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Spectral properties of Schrödinger operators on superconducting surfaces

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Abstract. In this work we focus on the characterization of the space $L^2(S; \mathbb{C})$ on Riemannian 2-manifolds S induced by a fixed magnetic vector potential \mathbf{A}_0 in the nonlinear Ginzburg-Landau (GL) superconductivity model. The linear differential operator governing the GL model is the surface Schrödinger operator $(i\nabla + A_0)^2$ on S. We obtain a complete orthonormal system in $L^2(S; \mathbb{C})$ from a collection of nontrivial solutions of the weak-form of the spectral problem associated with $(i\nabla + A_0)^2$. Then, after proving that any member of this basis satisfies a higher regularity condition, we conclude that each is also an eigenfunction of the strong-form of the surface Schrödinger operator, and must satisfy a natural Neumann condition over any nonempty component of the manifold boundary ∂S . These results form the theoretical foundations used to develop efficient computational tools for simulating the Langevin version of the surface GL model.

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Contents

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1. Introduction

Spectral properties of differential operators defined on Riemannian manifolds facilitate the understanding and efficient numerical simulation of physical processes described by mathematical models they govern. Eigenvalues and eigenfunctions of the Laplacian on manifolds (with and without boundaries) have been investigated for several decades, and provide important tools for the simulation and analysis of processes such as vibrations of drums and membranes, or stationary states of free quantum particles, see for example [\[20\]](#page-41-0) for an excellent survey and references therein.

The focus of this article is the investigation of spectral problems corresponding to Schrödinger operators that arise in a class of GL models for superconductivity in thin materials. The results are used to characterize the Lebesgue space of complex-valued, square-integrable functions on Riemannian 2-manifolds S that are taken to represent thin superconductors having rotational symmetry about the axis of a constant, externally-applied magnetic field. From standard gauge, scaling and approximation considerations this may be taken to be the system magnetic field, and equal to the curl of the magnetic vector potential $\mathbf{A}_0 = R \hat{\theta}$, where R represents distance from the z-axis, and $\hat{\theta}$ denotes the unit coordinate vector corresponding to the direction of increasing θ in a cylindrical-polar coordinate system. In this context, the GL system involves a single partial differential equation, which is nonlinear in the complex-valued order parameter, and is governed by the Schrödinger operator $(i \nabla + R \hat{\theta})^2$ on S. See references [\[6,](#page-40-1) [7,](#page-40-2) [12\]](#page-41-1) for further details regarding the particulars and validity of this GL model realization. In a future work, we implement a highly efficient finite element method to compute the eigenvalues and modes of the surface Schrödinger operator for use with advanced GL simulation techniques.

Our motivation is to provide an efficient computational and analysis framework for the investigation of nondeterministic critical phenomena in the Langevin version of the GL model [\[5,](#page-40-3) [10\]](#page-41-2). Deterministic GL systems have been widely used to study the formation of vortex configurations in thin superconductors that contain a Riemannian manifold $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$ $[2, 4, 6, 7, 13, 16, 17, 19]$. If such phenomena are essentially nondeterministic, as are evolutions of vortex configurations from ideal (superconducting or nonsuperconducting) initial states in highly symmetric systems, we rely on the Langevin extension of the GL model to complete the phenomenological context. Stochastic GL simulations in finite-dimensional subspaces that include high-frequency modes are therefore needed, and the symmetry in the systems we consider naturally supports the development of spectral methods. It turns out that methods based on the eigenfunctions of the surface Schrödinger operator

 $(i \nabla + R \hat{\theta})^2$, which are known only for simple choices of S such as the planar disk $[3, 19]$ $[3, 19]$, are highly efficient. Because the geometry of the superconductor may otherwise substantially influence the critical phenomena $[15]$, we use a generalized approach that allows for investigations of the model on any surface of revolution.

We take $S \subseteq \mathbb{R}^3$ to be a C^2 Riemannian 2-manifold (with or without boundary) that is open, bounded, connected, and given as the range of the parameterization

$$
\mathbf{x}(s,\theta) = [R(s)\cos\theta, R(s)\sin\theta, Z(s)], \quad s \in I, \theta \in [0, 2\pi), \tag{1.1}
$$

where $I \subseteq \mathbb{R}$ is an interval. In terms of this standard parameterization for S, we begin by deriving both weak and strong formulations for the surface Schrödinger operator. Then, from the collection of nontrivial solutions of the corresponding weakly-formulated spectral problem, we identify a complete orthonormal system for the space $L^2(S; \mathbb{C})$. In order to define finite-dimensional subspaces spanned by the elements of this basis that are suitable for simulations of the associated nonlinear GL and Langevin-Ginzburg-Landau (LGL) models, it is important to establish an additional regularity property. Specifically, in this work we also prove that every solution to the weakly-formulated Schrödinger spectral problem lies (at least) in the space $H^2(S; \mathbb{C})$. This last result is needed primarily to establish the spectral accuracy of the numerical simulation methods introduced in future articles, and is instrumental in demonstrating how these eigenfunctions, and their corresponding eigenvalues, can be efficiently represented and accurately approximated. To accomplish all of this, we next introduce some suitable constraints on S and (1.1) , then specify notational conventions that are used throughout the article. Some crucial results required by our analysis are included in the appendix.

1.1. Preliminaries. Whenever S has a boundary, we assume that each boundary point has a neighborhood in \overline{S} whose intersection with S is simply connected. We may choose the parametrization **x** so that the functions R and Z in $(1,1)$ have bounded, continuous derivatives through the second order on I^o and $\mathbf{x}|_{I^o \times [0,2\pi)}$ is a homeomorphism, where I^o denotes the interior of I . Suitable versions of our approach and analysis may be retained when differentiability assumptions are relaxed (when S is a right circular cone, for example). We take the left and right endpoints of the interval I in [\(1.1\)](#page-2-0) to be 0 and s_0 , respectively, where $s_0 > 0$. To integrate a function

$$
f\colon S\longrightarrow \mathbb{C}
$$

over S, we use (1.1) to obtain

$$
\int_{S} f dx = \int_{0}^{2\pi} \int_{0}^{s_0} f(\mathbf{x}(s,\theta)) |\mathbf{x}_s(s,\theta) \times \mathbf{x}_{\theta}(s,\theta)| ds d\theta
$$
\n
$$
= \int_{0}^{2\pi} \int_{0}^{s_0} f(\mathbf{x}(s,\theta)) R(s) \sqrt{R_s^2 + Z_s^2} ds d\theta.
$$
\n(1.2)

We assume that $R \ge 0$, so that $f = 1$ in [\(1.2\)](#page-3-1) gives the geometric area of S. For integrals on ∂S , we write

$$
\int_{\partial S} f \, dx = \int_{0}^{2\pi} f(\mathbf{x}(s,\theta)) R(s) \Big|_{s=0}^{s=s_0} d\theta,\tag{1.3}
$$

which yields zero whenever $\partial S = \emptyset$. Lastly, we shall always assume that **x** has been chosen so that

$$
\inf_{s \in I} \sqrt{R_s^2 + Z_s^2} > 0, \qquad \sup_{s \in I} \sqrt{R_s^2 + Z_s^2} < \infty. \tag{1.4}
$$

Throughout this article, the standard (conjugate symmetric) inner product in L^2 (S; C) is denoted by $\langle \cdot, \cdot \rangle_2$. For our weak formulation, it is convenient to introduce the real, symmetric inner product in $L^2(S; \mathbb{C})$ given by

$$
\langle u, v \rangle := \langle u, v \rangle_2 + \langle v, u \rangle_2, \quad u, v \in L^2(S; \mathbb{C}). \tag{1.5}
$$

If $\partial S \neq \emptyset$, we denote the associated real, symmetric inner product in $L^2(\partial S; \mathbb{C})$ as $\langle u, v \rangle_{\partial S}$. Let $\|\cdot\|_2$ and $\|\cdot\|_{1,2}$ denote, respectively, the standard norms in $L^2(S; \mathbb{C})$ and $H^1(S; \mathbb{C})$. We introduce the norm $\|\cdot\| = \sqrt{2} \|\cdot\|_2$, which is induced by the real, symmetric inner product $\langle \cdot, \cdot \rangle$ identified in [\(1.5\)](#page-3-2). For any domain X, the standard norm in $L^2(X; \mathbb{C})$ is denoted by $\|\cdot\|_{2,X}$, and we let $\|\cdot\|_X = \sqrt{2}\|\cdot\|_{2,X}$ be the norm induced by the real, symmetric inner product $\langle \cdot, \cdot \rangle_X$.

2. The Schrödinger operator on S

In this section we derive in detail the strong and weak formulations for the surface Schrödinger operator, as required for our investigations of the spectral problems.

2.1. Strong formulation of the Schrödinger operator on S. The vector-valued first-order operator $(i \nabla + R \hat{\theta})$ is specified by utilizing the standard definition of the gradient of a function defined on S . We first recall our parameterization for S in $(1,1)$, and use it to write the surface normal vector as

$$
\mathbf{n}(\mathbf{x}(s,\theta)) = \frac{\mathbf{x}_s \times \mathbf{x}_\theta}{|\mathbf{x}_s \times \mathbf{x}_\theta|} = \frac{[-Z_s \cos \theta, -Z_s \sin \theta, R_s]}{\sqrt{R_s^2 + Z_s^2}}, \quad \mathbf{x}(s,\theta) \in S. \tag{2.1}
$$

We work in a "thin" region $\Omega \subseteq \mathbb{R}^3$ containing S, and given by the parametric representation

$$
\boldsymbol{\rho}(\rho, s, \theta) = [R(s)\cos\theta, R(s)\sin\theta, Z(s)] + \rho \mathbf{n}(\mathbf{x}(s, \theta)), \tag{2.2}
$$

where the parameter ρ is restricted to the interval $(-\epsilon, \epsilon)$ for some sufficiently small $\epsilon > 0$. Given $u \in H^1(S; \mathbb{C})$, to work in Ω we need to extend u into the space $H^1(\Omega; \mathbb{C})$ such that the value of the extension and each of its first partial derivatives on S agrees almost everywhere with those of u . At this stage, we assume that such an extension is always possible provided ϵ is sufficiently small, and simply use u again to denote it. For the gradient of u , we must evaluate

$$
\nabla u = [u_x, u_y, u_z] - \mathbf{n} (\mathbf{n} \cdot [u_x, u_y, u_z]) \tag{2.3}
$$

on S. To evaluate the right hand side of [\(2.3\)](#page-4-0), we construct $|u_x, u_y, u_z|$ component by component. On Ω , from the chain rule we have

$$
u_x = u_s s_x + u_\rho \rho_x + u_\theta \theta_x, \tag{2.4}
$$

and from (2.2) we obtain the parametric equations

$$
x = \left(R - \frac{\rho Z_s}{\sqrt{R_s^2 + Z_s^2}}\right)\cos\theta,\tag{2.5a}
$$

$$
y = \left(R - \frac{\rho Z_s}{\sqrt{R_s^2 + Z_s^2}}\right) \sin \theta, \tag{2.5b}
$$

$$
z = Z + \frac{\rho R_s}{\sqrt{R_s^2 + Z_s^2}}.\tag{2.5c}
$$

From differentiation of the relation

$$
\left(R - \frac{\rho Z_s}{\sqrt{R_s^2 + Z_s^2}}\right)^2 = x^2 + y^2\tag{2.6}
$$

with respect to x , we find that

$$
\Big(R - \frac{\rho Z_s}{\sqrt{R_s^2 + Z_s^2}}\Big)\Big(R_s\Big(1 - \rho \frac{R_s Z_{ss} - Z_s R_{ss}}{(R_s^2 + Z_s^2)^{3/2}}\Big)s_x - \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}}\rho_x\Big) = x, \tag{2.7}
$$

while from the third relation in (2.5) we have

$$
Z_s \Big(1 - \rho \frac{R_s Z_{ss} - Z_s R_{ss}}{(R_s^2 + Z_s^2)^{3/2}} \Big) s_x + \frac{R_s}{\sqrt{R_s^2 + Z_s^2}} \rho_x = 0. \tag{2.8}
$$

To use results [\(2.7\)](#page-4-3) and [\(2.8\)](#page-5-0) on S, we evaluate them at $\rho = 0$ to obtain the system

$$
\begin{pmatrix}\nR_s & -\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \\
Z_s & \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}\n\end{pmatrix}\n\begin{pmatrix}\ns_x \\
\rho_x\n\end{pmatrix} = \begin{pmatrix}\n\cos\theta \\
0\n\end{pmatrix},
$$
\n(2.9)

whence we find the formulas

$$
s_x = \frac{R_s}{R_s^2 + Z_s^2} \cos \theta \quad \text{and} \quad \rho_x = -\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \cos \theta. \tag{2.10}
$$

From the relation

$$
\tan \theta = \frac{y}{x} \tag{2.11}
$$

on Ω , we find that

$$
\theta_x = -\frac{\sin \theta}{R}.\tag{2.12}
$$

Substituting results (2.10) and (2.12) into (2.4) now gives

$$
u_x = u_s \frac{R_s}{R_s^2 + Z_s^2} \cos \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \cos \theta - u_\theta \frac{\sin \theta}{R}.
$$
 (2.13)

For the second component, we proceed in a similar fashion. On Ω , we have

$$
u_y = u_s s_y + u_\rho \rho_y + u_\theta \theta_y. \tag{2.14}
$$

Differentiation with respect to y of (2.6) and the third equation in (2.5) , followed by evaluation on S , results in the system

$$
\begin{pmatrix}\nR_s & -\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \\
Z_s & \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}\n\end{pmatrix}\n\begin{pmatrix}\ns_y \\
\rho_y\n\end{pmatrix} =\n\begin{pmatrix}\n\sin \theta \\
0\n\end{pmatrix},
$$
\n(2.15)

from which we find that

$$
s_y = \frac{R_s}{R_s^2 + Z_s^2} \sin \theta \quad \text{and} \quad \rho_y = -\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \sin \theta. \tag{2.16}
$$

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After using (2.11) to find that

$$
\theta_y = \frac{\cos \theta}{R},\tag{2.17}
$$

from the substitution of $(2.16-2.17)$ $(2.16-2.17)$ into (2.14) we see that

$$
u_y = u_s \frac{R_s}{R_s^2 + Z_s^2} \sin \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \sin \theta + u_\theta \frac{\cos \theta}{R}.
$$
 (2.18)

Finally, for the third component we write

$$
u_z = u_s s_z + u_\rho \rho_z + u_\theta \theta_z. \tag{2.19}
$$

Differentiation of the third equation in (2.5) with respect to z gives

$$
Z_s \Big(1 - \rho \frac{R_s Z_{ss} - Z_s R_{ss}}{(R_s^2 + Z_s^2)^{3/2}} \Big) s_z + \frac{R_s}{\sqrt{R_s^2 + Z_s^2}} \rho_z = 1, \tag{2.20}
$$

while from (2.6) we have

$$
R_s \Big(1 - \rho \frac{R_s Z_{ss} - Z_s R_{ss}}{(R_s^2 + Z_s^2)^{3/2}} \Big) s_z - \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \rho_z = 0. \tag{2.21}
$$

At $\rho = 0$, from [\(2.20\)](#page-6-1)–[\(2.21\)](#page-6-2) we obtain the system

$$
\begin{pmatrix}\nR_s & -\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \\
Z_s & \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}\n\end{pmatrix}\n\begin{pmatrix}\ns_z \\
\rho_z\n\end{pmatrix} = \begin{pmatrix}\n0 \\
1\n\end{pmatrix},
$$
\n(2.22)

which gives

$$
s_z = \frac{Z_s}{R_s^2 + Z_s^2} \quad \text{and} \quad \rho_z = \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}.\tag{2.23}
$$

