# A Variational and Regularization Framework for Stable Strong Solutions of Nonlinear Boundary-Value Problems

Joseph W. Jerome*

**Key words:** Minimizer, regularization, boundary-value problems, stability, approximation, calculus of variations

**2020 AMS classification numbers:** 49J27, 49J50, 35Q92, 41A65, 47J07

**Abstract**

We study a variational approach introduced by S.D. Fisher and the author in the 1970s in the context of norm minimization for differentiable mappings occurring in nonlinear elliptic boundary value problems. It may be viewed as an abstract version of the calculus of variations. A strong hypothesis, initially limiting the scope of this approach, is the assumption of a bounded minimizing sequence in the least squares formulation. In this article, we employ regularization and invariant regions to overcome this obstacle. A consequence of the framework is the convergence of approximations for regularized problems to a desired solution. The variational method is closely associated with the implicit function theorem, and it can be jointly studied, so that continuous parameter stability is naturally deduced. A significant aspect of the theory is that the reaction term in a reaction-diffusion equation can be selected to act globally as in the steady Schrödinger-Hartree equation. Local action, as in the non-equilibrium Poisson-Boltzmann equation, is also included. Both cases are studied at length prior to the development of a general theory.

[1]Department of Mathematics, Northwestern University, Evanston, IL 60208.

# 1 Introduction.

During the 1960s and 1970s, considerable effort was directed toward applying the methods of nonlinear functional analysis to the theory of partial differential equations (PDE). The volumes of E. Zeidler, particularly [24, 25], discuss many of these results. An especially seminal study was the article by H. Brézis [3]. In [3], the concept of duality allowed the merger of monotone operator theory with weak solutions of PDE. In the ensuing decades, this has been an especially effective methodology. For a systematic study, see [21]. In this article, we describe results based upon a variational calculus developed by S.D. Fisher and the author in [7]. Related results may be found in [6] and [11].

These results, which may be viewed as an effective abstraction of the calculus of variations [20], form the starting point for the analysis of the present study. One of the advantages, as is the case for monotone operator theory and its extensions, is the decoupling from direct dependence upon fixed point theory. In the appendix, we discuss connections to fixed point theory, and the limitations of the latter. In addition, the hypotheses of the variational approach are naturally compatible with those of the implicit function theorem, and we obtain local continuous parametric solutions. The models envisioned here are generalized reaction-diffusion boundary-value problems. For these models, the reaction terms may act either locally or globally. For small-scale models, this is essential.

## 1.1 Prior results

We now summarize our prior results. Precise statements may be found in the appendix in section A.1. Suppose $T$ maps a reflexive Banach space $X$ into a normed linear space $Y$. We suppose the following.

1. $T$ maps weakly convergent sequences in $X$ onto weakly convergent sequences in $Y$.

2. If $U$ is the translate of a closed linear subspace $U_0$ of $X$, then there exists a bounded minimizing sequence in $X$ for
$$\alpha = \inf\{\|Tx\| : x \in U\}. \tag{1}$$
We understand the usual use of these terms. If these two conditions hold, there is a minimizer $x_0$ for the minimization problem (1) (cf. Theorem A.1).

3. If $Y = L^p$, $1 < p < \infty$, and if $T$ is continuous and Fréchet differentiable on $X$, then $\alpha = 0$, provided $L = T'(x_0)$ maps $U_0$ onto $L^p$ (cf. Theorem A.2).

Although these results are useful, they are limited by the assumption of a bounded minimizing sequence. This is the case for the partial differential equations of mathematical physics, and the associated boundary-value problems, the principal topic of application here. Fortunately, the framework here is accommodated by regularization, which does not alter the solution set when used in conjunction with the invariant interval property. This is not only technically advantageous, but facilitates the abstract computational procedures, expressed via least square approximation.

**Remark 1.1.** *Throughout this article, we assume that the spatial domain* $\Omega \subset \mathbb{R}^N$ *is bounded and connected, and possesses a* $C^2$ *boundary, and that the Euclidean dimension* $N$ *satisfies* $N = 1, 2, 3$. *In addition, we make use of standard Sobolev embedding theorems [1].*

### 1.2 Summary of the article

In sections four and five, we present a general theory, based upon the variational approach, for reaction-diffusion equations. Existence, uniqueness, approximation, and stability results are presented. Weak maximum principles and regularization enter fundamentally. In the following section two, we prepare for the general theory by examining the inhomogeneous Dirichlet boundary value problem for both the steady non-equilibrium Poisson-Boltzmann equation and the steady Schrödinger-Hartree equation. These equations depend locally, and globally, respectively, upon the solution in assembling charge. The steady Schrödinger-Hartree equation possesses a convolution term, and is an example of the general reaction-diffusion equation studied here. We illustrate the variational theory by deriving a strong solution in each case, which is unique for the non-equilibrium Poisson-Boltzmann equation and, under certain circumstances, for the steady Schrödinger-Hartree equation. In section three, we examine further properties, including stability as governed by the implicit function theorem. These results carry over to the general results of sections four and five. The coupling to the implicit function theorem requires uniqueness for solutions of the linearized problem. An appendix provides documentation for the variational calculus, and also includes a discussion of the alternative approach using the Leray-Schauder theorem. This approach yields existence theorems with weaker hypotheses.

## 2 Examples: Boundary-Value Problems of Mathematical Physics

Prior to describing the general theory, we study two important examples, which illustrate the role of the hypotheses. Some new insights and connections beyond an existence/uniqueness analysis are developed in this and the following section. The first example is that of a locally defined reaction term and the second example that of a globally defined reaction term.

## 2.1 Unique strong solution of the Poisson-Boltzmann equation

In its original formulation, the Poisson-Boltzmann equation was derived as an equilibrium model of anions and cations in solution in a neutral state. Equilibrium has the technical meaning here of zero total ionic current. Neutrality has the meaning that the anion and cation densities balance each other at zero potential. When interpreted in the context of electrochemistry, equilibrium has the usual meaning that the electrochemical potentials are constant throughout the solution. The simplest form of the equation is the neutral version $\Delta u - c \sinh u = 0$, for some positive constant $c$. This equation is more than a century old, and has application to several fields [8, 10]. The model has been studied analytically in [25, Sec. 27.8] in the framework of monotone operator theory. The one-dimensional boundary-value problem has been studied via explicit solutions in [16]. Additional studies of weak solutions of the equilibrium Poisson-Boltzmann equation have appeared in the literature [12, Ex. 3.2.1]; a weak solution was derived by methods of convex analysis.

The non-equilibrium model emerged later, particularly as part of the Poisson-Nernst-Planck system (PNP). The monograph [17] provides a useful reference for the interpretation for electrophysiology. If Boltzmann statistics are employed in the PNP system, with two ionic species of opposite parity, the three unknown functions are the electrostatic potential, and the ionic electrochemical potentials. When the anions and cations are replaced by electrons and holes in solid state devices, the latter system is the basis for the drift-diffusion semiconductor system [13]. The semiconductor model has features of geometry and structure not shared by the electrochemistry model. In the semiconductor literature, the electrochemical potentials are referred to as quasi-Fermi levels.

We now present the steady, non-equilibrium model studied here. It allows for the possibility of spatially dependent ionic currents. Consider, for example, a chemical system of anions and cations in solution, with densities expressed by Boltzmann statistics, contained in a domain $\Omega$. We require single monovalent species of anions and cations. The representation of the charge density may be consolidated into the form $f(x, u) = c(x) \sinh(u)$ for a strictly positive function $c$ which is assumed to belong to $C(\bar{\Omega})$. This is a neutrality model, with electrochemical potentials of equal magnitude and opposite sign. The function $c$ is formed as an exponential multiplier derived from the electrochemical potentials. The reciprocal of the dielectric constant is included as a factor in $c$. Nonconstant currents are predicted by the model, easily expressed if $c$ is smooth. Inhomogeneous Dirichlet boundary conditions are also specified. We provide a formal definition of an appropriate boundary-value problem for the electrostatic potential, and a corresponding strong solution $u$ in $H^2(\Omega)$.

