Spectral analysis for matrix Hamiltonian operators

Jeremy L. Marzuola¹ and Gideon Simpson²

¹ Department of Mathematics, University of North Carolina-Chapel Hill, Phillips Hall, Chapel Hill, NC 27599, USA
² Mathematics Department, University of Toronto, Toronto, ON, M5S 2E4, Canada

E-mail: marzuola@math.unc.edu and simpson@math.toronto.edu

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Abstract
In this work, we study the spectral properties of matrix Hamiltonians generated by linearizing the nonlinear Schrödinger equation about soliton solutions. By a numerically assisted proof, we show that there are no embedded eigenvalues for the three dimensional cubic equation. Although we focus on a proof of the 3D cubic problem, this work presents a new algorithm for verifying certain spectral properties needed to study soliton stability.

Source code for verification of our computations, and for further experimentation, is available at http://hdl.handle.net/1807/25174.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The nonlinear Schrödinger equation (NLS) in \( \mathbb{R} \times \mathbb{R}^d \),

\[
    i \psi_t + \Delta \psi + g(|\psi|^2)\psi = 0,
    \quad \psi(0, x) = \psi_0(x),
\]

appears in many different contexts. It arises as a leading order envelope approximation in nonlinear optics, Bose–Einstein condensates, and hydrodynamics. It is also intrinsically interesting as a canonical example of the competition between nonlinearity and dispersion.

1.1. Solitons

For appropriate choices of the nonlinearity \( g : \mathbb{R} \to \mathbb{R} \), the equation is known to possess soliton solutions, nonlinear bound states of (1.1) that arise from the ansatz

\[
    \psi(t, x) = e^{i\lambda t} R(x; \lambda),
\]
where \( \lambda > 0 \) is the soliton parameter. The soliton, \( R \), is a positive, radially symmetric, exponentially decaying solution of the nonlinear elliptic equation
\[
-\lambda R + \Delta R + g(|R|^2)R = 0.
\] (1.2)

Precise restrictions on \( g \) are given in [3], where the existence of the soliton is established by a variational formulation of the problem. One satisfactory nonlinearity is the monomial \( g(s) = s^\sigma \) with \( \sigma > 0 \). For these power nonlinearities, a scaling property of (1.2) permits us to take \( \lambda = 1 \). Additional details are given in the texts [32, 6], and references therein.

Solitons are of interest both in applications, as mechanisms for transporting information and energy, and intrinsically to nonlinear dispersive equations. Indeed, it is conjectured that any solution of (1.1) with appropriate nonlinearity that does not disperse as \( t \to \infty \) must eventually converge to a finite sum of stable solitons. This is referred to as the ‘soliton resolution’ conjecture, a notoriously difficult problem to formulate, see [33].

1.2. Stability

The stability of the solitons is a natural property to investigate, but first we must clarify what kind of stability we seek. Some of the first results on NLS concerned the orbital stability of the solitons. For NLS, a soliton solution is said to be orbitally stable if a perturbation thereof remains small in the \( H^1 \) norm, modulo the group of symmetries associated with the equation, i.e. translation in space. In [16, 36, 37], Weinstein and Grillakis, Shatah and Strauss determined that the question of orbital stability of NLS solitons could be reduced to computing the sign of
\[
\frac{d}{d\lambda} \int |R(x; \lambda)|^2 \, dx.
\] (1.3)

When this is positive, the solitons are orbitally stable; when it is negative, they are unstable.

Although these orbital stability results are quite elegant, they do not tell us what happens as \( t \to \infty \). In particular, orbital stability does not imply that the perturbation diminishes; the solution may perpetually oscillate about the soliton. For information on long time behaviour, we seek asymptotic stability, which generally states that a perturbation of the soliton converges to a (possibly different) bound state and radiation. In this work, we study certain details necessary for asymptotic stability.

Asymptotic stability is usually proven perturbatively. Writing \( \psi = e^{i\lambda t} (R(\cdot; \lambda) + \phi) \), the evolution of the perturbation, \( \phi \), is governed by
\[
\partial_t \begin{pmatrix} \phi \\ \phi^* \end{pmatrix} = i\mathcal{H} \begin{pmatrix} \phi \\ \phi^* \end{pmatrix} + \mathcal{F}(\phi, \phi^*) = i \begin{pmatrix} -\Delta + \lambda - V_1 \\ V_2 \\ V_1 - \lambda + V_2 \end{pmatrix} \begin{pmatrix} \phi \\ \phi^* \end{pmatrix} + \mathcal{F}(\phi, \phi^*). \] (1.4)