Since clearly

$$
\theta_z = 0,\tag{2.24}
$$

from [\(2.19\)](#page-6-3) we now see that

$$
u_z = u_s \frac{Z_s}{R_s^2 + Z_s^2} + u_\rho \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}.
$$
 (2.25)

Now, from [\(2.13\)](#page-5-6), [\(2.18\)](#page-6-4), [\(2.25\)](#page-6-5) and [\(2.1\)](#page-4-6) we have

$$
\mathbf{n} \cdot [u_x, u_y, u_z] = \frac{[-Z_s \cos \theta, -Z_s \sin \theta, R_s]}{\sqrt{R_s^2 + Z_s^2}} \cdot \left[u_s \frac{R_s}{R_s^2 + Z_s^2} \cos \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \cos \theta - u_\theta \frac{\sin \theta}{R}\right],
$$
\n
$$
u_s \frac{R_s}{R_s^2 + Z_s^2} \sin \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \sin \theta + u_\theta \frac{\cos \theta}{R},
$$
\n
$$
u_s \frac{Z_s}{R_s^2 + Z_s^2} + u_\rho \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}\right]
$$
\n
$$
= u_\rho.
$$
\n(2.26)

Returning to (2.3) , we get

$$
\nabla u = [u_x, u_y, u_z] - \mathbf{n}(\mathbf{n} \cdot [u_x, u_y, u_z])
$$

\n
$$
= \left[u_s \frac{R_s}{R_s^2 + Z_s^2} \cos \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \cos \theta - u_\theta \frac{\sin \theta}{R},
$$

\n
$$
u_s \frac{R_s}{R_s^2 + Z_s^2} \sin \theta - u_\rho \frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \sin \theta + u_\theta \frac{\cos \theta}{R},
$$

\n
$$
u_s \frac{Z_s}{R_s^2 + Z_s^2} + u_\rho \frac{R_s}{\sqrt{R_s^2 + Z_s^2}} \right]
$$

\n
$$
- \frac{\left[-Z_s \cos \theta, -Z_s \sin \theta, R_s\right]}{\sqrt{R_s^2 + Z_s^2}} u_\rho,
$$

\n(2.27)

and

$$
\nabla u = \left[u_s \frac{R_s}{R_s^2 + Z_s^2} \cos \theta - u_\theta \frac{\sin \theta}{R}, \frac{R_s}{R_s^2 + Z_s^2} \sin \theta + u_\theta \frac{\cos \theta}{R}, \frac{Z_s}{R_s^2 + Z_s^2} \right].
$$
\n(2.28)

After defining the unit coordinate vectors

$$
\hat{s} = \frac{\mathbf{x}_s}{|\mathbf{x}_s|} = \frac{[R_s \cos \theta, R_s \sin \theta, Z_s]}{\sqrt{R_s^2 + Z_s^2}}
$$
(2.29)

and

$$
\hat{\theta} = \frac{\mathbf{x}_{\theta}}{|\mathbf{x}_{\theta}|} = [-\sin \theta, \cos \theta, 0],
$$
\n(2.30)

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we see that

$$
\hat{s} \cdot \nabla u = \frac{u_s}{\sqrt{R_s^2 + Z_s^2}}\tag{2.31}
$$

and

$$
\hat{\theta} \cdot \nabla u = \frac{u_{\theta}}{R},\tag{2.32}
$$

so we write [\(2.28\)](#page-7-0) more conveniently as

$$
\nabla u = \hat{s} \frac{u_s}{\sqrt{R_s^2 + Z_s^2}} + \hat{\theta} \frac{u_\theta}{R}.
$$
 (2.33)

From [\(2.33\)](#page-8-0), we may finally write the (surface) operator $(i \nabla + R \hat{\theta})$ as

$$
(i\nabla + R\hat{\theta}) = \hat{s}\frac{i}{\sqrt{R_s^2 + Z_s^2}}\frac{\partial}{\partial s} + \hat{\theta}\Big(\frac{i}{R}\frac{\partial}{\partial \theta} + R\Big). \tag{2.34}
$$

To formulate $(i\nabla + R\hat{\theta})^2$ on S, we take $u \in H^2(S; \mathbb{C})$, and apply [\(2.34\)](#page-8-1) to $(i \nabla + R \hat{\theta})u$. Thus, we start from

$$
(i\nabla + R\hat{\theta})^2 u
$$

= $\left(\hat{s} \frac{i}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial}{\partial s} + \hat{\theta} \left(\frac{i}{R} \frac{\partial}{\partial \theta} + R\right)\right) \cdot \left(\hat{s} \frac{i u_s}{\sqrt{R_s^2 + Z_s^2}} + \hat{\theta} \left(\frac{i u_\theta}{R} + R u\right)\right),$ (2.35)

and keep in mind that the unit coordinate vectors \hat{s} and $\hat{\theta}$ are generally not constant. Working from [\(2.29\)](#page-7-1), we have

$$
\hat{s}_s = \left[\left(\frac{R_s}{\sqrt{R_s^2 + Z_s^2}} \right)_s \cos \theta, \left(\frac{R_s}{\sqrt{R_s^2 + Z_s^2}} \right)_s \sin \theta, \left(\frac{Z_s}{\sqrt{R_s^2 + Z_s^2}} \right)_s \right]
$$
\n
$$
= \frac{\mathfrak{N}}{(R_s^2 + Z_s^2)^{3/2}},
$$
\n(2.36)

where

$$
\mathfrak{N} = [(R_{ss}Z_s - R_sZ_{ss})Z_s \cos\theta, (R_{ss}Z_s - R_sZ_{ss})Z_s \sin\theta, (R_sZ_{ss} - R_{ss}Z_s)R_s]
$$

and observe, in particular, that

$$
\hat{s} \cdot \hat{s}_s = \frac{R_s Z_s (R_{ss} Z_s - R_s Z_{ss} + R_s Z_{ss} - R_{ss} Z_s)}{(R_s^2 + Z_s^2)^2} = 0. \tag{2.37}
$$

Therefore, the first of the four terms produced on the right hand side of (2.35) reads

$$
\begin{split}\n&\left(\hat{s}\frac{i}{\sqrt{R_s^2 + Z_s^2}}\frac{\partial}{\partial s}\right) \cdot \left(\hat{s}\frac{i u_s}{\sqrt{R_s^2 + Z_s^2}}\right) \\
&= -\left(\hat{s}\frac{1}{\sqrt{R_s^2 + Z_s^2}}\right) \cdot \frac{\partial}{\partial s} \left(\hat{s}\frac{u_s}{\sqrt{R_s^2 + Z_s^2}}\right) \\
&= -\left(\hat{s}\frac{1}{\sqrt{R_s^2 + Z_s^2}}\right) \cdot \left(\hat{s}_s\frac{u_s}{\sqrt{R_s^2 + Z_s^2}} + \hat{s}\frac{\partial}{\partial s}\left(\frac{u_s}{\sqrt{R_s^2 + Z_s^2}}\right)\right) \\
&= -\frac{1}{\sqrt{R_s^2 + Z_s^2}}\frac{\partial}{\partial s}\left(\frac{u_s}{\sqrt{R_s^2 + Z_s^2}}\right).\n\end{split} \tag{2.38}
$$

Next, by differentiation of (2.30) , we clearly see that

$$
\hat{\theta}_s = \mathbf{0},\tag{2.39}
$$

and since $\hat{s} \cdot \theta = 0$, we conclude that

$$
\left(\hat{s}\frac{i}{\sqrt{R_s^2 + Z_s^2}}\frac{\partial}{\partial s}\right) \cdot \left(\hat{\theta}\left(\frac{i u_\theta}{R} + R u\right)\right) = 0. \tag{2.40}
$$

Returning again to [\(2.29\)](#page-7-1), we have

$$
\hat{s}_{\theta} = \frac{\left[-R_s \sin \theta, R_s \cos \theta, 0\right]}{\sqrt{R_s^2 + Z_s^2}},\tag{2.41}
$$

and we notice here that

$$
\hat{\theta} \cdot \hat{s}_{\theta} = \frac{R_s}{\sqrt{R_s^2 + Z_s^2}}.
$$
\n(2.42)

Using [\(2.41](#page-9-0)[-2.42\)](#page-9-1), and (again) the fact that $\hat{s} \cdot \theta = 0$, the third term produced on the right hand side of (2.35) can be calculated as

$$
\hat{\theta}\left(\frac{i}{R}\frac{\partial}{\partial\theta}+R\right)\cdot\left(\hat{s}\frac{iu_s}{\sqrt{R_s^2+Z_s^2}}\right) = -\frac{\hat{\theta}}{R}\cdot\frac{\partial}{\partial\theta}\left(\hat{s}\frac{u_s}{\sqrt{R_s^2+Z_s^2}}\right)
$$

$$
=-\frac{\hat{\theta}}{R}\cdot\left(\hat{s}_\theta\frac{u_s}{\sqrt{R_s^2+Z_s^2}}\right)
$$
(2.43)
$$
=-\frac{R_s}{R(R_s^2+Z_s^2)}u_s.
$$

Finally, we refer back to (2.30) , and find that

$$
\hat{\theta}_{\theta} = [-\cos\theta, -\sin\theta, 0];\tag{2.44}
$$

here, we note the identity

$$
\hat{\theta} \cdot \hat{\theta}_{\theta} = 0. \tag{2.45}
$$

Thus, the last of the four terms produced by (2.35) is

$$
\hat{\theta}\Big(\frac{i}{R}\frac{\partial}{\partial\theta}+R\Big)\cdot\Big(\hat{\theta}\Big(\frac{i u_{\theta}}{R}+R u\Big)\Big)=-\frac{\hat{\theta}}{R}\cdot\frac{\partial}{\partial\theta}\Big(\hat{\theta}\frac{u_{\theta}}{R}\Big)+i2u_{\theta}+R^2 u
$$
\n
$$
=-\frac{u_{\theta\theta}}{R^2}+i2u_{\theta}+R^2 u.
$$
\n(2.46)

When substituting (2.38) , (2.40) , (2.43) and (2.46) into the right hand side of equation (2.35) , we therefore have

$$
(i\nabla + R\hat{\theta})^2 u = -\frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial}{\partial s} \left(\frac{u_s}{\sqrt{R_s^2 + Z_s^2}} \right)
$$

$$
-\frac{R_s}{R(R_s^2 + Z_s^2)} u_s - \frac{u_{\theta\theta}}{R^2} + i2u_{\theta} + R^2 u.
$$
(2.47)

Next, we describe a weak formulation for the surface Schrödinger operator.

2.2. Weak formulation of the of the Schrödinger operator on S**.** In this section, we establish a Green's identity for the surface Schrödinger operator that allows us to relate its weak and strong formulations in $L^2(S; \mathbb{C})$.

Theorem 2.1. Let $u \in H^2(S; \mathbb{C})$ and $v \in H^1(S; \mathbb{C})$. Then, the formula

$$
\langle (i\nabla + R\hat{\theta})u, (i\nabla + R\hat{\theta})v \rangle = \langle (i\nabla + R\hat{\theta})^2u, v \rangle + \langle (i\nabla + R\hat{\theta})u \cdot \hat{s}, iv \rangle_{\partial S} \tag{2.48}
$$

holds.

Proof. We begin by stating several intermediate results that are used in the proof. We have the following:

- (1) the mapping $(u, v) \mapsto \langle u, v \rangle$ of $L^2(S; \mathbb{C}) \times L^2(S; \mathbb{C}) \to \mathbb{R}$ is continuous;
- (2) the mapping $(u, v) \mapsto \langle u, v \rangle_{\partial S}$ of $L^2(\partial S; \mathbb{C}) \times L^2(\partial S; \mathbb{C}) \to \mathbb{R}$ is continuous;
- (3) the mapping $u \mapsto (i \nabla + R \hat{\theta}) u$ of $H^1(S; \mathbb{C}) \to L^2(S; \mathbb{C})$ is continuous;
- (4) the mapping $u \mapsto (i \nabla + R \hat{\theta})^2 u$ of $H^2(S; \mathbb{C}) \to L^2(S; \mathbb{C})$ is continuous;
- (5) the space $C^2(\overline{S}; \mathbb{C})$ is dense in $L^2(S; \mathbb{C}), H^1(S; \mathbb{C})$, and $H^2(S; \mathbb{C})$.

$$
(2.49)
$$

Establishing $(1 - 4)$ in (2.49) amounts to a straightforward exercise. Item (5) represents a classical result from the theory of Sobolev spaces, properly adapted for the domain S (for example, we may work from Theorem 3.22 in [\[1\]](#page-40-7)). Our approach is to begin by showing [\(2.48\)](#page-10-2) on the dense subspace $C^2(\bar{S}; \mathbb{C})$. Here, our parameterization assumptions allow us to use integration by parts, then [\(2.49\)](#page-10-1) may be applied to extract appropriate limits and complete the proof. So, let $u, v \in$ $C^2(\overline{S}; \mathbb{C})$. We begin by using [\(2.34\)](#page-8-1) with [\(1.2\)](#page-3-1) to write

$$
\langle (i\nabla + R\hat{\theta})u, (i\nabla + R\hat{\theta})v \rangle_{2} =
$$
\n
$$
= \int_{0}^{2\pi} \int_{0}^{S_{0}} \left(\hat{s} \frac{i}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s} + \hat{\theta} \left(\frac{i}{R} \frac{\partial u}{\partial \theta} + Ru \right) \right)
$$
\n
$$
\cdot \overline{\left(\hat{s} \frac{i}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial v}{\partial s} + \hat{\theta} \left(\frac{i}{R} \frac{\partial v}{\partial \theta} + Rv \right) \right)} R \sqrt{R_{s}^{2} + Z_{s}^{2}} ds d\theta
$$
\n
$$
= \int_{0}^{2\pi} \left(\int_{0}^{S_{0}} \frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s} \frac{\partial v}{\partial s}} ds \right) d\theta + \int_{0}^{S_{0}} \left(\int_{0}^{2\pi} \left(\frac{1}{R^{2}} \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} - i u \frac{\partial v}{\partial \theta} + i \frac{\partial u}{\partial \theta} \bar{v} + R^{2} u \bar{v} \right) d\theta \right) R \sqrt{R_{s}^{2} + Z_{s}^{2}} ds.
$$
\n(2.50)

Owed to the properties of u , v and \bf{x} , we can use integration by parts to evaluate the innermost integral in the first term on the right hand side of (2.50) . We get

$$
\int_{0}^{s_{0}} \frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s} \frac{\partial v}{\partial s}} ds
$$
\n
$$
= \frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s} \overline{v} \Big|_{s=0}^{s=s_{0}} - \int_{0}^{s_{0}} \frac{\partial}{\partial s} \Big(\frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s}} \Big) \overline{v} ds
$$
\n
$$
= \frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s} \overline{v} \Big|_{s=0}^{s=s_{0}}
$$
\n
$$
- \int_{0}^{s_{0}} \Big(\frac{R_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s}} + R \frac{\partial}{\partial s} \Big(\frac{1}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \frac{\partial u}{\partial s}} \Big) \Big) \overline{v} ds,
$$
\n(2.51)

and when applying (1.3) to (2.51) , we conclude that

$$
\int_{0}^{2\pi} \left(\int_{0}^{s_0} \frac{R}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \frac{\partial v}{\partial s} ds \right) d\theta
$$
\n
$$
= \int_{0}^{2\pi} \frac{R}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \overline{v} \Big|_{s=0}^{s=s_0} d\theta - \int_{0}^{2\pi} \int_{0}^{s_0} \Im \overline{v} R \sqrt{R_s^2 + Z_s^2} ds d\theta \qquad (2.52)
$$
\n
$$
= \int_{\partial S} \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \overline{v} dx - \int_{S} \Im \overline{v} dx,
$$

where

$$
\mathfrak{I} = \frac{R_s}{R(R_s^2 + Z_s^2)} \frac{\partial u}{\partial s} + \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial}{\partial s} \Big(\frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \Big).
$$