**Definition 2.1.** *The electrostatic potential $u$ will be required to satisfy $u \in H^2(\Omega)$ and to be a strong solution of the following potential equation:*

$$-\nabla^2 u + f(x, u) = 0. \tag{2}$$

*The sign reversal of $f$ is due to its lhs placement. Dirichlet boundary conditions are specified for $u$: For a fixed function $u_0 \in H^2(\Omega)$,*

$$\Gamma u = \text{bdy tr } u = \text{bdy tr } u_0 = \Gamma u_0. \tag{3}$$

We will analyze the example by positioning it within the framework described in the introduction.

The existence proof requires that the set of solutions of the regularized problem as defined below coincides with the solutions of the standard problem just defined. This is stated as Lemma 2.3.

Prior to introducing the regularization, we require the specification of an interval containing the range of $u$. If $\delta = \sup\{|\Gamma u_0(x)| : x \in \partial\Omega\}$, set $I_\delta = [-\delta, \delta]$. The subsequent theory will show that the range of $u$ lies in $I_\delta$ for a solution $u$. The regularization $\phi$ is incorporated into the definition of $T$, denoted $T_\phi$ in this case. We carry out the following steps.

1. Definition of $X, T_\phi, U$.
2. Properties of $T_\phi$, including minimizing sequences.
3. Surjectivity of its linearization $L$.

(1) The reflexive Banach space $X$ is identified with the Hilbert space $H^2(\Omega)$. Equivalent norms will be useful, particularly the norm identified in Lemma 2.1 to follow. The affine space $U$ is defined by the boundary trace of the definition. It can be characterized as the translate of the kernel of $\Gamma$ by $u_0$. The definition of $T_\phi$ depends upon a regularization, introduced to ensure the existence of a bounded minimizing sequence. Define

$$\Phi(\omega) = \begin{cases} 1, & |\omega| \le 1/2, \\ 1 - e^{-\frac{1}{\tan^2|\pi\omega/2|-1}}, & 1/2 < |\omega| < 1, \\ 0, & |\omega| \ge 1. \end{cases} \tag{4}$$

It is easily checked that $0 \le \Phi \in C_0^\infty(\mathbb{R})$, and $\Phi \equiv 1$ in $[-1/2, 1/2]$. For

$$\phi(y) = \Phi(y/(2\delta)), \tag{5}$$

define $T_\phi$ as follows. For $v \in U$,

$$T_\phi v = -\nabla^2 v + f(x, v\phi(v)). \tag{6}$$

- $T_\phi$ is well-defined from $U \subset H^2(\Omega)$ into $L^2(\Omega)$.

This follows since the composite operator defined by $f$ may be identified with a Nemytskii operator [25, Sec. 26.3], [18, 21]. Indeed, $f$ satisfies the continuity requirement and is at most of linear growth (in fact, bounded) because of the regularization, hence is $L^2$ continuous and locally bounded.

(2) Properties of $T_\phi$.

- $T_\phi$ maps every weakly convergent sequence in $H^2$ onto a weakly convergent sequence in $L^2$.

  To show this, we decompose $T_\phi$ into the sum of the Laplacian component $L_1$ and the component $L_2$ containing the composition with $f$. For linear operators, continuity is equivalent to weak continuity [24]. We consider the lower order component. By the compact embedding theorem, every weakly convergent sequence in $H^2$ is convergent in $L^2$. Strong convergence, and hence weak convergence, is implied by the Nemytskii property.

- Every minimizing sequence is bounded.

Suppose that $\{v_k\}$ is a minimizing sequence:

$$\lim_{k\to\infty} \|T_\phi v_k\|_{L^2} \to \alpha, \tag{7}$$

where

$$\alpha = \inf_{v\in U} \|T_\phi v\|_{L^2}. \tag{8}$$

Without loss of generality, we may assume that

$$\alpha \le \|T_\phi v_k\|_{L^2} \le \alpha + 1, \ \forall k. \tag{9}$$

We show that every such minimizing sequence is bounded in $H^2$. To do this, we make use of the following equivalent norm in $H^2$ (see the following Lemma 2.1):

$$\|h\|^2 = \|\nabla^2 h\|^2_{L^2} + \|\Gamma h\|^2_{W^{3/2,2}(\partial\Omega)}. \tag{10}$$

Since every member of the minimizing sequence is in $U$, and thus has a fixed boundary trace, it is enough to show that the Laplacian term is bounded. To do this, we isolate the Laplacian component of the sequence as follows.

$$\|\nabla^2 v_k\|_{L^2} \le \alpha + 1 + \|f(\cdot\,, \phi(v_k)v_k)\|_{L^2}. \tag{11}$$

The right hand side is bounded since the second argument of the function $f$ is evaluated on the fixed compact set $[-2\delta, 2\delta]$ , due to the cutoff function $\phi$.

It follows that there is a minimizer, $u$. We examine $T_\phi$ in order to show that $u$ solves the regularized problem.

- The mapping $T_\phi$ is continuously Fréchet differentiable on $H^2(\Omega)$.

It is enough [22] to show that $T_\phi$ is continuously Gâteaux differentiable. This involves two steps.

- $T'_\phi(v)$ exists as a bounded linear operator from $H^2$ to $L^2$ for each $v \in H^2$.
- $T'_\phi(v)$ is continuous in $v$ in the operator topology.

By implementing the definition of the Gâteaux derivative $T'_\phi(v) = L$, we obtain, for $f_u(x,u) = c(x)\cosh(u)$,

$$L\nu = -\nabla^2 \nu + f_u(\cdot\,, u\phi(u))[\nu\phi(u) + u\phi'(u)\nu]. \tag{12}$$

To prove that $L$ is bounded as stated, it suffices to show that

$$\|L\nu\|_{L^2} \leq C(u)\|\nu\|_{H^2},$$

where $C(u)$ is a positive constant depending on $u$. This is implied by the observation that the lower order component of $L$ has bounded multiplier coefficients.

In order to show that $T'_\phi$ is continuous, we must show that

$$\lim_{w \to v} \{ \sup_{\|\nu\|_{H^2} \leq 1} \|(L_w - L_v)\nu\|_{L^2} \} = 0. \tag{13}$$

Here, $L_v = T'_\phi(v), L_w = T'_\phi(w)$. Because the leading component of each derivative operator is linear, it suffices to examine the lower order component. The sequential equivalence of the limit allows a term by term analysis in the expansion of $(L_w - L_v)\nu$. The convergence of $w$ to $v$ in $H^2$ implies uniform convergence by the Sobolev embedding theorem. This uniform convergence is preserved under (uniformly) continuous composition by the derivative function. This establishes operator continuity.

- If $u$ is a minimizer, $L = L_u : U_0 \mapsto L^2$ is surjective.

We use a two step procedure. We first consider weak solutions, via the theory of pseudomonotone operators. By writing $L = L_1 + L_2$, where $L_1$ and $L_2$ act from $H^1_0$ to $H^{-1}$, we are able to identify $L$ as the strongly continuous perturbation of a monotone continuous operator, so that $L$ is a (bounded) pseudomonotone operator. Here, strongly continuous means that weakly convergent sequences are mapped onto convergent sequences. Also, $L$ is coercive since the lower order terms are uniformly bounded. These details are straightforward and detailed in Lemma 2.2 to follow. It follows that $Lv = h$, for $v \in H^1_0$ and given $h \in L^2$. We conclude that a weak solution exists.

For domains $\Omega$ considered here, the Poisson equation with homogeneous boundary conditions is uniquely solvable in $U_0 \subset H^2$ [9]. By again writing $L = L_1 + L_2$, where the term $L_1$ is the Laplacian component, we may solve uniquely for $w$, where $L_1 w = h - L_2 v$. A straightforward uniqueness argument allows us to conclude that $v = w$. Indeed, by subtraction, we obtain the weak solution for $w - v$ in terms of the Laplace equation with homogeneous boundary conditions. We conclude that $w - v = 0$, so that $v$ has the required regularity. Thus, $\alpha = 0$ and a solution of the *regularized* nonlinear boundary value problem exists. However, any solution of the regularized problem is a solution of the standard problem, and conversely. This is documented in Lemma 2.3 to follow. This concludes the existence analysis of the example.