The operator \( \mathcal{H} \) is the linearized (about a soliton) operator of NLS, and \( V_1 = g(R^2) + g'(R^2)R^2 \) and \( V_2 = g'(R^2)R^2 \); this is the matrix Hamiltonian. The perturbation \( \mathcal{F} \) contains the nonlinear interactions. We could have also decomposed the perturbation into real and imaginary parts, \( \phi = u + i v \), to get the evolution equation
\[
\partial_t \begin{pmatrix} u \\ v \end{pmatrix} = J L \begin{pmatrix} u \\ v \end{pmatrix} + G(u, v) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} L_+ & 0 \\ 0 & L_- \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + G(u, v), \] (1.5)

where \( L_\pm = -\Delta + \lambda - V_\pm \) and \( G \) contains the nonlinear terms. The potentials are \( V_+ = V_1 + V_2 \) and \( V_- = V_1 - V_2 \). The isometry between these two formulations permits us to go back and forth; we shall do this frequently.

Proofs of asymptotic stability typically require Strichartz estimates on the evolution operator of the form
\[
\|e^{itH}f\|_{L^6_t L^3_x} \lesssim \|f\|_{L^6_x}. \] (1.6)
With such estimates, (1.4) is shown to be dominated by the linear flow, permitting the nonlinear term to be treated as a perturbation. This strategy for NLS was initiated by Buslaev and Perelman [4], who studied the stability of a single soliton known to be orbitally stable. There approach has been followed in many works with various restrictions on the perturbations and assumptions on the nonlinearity. Additional assumptions on the spectrum of the linearized operator are also often necessary. As examples, we point the reader to Buslaev and Sulem [5], which generalizes the earlier work, and to Cuccagna and Rodnianski, Schlag, and Soffer [9, 25], who studied the stability of multiple soliton solutions. Schlag and Krieger and Schlag [18, 26], studied the stability on an orbitally unstable soliton, subject to constraints that mitigate the linear instability.

1.3. The spectrum

Dispersive estimates on $e^{itH}$ require careful considerations of the spectrum of $H, \sigma(H)$. Since the spectra of $H$ and JL are related by $\sigma(H) = i\sigma(JL)$, we can also study that operator. Generically, the spectrum of $H$ includes the points highlighted in figure 1. Using well-known results on relatively compact perturbations of differential operators, we can assert that the essential spectrum lies in $(-\infty, -\lambda] \cup [\lambda, \infty)$ [17, 24]. See [14] for a nice description of the essential spectrum for matrix Hamiltonian. By direct computation on JL, we can find a $2d + 2$ dimensional kernel; details are given in section 2.1.2. This implies the $2d + 2$ dimensional kernel of $H$.

Bound states corresponding to eigenvalues of $H$, along with resonances, can obstruct the necessary dispersive estimates. In many of the results on asymptotic stability, the authors explicitly assume:

1) $H$ has no eigenvalues in the essential spectrum. Eigenvalues contained in the essential spectrum are called embedded eigenvalues. These will be the focus of this work.

2) The only real eigenvalue in the spectral gap, $[-\lambda, \lambda]$, is zero.

3) The values $\pm\lambda$, the endpoints of the essential spectrum, are not resonances.

See section 2.1 for a discussion related to these conditions. These properties, which are often assumed, motivate two problems:

**Open Problem 1.1.** Prove that $H$ has no embedded eigenvalues.
Open Problem 1.2. Prove that \( \mathcal{H} \) has no endpoint resonances.

In this work we study \( \mathcal{H} \), and resolve the questions of embedded eigenvalues and endpoint resonances for some cases of \( (1.1) \). We believe our approach may provide a framework applicable to other problems. The question of gap eigenvalues is more subtle, as they may exist in subcritical problems where the soliton is orbitally stable; we will not address this here.

Remark 1.3. Krieger and Schlag [18] resolved these questions for 1D supercritical power nonlinearities using scattering theory ideas similar to those of Perelman [23]. Interestingly, our algorithm only works for a subset of supercritical monomial nonlinearities in 1D. The existence of both embedded eigenvalues and embedded resonances for operators of the form \( \mathcal{H} \) requires precise asymptotic matching with direct algebraic dependence upon the forms of the potentials. They are thus believed to be rare. However, in higher dimensions, neither can be ruled out analytically, even under strong assumptions on the symmetry, regularity and decay of the potentials. See Schlag’s discussion in [26].

Remark 1.4. Linearizing about the ground state soliton for the cubic NLS in 1D, which is \( L^2 \) subcritical, does actually result in endpoint resonances, see [7]. Despite this, asymptotic stability still holds due to the celebrated inverse scattering theory. In higher dimensions, as seen by [14], endpoint resonances result in weaker dispersive estimates that make proving asymptotic stability rather challenging.