Moving to the innermost integral in the second term on the right hand side of equa-tion [\(2.50\)](#page-11-0), because every integrand is periodic with respect to the θ parameter, from integration by parts we find here that

$$
\int_{0}^{2\pi} \left(\frac{1}{R^2} \frac{\partial u}{\partial \theta} \frac{\overline{\partial v}}{\partial \theta}\right) d\theta = -\int_{0}^{2\pi} \left(\frac{1}{R^2} \frac{\partial^2 u}{\partial \theta^2} \overline{v}\right) d\theta,\tag{2.53}
$$

and

$$
\int_{0}^{2\pi} \left(-iu \frac{\overline{\partial v}}{\partial \theta} + i \frac{\partial u}{\partial \theta} \bar{v} \right) d\theta = \int_{0}^{2\pi} \left(i 2 \frac{\partial u}{\partial \theta} \bar{v} \right) d\theta.
$$
 (2.54)

Together, (2.53) and (2.54) show that

$$
\int_{0}^{s_0} \left(\int_{0}^{2\pi} \left(\frac{1}{R^2} \frac{\partial u}{\partial \theta} \frac{\partial v}{\partial \theta} - i u \frac{\partial v}{\partial \theta} + i \frac{\partial u}{\partial \theta} \bar{v} + R^2 u \bar{v} \right) d\theta \right) R \sqrt{R_s^2 + Z_s^2} ds
$$
\n
$$
= \int_{S} \left(-\frac{1}{R^2} \frac{\partial^2 u}{\partial \theta^2} \bar{v} + i 2 \frac{\partial u}{\partial \theta} \bar{v} + R^2 u \bar{v} \right) dx.
$$
\n(2.55)

Substituting (2.52) and (2.55) into (2.50) , while recalling the Schrödinger formulation in (2.47) , leads to

$$
\langle (i\nabla + R\hat{\theta})u, (i\nabla + R\hat{\theta})v \rangle_2 = \int_{\partial S} \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \bar{v} \, dx + \langle (i\nabla + R\hat{\theta})^2 u, v \rangle_2.
$$
\n(2.56)

In a similar way, we have

$$
\overline{\langle (i\nabla + R\hat{\theta})u, (i\nabla + R\hat{\theta})v \rangle_2} = \int_{\partial S} \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} v \, dx + \overline{\langle (i\nabla + R\hat{\theta})^2u, v \rangle_2},\tag{2.57}
$$

and it follows that

$$
\langle (i\nabla + R\hat{\theta})u, (i\nabla + R\hat{\theta})v \rangle
$$

=
$$
\int_{\partial S} \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \bar{v} \, dx + \int_{\partial S} \frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} v \, dx + \langle (i\nabla + R\hat{\theta})^2 u, v \rangle
$$

=
$$
\int_{\partial S} \Big(\frac{i}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \Big) \bar{i} v \, dx + \int_{\partial S} \Big(\frac{i}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial u}{\partial s} \Big) i v \, dx
$$

+
$$
\langle (i\nabla + R\hat{\theta})^2 u, v \rangle
$$

=
$$
\langle (i\nabla + R\hat{\theta})u \cdot \hat{s}, iv \rangle_{\partial S} + \langle (i\nabla + R\hat{\theta})^2 u, v \rangle.
$$
 (2.58)

To generalize [\(2.58\)](#page-13-0), we use familiar continuity arguments. Let $u \in H^2(S; \mathbb{C})$, and $v \in H^1(S; \mathbb{C})$. By (5) from [\(2.49\)](#page-10-1), we may choose sequences $\{u_n\}$ and $\{v_n\}$ from $C^2(\overline{S}; \mathbb{C})$ such that $u_n \to u$ in $H^2(S; \mathbb{C})$, and $v_n \to v$ in $H^1(S; \mathbb{C})$. Using (1), (3) and (4) from [\(2.49\)](#page-10-1), we have, as $n \to \infty$,

$$
u_n \to u \text{ in } H^2(S; \mathbb{C}) \implies (i \nabla + R \hat{\theta})^2 u_n \to u \text{ in } L^2(S; \mathbb{C}) \text{ and}
$$

$$
(i \nabla + R \hat{\theta}) u_n \to u \text{ in } L^2(S; \mathbb{C}),
$$
 (2.59a)

and

$$
v_n \to v \text{ in } H^1(S; \mathbb{C}) \implies (i \nabla + R \hat{\theta}) v_n \to v \text{ in } L^2(S; \mathbb{C}) \text{ and}
$$

\n
$$
i v_n \to i v \text{ in } L^2(S; \mathbb{C}),
$$
\n(2.59b)

which together imply that

$$
\langle (i\nabla + R\,\hat{\theta})u_n, (i\nabla + R\,\hat{\theta})v_n \rangle \to \langle (i\nabla + R\,\hat{\theta})u, (i\nabla + R\,\hat{\theta})v \rangle, \qquad (2.60a)
$$

and

$$
\langle (i\nabla + R\,\hat{\theta}\,)^2 u_n, v_n \rangle \to \langle (i\nabla + R\,\hat{\theta}\,)^2 u, v \rangle \tag{2.60b}
$$

for the same such *n*. Moreover, (2) in [\(2.49\)](#page-10-1), when used with Theorem [A.1](#page-42-1) in the appendix, guarantees that

$$
\langle (i\nabla + R\,\hat{\theta}\,)u_n \cdot \hat{s}, iv_n \rangle_{\partial S} \to \langle (i\nabla + R\,\hat{\theta}\,)u \cdot \hat{s}, iv \rangle_{\partial S},\tag{2.61}
$$

and since [\(2.58\)](#page-13-0) gives, for all $n \in \mathbb{N}$,

$$
\langle (i\nabla + R\hat{\theta})u_n, (i\nabla + R\hat{\theta})v_n \rangle = \langle (i\nabla + R\hat{\theta})u_n \cdot \hat{s}, iv_n \rangle_{\partial S} + \langle (i\nabla + R\hat{\theta})^2 u_n, v_n \rangle,
$$

(2.62)
we obtain the result by letting $n \to \infty$ in (2.62).

With these Schrödinger formulations and results in place, we next detail some foundational spectral analysis.

3. Characterization of Schrödinger eigenmodes

Our essential results in this section are as follows:

- There is a complete orthonormal sequence in $L^2(S; \mathbb{C})$ consisting of eigenfunctions of the weakly-formulated spectral problem.
- e corresponding collection of eigenvalues is nonnegative, unbounded, and has no finite accumulation points.

To establish these facts, we start by considering the weakly-formulated spectral Schrödinger problem of finding all nonzero $v \in H^1(S; \mathbb{C})$ such that

$$
\langle (i \nabla + R \hat{\theta}) v, (i \nabla + R \hat{\theta}) w \rangle = \lambda \langle v, w \rangle, \tag{3.1}
$$

for all $w \in H^1(S; \mathbb{C})$ and some $\lambda \in \mathbb{R}$. For convenience, in the arguments that follow positive constants that do not depend on v or w (or a parameter h used later to define a difference operator in the next section) are denoted by K ; the value of K itself may vary according to the context, particularly in passing from one line to the next, or from one side of an equation or inequality to the other. We use subscript notation to fix the value of constants of this type, or to indicate their dependence on a particular parameter.

We proceed to show that an orthonormal basis for $L^2(S; \mathbb{C})$ can be formed from a collection of the solutions of (3.1) . Throughout this section, we work with the real, bilinear forms

$$
L: H^{1}(S; \mathbb{C}) \times H^{1}(S; \mathbb{C}) \longrightarrow \mathbb{R},
$$

\n
$$
(v, w) \longmapsto \langle (i \nabla + R \hat{\theta}) v, (i \nabla + R \hat{\theta}) w \rangle,
$$
\n(3.2)

and, for $\lambda \in \mathbb{R}$,

$$
L_{\lambda}: H^{1}(S; \mathbb{C}) \times H^{1}(S; \mathbb{C}) \longrightarrow \mathbb{R},
$$

\n
$$
(v, w) \longmapsto L(v, w) - \lambda \langle Ev, Ew \rangle,
$$
\n(3.3)

where

 $E: H^1(S; \mathbb{C}) \longrightarrow L^2(S; \mathbb{C})$

is the compact embedding operator obtained from Theorem $A.2$ in the appendix. The essential goals of present interest are formalized in the next theorem. After first establishing several necessary results, we return to its proof near the end of this section.

Theorem 3.1. Let L_{λ} be the form ([3.3](#page-14-3)). Then, there are countably infinite se- $\{a_j\} \subseteq [0, \infty)$ and $\{\psi_j\} \subseteq H^1(S; \mathbb{C}) \setminus \{0\}$ such that

- (a) $L_{\lambda_j}(\psi_j, v) = 0$ *for all* $v \in H^1(S; \mathbb{C}), j \in \mathbb{N}$;
- (b) $\{\lambda_i\}$ *is unbounded, and has no finite accumulation points;* (3.4)
- (c) $\{\psi_j\}$ is a complete orthonormal sequence for $L^2(S; \mathbb{C})$.

To prove Theorem [3.1](#page-15-0) we rely on the Lax-Milgram theorem, and utilize aspects of the theory of compact linear operators in Hilbert space. The essential results used are included in the appendix; we demonstrate next that these are applicable in the context of our problem.

The version of the Lax-Milgram theorem we require is stated, without proof, as Theorem $A.3$ in the appendix. The premises of this theorem are established next.

Theorem 3.2. Let $\mu < 0$. There is a constant $M > 0$ such that

$$
L_{\mu}(v, w) \le M \|v\|_{1,2} \|w\|_{1,2} \quad \text{for all } v, w \in H^1(S; \mathbb{C}). \tag{3.5}
$$

Proof. Let $v, w \in H^1(S; \mathbb{C})$. We work directly from the appropriate definitions, and find that

$$
L_{\mu}(v, w) = L(v, w) - \mu \langle Ev, Ew \rangle
$$

\n
$$
\leq |\langle (i \nabla + R \hat{\theta})v, (i \nabla + R \hat{\theta})w \rangle|
$$

\n
$$
+ |\mu| |\langle Ev, Ew \rangle|
$$

\n
$$
\leq |\langle i \nabla v, i \nabla w \rangle + \langle i \nabla v, \hat{\theta} Rw \rangle + \langle \hat{\theta} Rv, i \nabla w \rangle + \langle \hat{\theta} Rv, \hat{\theta} Rw \rangle|
$$
(3.6)
\n
$$
+ K \|Ev\| \|Ew\|
$$

\n
$$
\leq \|\nabla v\| \|\nabla w\| + \|\nabla v\| \|Rw\| + \|Rv\| \|\nabla w\|
$$

\n
$$
+ \|Rv\| \|Rw\| + K \|v\|_{1,2} \|w\|_{1,2}.
$$

Clearly the inequalities $\|\nabla v\| \leq \sqrt{2} \|v\|_{1,2}$ and $\|Rv\| \leq K \|v\|_{1,2}$ hold, and they remain valid when v is replaced by w . The result then follows.

A similar type of argument is used to verify the second needed premise.

Theorem 3.3. *Here are constants* $\mu < 0$ *and* $m > 0$ *such that*

$$
L_{\mu}(v, v) \ge m \|v\|_{1,2}^2 \quad \text{for all } v \in H^1(S; \mathbb{C}). \tag{3.7}
$$

Proof. Let $v \in H^1(S; \mathbb{C})$. We first work with $L(v, v)$, and find that

$$
L(v, v) = \langle (i\nabla + R\hat{\theta})v, (i\nabla + R\hat{\theta})v \rangle
$$

= $\langle i\nabla v, i\nabla v \rangle + 2\langle i\nabla v, \hat{\theta}Rv \rangle + \langle \hat{\theta}Rv, \hat{\theta}Rv \rangle$ (3.8)
= $\|\nabla v\|^2 + 2\langle i\nabla v, \hat{\theta}Rv \rangle + \|Rv\|^2$.

Thus, from (3.8) , Hölder's inequality, and previous results, we have

$$
2||v||_{1,2}^{2} = ||\nabla v||^{2} + ||v||^{2}
$$

= $L(v, v) - (2\langle i \nabla v, \hat{\theta} R v \rangle + ||Rv||^{2}) + ||v||^{2}$ (3.9)

$$
\leq L(v, v) + 2\sqrt{2}||v||_{1,2}||Rv|| + K||v||^{2}.
$$

Now [\(3.9\)](#page-16-1), Young's inequality, and the identity $||v||^2 = \langle Ev, Ev \rangle$ together show that

$$
2||v||_{1,2}^{2} \le L(v,v) + \epsilon ||v||_{1,2}^{2} + \frac{2}{\epsilon} ||Rv||^{2} + K||v||^{2}
$$

\n
$$
\le L(v,v) + \epsilon ||v||_{1,2}^{2} + K_{\epsilon} \langle Ev, Ev \rangle
$$

\n
$$
= L_{-\kappa_{\epsilon}}(v,v) + \epsilon ||v||_{1,2}^{2}
$$
\n(3.10)

for arbitrary $\epsilon > 0$. We take any such $\epsilon < 2$, and find that the result then follows from [\(3.10\)](#page-16-2), with $m = 2 - \epsilon$ and $\mu = -K_{\epsilon}$. \Box

With μ < 0 as specified in Theorem [3.3,](#page-16-3) we use Theorem [A.3](#page-42-3) from the appendix to obtain a linear bijection

$$
A\colon H^1(S; \mathbb{C}) \longrightarrow H^{-1}(S; \mathbb{C})
$$

such that

$$
L_{\mu}(v, w) = (F, w) \text{ for all } w \in H^{1}(S; \mathbb{C}) \iff F = Av.
$$
 (3.11)

Moreover, since the same theorem guarantees that both A and A^{-1} are bounded, it follows that both are continuous.

From the mapping A^{-1} , we need to construct a suitable compact, self-adjoint operator in $L^2(S; \mathbb{C})$. We first obtain an adjoint for the compact embedding E with the help of the Riesz representation theorem. By Theorem 2.44 (or 1.12) from [\[1\]](#page-40-7), we identify the space $L^2(S; \mathbb{C})$ with its normed dual, which in turn allows us to find $E^*: L^2(S; \mathbb{C}) \to H^{-1}(S; \mathbb{C})$ such that

$$
(E^*v, w) = \langle v, Ew \rangle
$$
 for $v \in L^2(S; \mathbb{C}), w \in H^1(S; \mathbb{C}).$ (3.12)

By standard concepts from functional analysis, we know that E^* is a continuous injection, and its range is dense in $H^{-1}(S; \mathbb{C})$. Moreover, the composite mapping $EA^{-1}E^*$ in $L^2(S; \mathbb{C})$ is compact, being a composition of compact and continuous operators. To show that it is also self-adjoint, we make use of the next theorem.