**Lemma 2.1.** *An equivalent norm on $H^2$ is given by (10).*

*Proof.* We will use a conclusion of the open mapping theorem, since the standard norm dominates the norm defined by (10). It is sufficient to show that $H^2$ is complete with the norm given by (10). Thus, if $\{v_k\}$ is a Cauchy sequence in this norm, we conclude that $-\Delta v_k$ is Cauchy in $L^2$, with limit $y$. Furthermore, the trace sequence $\Gamma v_k = \sigma_k$ converges to $\sigma$ in $W^{3/2,2}(\partial\Omega)$. Completeness thus reduces to the unique solution of the Poisson equation for given $y, \sigma$. Let $\sigma_{\mathrm{e}}$ designate the extension, unique up to elements of the kernel of $\Gamma$, of $\sigma$ to an $H^2(\Omega)$ function. We first establish a weak solution of the Poisson boundary value problem, and then use PDE theory to argue for greater regularity. For the first part, we introduce a quadratic functional $Q(v)$, defined on a hyperplane $\mathcal{U}$, and establish a minimum for $Q$. Here, $\mathcal{U}$ is the translate by $\sigma_{\mathrm{e}}$ within $H^1$ of $H^1_0$, and $Q$ is the quadratic functional acting on $\mathcal{U}$ defined by

$$Q(v) = \int_\Omega |\nabla v|^2 \, dx - 2 \int_\Omega yv \, dx. \tag{14}$$

The minimization of $Q$ over $\mathcal{U}$ is represented as a convex, continuous minimization problem. These properties are evident. To see that $Q$ is coercive, write the decomposition of elements of $\mathcal{U}$ in terms of the the sum of $\sigma_{\mathrm{e}}$ and an element in $H^1_0$, then use the equivalent gradient seminorm. It follows from standard theory [5] that $Q$ has a minimizer. Standard arguments show that any minimizer is a weak solution in the sense defined by [9]. This is as far as variational calculus can take us. However, the regularity theory of PDE can now be invoked [9, Sec. 8.4] to bootstrap from $H^1$ regularity to $H^2$ regularity. □

**Lemma 2.2.** *Define the functional $L = L_1 + L_2 : H^1_0 \mapsto H^{-1}$, for $\nu \in H^1$, by*

$$\langle L_1 \nu, \psi \rangle = (\nabla \nu, \nabla \psi)_{L^2} \tag{15}$$

$$\langle L_2 \nu, \psi \rangle = (f_u(\cdot\,, u\phi(u))[\nu\phi(u) + u\phi'(u)\nu], \psi)_{L^2}. \tag{16}$$

*Then the following hold.*

1. *$L_1$ is monotone and continuous.*
2. *$L_2$ is strongly continuous.*
3. *$L$ is bounded and pseudomonotone.*
4. *$L$ is coercive.*

*In particular, $L$ is surjective in the weak sense.*

*Proof.* The conclusion that $L$ is surjective is proven in [25, Th. 27.A and Prop. 27.6]. We now verify the statements. Property (1) is routine. For property (2), we observe that, if a sequence is weakly convergent in $H^1_0$, it is strongly convergent in $L^2$. This is preserved under multiplication by bounded multipliers. As previously observed, the operator $L_2$ has the Nemytskii property. In particular, $L_2$ is strongly continuous. For (3), the pseudomonotone property is a standard result [25]. The boundedness of $L_1$ is immediate from the Schwarz inequality.

The boundedness of $L_2$ follows from the bounded multiplier property. We now verify coerciveness (4). Suppose $\|\nu\|_{H_0^1} \to \infty$. By absorbing the $L^2$ term involving $\nu$ into the gradient term, one bounds the $H_0^1$ norm from below by a constant. Coerciveness is immediate. □

**Lemma 2.3.** *The solution set for the regularized problem is exactly equal to that of the standard problem.*

*Proof.* The proof depends upon the fact that solutions of both problems satisfy the same weak maximum principle:

$$\|v\|_{L^\infty} \leq \delta. \tag{17}$$

We provide details in the case when $v$ satisfies the regularized equation; the other case is identical. Consider the weak formulation of the regularized equation with test functions $\psi_1 = (v-\delta)^+, \psi_2 = (v+\delta)^-$. These functions have zero boundary trace since the support of the boundary values is contained in $I_\delta = [-\delta, \delta]$. We claim that the test functions are zero. We show this as follows. If $\psi_1 = (v-\delta)^+$ is selected as test function, we have

$$0 = \int_\Omega |\nabla(v-\delta)^+|^2 \, dx + \int_\Omega f(x, v\phi(v))(v-\delta)^+ \, dx, \tag{18}$$

where both terms are nonnegative. For the second term, this is implied by the sign-preserving property of $f$ relative to its second argument: sinh is an odd function. For the first term, a standard formula has been used for the derivative of a Lipschitz function [9]. We conclude that $\psi_1 = 0$. The proof is similar to show that $\psi_2 = 0$. We have thus established the weak maximum principle for solutions of the regularized problem. It follows that $v\phi(v) = v$. The proof for the standard equation is identical. □

**Theorem 2.1.** *Existence and uniqueness hold for the Poisson-Boltzmann boundary-value problem as defined in Definition 2.1.*

*Proof.* Existence for the regularized problem has been demonstrated by the preceding arguments. Lemma 2.3 implies existence as defined in Definition 2.1. Uniqueness is obtained by a monotonicity argument applied to the integrated version of the boundary-value problem as given in Definition 2.1. By considering the difference $w$ of two possible solutions, one first concludes that $\Delta w = 0$, with the boundary trace of $w$ equal to zero. It follows that $w = 0$. □

## 2.2 The steady Schrödinger-Hartree equation in $\mathbb{R}^3$

This equation may be viewed as the steady form of the corresponding equation of density functional theory [23] when the correlation-exchange potential is assumed negligible. It describes a bounded quantum system of non-interacting electrons. The unknown orbital $\psi$ is real-valued here, since we impose real boundary values. It is a direct calculation to show that $\psi$ is real. We assume that $\psi$ is scalar-valued, but the argument generalizes to the multi-orbital case. We are not aware of any other analysis of this model as formulated here. Versions of the time-dependent model have been analyzed in [4] and [15].

**Definition 2.2.** *The orbital $\psi$ will be required to satisfy $\psi \in H^2(\Omega)$ and to be a strong solution of the following equation:*

$$-\nabla^2\psi + (W * |\psi|^2)\psi = 0. \tag{19}$$

*Here, $W$ is the potential, $W(x) = 1/|x|$. The electronic charge is the integral $\int_\Omega |\psi|^2 dx$, and the Hartree potential is the standard convolution, $W * |\psi|^2$. We have chosen units in which $\hbar^2/(2m) = 1$, where $m$ is the electron effective mass. Dirichlet boundary conditions are specified for $\psi$: For a fixed function $\psi_0 \in H^2(\Omega)$,*

$$\Gamma\psi = \text{bdy tr } \psi = \text{bdy tr } \psi_0 = \Gamma\psi_0. \tag{20}$$

The template for how to proceed has been established in the analysis of the previous example. The meaning of $X$ and $U$ is retained. As previously, regularization is employed. We define

$$T_\phi\omega = -\Delta\omega + W * (|\omega\phi(\omega)|^2)\omega\phi(\omega), \tag{21}$$

for $\omega \in U$. We establish the existence of a minimizer by showing that $T_\phi$ preserves weak convergence, and by deriving a bounded minimizing sequence.

- $T_\phi$ is weakly continuous

The Laplacian preserves weak convergence. The lower order part is written as the product of the Hartree potential $W * |\phi(\omega)\omega|^2$ and the term $\omega\phi(\omega)$. If $\omega_n \rightharpoonup \omega$ in $H^2$, the sequence converges strongly in $L^2$, and each of the sequences $W * |\phi(\omega_n)\omega_n|^2$ and $\omega_n\phi(\omega_n)$ is strongly convergent in $L^2$. This is due to the Nemytskii property associated with $\phi(\omega_n)\omega_n$, so that this sequence is $L^2$ convergent; Young's inequality propagates this convergence to the Hartree potential sequence. Both sequences are pointwise bounded. It follows [14] that the product converges weakly in $L^2$.

- Every minimizing sequence is bounded.

The approach of the previous example is effective here also. One uses the equivalent $H^2$ norm, so that it suffices to bound the Laplacian. By design, the lower order terms are pointwise bounded, hence bounded in $L^2$. An argument similar to that for the preceding example then gives the bound for the Laplacian.