Remark 1.5. In Cuccagna and Pelinovsky and Cuccagna, Pelinovsky and Vougalter [10, 11], it is shown that embedded eigenvalues of positive Krein signature in 1D can be dispersion managed via a Fermi golden rule approach, and that this is a generic assumption. However, it is unknown if this can be extended to higher dimensions and embedded eigenvalues still complicate the analysis. Hence, it may be simpler to prove their absence.

1.4. Main results

The main result of this work is

Theorem 1. The linearized operator of the focusing 3D cubic NLS has no embedded eigenvalues and no endpoint resonances.

Although this is but one example, we contend that our approach can be applied to other problems. Indeed, we establish the same results for the 1D problem with the nonlinearities \( g(s) = s^{2.5} \) and \( g(s) = s^3 \). Extensions are also discussed in section 5.

Our theorem hinges on a so-called spectral property based on the linearized operator\(^3\). Generically, this property can be formulated as:

**Definition 1.6 (The generalized spectral property).** Let \( d \geq 1 \). Given \( L_{\pm} \) and a skew-adjoint operator \( \Lambda \), consider the two real Schrödinger operators

\[
L_+ = -\Delta + \mathcal{V}_+, \quad L_- = -\Delta + \mathcal{V}_-,
\]

defined by the commutator relations

\[
L_{\pm} f = \frac{1}{2} [L_{\pm}, \Lambda] f = \frac{1}{2} [L_{\pm} \Lambda f - \Lambda L_{\pm} f].
\]

Let the real quadratic form for \( z = (u, v)^T \in H^1 \times H^1 \) be

\[
\mathcal{B}(z, z) = \mathcal{B}_+(u, u) + \mathcal{B}_-(v, v) = \langle L_+ u, u \rangle + \langle L_- v, v \rangle.
\]

\(^3\) Any property on the spectrum of a linear operator is a spectral property. This moniker is due to Merle and Raphaël, in their study of blow-up [15, 21].
The system is said to satisfy a spectral property on the subspace $\mathcal{U} \subseteq H^1 \times H^1$ if there exists a universal constant $\delta_0 > 0$ such that $\forall z \in \mathcal{U}$,

$$B(z, z) \geq \delta_0 \int (|\nabla z|^2 + e^{-|y||z|^2}) \, dy.$$  

In this work, the skew adjoint operator is

$$\Lambda f \equiv \frac{d}{2} f + x \cdot \nabla f = \frac{d}{d\lambda} \left[ \lambda \frac{d}{d\lambda} f(\lambda x) \right].$$  

(1.7)

The potentials in $L_{\pm}$ become

$$V_{\pm} = \frac{1}{2} x \cdot \nabla V_{\pm}.$$  

(1.8)

This choice of $\Lambda$ has particular significance for the $L^2$ critical equation, though we employ it in supercritical problems. This (mis)application is discussed in section 5.

Our results rely on the key observation of Perelman [22] that

**Theorem 2.** Given the $J\Lambda L$ operator, assume the spectral property of definition 1.6 applies to $L_{\pm}$. Then $J\Lambda L$ has no embedded eigenvalues on the subspace $\mathcal{U}$.

**Proof.** Let us assume we have an embedded eigenstate $z_{em} = (u_{em}, v_{em})^T \in \mathcal{U}$ corresponding to eigenvalue $i\tau_{em}$, $\tau_{em} > \lambda_0$. Then,

$$L_- v_{em} = i\tau_{em} u_{em}, \quad L_+ u_{em} = -i\tau_{em} v_{em}.$$  

Plugging into the form

$$B(z_{em}, z_{em}) = \langle L_+ u_{em}, u_{em} \rangle + \langle L_- v_{em}, v_{em} \rangle$$  

$$= \frac{1}{2} \left[ \langle \Lambda u_{em}, L_+ u_{em} \rangle + \langle L_+ u_{em}, \Lambda u_{em} \rangle \right]$$  

$$+ \frac{1}{2} \left[ \langle \Lambda v_{em}, L_- v_{em} \rangle + \langle L_- v_{em}, \Lambda v_{em} \rangle \right]$$  

$$= \frac{1}{2} \left[ i\tau_{em} \langle \Lambda u_{em}, v_{em} \rangle - i\tau_{em} \langle v_{em}, \Lambda u_{em} \rangle \right]$$  

$$+ \frac{1}{2} \left[ -i\tau_{em} \langle \Lambda v_{em}, u_{em} \rangle + i\tau_{em} \langle u_{em}, \Lambda v_{em} \rangle \right]$$  

$$= \frac{i\tau_{em}}{2} \left[ \langle \Lambda u_{em}, v_{em} \rangle - \langle v_{em}, \Lambda u_{em} \rangle + \langle v_{em}, \Lambda u_{em} \rangle - \langle \Lambda u_{em}, v_{em} \rangle \right] = 0. \quad \Box$$  

We note that this holds not just for embedded eigenvalues, but for any purely imaginary eigenvalue. Thus, if the spectral property holds, we are assured that there are no imaginary eigenvalues on the designated subspace. In this way, we can actually rule out gap spectrum away from the origin for a certain class of problems, superseding the results of [12]. Furthermore, we note that the spectral property also rules out endpoint resonances, which are perfectly bounded functions in the equivalent weak formulation of the resulting bilinear forms. The subspace $\mathcal{U}$ is constructed in section 2.