Theorem 3.4. *Let* $\hat{A} = (E^*)^{-1}AE^{-1}$ *. Then,*

(1) $\mathcal{R}(\hat{A}) = L^2(S; \mathbb{C});$ (2) \hat{A} *is densely defined in* $L^2(S; \mathbb{C});$ (3) \hat{A} is symmetric in $L^2(S; \mathbb{C})$. (3.13)

Therefore, the inverse operator $\hat{A}^{-1} = EA^{-1}E^*$ *is self-adjoint.*

Proof. The last conclusion follows from $(1-3)$, together with [\[18\]](#page-41-8), Theorem 13.11. For (1), since A is a surjection we have $\mathcal{R}(E^*) \subseteq \mathcal{D}(A^{-1})$, and clearly the identification

$$
\mathcal{R}(A^{-1}) = \mathcal{D}(A) = H^1(S; \mathbb{C}) = \mathcal{D}(E)
$$

is valid; thus $\mathcal{D}(\hat{A}^{-1}) = L^2(S; \mathbb{C})$, whence $\mathcal{R}(\hat{A}) = L^2(S; \mathbb{C})$. To see (2), we note that $\mathcal{R}(E^*)$ is dense in $\mathcal{D}(A^{-1})$, so by continuity $\mathcal{R}(A^{-1}E^*)$ is dense in $H^1(S; \mathbb{C})$, the domain of E. Thus, again by continuity, $\mathcal{R}(\hat{A}^{-1})$ is dense in $E(H^1(S; \mathbb{C}))$, which is itself dense in $L^2(S; \mathbb{C})$, so $\mathcal{R}(\hat{A}^{-1})$ is dense in $L^2(S; \mathbb{C})$ as needed. To show (3), we need to verify that $\langle \hat{A}v, w \rangle = \langle v, \hat{A}w \rangle$ for all $v, w \in \mathcal{D}(\hat{A})$. For such v and w, we find with the help of (3.12) and (3.11) that

$$
\langle \hat{A}v, w \rangle = \langle (E^*)^{-1} A E^{-1} v, w \rangle
$$

=\langle (E^*)^{-1} A E^{-1} v, E E^{-1} w \rangle
= (E^*(E^*)^{-1} A E^{-1} v, E^{-1} w) (3.14)
= (A E^{-1} v, E^{-1})
= L_{\mu} (E^{-1} v, E^{-1} w).

When remembering that the form $\langle \cdot, \cdot \rangle$ is symmetric, we recognize by similar arguments that

$$
\langle v, \hat{A}w \rangle = \langle v, (E^*)^{-1} A E^{-1} w \rangle = \langle (E^*)^{-1} A E^{-1} w, v \rangle = L_{\mu}(E^{-1} w, E^{-1} v), \tag{3.15}
$$

whence the fact that L_{μ} is itself symmetric allows the result.

The proof of Theorem 3.1 can now be easily assembled.

[3.1.](#page-15-0) Proof of Theorem 3.1. We begin by utilizing some classical results from the theory of compact linear operators in Hilbert space. Since \hat{A}^{-1} is compact, self-adjoint, nontrivial, and clearly not of finite rank, we apply Theorem [A.4](#page-43-1) to identify the eigen-sequences

$$
\{\tilde{\lambda}_j\} \subseteq \mathbb{R} \quad \text{and} \quad \{\tilde{\psi}_j\} \subseteq L^2(S; \mathbb{C}) \setminus \{0\},\tag{3.16}
$$

where

$$
\hat{A}^{-1}\tilde{\psi}_j = \tilde{\lambda}_j \tilde{\psi}_j \quad \text{for all } j \in \mathbb{N} \tag{3.17}
$$

 \Box

and $\{\tilde{\psi}_j\}$ is a complete orthonormal system for $L^2(S;\mathbb{C})$. To specify $\{\lambda_j\}$, we notice that \hat{A}^{-1} is nonsingular, and consequently that $\{\tilde{\lambda}_j\} \subseteq \mathbb{R} \setminus \{0\}$, then make the assignment

$$
\lambda_j = \tilde{\lambda}_j^{-1} + \mu, \quad j \in \mathbb{N}.\tag{3.18}
$$

Next, it is clear that $\mathcal{R}(\widehat{A}^{-1}) \subseteq \mathcal{R}(E)$, and since [\(3.17\)](#page-18-0) implies that $\{\widetilde{\psi}_j\} \subseteq \mathcal{R}(\widehat{A}^{-1})$, each $\widetilde{\psi}_j \in \mathcal{R}(E)$ and we may identify $\{\psi_j\} \subseteq H^1(S; \mathbb{C}) \setminus \{0\}$ through the assignment

$$
\psi_j = E^{-1} \tilde{\psi}_j, \quad j \in \mathbb{N}.
$$
\n(3.19)

Here $\widetilde{\psi}_j = \psi_j$ in $L^2(S; \mathbb{C})$, so it is clear that $\{\psi_j\}$ is itself a complete orthonormal system for $L^2(S; \mathbb{C})$. To show (a) in [\(3.4\)](#page-15-1), we let $j \in \mathbb{N}$, $v \in H^1(S; \mathbb{C})$, and first write (3.17) as

$$
\tilde{\psi}_j + (\mu - \lambda_j)\hat{A}^{-1}\tilde{\psi}_j = 0 \quad \text{in } L^2(S; \mathbb{C}).
$$
\n(3.20)

Using the formula for \hat{A}^{-1} from Theorem [3.4,](#page-17-1) we have

$$
\widetilde{\psi}_j + (\mu - \lambda_j) E A^{-1} E^* \widetilde{\psi}_j = 0, \qquad (3.21)
$$

and after applying AE^{-1} on the left we get

$$
A\psi_j + (\mu - \lambda_j)E^* E \psi_j = 0 \quad \text{in } H^{-1}(S; \mathbb{C}).
$$
 (3.22)

Evaluating both sides of (3.22) at v gives

$$
(A\psi_j, v) + (\mu - \lambda_j)(E^* E \psi_j, v) = 0,
$$
\n(3.23)

to which we apply (3.11) and (3.12) to obtain

$$
L_{\mu}(\psi_j, v) + (\mu - \lambda_j) \langle E \psi_j, E v \rangle = 0. \tag{3.24}
$$

Using (3.3) , we see from (3.24) that

$$
L_{\lambda_j}(\psi_j, v) = 0. \tag{3.25}
$$

To see that $\{\lambda_i\} \subseteq [0,\infty)$, we use $v = \psi_i$ in [\(3.25\)](#page-19-2) for any $j \in \mathbb{N}$ and find that

$$
L(\psi_j, \psi_j) - \lambda_j \langle E\psi_j, E\psi_j \rangle = 0, \qquad (3.26)
$$

whence

$$
0 \leq ||(i\nabla + R\hat{\theta})\psi_j||^2 = L(\psi_j, \psi_j) = \lambda_j \langle E\psi_j, E\psi_j \rangle = \lambda_j ||\psi_j||^2 = \lambda_j. \tag{3.27}
$$

Lastly, (b) in (3.4) follows from implication (3) in $(A.7)$ and our application of Theorem $A.4$ above, combined with identification (3.18) . This completes the proof.

In the next section, we establish that the elements of the sequence $\{\psi_i\}$ belong to $H^2(S; \mathbb{C})$, are strong Schrödinger eigenfunctions, and satisfy a natural Neumann boundary condition.

4. Regularity properties and implications

An essential ingredient in the theoretical and computational approaches we rely upon is the knowledge that each of the members of any sequence $\{\psi_i\}$ obtained from Theorem [3.1](#page-15-0) in fact lie in the space $H^2(S; \mathbb{C})$. To demonstrate this, a judicious modification of the "tangential differential quotients" technique used in $[11]$ to establish elliptic smoothness properties for problems on open sets in Euclidean space is made. This requires the use of homeomorphic mappings between subsets of \mathbb{R}^2 and S which effectively "straighten out" the manifold boundary, whenever one is present. As a consequence, to obtain the desired results on any admissible S, we must work separately on subsets that either do, or do not, contain points in the z-axis. To see why, notice that our default parameterization alone does not suit our purposes whenever S intersects the z -axis, due to its lack of invertibility. On the other hand, it is exactly appropriate near any component of ∂S , since here $\hat{\theta}$ always gives the appropriate tangential direction we require.

At this stage we need to identify several types of subsets of S, along with special functions associated with them, in terms of some positive number ϵ . The set of all points in S that are less than ϵ from the z-axis is denoted by S_{ϵ} ; that is

$$
S_{\epsilon} = \{ (x, y, z) \in S : x^2 + y^2 < \epsilon^2 \}. \tag{4.1}
$$

A component of some S_{ϵ} that intersects the z-axis, is a proper subset of S, on whose closure we have $\hat{n} \cdot \hat{z} \neq 0$, is called a *polar cap*. Such a set containing the point $(0, 0, z_k) \in \mathbb{R}^3$ would be written as S_{ϵ}^k , where k might be any convenient indexing integer. Given a polar cap S_{ϵ}^{k} , we can obtain a *polar cutoff function* $\zeta \in C_0^\infty(S; \mathbb{R})$ associated with it that satisfies the following conditions:

- (1) $\zeta|_{S_{\epsilon}^k} = 1;$ $\ddot{\epsilon}$ (4.2)
- (2) for some $\epsilon' > 0$, ζ has compact support in the polar cap $S_{\epsilon+\epsilon'}^k$.

We call the polar cap $S_{\epsilon+\epsilon'}^k$ identified in (2) from [\(4.2\)](#page-20-0) the *polar support* of ζ associated with S_{ϵ}^{k} . Next, whenever the interior of the complement in S of some S_{ϵ} is connected, we call it a *nonpolar component*, and denote it by S_{ϵ}^{c} . With any such set we may associate a *nonpolar cutoff function*, taken as some $\zeta \in$ C_0^{∞} (S; R) for which the following hold:

(1) $\zeta|_{S_{\epsilon}^c} = 1;$ ϵ (2) whenever $(0, 0, z_k) \in S$, there is positive $\epsilon' < \epsilon$ such that $\zeta|_{S_{\epsilon'}^k} = 0$. (4.3)

We call the interior of the compliment in S of the union of the polar caps S_{ϵ}^k identified in (2) from [\(4.3\)](#page-20-1) the *nonpolar support* of ζ associated with S_{ϵ}^c (we take S itself whenever there are no poles). We note that this set is necessarily connected, and contains the closure of S_{ϵ}^{c} . We assert the existence of the cutoff functions described in [\(4.2](#page-20-0)[-4.3\)](#page-20-1), along with their associated supports, for any instance of either a polar cap or nonpolar component without including available proofs. With these terms and definitions at hand, our regularity arguments for the general case can be carried out by using exactly one nonpolar component of S, along with at most two polar caps which overlap it.

The work in this section will require the use of more than one type of parameterization for subsets of S. For this reason, we shall at times revert to writing A_0 for our fixed magnetic vector potential, particularly whenever the result of interest is applicable independent of the parameterization choice.

We begin by showing that any z-intercept in the domain is contained in a polar cap on which the needed regularity condition holds.

Theorem 4.1. *Suppose that* $(0, 0, z_0) \in S$, $\psi \in H^1(S; \mathbb{C})$, $\lambda \in [0, \infty)$ and

$$
L_{\lambda}(\psi, v) = 0 \quad for all $v \in H^1(S; \mathbb{C}).$ (4.4)
$$

Then, for every polar cap $S^0_\epsilon \subseteq S$, we have $\psi \in H^2(S^0_\epsilon;\mathbb{C})$.

The proof of Theorem [4.1](#page-20-2) (and subsequent arguments) requires several background results, which we present next in the following lemmas.

Lemma 4.2. *Suppose that* $\psi \in H^1(S; \mathbb{C})$ *and* $\lambda \in [0, \infty)$ *together satisfy* ([4.4](#page-20-3)), $U \subseteq S$ *is the polar (nonpolar) support of a polar (nonpolar) cutoff function* ζ *associated with some polar cap (nonpolar component) in* S, and let $u = \zeta \psi$. *Then, for all* $v \in H^1(S; \mathbb{C})$ *we have*

$$
\langle (i\nabla + \mathbf{A}_0)u, (i\nabla + \mathbf{A}_0)v \rangle_U - \lambda \langle u, v \rangle_U \le K ||v||_U. \tag{4.5}
$$

Proof. Let $v \in H^1(S; \mathbb{C})$. From the product rule, we get

$$
(i\nabla + \mathbf{A}_0)u = (i\nabla + \mathbf{A}_0)(\zeta\psi) = \zeta(i\nabla + \mathbf{A}_0)\psi + i\psi\nabla\zeta
$$
 (4.6)

to obtain the formula

$$
\zeta(i\nabla + \mathbf{A}_0)\psi = (i\nabla + \mathbf{A}_0)u - i\psi\nabla\zeta,
$$
\n(4.7)

which is valid a.e. on S. We next work from the equation $L_{\lambda}(\psi, \zeta v) = 0$. Since

$$
(i\nabla + \mathbf{A}_0)(\zeta v) = \zeta(i\nabla + \mathbf{A}_0)v + iv\nabla\zeta,
$$
\n(4.8)

it follows that

$$
\langle (i\nabla + \mathbf{A}_0)\psi, (i\nabla + \mathbf{A}_0)(\zeta v) \rangle
$$

= \langle \zeta(i\nabla + \mathbf{A}_0)\psi, (i\nabla + \mathbf{A}_0)v \rangle - \langle i\nabla \zeta(i\nabla + \mathbf{A}_0)\psi, v \rangle. (4.9)

It is clear that

$$
\langle \psi, \zeta v \rangle = \langle u, v \rangle, \tag{4.10}
$$

so [\(4.7\)](#page-21-0), [\(4.9\)](#page-21-1), and [\(4.10\)](#page-21-2), and the L_{λ} -identity noted above together give

$$
L_{\lambda}(u,v) = \langle i \psi \nabla \zeta, (i \nabla + \mathbf{A}_0)v \rangle + \langle i \nabla \zeta (i \nabla + \mathbf{A}_0)\psi, v \rangle. \tag{4.11}
$$

To the first term on the right hand side of (4.11) we apply Theorem [A.5](#page-43-3) in the appendix, and find that

$$
\langle i\,\psi\,\nabla\zeta, (i\,\nabla + \mathbf{A}_0)v \rangle = \langle i(i\,\nabla + \mathbf{A}_0)(\psi\,\nabla\zeta), v \rangle
$$

=\langle i\,\nabla\zeta(i\,\nabla + \mathbf{A}_0)\psi, v \rangle - \langle \psi\,\Delta\zeta, v \rangle, (4.12)

whence (4.12) substituted into (4.11) yields

$$
L_{\lambda}(u,v) = 2\langle i \nabla \zeta(i \nabla + \mathbf{A}_0)\psi, v \rangle - \langle \psi \Delta \zeta, v \rangle.
$$
 (4.13)

Utilizing the properties of ζ allows us to restrict the domain of integration on both sides of (4.13) to U, which in turn leads to the inequality

$$
\langle (i\nabla + \mathbf{A}_0)u, (i\nabla + \mathbf{A}_0)v \rangle_U - \lambda \langle u, v \rangle_U
$$

\n
$$
\leq 2|\langle \nabla \zeta(i\nabla + \mathbf{A}_0)\psi, v \rangle_U| + |\langle \psi \Delta \zeta, v \rangle_U|.
$$
\n(4.14)

The properties of ζ and ψ allow for the use of Hölder's inequality to obtain [\(4.5\)](#page-21-6) from [\(4.14\)](#page-22-0). \Box

Two slightly different discrete integration by parts formulas are listed next. These are stated in terms of the difference operator $\delta_{\hat{w}}^h$, which we define for functions mapping \mathbb{R}^2 into C. Given such a function f, some $h \neq 0$, and a unit vector $\hat{w} \in \mathbb{R}^2$, we let

$$
\delta_{\hat{w}}^h f(\mathbf{x}) = \frac{f(\mathbf{x} + \hat{w}h) - f(\mathbf{x})}{h}, \quad \mathbf{x} \in \mathbb{R}^2.
$$
 (4.15)

When working on a polar support, a standard proof that we will not repeat here is available; indeed the following lemma amounts to a straightforward adaptation of a result from Section 5:8:2 of [\[9\]](#page-41-10).