- The Gâteaux derivative and the Fréchet derivative

The Gâteaux derivative of $T_\phi$, which is a directional derivative with respect to an arbitrary function $\chi \in H^2$, is computed by direct use of the rules of differentiation, including the derivative of integrals with respect to a parameter. One obtains for the derivative operator $L = T'_\phi(\omega)$ at $\omega \in H^2$:

$$L\chi = -\Delta\chi + W * |\omega\phi(\omega)|^2[\omega\phi'(\omega)\chi + \phi(\omega)\chi] + 2\omega W * (\omega\phi(\omega)[\omega\phi'(\omega)\chi + \phi(\omega)\chi]). \tag{22}$$

We observe that $L$ is a bounded linear operator from $H^2$ to $L^2$. Indeed, it acts as a two-part perturbation of the Laplacian. The perturbation analysis is assisted by the standard convolution inequality,

$$\|W * h\|_{L^\infty} \leq \|W\|_{L^1} \|h\|_{L^\infty}, \tag{23}$$

which is derived as the limiting version of Young's inequality. Here, the $L^1$ norm of $W$ is computed on a closed ball, centered at the origin, of radius equal to the diameter of $\Omega$. By use of the inequality, one sees that one part of the perturbation involves $\chi$ multiplied by a pointwise bounded product. For the other part, notice that $\omega$ is a bounded multiplier and that the convolution is computed of $\chi$ with a bounded multiplier. The convolution inequality may be used to infer a bound in terms of $\chi$.

The uniform operator continuity of the derivative depends on the corresponding properties of the perturbation of the Laplacian. We hold $\chi$ and $\omega$ fixed, and allow $\xi \to \omega$. Consider the $L^2$ estimation of $(T'_\phi(\xi) - T'_\phi(\omega))(\chi)$. Since similar methods are used in a term by term analysis, for brevity, we select one such term for a detailed analysis. Specifically, we estimate

$$E(\omega, \xi) := W * |\xi\phi(\xi)|^2 [\xi\phi'(\xi)]\chi - W * |\omega\phi(\omega)|^2 [\omega\phi'(\omega)]\chi \tag{24}$$

by the following standard method:

$$E = E_1 + E_2, \tag{25}$$

where

$$\begin{aligned} E_1 &:= W * |\xi\phi(\xi)|^2 [\xi\phi'(\xi)\chi] &-& \quad W * |\xi\phi(\xi)|^2 [\omega\phi'(\omega)\chi] \\ E_2 &:= W * |\xi\phi(\xi)|^2 [\omega\phi'(\omega)\chi] &-& \quad W * |\omega\phi(\omega)|^2 [\omega\phi'(\omega)\chi]. \end{aligned} \tag{26}$$

We can obtain $L^\infty$ estimates for both $E_1$ and $E_2$ which imply the desired $L^2$ estimates. One requires the standard convolution inequality (23). One obtains

$$\|E_1\|_{L^\infty} \leq \|W * |\xi\phi(\xi)|^2\|_{L^\infty} \|\xi\phi'(\xi) - \omega\phi'(\omega)\|_{L^\infty} \|\chi\|_{L^\infty}. \tag{27}$$

We now make use of the continuous embedding of $H^2$ into $C(\bar{\Omega})$. For continuity purposes, we may assume that $\xi$ is in a bounded neighborhood of $\omega$. In particular, as $\xi \to \omega$, the convolution term remains bounded, and $\|\xi\phi'(\xi) - \omega\phi'(\omega)\|_{L^\infty} \to 0$. This completes the analysis of $E_1$.

The principal term in the estimation of $E_2$ is the convolution difference term. After some simplification, we have for the convolution difference:

$$\|W * [|\xi\phi(\xi)|^2 - |\omega\phi(\omega)|^2]\|_{L^\infty}. \tag{28}$$

Within the convolution, one expresses the difference of squares as a factored product $hg$, with $h = |\xi\phi(\xi)| - |\omega\phi(\omega)|$ and $g = |\xi\phi(\xi)| + |\omega\phi(\omega)|$. By the Sobolev embedding theorem referenced earlier, convergence in $H^2$ implies uniform convergence of the expression $h$ to 0. All other terms, including $g$ remain uniformly bounded. This completes the analysis for $E_2$.

- Denote a minimizer by $\psi$. Then

$$L\chi = T'_{\phi}(\psi)\chi = g \tag{29}$$

has a solution $\chi \in U_0, \forall g \in L^2$.

The proof follows that of the surjectivity analysis for the Poisson-Boltzmann equation. Specifically, the conditions of Lemma 2.2 are satisfied. Inequality (23) is used in a fundamental way. Since the reaction term of the Schrödinger-Hartree equation is sign-preserving in its second argument, we may apply Lemma 2.3 to obtain the following.

**Theorem 2.2.** *Existence holds for the steady Schrödinger-Hartree boundary-value problem. Uniqueness holds under the conditions of Corollary 4.1 to follow.*

# 3 Further Properties of the Examples: Stability

In section five, we will examine the application of the implicit function theorem to verify the stability of the solution dependence upon perturbations of the rhs of the given reaction-diffusion equation in the general case. The purpose of the present section is to illustrate how this is carried out for the Poisson-Boltzmann equation. It is seen as providing additional clarity for the results of section five. We define the appropriate mappings in the next section for both the Poisson-Boltzmann and Schrödinger-Hartree equations. As described later in the article, the implicit function theorem can be applied to the Schrödinger-Hartree equation when uniqueness holds. Here, we restrict consideration in section 3.2 to the Poisson-Boltzmann equation since no further hypotheses are required.

## 3.1 Reformulation without regularization

We define the reformulations as follows.

**Definition 3.1.** *The Poisson-Boltzmann mapping* $T_{\mathrm{PB}}$ *is given as*

$$T_{\mathrm{PB}}\, v = -\Delta v + f(\cdot\,, v), \quad v \in H^2(\Omega). \tag{30}$$

*The steady Schrödinger-Hartree mapping* $T_{\mathrm{SH}}$ *is given as*

$$T_{\mathrm{SH}}\, \omega = -\Delta\omega + (W * |\omega|^2)\omega, \;\; \omega \in H^2(\Omega). \tag{31}$$

*Here,* $f(x,u) = c(x)\sinh(x)$ *in (30) and* $W(x) = 1/|x|$ *in (31), with* $N = 3$.

**Theorem 3.1.** *The following statements are valid.*

1. *For* $T = T_{\mathrm{PB}}$ *and* $T = T_{\mathrm{SH}}$ *,*

$$\alpha = \min\{\|Tx\| : x \in U\} = 0. \tag{32}$$

*When uniqueness holds, the minimum is uniquely attained by the solution of the corresponding boundary-value problem.*

2. *The mappings $T_{\rm PB}$ and $T_{\rm SH}$ are continuously Fréchet differentiable on $H^2$. They are given explicitly by:*

$$
\begin{aligned}
{T_{\rm PB}}'(v)(\eta) &= -\Delta\eta + f_u(\cdot\,, v)\eta, \quad v, \eta \in H^2, && (33)\\
{T_{\rm SH}}'(\omega)(\chi) &= -\Delta\chi + 2W * (\omega\chi)\omega + (W * |\omega|^2)\chi, \;\; \omega, \chi \in H^2. && (34)
\end{aligned}
$$

3. *For $T = T_{\rm PB}$ and $T = T_{\rm SH}$ , the derivative mappings at the respective solutions of the boundary-value problems are bijective (resp. surjective), as linear mappings of $U_0$ into $L^2$.*

*Proof.* The first statement follows from Theorems 2.1 and 2.2, resp. The second statement uses the direct representations of $T'_{\rm PB}$ and $T'_{\rm SH}$ , obtained by standard directional differentiation. However, to complete the argument, it must be shown that the stated formulas define bounded linear operators, and that uniform operator continuity holds. The first of these properties depends upon the Sobolev embedding theorem into $C(\bar{\Omega})$. As a result, the multipliers of the lower order terms are pointwise bounded for both examples. An argument for the uniform operator continuity can be constructed along the lines of the case of $T'_\phi$ in the previous sections. As is evident, the analysis is simpler here. For the Poisson-Boltzmann example, one uses the uniform continuity in the second argument of the function $f_u(x, u) = c(x)\cosh(u)$ on compact sets to examine the lower order term. This reduction is due to the local nature of continuity, and the embedding theorem. For the steady Schrödinger-Hartree example, the inequality (23) is used. The details are similar to those of the earlier analysis.

