \( w_{\epsilon_k} \to w \) 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 eq. (B.4) 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 \((r + \epsilon_k)y''_{\epsilon_k} \xrightarrow{k \to \infty} Y \) in \( C([0, T]; \mathbb{R}) \), possibly after relabelling the subsequence, and follows \( y''_{\epsilon_k} \xrightarrow{k \to \infty} \frac{Y(r)}{r} \) in \( C([\delta, T]; \mathbb{R}) \) for every \( \delta > 0 \), and therefore 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 eq. (B.5) 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 \( y_{\epsilon_k} \) is a classical solution to eq. (B.4), it is also a weak solution. Writing eq. (B.4) in the weak form, integrating by parts, and taking \( k \to \infty \), we obtain \( ry'' + Ay' + \tilde{\kappa}^2 r \sinh y = \lambda \) 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 eq. (B.4) and the uniform convergence of \( y_{\epsilon_k} \) 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 \( y_{\epsilon_k} \xrightarrow{k \to \infty} y' \) uniformly on compact subsets of \((0, T)\) for \( j = 0, 1, 2 \). Taking \( k \to \infty \) from eq. (B.4), 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 \( y \in C^\infty_{loc}(\mathbb{R}; \mathbb{R}) \).

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

\[
\int_0^T y''_{\epsilon_k} \phi = -\int_0^T y'_{\epsilon_k} \phi' - \int_0^T y' \phi' = \int_0^T y'' \phi.
\]

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 \( y_{\epsilon_k} \xrightarrow{k \to \infty} y' \) for every \( \delta > 0 \), we conclude that \( \delta \) could be taken to be zero. In particular, \( y'(0) = \lim_{k \to \infty} y'_{\epsilon_k}(0) = 0 \).

Finally from the phase portrait analysis, the solution \( (y(r), w(r)) \) exhibits an oscillatory behavior in \( \mathbb{R}^2 \); however, note that in the non-autonomous case, the solution curve does not lie in any curves of constant Hamiltonian due to the \( y' \) term. Since every closed curve of constant Hamiltonian contains the global minimum \( (\sinh^{-1}(\frac{\lambda}{\kappa^2}), 0) \), there exists \( \{R_n\}_{n=1}^\infty \) such that \( 0 < R_n < R_{n+1}, R_n \xrightarrow{n \to \infty} \infty \) such that \( y(R_n) = 0 \).

\( \square \)

**Remark B.1.** For \( d = 3 \), eq. (B.1) with \( \kappa = 1 \) 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

\[
ry'' + 2y' + ry = 0.
\]
The two linearly independent solutions are given by
\[ j_0(r) = \frac{\sin r}{r}, \quad y_0(r) = \frac{\cos r}{r}. \]

We give plots comparing the linear and nonlinear solutions for \( d = 3 \).

Figure 4: Comparison of solutions to eq. (B.1) and its corresponding linearization.

Remark B.2. Intuitively, this non-uniqueness stems from the non-coercivity of the nonlinear operator \( T u := -\epsilon \Delta u + \kappa^2 \sinh u \) when \( \epsilon, \kappa \) do not satisfy \( \epsilon, \kappa > 0 \). Indeed, our choice of nonlinearity is beyond the scope of those discussed in [18] that studies the uniqueness of radial solution to \( \Delta u + f(u) = 0 \) when \( f'(0) < 0 \).

As a simple example, let \( \epsilon = 1, \kappa = i \) and consider the linearized equation \( u'' + u = 0 \) in \( x \in (0, \pi) \) with the boundary condition \( u(0) = u(\pi) = 0 \). Then, we have an uncountable family of solutions \( \{ A \sin x \}_{A \in \mathbb{R}} \).

However, it turns out that uniqueness can be salvaged if we drop the lower orders terms of \( \sinh(u) \). We state a result whose proof, based on the Derrick-Pohozaev identity, is easily adapted from that of [12, Section 9.4, Theorem 1]; compare this to proposition B.1.

Let \( d \geq 3 \) and \( N_0 > \frac{d+2}{d-2} \) be an odd integer. Suppose \( u \in C^2(\Omega) \) is a classical solution to
\[
-\Delta u = \sum_{N \geq N_0, N \text{ odd}} \frac{u^N}{N!}, \quad x \in \Omega
\]
\[ u = 0, \quad x \in \partial \Omega, \]
where \( \Omega \) is a star-shaped domain containing \( 0 \in \mathbb{R}^d \) with \( \partial \Omega \in C^1 \). Then, \( u = 0 \) in \( \overline{\Omega} \).

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