Lemma 4.3. Let $\hat{w} \in \mathbb{R}^2$ be a unit vector, let $V \subseteq \mathbb{R}^2$ be open, and let

 $u, v \colon \mathbb{R}^2 \longrightarrow \mathbb{C}.$

Suppose that $u, v \in L^2(V; \mathbb{C})$, and that v has compact support in V. Then, for all *nonzero h of sufficiently small absolute value we have*

$$
\langle u, \delta^h_{\hat{w}} v \rangle_V = -\langle \delta^{-h}_{\hat{w}} u, v \rangle_V. \tag{4.16}
$$

On a nonpolar support, in accordance with the method of tangential difference quotients we shall only require a $\hat{w} = \hat{\theta}$ version of [\(4.16\)](#page-22-1). Periodicity in the θ -parameter allows us to relax the requirements in Lemma [4.3](#page-22-2) somewhat. Moreover, due to the rotational symmetry of S , we are able to more conveniently state the result in terms of a surface inner product.

Lemma 4.4. Let $U \subseteq S$ be a nonpolar support in S, and let $u, v \in L^2(U; \mathbb{C})$. *en, for all nonzero* h *we have*

$$
\langle u, \delta^h_{\hat{\theta}} v \rangle_U = -\langle \delta^{-h}_{\hat{\theta}} u, v \rangle_U. \tag{4.17}
$$

Proof. Let $h \neq 0$. We may assume that U is given by the standard parameterization on $J \times [0, 2\pi)$, where $J \subseteq I$ is an interval. Also, working from the parametric versions of u and v on this domain, we use their known 2π -periodicity in θ to extend each to $J \times \mathbb{R}$ in the natural way. Let us first suppose that u and v lie in $C^k(\overline{U};\mathbb{C})$, for each $k \in \mathbb{N}_0$. In terms of the standard parameterization of S, from (4.15) we obtain

$$
\delta_{\hat{\theta}}^h v(s,\theta) = \frac{v(s,\theta+h) - v(s,\theta)}{h}
$$
 (4.18a)

and

$$
\delta_{\hat{\theta}}^{-h}u(s,\theta) = -\frac{u(s,\theta - h) - u(s,\theta)}{h}.
$$
\n(4.18b)

Since u and v are both periodic in θ , we find that each term in each of the quo-tients in [\(4.18\)](#page-23-0), along with the quotients themselves, also lie in $C^k(\overline{U}; \mathbb{C})$, for each $k \in \mathbb{N}_0$. The first terms of the left and right hand sides of [\(4.17\)](#page-22-4), respectively, can be written as

$$
\int\limits_{U} u \, \overline{\delta_{\hat{\theta}}^{h} v} \, dx = \int\limits_{J} \left(\int\limits_{0}^{2\pi} u(s, \theta) \, \frac{\overline{v}(s, \theta + h) - \overline{v}(s, \theta)}{h} d\theta \right) R \sqrt{R_s^2 + Z_s^2} ds \quad (4.19)
$$

and

$$
-\int\limits_{U} \delta_{\hat{\theta}}^{-h} u \,\bar{v} \,dx = \int\limits_{J} \left(\int\limits_{0}^{2\pi} \frac{u(s,\theta - h) - u(s,\theta)}{h} \bar{v}(s,\theta) \,d\theta \right) R \sqrt{R_s^2 + Z_s^2} ds, \tag{4.20}
$$

so we have

$$
\int_{U} u \overline{\delta_{\hat{\theta}}^{h} v} dx + \int_{U} \delta_{\hat{\theta}}^{-h} u \overline{v} dx
$$
\n
$$
= \frac{1}{h} \int_{J} \left(\int_{0}^{2\pi} u(s, \theta) \overline{v}(s, \theta + h) - u(s, \theta - h) \overline{v}(s, \theta) d\theta \right) R \sqrt{R_{s}^{2} + Z_{s}^{2}} ds.
$$
\n(4.21)

If we focus on the second term in the inner integral on the right hand side of [\(4.21\)](#page-23-1), when substituting $\theta + h$ for θ and invoking periodicity we find that

$$
\int_{0}^{2\pi} u(s,\theta - h)\bar{v}(s,\theta) \,d\theta = \int_{0}^{2\pi} u(s,\theta)\bar{v}(s,\theta + h) \,d\theta,\tag{4.22}
$$

which when taken with (4.21) implies that

$$
\int\limits_{U} u \, \overline{\delta_{\hat{\theta}}^{h} v} \, dx + \int\limits_{U} \delta_{\hat{\theta}}^{-h} u \, \overline{v} \, dx = 0. \tag{4.23}
$$

A similar argument shows that

$$
\int\limits_{U} \overline{u} \, \delta^h_{\hat{\theta}} v \, dx + \int\limits_{U} \overline{\delta_{\hat{\theta}}^{-h} u} \, v \, dx = 0, \tag{4.24}
$$

then (4.23) and (4.24) together imply (4.17) . Finally, we extend this result by continuity to admit arguments from $L^2(U; \mathbb{C})$, and the proof is complete. \Box

We next include some difference quotient inequalities, again adapted from standard results widely available in many sources from the partial differential equations literature.

Lemma 4.5. *Let* $\hat{w} \in \mathbb{R}^2$ *be a unit vector, let* $V \subseteq \mathbb{R}^2$ *be open, let* $u: \mathbb{R}^2 \to \mathbb{C}$ *, and* suppose that *u* has compact support in V *.* If $u \in H^1(V; \mathbb{C})$, then for all nonzero h *of suciently small absolute value we have*

$$
\|\delta_{\hat{w}}^h u\|_{V} \le K \|\partial_{\hat{w}} u\|_{V},\tag{4.25}
$$

where $\partial_{\hat{w}} u$ *is the directional derivative of* u *along* \hat{w} *. On the other hand, if* $u \in$ $L^2(V; \mathbb{C})$ and $\|\delta^h_{\hat{w}}u\|_V \leq K_1$ for all nonzero h of sufficiently small absolute value, *then* $u \in H^1(V; \mathbb{C})$ and

$$
\|\partial_{\hat{w}} u\|_{V} \le K_1. \tag{4.26}
$$

Lemma [4.5](#page-24-2) will be used when working on a polar support. On a nonpolar support, again we need only work with $\delta^h_{\hat{\theta}} u$, and can again omit the compact support requirement.

Lemma 4.6. Let $U \subseteq S$ be a nonpolar support in S, given by the standard param*eterization on some* $V = J \times [0, 2\pi)$ where $J \subseteq I$ *is an interval. If* $u \in H^1(V; \mathbb{C})$, then after extending u to the domain $J \times \mathbb{R}$ by periodicity in the natural way, for *all nonzero* h *we have*

$$
\|\delta_{\hat{\theta}}^h u\|_{V} \le K \left\|\frac{\partial u}{\partial \theta}\right\|_{V}.
$$
\n(4.27)

On the other hand, if $u \in L^2(V; \mathbb{C})$ *and after periodically extending u to the* d omain $J \times \mathbb{R}$ we have $\|\delta^h_{\hat{\theta}} u\|_V \leq K_1$ for all nonzero h , then $u \in H^1(V;\mathbb{C})$ and

$$
\left\|\frac{\partial u}{\partial \theta}\right\|_{V} \le K_{1}.\tag{4.28}
$$

As mentioned, the standard surface parameterization is not suitable for analysis within polar caps in S. In these cases, we shall work instead with a mapping of the form

$$
\mathbf{x}(p,q) = [p,q, Z(p,q)],\tag{4.29}
$$

where $Z: \mathbb{R}^2 \to \mathbb{R}$. By definition, any polar cap in S can be parameterized by restricting a function of the form [\(4.29\)](#page-25-0) to some open, circular disk $D \subseteq \mathbb{R}^2$ centered at the origin. Moreover, since polar caps are surfaces of revolution with respect to the z-axis, we must have

$$
qZ_p = pZ_q \quad \text{on } D. \tag{4.30}
$$

Furthermore, the properties of S allow us to assume that $Z \in C^2(\overline{D}; \mathbb{R})$. Now, by following a procedure analogous to that demonstrated in Section [2,](#page-3-0) we can express the gradient of a function v defined on a polar cap parameterized through some instance of (4.29) as

$$
\nabla v = \frac{\hat{p}}{\sqrt{1 + Z_p^2}} \Big(v_p + \frac{2Z_p Z_q}{1 + Z_p^2 + Z_q^2} v_q \Big) + \frac{\hat{q}}{\sqrt{1 + Z_q^2}} \Big(\frac{2Z_p Z_q}{1 + Z_p^2 + Z_q^2} v_p + v_q \Big),\tag{4.31}
$$

where

$$
\hat{p} = \frac{\hat{x} + \hat{z}Z_p}{\sqrt{1 + Z_p^2}}, \text{ and } \hat{q} = \frac{\hat{y} + \hat{z}Z_q}{\sqrt{1 + Z_q^2}}.
$$
\n(4.32)

When using this parameterization for integration, we include the surface element

$$
\sqrt{1 + Z_p^2 + Z_q^2},\tag{4.33}
$$

which enjoys the useful property of being bounded above and below on D by positive constants. Also, we have the following:

Lemma 4.7. Let U be a polar support in S, parameterized on some disk $D \subseteq \mathbb{R}^2$ *through (*[4.29](#page-25-0)*).*

1. If
$$
v \in L^2(U; \mathbb{C})
$$
, then its parametric composition lies in $L^2(D; \mathbb{C})$, and
2. If $v \in H^1(U; \mathbb{C})$, then its parametric composition lies in $H^1(D; \mathbb{C})$.
(4.34)

Proof. To show 1, we let $v \in L^2(U; \mathbb{C})$ and find that

$$
||v||_D^2 = 2 \int_D |v|^2 dx
$$

\n
$$
\leq 2 \int_D \sqrt{1 + Z_p^2 + Z_q^2} |v|^2 dx
$$

\n
$$
= 2 \int_U |v|^2 dx
$$

\n
$$
= ||v||^2 < \infty.
$$

\n(4.35)

For 2, we let $v \in H^1(U; \mathbb{C})$ and make use of the formulas

$$
v_p = v_x + v_z Z_p
$$
 and $v_q = v_y + v_z Z_q$. (4.36)

We then have

$$
||v_p||_D^2 = 2 \int_D |v_x + v_z Z_p|^2 dx
$$

\n
$$
\leq K \int_D \sqrt{1 + Z_p^2 + Z_q^2} (|v_x|^2 + |v_z|^2) dx
$$

\n
$$
\leq K \Biggl(\int_U |v_x|^2 dx + \int_U |v_z|^2 dx\Biggr)
$$

\n
$$
< \infty.
$$
\n(4.37)

In a similar way, we find that $||v_q||$ 2 $_D^2 < \infty$, which together with [\(4.37\)](#page-26-0) and [\(4.35\)](#page-26-1) implies the result.

We shall make use of the ellipticity condition established in the next lemma.

Lemma 4.8. Let U be a polar support in S, parameterized on some disk $D \subseteq \mathbb{R}^2$ *through* ([4.29](#page-25-0)), and let $v \in H^1(U; \mathbb{C})$. Then, we have

$$
|\nabla v|^2 \ge K(|v_p|^2 + |v_q|^2) \quad a.e. \text{ on } D. \tag{4.38}
$$

Proof. By Part 2 of Lemma [4.7,](#page-25-1) we know that the parameterized version of v lies in $H^1(D; \mathbb{C})$. Working a.e. on D, we first seek to show that

$$
|\nabla v|^2 \ge K(|f|^2 + |g|^2),\tag{4.39}
$$

where

$$
f = v_p + \frac{2Z_p Z_q}{1 + Z_p^2 + Z_q^2} v_q \quad \text{and} \quad g = \frac{2Z_p Z_q}{1 + Z_p^2 + Z_q^2} v_p + v_q. \tag{4.40}
$$

By [\(4.31\)](#page-25-2) and [\(4.32\)](#page-25-3), we get

$$
|\nabla v|^2 = \frac{1}{1 + Z_p^2} |f|^2 + \frac{1}{1 + Z_q^2} |g|^2 + \frac{Z_p Z_q}{(1 + Z_p^2)(1 + Z_q^2)} (f\bar{g} + \bar{f}g). \tag{4.41}
$$

An application of the formula

$$
\pm ab(c\bar{d} + \bar{c}d) \ge -(a^2|c|^2 + b^2|d|^2), \quad a, b \in \mathbb{R} \text{ and } c, d \in \mathbb{C}, \qquad (4.42)
$$

to the last term on the right hand side of [\(4.41\)](#page-27-0) shows that

$$
|\nabla v|^2 \ge \frac{1}{1 + Z_p^2} |f|^2 + \frac{1}{1 + Z_q^2} |g|^2 - \frac{Z_p^2}{(1 + Z_p^2)^2} |f|^2 - \frac{Z_q^2}{(1 + Z_q^2)^2} |g|^2
$$

=
$$
\frac{1}{(1 + Z_p^2)^2} |f|^2 + \frac{1}{(1 + Z_q^2)^2} |g|^2,
$$
 (4.43)

whence [\(4.39\)](#page-27-1) holds since Z_p and Z_q are bounded on D. To complete the proof, it is enough to now establish that

$$
|f|^{2} + |g|^{2} \ge K(|v_{p}|^{2} + |v_{q}|^{2})
$$
\n(4.44)

a.e. on D. From the formulas

$$
|f|^{2} = |v_{p}|^{2} + \frac{4Z_{p}^{2}Z_{q}^{2}}{(1 + Z_{p}^{2} + Z_{q}^{2})^{2}}|v_{q}|^{2}
$$

+
$$
sgn(Z_{p}Z_{q})\frac{2|Z_{p}||Z_{q}|}{1 + Z_{p}^{2} + Z_{q}^{2}}(v_{p}\overline{v_{q}} + \overline{v_{p}}v_{q})
$$
(4.45)

and

$$
|g|^{2} = \frac{4Z_{p}^{2}Z_{q}^{2}}{(1+Z_{p}^{2}+Z_{q}^{2})^{2}}|v_{p}|^{2} + |v_{q}|^{2}
$$

+
$$
\text{sgn}(Z_{p}Z_{q})\frac{2|Z_{p}||Z_{q}|}{1+Z_{p}^{2}+Z_{q}^{2}}(v_{p}\overline{v_{q}} + \overline{v_{p}}v_{q}),
$$
(4.46)

it follows that

$$
|f|^{2} + |g|^{2} = \left(1 + \frac{4Z_{p}^{2}Z_{q}^{2}}{(1 + Z_{p}^{2} + Z_{q}^{2})^{2}}\right)(|v_{p}|^{2} + |v_{q}|^{2})
$$

+
$$
sgn(Z_{p}Z_{q}) \frac{4|Z_{p}||Z_{q}|}{1 + Z_{p}^{2} + Z_{q}^{2}}(v_{p}\overline{v_{q}} + \overline{v_{p}}v_{q}).
$$
 (4.47)

Another application of [\(4.42\)](#page-27-2) then gives

$$
|f|^{2} + |g|^{2} \ge \left(1 + 4\left[\left(\frac{|Z_{p}| |Z_{q}|}{1 + Z_{p}^{2} + Z_{q}^{2}}\right)^{2} - \frac{|Z_{p}| |Z_{q}|}{1 + Z_{p}^{2} + Z_{q}^{2}}\right]\right)(|v_{p}|^{2} + |v_{q}|^{2}),\tag{4.48}
$$

and upon completing the square we obtain

$$
|f|^2 + |g|^2 \ge K \Big(\frac{|Z_p||Z_q|}{1 + Z_p^2 + Z_q^2} - \frac{1}{2} \Big)^2 (|v_p|^2 + |v_q|^2). \tag{4.49}
$$

Since

$$
\Big(\frac{|Z_p||Z_q|}{1+Z_p^2+Z_q^2}-\frac{1}{2}\Big)^2
$$

has a positive lower bound on D, we obtain [\(4.44\)](#page-27-3) and the proof is complete. \Box

We next present several lemmas that allow for the isolation of critical terms in the product

$$
\langle (i\nabla + \mathbf{A}_0)u, (i\nabla + \mathbf{A}_0)(-\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u) \rangle_U \tag{4.50}
$$

whenever u, U is a pairing of the polar type indicated in Lemma [4.2,](#page-21-7) and $\hat{w} = \hat{p}$ or \hat{q} . In [\(4.50\)](#page-28-0) and what follows, we use the more general representation of the magnetic vector potential A_0 , rather than its realization in the standard parameterization. We work from the formula

$$
\langle (i \nabla + \mathbf{A}_0)u, (i \nabla + \mathbf{A}_0)(-\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u) \rangle_U
$$

= -\langle \nabla u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u) \rangle_U - \langle i \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U
+ \langle i \mathbf{A}_0 u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u) \rangle_U - \langle |\mathbf{A}_0|^2 u, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U, (4.51)

and carry out in each of the four terms on the right hand side a discrete integration by parts, as needed in order to use (4.5) to find bounds sufficient to conclude higher regularity in polar regions.