For the third statement, we observe that surjectivity is incorporated into the existence analysis of the variational method; in other words, previous arguments apply. The injectivity of the linearized Poisson-Boltzmann mapping is a consequence of the monotonicity of $f$ in its second argument. This implies that the difference of any two solutions is a harmonic function with vanishing boundary values, hence is zero. □

## 3.2 Solution sets: The implicit function theorem

The operator calculus naturally leads to possible applications of the implicit function theorem in Hilbert space In the Poisson-Boltzmann model, we consider small perturbations in the permanent charge, taken as zero in the model as defined. These perturbations are denoted by $h$. The implicit function theorem is designed to cover this in terms of a continuous solution result. Note that this is much stronger than an existence result. We do not consider perturbations of the boundary condition. More precisely, we require that the solution set, depending locally on $h$, remain in the hyperplane $U$ which is the translate of the zero trace subspace $U_0$ of $H^2$. A precise statement of the implicit function theorem may be found in [24, Theorem 4.B, p. 150]i (see also Theorem A.3 of the appendix). In order to align our framework with the classical theory, we formulate the following.

**Definition 3.2.** *Designate by $u$ the unique solution of the Poisson-Boltzmann boundary-value problem, and define $w_0 = u - u_0$. Set*

$$\mathcal{H} = L^2 \times U_0, \tag{35}$$

*and $S : \mathcal{H} \to L^2$ by*

$$S(h, w) = T_{\mathrm{PB}}\,(w + u_0) - h. \tag{36}$$

**Lemma 3.1.** *$S$ satisfies the following properties.*

1. *$S(0, w_0) = 0$, and $S$ is continuous at $(0, w_0)$. In fact, $S$ is continuous on $\mathcal{H}$.*
2. *The derivative $S_w$ of $S$ with respect to $w$ exists on $\mathcal{H}$ and is continuous at $(0, w_0)$.*
3. *$S_w(0, w_0)$ is bijective from $U_0$ to $L^2$.*

*Proof.* Each of these properties is a slight extension of previously derived results. This is due to the way in which $h$ enters into the definition of $S$. □

We now have established a framework for the stability result.

**Proposition 3.1.** *The boundary-value problem for the Poisson-Boltzmann equation is consistent and stable. In the hyperplane $U$ in $H^2$, there is a local continuous solution, $u(h)$, with $u(0) = u$, for the equation,*

$$T_{\mathrm{PB}} u(h) = h. \tag{37}$$

*Here, $h$ is in a closed $L^2$-ball $\mathcal{B}$, centered at the origin.*

*Proof.* The preceding lemma 3.1 provides the necessary hypotheses required for an application of the implicit function theorem, given as Theorem A.3 in the appendix. Notice that $S_w$ can be identified with the derivative of $T_{\mathrm{PB}}$. The definition of $S$ in terms of $T$ yields the result. □

A similar result holds for the steady Schrödinger-Hartree equation when the condition for uniqueness holds, as specified in Corollary 4.1.

# 4 Generalized Reaction-Diffusion Equations

The traditional understanding of reaction-diffusion equations or systems has been to identify the so-called vector fields as acting locally, as in the case of the Poisson-Boltzmann equation. However, as the steady Schrödinger-Hartree equation indicates, the reaction terms may act globally. Any quantum mechanical model exhibits this global behavior. A theory is outlined here which includes both possibilities.

## 4.1 Existence and uniqueness

We maintain the assumption of a $C^2$ bounded domain in $\mathbb{R}^N, N = 1, 2, 3$. We consider the following.

**Definition 4.1.** *We define two categories of boundary-value problems, depending on locally and globally defined reaction terms.*

1. *The local reaction term $\mathcal{F}_\ell$ satisfies*

$$\mathcal{F}_\ell(u) = F(x, u) = \sum_{j=1}^{J} a_j(x) f_j(u), \tag{38}$$

   *where $0 \le a_j \in C(\bar{\Omega}), j = 1, \dots, J$, and $f_j \in C^1, j = 1, \dots, J$.*

2. *The global reaction term $\mathcal{F}_g$ satisfies*

$$\mathcal{F}_g = \mathcal{L}(g(u))u, \tag{39}$$

   *where $\mathcal{L}$ is a positive continuous linear operator on $C(\bar{\Omega})$ and $g$ has continuous directional derivatives on $H^2$ with range in $C(\bar{\Omega})$.*

*Consider the boundary value problem:*

$$-\nabla^2 u + \mathcal{F}(u) = 0, \tag{40}$$

*where $\mathcal{F}$ assumes either the local or global form. As previously, for a fixed function $u_0 \in H^2(\Omega)$, we require*

$$\Gamma u = \text{bdy tr } u = \text{bdy tr } u_0 = \Gamma u_0. \tag{41}$$

*Finally, we set $\delta = \sup\{|\Gamma u_0(x)| : x \in \partial\Omega\}$.*

**Definition 4.2.** *The interval $I_\delta = [-\delta, \delta]$, containing the support of the boundary data, is called invariant for $\mathcal{F}_\ell$ if, for the real variable $u$, $F(x, u) \ge 0$ (resp. $\le 0$) whenever $u \ge 0$ (resp. $u \le 0$), for all $x \in \bar{\Omega}$. It is invariant for $\mathcal{F}_g$ if $g$ is nonnegatively valued.*

**Theorem 4.1** (Existence)**.** *Consider the boundary value problem of Definition 4.1. If $I_\delta$ is an invariant interval for $\mathcal{F}$, then a solution exists in $U$ in both cases.*

*Proof.* As was the case for each of the two examples, we make the replacement $u \to u\phi(u)$ in the reaction term, and define

$$T_\phi(u) = -\Delta u + \mathcal{F}(u\phi(u)). \tag{42}$$

$U_0$ and $U$ are defined as previously. Since the lower order part is a Nemytskii operator with a pointwise bounded range, we conclude that $T_\phi$ is weakly continuous and possesses a bounded minimizing sequence. For the latter, we use the equivalent norm given by Lemma 2.1. The details here closely follow the corresponding analysis of the Poisson-Boltzmann equation with the replacement $f(\cdot\,,u) \mapsto F(\cdot\,,u)$, and the steady Schrödinger-Hartree equation with the replacement $W * (|u|^2)u \mapsto \mathcal{L}(g(u))u$. Notice that the hypotheses on $\mathcal{L}$ and $g$ are intended to generalize the use of the inequality (23). It follows then that a minimizer exists for the extremal problem,

$$\alpha = \min\{\|T_\phi v\| : v \in U\}. \tag{43}$$

We demonstrate, as previously, that $\alpha = 0$. This requires the continuous differentiability of $T_\phi$ and the surjectivity of the linear operator,

$$L(v) = T'_\phi(v) : U_0 \mapsto L^2, \tag{44}$$

if $v = u$ is a minimizer. The formal representations are straightforward:

$$L\eta = -\Delta\eta + F_u(\cdot\,, v\phi(v))[\phi(v)\eta + v\phi'(v)\eta], \tag{45}$$

for $\mathcal{F} = \mathcal{F}_\ell$, where $F_u$ denotes differentiation in the second argument, and

$$L\eta = -\Delta\eta + \mathcal{L}g(v\phi(v))[v\phi'(v)\eta + \phi(v)\eta] + v\mathcal{L}(g'(v\phi(v))[v\phi'(v)\eta + \phi(v)\eta]) \tag{46}$$

for $\mathcal{F} = \mathcal{F}_g$. Here, $g'$ is the classical derivative.

Note that in each case, the lower order parts of the representations are continuous and pointwise bounded as real functions. Therefore, they are Nemytskii operators on $L^2$, and it follows that the directional derivatives exist as bounded operators from $H^2$ to $L^2$. Uniform operator continuity in the variable $v$ requires a term-by-term analysis, as discussed for the proofs of the examples. Since the same analysis applies here, we shall not repeat it. Continuous Fréchet differentiability is the result.