Lemma 4.9. Let U be a polar support in S, $\hat{w} \in \mathbb{R}^2$ be a unit vector, $u \in$ $H¹(U; \mathbb{C})$, and suppose that u has compact support in U. Then, for all nonzero h of sufficiently small absolute value we have

$$
|\langle |\mathbf{A}_0|^2 u, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U| \le K. \tag{4.52}
$$

Proof. We first obtain a parameterization of the form (4.29) that yields U on some open disk $D \subseteq \mathbb{R}^2$. Since u has compact support in U, its parametric version has compact support in D . We extend this function by assigning the value of 0 outside of D , and with the help of Lemma [4.7](#page-25-1) know that what results must belong to $H^1(D; \mathbb{C})$. Of course $\sqrt{1+Z_p^2+Z_q^2}|\mathbf{A}_0|^2u$ enjoys the same properties, so when applying Lemma 4.3 and Hölder's inequality we find that

$$
\begin{split} |\langle |\mathbf{A}_{0}|^{2} u, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u \rangle_{U}| &= \left| \langle \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} |\mathbf{A}_{0}|^{2} u, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u \rangle_{D} \right| \\ &= \left| \langle \delta_{\hat{w}}^{h} (\sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} |\mathbf{A}_{0}|^{2} u), \delta_{\hat{w}}^{h} u \rangle_{D} \right| \\ &\leq \left\| \delta_{\hat{w}}^{h} (\sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} |\mathbf{A}_{0}|^{2} u) \right\|_{D} \left\| \delta_{\hat{w}}^{h} u \right\|_{D} \end{split} \tag{4.53}
$$

for all nonzero h of sufficiently small absolute value. Now, an application of (4.25) from Lemma [4.5](#page-24-2) to each of the two resulting factors on the right hand side of [\(4.53\)](#page-29-0) \Box yields the result.

The bounding criteria of the next two terms on the right hand side of (4.51) are conveniently combined in the next lemma.

Lemma 4.10. Let U be a polar support in S parameterized on some disk $D \subseteq \mathbb{R}^2$ through ([4.29](#page-25-0)), let $\hat{w} \in \mathbb{R}^2$ *be a unit vector,* $u \in H^1(U; \mathbb{C})$ *, and suppose that* u *has compact support in U. Then, for each* $\epsilon > 0$ *we have*

$$
|\langle i \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U - \langle i \mathbf{A}_0 u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u) \rangle_U|
$$

\n
$$
\leq K_{\epsilon} + \epsilon (\|\delta_{\hat{w}}^h u_p\|_D^2 + \|\delta_{\hat{w}}^h u_q\|_D^2)
$$
\n(4.54)

for all nonzero h of sufficiently small absolute value.

Proof. Let $\epsilon > 0$. It is convenient to use the representation

$$
\nabla v = \mathbf{f} v_p + \mathbf{g} v_q,\tag{4.55}
$$

where from (4.31) we identify

$$
\mathbf{f} = \hat{p} \frac{1}{\sqrt{1 + Z_p^2}} + \hat{q} \frac{2Z_p Z_q}{\sqrt{1 + Z_q^2} (1 + Z_p^2 + Z_q^2)},
$$
(4.56)

and

$$
\mathbf{g} = \hat{q} \frac{1}{\sqrt{1 + Z_q^2}} + \hat{p} \frac{2Z_p Z_q}{\sqrt{1 + Z_p^2} (1 + Z_p^2 + Z_q^2)}.
$$
(4.57)

As in our last proof, we reason that since u has compact support in U, its parametric version has compact support in D ; we then extend this function by assigning the value of 0 outside of D, and the result belongs to $H^1(D; \mathbb{C})$ by Lemma [4.7.](#page-25-1) Beginning with the second term in the absolute value on the left hand side of [\(4.54\)](#page-29-1), since both $i\sqrt{1+Z_p^2+Z_q^2\mathbf{A}_0u\cdot\mathbf{f}}$ and $i\sqrt{1+Z_p^2+Z_q^2\mathbf{A}_0u\cdot\mathbf{g}}$ belong to $H^1(D;\mathbb{C})$ with compact support in D , Lemma [4.3](#page-22-2) and Hölder's inequality allow that

$$
|\langle i \mathbf{A}_{0} u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u) \rangle_{U}|
$$
\n
$$
= |\langle i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u, \mathbf{f} (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u)_{p} + \mathbf{g} (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u)_{q} \rangle_{D}|
$$
\n
$$
\leq |\langle i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{f}, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u_{p} \rangle_{D}|
$$
\n
$$
+ |\langle i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{g}, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u_{q} \rangle_{D}|
$$
\n
$$
\leq |\langle \delta_{\hat{w}}^{h} (i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{f}), \delta_{\hat{w}}^{h} u_{p} \rangle_{D}|
$$
\n
$$
+ |\langle \delta_{\hat{w}}^{h} (i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{g}), \delta_{\hat{w}}^{h} u_{q} \rangle_{D}|
$$
\n
$$
\leq |\delta_{\hat{w}}^{h} (i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{f})|_{D} |\delta_{\hat{w}}^{h} u_{p}||_{D}
$$
\n
$$
+ |\delta_{\hat{w}}^{h} (i \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \mathbf{A}_{0} u \cdot \mathbf{g})|_{D} |\delta_{\hat{w}}^{h} u_{q}||_{D}
$$

for all nonzero h of sufficiently small absolute value. After using Lemma 4.5 to find bounds for the first factor in each resulting term, then applying Young's inequality, we may conclude for all such h that

$$
|\langle i\mathbf{A}_0 u, \nabla(\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u)\rangle_U| \le K_{1,\epsilon} + \frac{\epsilon}{2} (\|\delta_{\hat{w}}^h u_p\|_D^2 + \|\delta_{\hat{w}}^h u_q\|_D^2). \tag{4.59}
$$

Moving to the next term, since the parametric version of ∇u has compact support in D, so must $i\sqrt{1+Z_p^2+Z_q^2}\nabla u\cdot\mathbf{A_0}$, and we can again apply Lemma [4.3](#page-22-2) to find that

$$
|\langle i \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U| = |\langle i \sqrt{1 + Z_p^2 + Z_q^2} \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_D|
$$

= $|\langle \delta_{\hat{w}}^h (i \sqrt{1 + Z_p^2 + Z_q^2} \nabla u \cdot \mathbf{A}_0), \delta_{\hat{w}}^h u \rangle_D|.$ (4.60)

Here, we assert that, a.e. on D,

$$
\delta_{\hat{w}}^{h}(i\sqrt{1+Z_{p}^{2}+Z_{q}^{2}}\nabla u\cdot\mathbf{A}_{0})=F_{1}u_{p}+F_{2}u_{q}+F_{3}\delta_{\hat{w}}^{h}u_{p}+F_{4}\delta_{\hat{w}}^{h}u_{q},\quad(4.61)
$$

where

$$
F_1 = i\left[\sqrt{1+Z_p^2+Z_q^2}\mathbf{A}_0\cdot\delta_{\hat{w}}^h\mathbf{f} + \mathbf{f}\cdot\delta_{\hat{w}}^h\left(\sqrt{1+Z_p^2+Z_q^2}\mathbf{A}_0\right)\right],\tag{4.62a}
$$

$$
F_2 = i\left[\sqrt{1+Z_p^2+Z_q^2}\mathbf{A}_0\cdot\delta_{\hat{w}}^h\mathbf{g} + \mathbf{g}\cdot\delta_{\hat{w}}^h(\sqrt{1+Z_p^2+Z_q^2}\mathbf{A}_0)\right],\qquad(4.62b)
$$

$$
F_3 = i\sqrt{1 + Z_p^2 + Z_q^2} \mathbf{A}_0 \cdot \mathbf{f},\tag{4.62c}
$$

and

$$
F_4 = i\sqrt{1 + Z_p^2 + Z_q^2} \mathbf{A}_0 \cdot \mathbf{g}.
$$
 (4.62d)

It follows that

$$
\sup_{x \in D} |F_j| \le K, \quad j = 1, 2, 3, 4,
$$
\n(4.63)

whence from (4.60) we obtain

$$
|\langle i \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U| \leq K \|\delta_{\hat{w}}^h u\|_D (\|u_p\|_D + \|u_q\|_D + \|\delta_{\hat{w}}^h u_p\|_D + \|\delta_{\hat{w}}^h u_q\|_D)
$$
\n(4.64)

for all nonzero h of sufficiently small absolute value. Now Lemma 4.5 , the properties of u , and Young's inequality together allow that

$$
|\langle i \nabla u \cdot \mathbf{A}_0, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u \rangle_U| \le K_{2,\epsilon} + \frac{\epsilon}{2} (\|\delta_{\hat{w}}^h u_p\|_D^2 + \|\delta_{\hat{w}}^h u_q\|_D^2),\tag{4.65}
$$

which when combined with [\(4.59\)](#page-30-1) and the triangle inequality yields the result. \Box

Regarding the highest order term in [\(4.51\)](#page-28-1), we have the following:

Lemma 4.11. Let U be a polar support in S parameterized on some disk $D \subseteq \mathbb{R}^2$ through ([4.29](#page-25-0)), let $\hat{w} \in \mathbb{R}^2$ *be a unit vector,* $u \in H^1(U; \mathbb{C})$ *, and suppose that* u *has compact support in U. Then, for all nonzero h of sufficiently small absolute value we have*

$$
K_1(\|\delta_{\hat{w}}^h u_p\|_D^2 + \|\delta_{\hat{w}}^h u_q\|_D^2) \le -\langle \nabla u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u) \rangle_U + K_2. \tag{4.66}
$$

Proof. As in the previous lemmas, we can apply Lemma [4.3](#page-22-2) to obtain

$$
-\langle \nabla u, \nabla (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u) \rangle_{U}
$$

\n
$$
= -\langle \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \nabla u, \mathbf{f} (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u)_{p} + \mathbf{g} (\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u)_{q} \rangle_{D}
$$

\n
$$
= -\langle \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \nabla u \cdot \mathbf{f}, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u_{p} \rangle_{D}
$$

\n
$$
-\langle \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \nabla u \cdot \mathbf{g}, \delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u_{q} \rangle_{D}
$$

\n
$$
= \langle \delta_{\hat{w}}^{h} (\sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \nabla u \cdot \mathbf{f}), \delta_{\hat{w}}^{h} u_{p} \rangle_{D}
$$

\n
$$
+ \langle \delta_{\hat{w}}^{h} (\sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} \nabla u \cdot \mathbf{g}), \delta_{\hat{w}}^{h} u_{q} \rangle_{D}
$$

\n(4.67)

for all h of sufficiently small absolute value, where we used (4.55) – (4.57) to represent the gradient of the second difference quotient of u on U . Applying the product rule of difference quotients, a.e. on D we have

$$
\delta_{\hat{w}}^h \left(\sqrt{1 + Z_p^2 + Z_q^2} \nabla u \cdot \mathbf{f} \right) = F + \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{f} \cdot \nabla (\delta_{\hat{w}}^h u) \tag{4.68a}
$$

and

$$
\delta_{\hat{w}}^h \left(\sqrt{1 + Z_p^2 + Z_q^2} \nabla u \cdot \mathbf{g} \right) = G + \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{g} \cdot \nabla (\delta_{\hat{w}}^h u), \tag{4.68b}
$$

where

$$
F = \delta_{\hat{w}}^h \left(\sqrt{1 + Z_p^2 + Z_q^2} \mathbf{f} \right) \cdot \nabla u + \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{f} \cdot (u_p \delta_{\hat{w}}^h \mathbf{f} + u_q \delta_{\hat{w}}^h \mathbf{g})
$$
 (4.69a) and

$$
G = \delta_{\hat{w}}^h \left(\sqrt{1 + Z_p^2 + Z_q^2} \mathbf{g} \right) \cdot \nabla u + \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{g} \cdot (u_p \delta_{\hat{w}}^h \mathbf{f} + u_q \delta_{\hat{w}}^h \mathbf{g}).
$$
\n(4.69b)

Owed to the properties of f , g , Z and u , we assert here that

$$
|\langle F, \delta_{\hat{w}}^h u_p \rangle_D| \le K \|\delta_{\hat{w}}^h u_p\|_D, \text{ and } |\langle G, \delta_{\hat{w}}^h u_q \rangle_D| \le K \|\delta_{\hat{w}}^h u_q\|_D. \tag{4.70}
$$

Now, when combining [\(4.70\)](#page-32-0) with [\(4.67\)](#page-31-0) and [4.68\)](#page-32-1) and applying Young's inequality, we find that

$$
\begin{split} \left\langle \sqrt{1+Z_{p}^{2}+Z_{q}^{2}}\mathbf{f}\cdot\nabla(\delta_{\hat{w}}^{h}u),\delta_{\hat{w}}^{h}u_{p}\right\rangle _{D}+\left\langle \sqrt{1+Z_{p}^{2}+Z_{q}^{2}}\mathbf{g}\cdot\nabla(\delta_{\hat{w}}^{h}u),\delta_{\hat{w}}^{h}u_{q}\right\rangle _{D} \\ \leq-\left\langle \nabla u,\nabla(\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^{h}u)\right\rangle _{U}+K_{\epsilon}+\epsilon(\|\delta_{\hat{w}}^{h}u_{p}\|_{D}^{2}+\|\delta_{\hat{w}}^{h}u_{q}\|_{D}^{2}) \end{split} \tag{4.71}
$$

for all nonzero h of sufficiently small absolute value, where $\epsilon > 0$ is arbitrary. But,

$$
\langle \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{f} \cdot \nabla(\delta_{\hat{w}}^h u), \delta_{\hat{w}}^h u_p \rangle_D + \langle \sqrt{1 + Z_p^2 + Z_q^2} \mathbf{g} \cdot \nabla(\delta_{\hat{w}}^h u), \delta_{\hat{w}}^h u_q \rangle_D
$$

=\langle \sqrt{1 + Z_p^2 + Z_q^2} \nabla(\delta_{\hat{w}}^h u), \nabla(\delta_{\hat{w}}^h u) \rangle_D
= 2 \int \sqrt{1 + Z_p^2 + Z_q^2} |\nabla(\delta_{\hat{w}}^h u)|^2 dx
\ge \int \int |\nabla(\delta_{\hat{w}}^h u)|^2 dx, \tag{4.72}

then an application of Lemma [4.8](#page-26-2) in the case $v = \delta_{\hat{w}}^h u \in H^1(U; \mathbb{C})$ allows us to combine [\(4.71\)](#page-32-2) with [\(4.72\)](#page-32-3) to complete the proof.