Lemma 2.2 is designed to verify the required surjectivity. It follows that the regularized problem is solvable. Finally, Lemma 2.3 is valid here due to the sign-preserving property built into the invariant interval hypothesis. This implies that the solution set for the regularized problem is the same as for the original problem. □

**Remark 4.1.** *There are uniqueness results which hold for both cases under certain assumptions. Both involve comparisons with the smallest eigenvalue of the Laplacian. We present them in turn, The abbreviations LRT (resp. GRT) represent local (resp. global) reaction terms. An essential fact for the proofs is the property that any solution satisfying Definition 4.1 must have range in $I_\delta$ if the latter is an invariant interval containing the range of the boundary data.*

**Proposition 4.1** (Uniqueness: LRT)**.** *Define $\delta$ as previously, and set $A = \max_{x\in\bar{\Omega}, j=1,\dots,J} a_j(x)$. If $\frac{df_j}{dy}$ is decomposed as $\frac{df_j}{dy} = (\frac{df_j}{dy})^+ - (\frac{df_j}{dy})^-$, set*

$$\theta = A \max_{y\in I_\delta} \sum_{j=1}^{J} |(df_j/dy(y))^-|. \tag{47}$$

*If the smallest eigenvalue of $-\Delta$ as a self-adjoint operator on $U_0 \subset L^2$ is denoted $\lambda_1$, then the solution for the local problem is unique if $\lambda_1 > \theta$.*

*Proof.* Suppose that $u$ and $v$ are solutions of the local system with $\mathcal{F} = F$, and set $w = u - v$. Note that $w \in U_0$. For notational purposes denote by $\Omega_-$ the set on which $F(\cdot\,, u) - F(\cdot\,, v)$ and $(u - v)$ are oppositely signed. By the mean value theorem, it follows that

$$\begin{aligned} 0 &= \int_\Omega (-\Delta(u-v))(u-v)\,dx + \int_\Omega (F(\cdot\,,u) - F(\cdot\,,v))(u-v)\,dx \\ &\geq \int_\Omega (-\Delta(u-v))(u-v)\,dx - \theta \int_{\Omega_-} (u-v)(u-v)\,dx \\ &\geq \lambda_1 \|u-v\|_{L^2}^2 - \theta \|u-v\|_{L^2}^2 \geq 0. \end{aligned} \tag{48}$$

Here, we have used the property of subadditivity for the operation of taking the negative part, as applied to the sum defining $F$. It follows that $(\lambda_1 - \theta)\|w\|_{L^2}^2 = 0$ so that $w = 0$. □

**Proposition 4.2** (Uniqueness: GRT)**.** *Define $\delta$ as previously, and consider the restriction of $g$ to $I_\delta$. Set $\tau = \max_{y \in I_\delta} |g'(y)|$. In addition to the assumptions previously stated for $\mathcal{L}$ and $g$ in Definition 4.1, assume:*

1. *$\mathcal{L}$ is a bounded linear operator on $L^2$.*
2. *$\mathcal{L}g(u) \geq 0$ for $u \in C(\bar{\Omega})$.*

*Then the solution is unique if*

$$\lambda_1 > \|\mathcal{L}\|_{L^2} \tau \delta. \tag{49}$$

*Proof.* We begin as in the previous proof. Suppose that $u$ and $v$ are solutions of the global system with $\mathcal{F}(u) = (\mathcal{L}g(u))u$, and set $w = u - v$. Note that $w \in U_0$.

$$\begin{aligned} 0 &= \int_\Omega (-\Delta(u-v))(u-v)\,dx + \int_\Omega (\mathcal{F}(u) - \mathcal{F}(v))(u-v)\,dx \\ &= \int_\Omega (-\Delta(u-v))(u-v)\,dx + \int_\Omega (\mathcal{L}g(u))(u-v)^2\,dx \\ &+ \int_\Omega (\mathcal{L}g(u) - \mathcal{L}g(v))v(u-v)\,dx \\ &\geq \int_\Omega (-\Delta(u-v))(u-v)\,dx - \int_\Omega |\mathcal{L}g(u) - \mathcal{L}g(v)|\,|v|\,|u-v|\,dx \\ &\geq \int_\Omega (-\Delta(u-v))(u-v)\,dx - \|\mathcal{L}\|_{L^2}\delta\|g(u) - g(v)\|_{L^2}\|u-v\|_{L^2} \\ &\geq \lambda_1\|u-v\|_{L^2}^2 - \|\mathcal{L}\|_{L^2}\delta\tau\|u-v\|_{L^2}^2 \\ &\geq 0. \end{aligned} \tag{50}$$

Here we have used the hypothesis (49). □

**Corollary 4.1.** *The solution of the steady Schrödinger-Hartree boundary value problem is unique if the boundary data are sufficiently small. More precisely uniqueness holds if*

$$\delta < \sqrt{\frac{\lambda_1}{2\|W\|_{L^1}}}. \tag{51}$$

*Proof.* If we define $\mathcal{L}(h) = W * h$, and $g(u) = |u|^2$, then we retrieve the steady Schrödinger-Hartree boundary value problem. The substitutions,

$$\|\mathcal{L}\|_{L^2} \leq \|W\|_{L^1}, g'(\mu) = 2\mu, \tag{52}$$

give the result when the proposition is applied. □

## 4.2 Convergence of approximations

Least squares methods for linear problems are well established in the literature. This includes the field of linear elliptic boundary-value problems, and finite element approximation procedures. Beginning in [2], J.H. Bramble and his collaborators have studied these methods over several decades, including applications to linear elasticity and electromagnetism. Although the work is too extensive to be cited here, it confirms the viability of the method. We are not aware of any systematic study for a nonlinear approximation theory. The following proposition is a step in that direction.

Suppose that $\{\mathcal{P}_n\}$ and $\{\mathcal{Q}_n\}$ are given sequences of finite dimensional approximation spaces with the properties that their unions are dense in $H^2$ and $U_0 \subset H^2$, respectively. We have the following.

**Proposition 4.3.** *In both cases of Definition 4.2 when uniqueness holds, we have the following. Included are the examples discussed earlier. If*

$$\alpha_n = \inf\{\|T_\phi(P_n u_0 + q_n)\| : q_n \in \mathcal{Q}_n\}, \tag{53}$$

*then the infimum is assumed for each $n$ by an approximation $u_n$, and the sequence $\alpha_n$ converges to zero. Also, $u_n \to u$ in $H^2$.*

*Proof.* The existence of a minimizer $u_n$ follows the argument for $u$ itself. We now argue that $\alpha_n \to 0$. Indeed,

$$\alpha_n \leq \alpha_n' = \|T_\phi u_n'\|, \tag{54}$$

where $u_n' = P_n u + Q_n u$. Since $u_n' \to u$, it follows by continuity that $\alpha_n' \to 0$. The squeeze lemma implies the result.

In order to prove $H^2$ convergence, We show that any subsequence $\{u_k\}$ of $\{u_n\}$ has a further subsequence $\{u_{k_j}\}$ which converges to $u$ in $H^2$. We will make use of the equivalent norm in $H^2$. By the earlier part of the proof,

$$T_\phi u_k \to 0, \text{ in } L^2, \tag{55}$$

so that this sequence is bounded in $L^2$. If $L_2$ denotes the lower order operator part of $T_\phi$, then $L_2 u_k$ is bounded in $L^2$ by the use of the regularization. It follows that the Laplacian sequence $-\Delta u_k$ is also bounded. Recall that the sequence $\{u_k\}$ has boundary trace which defines a bounded sequence in $W^{3/2,2}(\partial\Omega)$, so that $\{u_k\}$ is bounded in $H^2$. It follows that there is a weakly convergent subsequence, $\{u_{k_j}\}$, with weak limit $u^*$ in $H^2$. Thus, $-\Delta u_{k_j}$ is weakly convergent in $L^2$ to $-\Delta u^*$. However, this convergence is actually $L^2$ convergence. Indeed, we can exhibit the terms of this sequence algebraically as the difference of two strongly convergent sequences: $T_\phi u_{k_j}$ and $L_2(u_{k_j})$. The latter convergence is a consequence of the compact embedding, coupled with the Nemytskii property of the lower order term. Altogether, by use of Lemma 2.1 and the trace convergence, we conclude that $u_{k_j}$ converges to $u^*$ in $H^2$. By use of the continuity of $T_\phi$ and the uniqueness of limits it follows that $T_\phi(u^*) = 0$, so that $u^*$ is a solution of the boundary value problem. By uniqueness, $u^* = u$. We conclude that $u_{k_j}$ converges to $u$ in $H^2$. This completes the proof. □

# 5 Stability and the Implicit Function Theorem

The usual interpretation of a well-posed problem, dating at least to Hadamard, is the continuous dependence of a unique solution with respect to parameters. In this article, we study solution stability with respect to perturbations of the rhs of the reaction-diffusion equation around zero.