The framework needed to prove Theorem 4.1 is now in place.

[4.1.](#page-20-2) Proof of Theorem 4.1. Given a polar cap S^0_ϵ , we first obtain a polar support U containing it, along with a corresponding polar cutoff function ζ . It is clear that the function u specified in Lemma [4.2](#page-21-7) is an element of $H^1(S; \mathbb{C})$, and if $\hat{w} \in \mathbb{R}^2$ is a unit vector, then using [\(4.5\)](#page-21-6) at $v = -\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^h u$ gives

$$
\langle (i\nabla + \mathbf{A}_0)u, (i\nabla + \mathbf{A}_0)(-\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u) \rangle_U = \lambda \langle u, -\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u \rangle_U + K \|\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u\|_U
$$
\n(4.73)

for all nonzero h of sufficiently small absolute value. Let us obtain a parameteri-zation of the form [\(4.29\)](#page-25-0) that yields U on some open disk $D \subseteq \mathbb{R}^2$. In the usual way, since u has compact support in U , its parametric version has compact support in D . We extend this function by assigning the value of 0 outside of D , then Lemma [4.7](#page-25-1) shows that the result belongs to $H^1(D; \mathbb{C})$. Using an argument similar to that detailed in Lemma 4.9 , we find a bound for the absolute value of the first term on the right hand side of (4.73) , apply Lemma [4.5](#page-24-2) to the second, then use Young's inequality to get

$$
\langle (i\nabla + \mathbf{A}_0)u, (i\nabla + \mathbf{A}_0)(-\delta_{\hat{w}}^{-h}\delta_{\hat{w}}^h u) \rangle_U \leq K + \frac{K_1}{4} \|\delta_{\hat{w}}^h\partial_{\hat{w}}u\|_D^2 \tag{4.74}
$$

for all such h , where K_1 is identified in [\(4.66\)](#page-31-1) after an appropriate application of Lemma 4.11 . Using Lemmas $4.9-4.11$ $4.9-4.11$ in conjunction with (4.51) , we then find by [\(4.74\)](#page-33-1) that

$$
\frac{K_1}{2}(\|\delta^h_{\hat{w}}u_p\|_D^2 + \|\delta^h_{\hat{w}}u_q\|_D^2) \leq K + \frac{K_1}{4}\|\delta^h_{\hat{w}}\partial_{\hat{w}}u\|_D^2, \tag{4.75}
$$

which when applied in the cases $\hat{w} = \hat{p}$ and $\hat{w} = \hat{q}$ shows that each of the quantities

$$
\|\delta_{\hat{p}}^h u_p\|_D^2, \quad \|\delta_{\hat{p}}^h u_q\|_D^2, \quad \|\delta_{\hat{q}}^h u_p\|_D^2, \quad \|\delta_{\hat{q}}^h u_q\|_D^2 \tag{4.76}
$$

are bounded independent of h , provided h is nonzero and of sufficiently small absolute value. We can now make a standard convergence argument. We choose any sequence $\{h_k\}$ convergent to zero from nonzero h of sufficiently small absolute value for which the above bounding criteria hold, then use weak sequential precompactness to extract weakly convergent subsequences from each of the corresponding sequences $\{\delta_p^{h_k}\}$ $_{\hat{p}}^{h_{k}}u_{p}\},$ $\{\delta_{\hat{p}}^{h_{k}}$ $_{\hat{p}}^{h_k}u_q \}, \ \{\delta^{h_k}_{\hat{q}}$ $\{\delta^{h_k}_{\hat{q}}\}_{\hat{q}}$ and $\{\delta^{h_k}_{\hat{q}}\}$ $\binom{n_k}{q}$ in the space $L^2(D; \mathbb{C})$. According to the definition of partial derivatives, the corresponding limits are clearly equal respectively to u_{pp} , u_{pq} , u_{qp} and u_{qq} in the same space (actually $u_{pq} = u_{qp}$ here), and we already know that $u \in H^1(D; \mathbb{C})$, so it follows that $u \in H^2(D; \mathbb{C})$. With this result at hand, it is no trouble to show that each of the nine second order partial derivatives of u with respect to the standard Euclidean coordinates belongs to the space $L^2(U; \mathbb{C})$. We rely upon the expressions

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$$
p_x = \frac{1 + Z_q^2}{1 + Z_p^2 + Z_q^2}, \quad p_y = \frac{Z_p Z_q}{1 + Z_p^2 + Z_q^2},
$$
(4.77a)

$$
p_z = \frac{Z_p}{1 + Z_p^2 + Z_q^2}, \quad q_x = \frac{Z_p Z_q}{1 + Z_p^2 + Z_q^2},
$$
(4.77b)

$$
q_y = \frac{1 + Z_p^2}{1 + Z_p^2 + Z_q^2}, \quad q_z = \frac{Z_q}{1 + Z_p^2 + Z_q^2},
$$
(4.77c)

all of which belong to the space $C^1(\overline{D}; \mathbb{C})$, and use the chain rule. For example, since a.e. on D we have

$$
u_{zy} = u_{zp}p_y + u_{zq}q_y
$$

= $(u_p p_z + u_q q_z)_{p} p_y + (u_p p_z + u_q q_z)_{q} q_y$
= $(u_{pp} p_z + u_p p_{zp} + u_{qp} q_z + u_q q_{zp}) p_y$
+ $(u_{pq} p_z + u_p p_{zq} + u_{qq} q_z + u_q q_{zq}) q_y,$ (4.78)

it is clear that

$$
|u_{zy}|^2 \le K(|u_{pp}|^2 + |u_{pq}|^2 + |u_{qp}|^2 + |u_{qq}|^2 + |u_p|^2 + |u_q|^2)
$$
 (4.79)

a.e. on D . Multiplying both sides of (4.79) by twice the surface element and integrating over D then shows that

$$
||u_{zy}||_{U}^{2} = 2 \int_{U} |u_{zy}|^{2} dx = 2 \int_{D} \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} |u_{zy}|^{2} dx
$$

\n
$$
\leq K \int_{D} \sqrt{1 + Z_{p}^{2} + Z_{q}^{2}} (|u_{pp}|^{2} + |u_{pq}|^{2} + |u_{qp}|^{2} + |u_{q}|^{2}) dx
$$

\n
$$
\leq K \int_{D} (|u_{pp}|^{2} + |u_{pq}|^{2} + |u_{qp}|^{2} + |u_{qq}|^{2} + |u_{p}|^{2} + |u_{q}|^{2}) dx
$$

\n
$$
< \infty,
$$

\n(4.80)

so that $u_{zy} \in L^2(U; \mathbb{C})$. Lastly, the conclusion that actually $\psi \in H^2(S^0_{\epsilon}; \mathbb{C})$ follows because $S_{\epsilon}^0 \subseteq U$, and $u|_{S_{\epsilon}^0} = \psi$. This completes the proof.

It remains to complete similar analysis with respect to nonpolar components in S . For this, we have a corresponding version of Theorem [4.1.](#page-20-2)

Theorem 4.12. *Suppose that* $\psi \in H^1(S; \mathbb{C})$, $\lambda \in [0, \infty)$ *and*

$$
L_{\lambda}(\psi, v) = 0 \quad \text{for all } v \in H^{1}(S; \mathbb{C}). \tag{4.81}
$$

Then, for every nonpolar component $S_{\epsilon}^c \subseteq S$, we have $\psi \in H^2(S_{\epsilon}^c; \mathbb{C})$.

The majority of the framework needed to prove Theorem [4.12](#page-35-0) has already been established, we need only supply a few intermediate results to allow for the convenient resolution the term

$$
\langle (i\nabla + R\,\hat{\theta}\,)u, (i\nabla + R\,\hat{\theta}\,)(-\delta_{\hat{\theta}}^{-h}\delta_{\hat{\theta}}^{h}u) \rangle_{U},\tag{4.82}
$$

when $U \subseteq S$ is a nonpolar component and u is as given in Lemma [4.2.](#page-21-7) We henceforth use the standard parameterization of S, and restrict it to a domain $V =$ $J \times [0, 2\pi)$ for $J \subseteq I$ on which it yields U, and we write $R \theta$ instead of \mathbf{A}_0 . First, a more convenient representation of [\(4.82\)](#page-35-1) is needed. We let $h \neq 0$, and recall (2.34) to find that

$$
\langle (i \nabla + R \hat{\theta})u, (i \nabla + R \hat{\theta})(-\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u) \rangle_{U}
$$

= $-\langle \frac{u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}}}, \frac{\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}} \rangle_{U} - \langle \frac{u_{\theta}}{R}, \frac{\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u_{\theta}}{R} \rangle_{U}$
- $\langle Ru, R(\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u) \rangle_{U} - \langle i u_{\theta}, \delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u \rangle_{U} - \langle u, i (\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u_{\theta}) \rangle_{U},$ (4.83)

then apply [\(4.17\)](#page-22-4) from Lemma [4.4](#page-22-5) to each of the resulting terms to get

$$
\langle (i \nabla + R \hat{\theta}) u, (i \nabla + R \hat{\theta}) (-\delta_{\hat{w}}^{-h} \delta_{\hat{w}}^{h} u) \rangle_{U}
$$

= $\langle \frac{\delta_{\hat{\theta}}^{h} u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}}}, \frac{\delta_{\hat{\theta}}^{h} u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}}} \rangle_{U} + \langle \frac{\delta_{\hat{\theta}}^{h} u_{\theta}}{R}, \frac{\delta_{\hat{\theta}}^{h} u_{\theta}}{R} \rangle_{U}$
+ $\langle R \delta_{\hat{\theta}}^{h} u, R \delta_{\hat{\theta}}^{h} u \rangle_{U} + 2 \langle i \delta_{\hat{\theta}}^{h} u_{\theta}, \delta_{\hat{\theta}}^{h} u \rangle_{U}.$ (4.84)

With the goal of applying the nonpolar version of (4.5) , we need to bound the highest order terms in [\(4.84\)](#page-35-2) from below, and the lowest order terms from above. To manage to last two terms on the right hand side of [\(4.84\)](#page-35-2), with the help of Lemma 4.4 we find the inequality

$$
|\langle R\delta_{\hat{\theta}}^{h}u, R\delta_{\hat{\theta}}^{h}u\rangle_{U} + 2\langle i\delta_{\hat{\theta}}^{h}u_{\theta}, \delta_{\hat{\theta}}^{h}u\rangle_{U}| \leq K(\|\delta_{\hat{\theta}}^{h}u\|_{V}^{2} + \|\delta_{\hat{\theta}}^{h}u\|_{V}\|\delta_{\hat{\theta}}^{h}u_{\theta}\|_{V})
$$

\n
$$
\leq K(1 + \|\delta_{\hat{\theta}}^{h}u_{\theta}\|_{V})
$$

\n
$$
\leq K + \nu \|\delta_{\hat{\theta}}^{h}u_{\theta}\|_{V}^{2},
$$
\n(4.85)

which is valid for arbitrary $v > 0$. Regarding the first two terms of [\(4.84\)](#page-35-2), since both

$$
\frac{R}{\sqrt{R_s^2 + Z_s^2}} \quad \text{and} \quad \sqrt{R_s^2 + Z_s^2}
$$

can be bounded from below by a positive constant on V , the domain for the standard parameterization of U , we have

$$
\begin{split}\n&\left\langle \frac{\delta_{\hat{\theta}}^{h} u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}}}, \frac{\delta_{\hat{\theta}}^{h} u_{s}}{\sqrt{R_{s}^{2} + Z_{s}^{2}}}\right\rangle_{U} + \left\langle \frac{\delta_{\hat{\theta}}^{h} u_{\theta}}{R}, \frac{\delta_{\hat{\theta}}^{h} u_{\theta}}{R}\right\rangle_{U} \\
&= \left\langle \frac{R}{\sqrt{R_{s}^{2} + Z_{s}^{2}}} \delta_{\hat{\theta}}^{h} u_{s}, \delta_{\hat{\theta}}^{h} u_{s}\right\rangle_{V} + \left\langle \sqrt{R_{s}^{2} + Z_{s}^{2}} \delta_{\hat{\theta}}^{h} u_{\theta}, \delta_{\hat{\theta}}^{h} u_{\theta}\right\rangle_{V} \\
&\geq K_{1}(\|\delta_{\hat{\theta}}^{h} u_{s}\|_{V}^{2} + \|\delta_{\hat{\theta}}^{h} u_{\theta}\|_{V}^{2}).\n\end{split} \tag{4.86}
$$

When evaluating [\(4.5\)](#page-21-6) at $v = -\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u$, by employing [\(4.85\)](#page-35-3) and [\(4.86\)](#page-36-0) and using Young's inequality we get

$$
K_1(\|\delta_\theta^h u_s\|_V^2 + \|\delta_\theta^h u_\theta\|_V^2)
$$

\n
$$
\leq K + \lambda \langle u, -\delta_\theta^{-h} \delta_\theta^h u \rangle_U + \nu (\|\delta_\theta^h u_\theta\|_U^2 + \|\delta_\theta^{-h} \delta_\theta^h u\|_U^2).
$$
\n(4.87)

Here, it easily follows that

$$
|\lambda \langle u, -\delta_{\hat{\theta}}^{-h} \delta_{\hat{\theta}}^{h} u \rangle_{U}| \leq K \quad \text{and} \quad \|\delta_{\hat{\theta}}^{h} u_{\theta}\|_{U}^{2} \leq K \|\delta_{\hat{\theta}}^{h} u_{\theta}\|_{V}^{2}, \tag{4.88}
$$

and we can use [\(4.27\)](#page-24-4) from Lemma [4.6](#page-24-5) to conclude that

$$
\|\delta_{\hat{\theta}}^{-h}\delta_{\hat{\theta}}^{h}u\|_{U}^{2} \leq K\|\delta_{\hat{\theta}}^{-h}\delta_{\hat{\theta}}^{h}u\|_{V}^{2} \leq K\|\delta_{\hat{\theta}}^{h}u_{\theta}\|_{V}^{2}.
$$
 (4.89)

After substituting (4.88) and (4.89) into (4.87) , and making a proper choice of ν relative to the constant K_1 on its left hand side, we arrive at the result

$$
\|\delta_{\hat{\theta}}^h u_s\|_V^2 + \|\delta_{\hat{\theta}}^h u_{\theta}\|_V^2 \le K,\tag{4.90}
$$

which is used to establish the following lemma.