We begin with a remark concerning the relevant mappings and their Fréchet derivative expressions when computed at a solution.

**Remark 5.1.** *At a solution $u$, $T_\phi$ reduces to $T$, where*

$$Tv = -\Delta v + \mathcal{F}(v), \tag{56}$$

*and $\mathcal{F}$ may assume either of the two forms (38) or (39). Similarly, in the cases when the Fréchet derivative $L = T'(u)$ is computed at a solution $u$, we have the following simplified expressions.*

$$L\eta = -\Delta\eta + F_v(\cdot\,, u)\eta \tag{57}$$

*for $\mathcal{F} = \mathcal{F}_\ell$, where $F_v$ denotes the derivative with respect to the second argument, and*

$$L\eta = -\Delta\eta + \mathcal{L}(g(u))\eta + u\mathcal{L}(g'(u)\eta) \tag{58}$$

*for $\mathcal{F} = \mathcal{F}_g$, where $g'$ is the classical derivative.*

The following proposition gives sufficient conditions for the uniqueness of the linearized problems at the solutions. In each case, the conditions are crucial for the application of the implicit function theorem used to infer stability.

**Proposition 5.1.** *Suppose that the hypothesis on $\theta$ in Proposition 4.1 holds. Then, for the case $\mathcal{F} = \mathcal{F}_\ell$, the solution of $L\eta = \chi, \eta \in U_0$, is unique. Suppose that hypotheses (1) and (2) of Proposition 4.2 hold. Then, for the case $\mathcal{F} = \mathcal{F}_g$, the solution of $L\eta = \chi, \eta \in U_0$, is unique.*

*Proof.* Consider the case $\mathcal{F} = \mathcal{F}_\ell$. Suppose that $L\omega = 0$, We must show that $\omega = 0$. One has:

$$\begin{aligned} 0 &= \int_\Omega (-\Delta\omega)\omega \, dx + \int_\Omega F_u(\cdot\,, u)\omega^2 \, dx \\ &\geq \int_\Omega (-\Delta\omega)\omega \, dx - \theta \int_\Omega \omega^2 \, dx \geq 0. \end{aligned} \tag{59}$$

As seen previously, this implies $\omega = 0$, since $\theta < \lambda_1$.

Consider the case $\mathcal{F} = \mathcal{F}_g$. Suppose that $L\omega = 0$. Thus,

$$\begin{aligned} 0 &= \int_\Omega (-\Delta\omega)\omega \, dx + \int_\Omega (\mathcal{L}g(u))\omega^2 \, dx + \int_\Omega u\mathcal{L}(g\prime(u)\omega)\omega \, dx \\ &\geq \int_\Omega (-\Delta\omega)\omega \, dx + \int_\Omega u\mathcal{L}(g\prime(u)\omega)\omega \, dx \\ &\geq \int_\Omega (-\Delta\omega)\omega \, dx - \int_\Omega |u| \, |\mathcal{L}(g\prime(u)\omega)| \, |\omega| \, dx \\ &\geq \lambda_1 \|\omega\|_{L^2}^2 - \|\mathcal{L}\|_{L^2} \delta\tau \|\omega\|_{L^2}^2 \\ &\geq 0. \end{aligned} \tag{60}$$

We conclude that $\omega = 0$ and that uniqueness holds. $\square$

We now consider the use of the implicit function theorem in the study of stability. This generalizes the earlier results of section three. The following definition sets the classical framework.

**Definition 5.1.** *Set*

$$\mathcal{H} = L^2 \times U_0, \tag{61}$$

*and define* $S : \mathcal{H} \to L^2$ *by*

$$S(h, w) = T(w + u_0) - h. \tag{62}$$

We have the following result.

**Theorem 5.1.** *Consider the boundary-value problem,*

$$-\nabla^2 u(h) + \mathcal{F}(u(h)) = h, \; u \in U. \tag{63}$$

*Under the existence hypotheses as specified in Theorem 4.1, and the uniqueness hypotheses of this section, as specified in Proposition 5.1, there is a local solution set depending continuously upon $h$. In particular, the boundary-value problem defined in Definition 4.1 is stable around zero in terms of a local continuous solution set $u(h)$.*

*Proof.* The bijective property of the linear mapping $T'(u)$ has been established in Proposition 5.1 and in the existence analysis. This may be reinterpreted in terms of the mapping $S$. Lemma 3.1 indicates the remaining properties of $S$, and by extension $T$, required for an application of the implicit function theorem (Theorem A.3). These properties are based on slight variants of the existence analysis. $\square$

## 6 Summary Remarks

As mentioned in the introduction, nonlinear functional analysis had developed in the 1960s to a level of mathematical maturity which allowed researchers to derive significant applications to the field of nonlinear partial differential equations. These studies continued well into the 1970s. Although the monograph [7] was principally directed toward the intersection of optimization and approximation theory, with special emphasis on spline functions, some of the tools developed there are applicable to differential equations and least squares methods. These results are derived in chapters 1–3. The chief limitation is the assumption of a bounded minimizing sequence. When this is established, a version of the classical approach of the calculus of variations is possible, through the identification of a minimizer. If the linearized problem is solvable, the minimizer is identified with a solution of the original operator equation.

In order to overcome the severity of the hypothesis of a bounded minimizing sequence, a regularization is introduced, which permits an estimation separation between higher and lower order terms. In the application to boundary-value problems, the existence of an invariant interval allows the minimizer of the regularized problem to be identified with the classical solution.

The article addresses issues of existence, uniqueness, approximation, and stability of solutions of reaction-diffusion boundary-value problems. A novelty of the theory is the inclusion of equations containing a reaction term with global dependence on the solution. This is in the spirit of quantum mechanics. The steady Schrödinger-Hartree equation is studied as an example.

There are two features of the least squares approximation theory introduced here. One is the generality of the approximation spaces. The other is the fact that the approximations, although defined by equations including the regularization, converge to the unique strong solution.

If one is interested only in the existence of solutions, the Leray-Schauder theorem requires fewer hypotheses. We will discuss this in the appendix. However, even in this case, the analysis is facilitated by the regularization. Our goal is broader, and includes stability and approximation. However, the alternate approach, making use of fixed point theory, and using numerical fixed points, is the so-called Krasnosel'skii calculus [19], which requires operator differentiation. In this sense, the assumptions of the two approaches are comparable.

The uniqueness results allow for departure from monotonicity in the reaction terms, as measured relative to the smallest eigenvalue of the Laplacian. In particular, it allows for a precise statement in the case of a globally dependent reaction term. As presented here, the uniqueness is tied to the approximation results. Moreover, the theory allows for small negative nonlinear perturbations of the Poisson-Boltzmann charge distribution.

Definition 4.2 describes an invariant interval. It plays a fundamental role in the article because the range of the solution is contained in the invariant interval provided the latter contains the range of the boundary values.

Among the open problems are the weakening of the hypothesis of a smoothly bounded domain and the extension from equations to systems.

# A Appendix

## A.1 Calculus of variations

We begin with a precise discussion of the underlying theory. The first result is a special case of [11, Th. 2].

**Theorem A.1.** *Suppose that $X$ is a reflexive Banach space, $Y$ is a normed linear space, and $U_0$ is a closed subspace of $X$. Suppose that $U$ is the translate of $U_0$ by a fixed element $u_0$ of $X$, and that*

$$T : U \mapsto Y, \tag{64}$$

*satisfies the following two conditions.*

1. *$T$ is weakly continuous: if $v_k \rightharpoonup v$, then $Tv_k \rightharpoonup Tv$.*
2. *If*
$$\alpha = \inf\{\|Tv\| : v \in U\}, \tag{65}$$
*there is a bounded sequence $\{v_k\}$ such that $\|Tv_k\| \to \alpha$.*

*Then there is a minimizer $u$:*

$$\alpha = \|Tu\|. \tag{66}$$

The next result provides a sufficient condition for the minimizer to be a solution of the appropriate equation. This is a special case of [7, Theorem 3.1].