Lemma 4.13. *Under the premises of a nonpolar instance of Lemma* [4.2](#page-21-7)*, where* U *is given on V by the standard parameterization of S*, we have $u \in H^2(V; \mathbb{C})$.

Proof. We conclude that $u \in H^1(V; \mathbb{C})$ from the inequality

$$
\int_{V} (|u_{s}|^{2} + |u_{\theta}|^{2} + |u|^{2}) dx
$$
\n
$$
\leq K \int_{V} R \sqrt{R_{s}^{2} + Z_{s}^{2}} (|u_{s}|^{2} + |u_{\theta}|^{2} + |u|^{2}) dx
$$
\n
$$
= K \int_{U} (|u_{x} R_{s} \cos \theta + u_{y} R_{s} \sin \theta + u_{z} Z_{s}|^{2} + |u|^{2}) dx
$$
\n
$$
\leq K \int_{U} (|u_{x}|^{2} + |u_{y}|^{2} + |u_{z}|^{2} + |u|^{2}) dx < \infty,
$$
\n(4.91)

which is valid because $u \in H^1(U; \mathbb{C})$, and the surface element $R\sqrt{R_s^2 + Z_s^2}$ can be bounded from below by a positive constant. Next, we let $h \neq 0$, then use [\(4.90\)](#page-36-4) along with a standard convergence argument that mimics that following [\(4.76\)](#page-33-2) in the proof of Theorem [4.1,](#page-20-2) to conclude that $u_{\theta\theta}$, $u_{\theta s}$ and $u_{s\theta}$ belong to $L^2(V; \mathbb{C})$. It remains only to show that u_{ss} lies in the same space; for this we let $v \in H^1(S; \mathbb{C})$ and recall [\(4.13\)](#page-21-5). We have

$$
\left\langle \frac{u_s}{R_s^2 + Z_s^2}, v_s \right\rangle_U + \left\langle \frac{u_\theta}{R^2}, v_\theta \right\rangle_U + \left\langle (R^2 - \lambda)u, v \right\rangle_U + \left\langle i u_\theta, v \right\rangle_U - \left\langle i u, v_\theta \right\rangle_U = - \left\langle (1 - i) \nabla \zeta (i \nabla + R \hat{\theta}) \psi + \psi \Delta \zeta, v \right\rangle_U, \tag{4.92}
$$

and integration by parts in the second and fifth terms on the left hand side of (4.92) then gives

$$
\left\langle \frac{u_s}{R_s^2 + Z_s^2}, v_s \right\rangle_U
$$
\n
$$
= \left\langle \frac{u_{\theta\theta}}{R^2} - i2u_{\theta} - (R^2 - \lambda)u - (1 - i)\nabla \zeta (i\nabla + R\hat{\theta})\psi - \psi \Delta \zeta, v \right\rangle_U.
$$
\n(4.93)

By definition, (4.93) implies that

$$
\left(\frac{u_s}{R_s^2 + Z_s^2}\right)_s = -\left(\frac{u_{\theta\theta}}{R^2} - i2u_{\theta}\right) - (R^2 - \lambda)u - (1 - i)\nabla\xi(i\nabla + R\hat{\theta})\psi - \psi\Delta\xi\right) \in L^2(U; \mathbb{C}).
$$
\n(4.94)

It follows from [\(4.94\)](#page-37-2) and the properties of the surface parameterization that $u_{ss} \in$ $L^2(U; \mathbb{C})$, then the inequality

$$
\int\limits_V |u_{ss}|^2 \ dx \le K \int\limits_U |u_{ss}|^2 \ dx \tag{4.95}
$$

 \Box

shows that its parametric composition lies in $L^2(V; \mathbb{C})$.

The proof of Theorem 4.12 can now be completed.

4.2. Proof of Theorem [4.12.](#page-35-0) Given a nonpolar component S_{ϵ}^{c} in S, we pick a nonpolar support U containing it, a corresponding nonpolar cutoff function ζ , then proceed to work on a domain V on which U is specified through the standard parameterization of S. To the function $u = \zeta \psi$ we apply Lemma [4.13](#page-37-3) to conclude that $u \in H^2(V; \mathbb{C})$, then rely on the properties of the mappings $s_x, s_y, s_z, \theta_x, \theta_y$ and θ _z given in [\(2.10\)](#page-5-1), [\(2.12\)](#page-5-2), [\(2.16\)](#page-5-4), [\(2.17\)](#page-6-0), [\(2.23\)](#page-6-6), and [\(2.24\)](#page-6-7), as well as those of the surface element $R\sqrt{R_s^2 + Z_s^2}$, to find that each of the nine second order partial derivatives of u with respect to x, y or z belongs to $L^2(U; \mathbb{C})$. In particular, since U is a nonpolar support, we know that $R \neq 0$ on V, which means that the mappings s_x , s_y , s_z , θ_x , θ_y and θ_z are all bounded from above by a positive constant, and that the surface element can be bounded from below by a positive constant. Furthermore, since the derivatives of s_x , s_y , s_x , θ_x , θ_y , and θ_z are bounded and continuous on I^o , an argument of the type given in (4.78) – (4.80) for the polar case holds equally well in all cases. The conclusion that actually $\psi \in H^2(S^c_{\epsilon}; \mathbb{C})$ again follows because $S_{\epsilon}^c \subseteq U$, and $u|_{S_{\epsilon}^c} = \psi$. We now can produce our global regularity result.

Theorem 4.14. *Suppose that* $\psi \in H^1(S; \mathbb{C})$, $\lambda \in [0, \infty)$ and ([4.81](#page-35-4)) holds. Then, *we have* $\psi \in H^2(S; \mathbb{C})$ *.*

Proof. We assert that any admissible S can be covered by one nonpolar component, along with at most two polar caps that overlap it in a set of nonzero measure. The result follows by Theorem 4.1 , Theorem 4.12 , and the sub-additivity of integration in S. □

Theorem [4.14](#page-38-0) provides the foundation for the theoretical and numerical arguments that apply to the deterministic and stochastic GL models considered in our future work. We close this article with an important corollary wherein a natural boundary condition satisfied by the basis functions is identified.

Corollary 4.15. *Suppose that* $\psi \in H^1(S; \mathbb{C}) \setminus \{0\}$, $\lambda \in [0, \infty)$ and ([4.81](#page-35-4)) holds. *Filterally is an eigenfunction of* $(i\nabla + R\hat{\theta})^2$ *with corresponding eigenvalue* λ *, and*

$$
\frac{\partial \psi}{\partial s} = 0 \quad \text{in } L^2(\partial S; \mathbb{C}) \tag{4.96}
$$

whenever $\partial S \neq \emptyset$ *.*

Proof. First, we rely upon the assertion that the space $C_0^{\infty}(S; \mathbb{C})$ of smooth functions with compact support in S is dense in $L^2(S; \mathbb{C})$. Let $v \in L^2(S; \mathbb{C})$, and pick any sequence $\{v_k\} \subseteq C_0^\infty(S; \mathbb{C})$ convergent to v. Rewriting [\(4.81\)](#page-35-4) at any v_k gives

$$
\langle (i\nabla + R\hat{\theta})\psi, (i\nabla + R\hat{\theta})v_k \rangle = \lambda \langle \psi, v_k \rangle, \tag{4.97}
$$

and since $\psi \in H^2(S; \mathbb{C})$ by Theorem [4.14,](#page-38-0) we may apply [\(2.48\)](#page-10-2) from Theorem [2.1](#page-10-4) to get

$$
\langle (i\nabla + R\,\hat{\theta})^2 \psi, v_k \rangle + \langle (i\nabla + R\,\hat{\theta}) \psi \cdot \hat{s}, iv_k \rangle_{\partial S} = \langle \lambda \psi, v_k \rangle. \tag{4.98}
$$

If $\partial S = \emptyset$, the second term on the left hand side of [\(4.98\)](#page-39-0) clearly vanishes. If instead the boundary is nonempty, we get the same result because $v_k|_{\partial S} = 0$, so in any event from [\(4.98\)](#page-39-0) we obtain

$$
\langle (i \nabla + R \hat{\theta})^2 \psi, v_k \rangle = \langle \lambda \psi, v_k \rangle. \tag{4.99}
$$

Letting $k \to \infty$ in [\(4.99\)](#page-39-1) gives

$$
\langle (i\nabla + R\,\hat{\theta}\,)^2 \psi, v \rangle = \langle \lambda \psi, v \rangle, \tag{4.100}
$$

which shows that

$$
(i\nabla + R\hat{\theta})^2 \psi = \lambda \psi \quad \text{in } L^2(S; \mathbb{C}). \tag{4.101}
$$

It remains to establish [\(4.96\)](#page-39-2). To this end, we will rely upon the fact that the space $C^2(\partial S; \mathbb{C})$ is dense in $L^2(\partial S; \mathbb{C})$. Let us suppose that $\partial S \neq \emptyset$, let $v \in L^2(\partial S; \mathbb{C})$, and choose a sequence $\{v_k\}$ from $C^2(\partial S; \mathbb{C})$ that is convergent to v. Using the continuous right inverse afforded by Theorem [A.1,](#page-42-1) we extend each v_k to the space $H^1(S; \mathbb{C})$, then [\(4.81\)](#page-35-4) together with Theorem [2.1](#page-10-4) again gives [\(4.98\)](#page-39-0). On the other hand, according to our argument above, we also know that

$$
\langle (i \nabla + R \hat{\theta})^2 \psi, v_k \rangle = \langle \lambda \psi, v_k \rangle, \tag{4.102}
$$

and so can conclude that

$$
\langle (i\nabla + R\ddot{\theta})\psi \cdot \hat{s}, iv_k \rangle_{\partial S} = 0 \tag{4.103}
$$

for each k. Letting $k \to \infty$ then shows that

$$
\langle (i\nabla + R\hat{\theta})\psi \cdot \hat{s}, iv \rangle_{\partial S} = 0, \tag{4.104}
$$

or equivalently that

$$
\langle -i(i\nabla + R\hat{\theta})\psi \cdot \hat{s}, v \rangle_{\partial S} = 0. \tag{4.105}
$$

⊓

Since v was arbitrarily chosen, when recalling (2.34) we see that

$$
\frac{1}{\sqrt{R_s^2 + Z_s^2}} \frac{\partial \psi}{\partial s} = -i (i \nabla + R \hat{\theta}) \psi \cdot \hat{s} = 0 \quad \text{in } L^2(\partial S; \mathbb{C}), \tag{4.106}
$$

which implies (4.96) in light of the properties of R and Z.

We note that the converse of Corollary [4.15](#page-38-1) also clearly holds, after a simple ap-plication of Theorem [2.1.](#page-10-4)

In a future work we describe and implement an arbitrary order, dimensionally reduced technique for the numerical computation of the eigenvalues and eigenfunctions of the surface Schrödinger operator.

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A. Referenced theorems

Theorem A.1. *Let* $\partial S \neq \emptyset$ *. Then, the trace mapping*

$$
\gamma: C^2(\overline{S}; \mathbb{C}) \longrightarrow C^2(\partial S; \mathbb{C}) \times C^1(\partial S; \mathbb{C}),
$$

\n
$$
u \longmapsto (u|_{\partial S}, \frac{\partial u}{\partial S}|_{\partial S}),
$$
\n(A.1)

extends by continuity to a continuous, linear, surjective mapping

$$
\tilde{\gamma}: H^2(S; \mathbb{C}) \longrightarrow H^{3/2}(\partial S; \mathbb{C}) \times H^{1/2}(\partial S; \mathbb{C}). \tag{A.2}
$$

Moreover, \tilde{v} has a continuous right inverse.

Comments on Proof. This version of the trace theorem represents an appropriate adaption of a classical result. Since S is locally Euclidean, the proof of an analogous theorem, applicable in a suitable space of real-valued functions defined on a sufficiently regular open domain in \mathbb{R}^2 , can be used to establish the result. A classical example of such a theorem can be found in [\[14\]](#page-41-11), while a more modern approach is given in [\[1\]](#page-40-7). П

Theorem A.2. *For* $j = 0, 1$ *we have the compact embedding*

$$
H^{j+1}(S; \mathbb{C}) \longrightarrow H^j(S; \mathbb{C}). \tag{A.3}
$$

Comments on Proof. This represents a version of the Rellich–Kondrachov theo-rem, stated as Theorem 6.3 in [\[1\]](#page-40-7), adapted for the manifold domain S . \Box

Theorem A.3. Let L_{λ} be the real, bilinear form specified in ([3.3](#page-14-3)), $\mu < 0$, and *suppose that the following conditions hold:*

(a) there is $M > 0$ such that

$$
L_{\mu}(u,v) \le M \|u\|_{1,2} \|v\|_{1,2} \quad \text{for all } u, v \in H^1(S; \mathbb{C}); \tag{A.4}
$$

(b) there is $m > 0$ such that

$$
L_{\mu}(u, u) \ge m \|u\|_{1,2}^2 \quad \text{for all } u \in H^1(S; \mathbb{C}). \tag{A.5}
$$

Then, for any $F \in H^{-1}(S; \mathbb{C})$ there is a unique $f \in H^1(S; \mathbb{C})$ such that

$$
L_{\mu}(f, v) = (F, v) \quad \text{for all } v \in H^{1}(S; \mathbb{C}).
$$
 (A.6)

The mapping $f \mapsto F$ *defined by* ([A.6](#page-42-4)) is a bounded linear bijection of $H^1(S; \mathbb{C})$ *onto* $H^{-1}(S; \mathbb{C})$, and the corresponding inverse mapping $F \to f$ is bounded.

Comments on Proof. This is the real, bilinear version of Theorem IV.1.1, with respect to L_{μ} on the space $H^1(S; \mathbb{C})$, as stated in [\[8\]](#page-41-12). \Box

Theorem A.4. Let T be a compact, self-adjoint, nontrivial linear mapping in $L^2(S; \mathbb{C})$ that is not of finite rank, and let $\sigma_p(T)$ denote the point spectrum of T. *Fhen, we have the following:*

(1)
$$
\sigma_p(T) \subseteq \mathbb{R}
$$
;
\n(2) $\sigma_p(T)$ is countably infinite;
\n(3) $(\sigma_p(T))' = \{0\}$.
\n(4.7)

The geometric multiplicity of each eigenvalue in $\sigma_p(T)$ is finite, and when repeat*ing the elements of* $\sigma_p(T)$ *according to their geometric multiplicities, there is a corresponding collection of eigenvectors of* T *that is a complete orthonormal set* in $L^2(S; \mathbb{C})$.

Notes. The point spectrum of T is, by definition, the set of all eigenvalues of T . Here $(\sigma_p(T))'$ denotes the derived set of $\sigma_p(T)$; thus (2) in [\(A.7\)](#page-43-2) above states that the eigenvalues of T accumulate at 0, and only at 0. \Box

Comments on Proof. This theorem combines instances of both Theorem II.5.2 and Corollary II.5:3 from [\[8\]](#page-41-12), and is a classical result for compact linear operators in Hilbert space. \Box

Theorem A.5. *If* $u \in H_0^1(S; \mathbb{C})$ and $v \in H^1(S; \mathbb{C})$, then

$$
\langle u, (i\nabla + R\hat{\theta})v \rangle = \langle (i\nabla + R\hat{\theta})u, v \rangle.
$$
 (A.8)

Comments on Proof. A procedure very similar to that outlined in the proof of Theorem [2.1](#page-10-4) yields this result. □

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