**Theorem A.2.** *Let $T$ be a continuous, Fréchet differentiable mapping from a Banach space $X$ into $L^p(\Omega)$, for $1 < p < \infty$. Let $U_0, U, \alpha$, be defined as in the previous theorem and suppose a minimizer $u$ exists. If the linear operator $L = T'(u)$ satisfies $LU_0$ is closed, then the following holds. There is a function $g \in L^q$, with $1/p + 1/q = 1$, such that:*

1. *$\int_\Omega gf \, dx = 0, \forall f \in U_0$,*
2. *$\alpha = \int_\Omega gTu \, dx$.*

*In particular, if $LU_0 = L^p$, then $\alpha = 0$ and $Tu = 0$.*

## A.2 Implicit function theorem

The following theorem represents the part of [24, Th. 4.B] which has been used in this article, viz. , statements (a) and (c). The notation here adapts the result to the current article.

**Theorem A.3.** *Suppose that:*

1. *$X, Y, Z$ are Banach spaces, $(x_0, y_0) \in X \times Y$, $\mathcal{O}$ is an open neighborhood of $(x_0, y_0)$,and $S : \mathcal{O} \mapsto Z$ satisfies*
$$S(x_0, y_0) = 0. \tag{67}$$

2. *The partial derivative operator $S_y$ exists as a Fréchet derivative on $\mathcal{O}$, and the linear operator $S_y(x_0, y_0)$ is bijective.*

3. *$S$ and $S_y$ are continuous at $(x_0, y_0)$.*

*Then the following hold.*

(a) *Existence and uniqueness: There exist positive numbers $r_0$ and $r$ such that, for every $x \in X$ satisfying $\|x - x_0\| \leq r_0$, there is exactly one $y(x) \in Y$ satisfying $\|y(x) - y_0\| \leq r$ and $S(x, y(x)) = 0$.*

(c) *Continuity: If $S$ is continuous in a neighborhood of $(x_0, y_0)$, then $y(x)$ is continuous in a neighborhood of $x_0$.*

## A.3 An alternative approach via fixed point theory

We consider in this section an alternative characterization in terms of a fixed point for the cases described in Definition 4.1. For concreteness we discuss the first case. A similar result holds for the second case. We denote by $-\Delta_0$ the restriction of the Laplacian to $U_0$, and its inverse by $(-\Delta_0)^{-1}$. These act as bounded linear operators between $U_0$ and $L^2$, respectively.

**Definition A.1.** *Denote by $u_0^*$ the harmonic function with boundary trace equal to the boundary trace of $u_0$. Define, for $v \in L^2$,*

$$\mathcal{T}_\phi v = -(-\Delta_0)^{-1}(F(\cdot\,, v\phi(v)) + u_0^*. \tag{68}$$

We have the following.

**Proposition A.1.** *The function $u$ satisfies $T_\phi(u) = 0$ if and only if $u$ is a fixed point of $\mathcal{T}_\phi$. Moreover, $u\phi(u) = u$ for this function, so that it satisfies the given boundary value problem*

*Proof.* The equivalence of the fixed point formulation and the zero for $T_\phi$ results from an application of $\Delta_0$ or its inverse. Note that the fixed point mapping must be considered on $L^2$. The other statements are slight variations of those already discussed. □

**Remark A.1.** *A standard approach to existence of solutions is to employ the Leray-Schauder theorem [9] to $\mathcal{T}_\phi$ as an operator on $L^2$. Continuity is a consequence of the Nemytskii property, induced by $\phi$. Compactness follows from the Sobolev embedding theorem. A standard energy argument establishes the boundedness of the homotopy of fixed points of the mappings $t\mathcal{T}_\phi$ for $0 \leq t \leq 1$. Arguments similar to those of Lemma 2.3 of the current article are required to show that such a fixed point corresponds to a desired solution of the equation (38). Because of the requirement of differentiability, the variational approach requires more hypotheses than the approach involving the Leray-Schauder theorem. However, the fixed point approach is not directly compatible with the stability associated with the implicit function theorem. Moreover, if one wishes to establish a joint existence/approximation theory, then the hypotheses are comparable, as is seen from the Krasnosel'skii calculus [19].*

## References


[1] R. Adams and J. Fournier, *Sobolev Spaces*, 2nd. ed. Pure and Applied Mathematics, 140, Elsevier/Academic Press, Amsterdam, 2003.

[2] J.H. Bramble and A. Schatz, Rayleigh-Ritz-Galerkin methods for Dirichlet's problem using subspaces without boundary conditions. Comm. Pure Appl. Math. **23** (1970), 658-675.

[3] H. Brézis, Équations et inéquations non linéaires dans les espaces vectoriels en dualité. Ann. Inst. Fourier **18** (1968), 115-175.

[4] E. Cancès and C. Le Bris, On the time-dependent Hartree-Fock equations with a classical nuclear nonlinear dynamics. Math. Models Meth. Appl. Sci. **9** (1999), 963-990.

[5] I. Ekeland and R. Temam, *Convex Analysis and Variational Problems.* Classics in Applied Mathematics, 28, SIAM, Philadelphia, 1999.

[6] S.D. Fisher, Solutions of some non-linear variational problems in $L^\infty$ and the problem of minimum curvature. Arch. Rational Mech. Anal. **61** (1976), no. 3, 291-305.

[7] S.D. Fisher and J.W. Jerome, *Minimum Norm Extremals in Function Spaces.* Springer Lecture Series in Mathematics 479, Berlin, 1975.

[8] F. Fogolari, A. Brigo, and N. Molinari, The Poisson-Boltzmann equation for biomolecular electrostatics: a tool for structural biology. J. Molec. Recognit. **15** (6)(2002), 377-392. .

[9] D. Gilbarg and N. Trudinger, *Elliptic Partial Differential Equations of Second Order.* Classics in Mathematics, Springer-Verlag, Berlin, 2001.

[10] J.N. Israelachvili, *Intermolecular and Surface Forces*, 3rd. ed. Burlington: Academic, 2011.

[11] J.W. Jerome, Minimization problems and linear and nonlinear spline functions I: Existence. SIAM J. Numer. Anal. **10** (1973), 808-819.

[12] J.W. Jerome, *Approximation of Nonlinear Evolution Equations.* Academic Press, Orlando, 1983.

[13] J.W. Jerome, Consistency of semiconductor modeling: An existence/stability analysis for the stationary Van Roosbroeck system. SIAM J. Appl. Math. **45** (1985), 565-590.

[14] J.W. Jerome, A trapping principle and convergence result for finite element solutions of steady reaction/diffusion systems. Numer. Math. **109** (2008), 121-142.

[15] J.W. Jerome and E. Polizzi, Discretization of time-dependent quantum systems: real-time propagation of the evolution operator. Applicable Anal. **93** (2014), 2574-2597.

[16] K. Johannessen, The exact solution to the one-dimensional Poisson-Boltzmann equation with asymmetric boundary conditions. J. Math. Chem. **52**(2014), 504-507.

[17] J. Keener and J. Sneyd, *Mathematical Physiology.* Interdisciplinary Mathematics, vol. 8, Springer-Verlag, New York, 1998.

[18] M. Krasnosel'skii, *Topological Methods in the Theory of Non-Linear Integral Equations.* Pergamon Press, 1964.

[19] M.A. Krasnosel'skii, G.M. Vainikko, P.P. Zabreiko, Ya.B. Rititskii, and V.Ya. Stetsenko, *Approximate Solution of Operator Equations.* Wolters-Noordhoff, Groningen, 1972.

[20] C.B. Morrey, Jr. , *Multiple Integrals in the Calculus of Variations.* Die Grundlehren der mathematischen Wissenschaften, Volume 130, Springer-Verlag, New York, 1966. Reprinted, 2008.

[21] R. Showalter, *Monotone Operators in Banach Space and Nonlinear Partial Differential Equations.* Mathematical Surveys and Monographs 49, American Mathematical Society, Providence, 1997.

[22] R. Tapia, The differentiation and integration of nonlinear operators. In, L.B. Rall (ed.)it Nonlinear Functional Analysis and Applications. Academic Press, New New York 1971, 45-101.

[23] C.A. Ullrich, *Time Dependent Density Functional Theory.* Oxford University Press, 2012.

[24] E. Zeidler, *Nonlinear Functional Analysis and its Applications* I. Springer, 1985.

[25] E. Zeidler, *Nonlinear Functional Analysis and its Applications* II/B. Springer, 1990.