Separately, we establish that for 3D NLS with nonlinearities that support solitons, one need only test for embedded eigenvalues that are:

- Near the endpoints of the essential spectrum,
- On a sufficiently low spherical harmonic.
In appendix A we give a proof of the following result using positive commutator arguments otherwise known as Mourre estimates:

**Theorem 3.** Given a Hamiltonian $H$, there exists some $M > 0$ such that for $|\mu| > M$, there are no solutions $u_\mu$ such that

$$Hu_\mu = \mu u_\mu.$$

For $d \geq 2$, there exists a $K > 0$ such that if an embedded eigenstate, $u_\mu$, exists, it is only supported on spherical harmonics below $K$.

**Remark 1.7.** Such results are well known using resolvent estimate techniques; however, our approach provides easily computable limits on $M$ and $K$ in terms of the soliton solution.

### 1.5. Organization of results

In section 2.1, we review some well-known properties of the linearized operator and some results of Erdogan and Schlag [14] who prove properties of the discrete spectrum and the absence of embedded resonances. In section 3, we prove an appropriate spectral property as in definition 1.6, based on the work in Fibich et al [15]. Perelman’s observation then rules out embedded eigenvalues and endpoint resonances. This proves theorem 2. In section 5, we discuss limitations and possible extensions of our approach.

In appendix A, we use Mourre multipliers to eliminate large embedded eigenvalues and large spherical harmonics from the expansion of an embedded eigenvalue. Although these results have been known via resolvent methods for some time, we aim to collect as much analytic information about the spectrum as possible, providing bounds for future estimates and computations. Appendix B provides proofs of some helpful ODE results. An overview of our numerical methods with benchmarks is then presented in appendix C.

## 2. Spectral properties of the linearized Hamiltonian

We now give more detailed and formal statements on the spectral properties of the operators.

### 2.1. A survey of results on the spectrum of $\mathcal{H}$

#### 2.1.1. Generic results on the spectrum of $\mathcal{H}$

We formalize the heuristic discussion from section 1 by collecting a number of prior results on the spectrum of linearized Hamiltonian operators in the the following theorem. Many of the results are nicely collected in several references, see for instance [12, 14, 26]. Let us write the operator as

$$\mathcal{H} = \mathcal{H}_0 + V = \begin{bmatrix} -\Delta + \lambda & 0 \\ 0 & -\Delta + \lambda \end{bmatrix} + \begin{bmatrix} -V_1 & -V_2 \\ V_2 & V_1 \end{bmatrix}.$$

**Theorem 4 (Erdogan–Schlag).** Assume there are no embedded eigenvalues in the continuous spectrum of $\sigma(\mathcal{H})$, then

- The essential spectrum of $\mathcal{H}$ equals $(-\infty, -\lambda] \cup [\lambda, \infty)$;
- $\sigma(\mathcal{H}) = -\sigma(\mathcal{H}) = \sigma(\mathcal{H}^*)$ and $\sigma(\mathcal{H}) \subset \mathbb{R} \cup i\mathbb{R}$;
- The discrete spectrum consists of eigenvalues $\{z_j\}_{j=1}^N$, $0 \leq N \leq \infty$, of finite multiplicity. For each $z_j \neq 0$, the algebraic and geometric multiplicities coincide and $\text{Ran}(\mathcal{H} - z_j)$ is closed.
In addition, if $V_1$ and $V_2$ decay sufficiently rapidly at infinity, then on the space

$$X_\sigma = L^{2,\sigma} \times L^{2,\sigma}, \quad L^{2,\sigma} = \{ f | |x|^{\sigma} f \in L^2 \}$$

for any $\mu$ such that $|\mu| > \lambda$, the operator $(H_0 - (\mu \pm i0))^{-1}V : X^{-1} \rightarrow X^{-1}$ is compact, and

$$I + (H_0 - (\mu \pm i0))^{-1}V$$

is invertible.

These results rely on resolvent estimates and an argument akin to a restriction theorem from harmonic analysis. This strategy closely emulates the bootstrapping argument of Agmon for scalar operators [1].

2.1.2. Results on the discrete spectrum of $\mathcal{H}$. We wish to show that the spectrum of $\mathcal{H}$ when linearized about the ground state has the discrete spectral decomposition displayed in figure 1. Namely, the following result holds

**Theorem 5.** The only discrete eigenvalue for $\mathcal{H}$ in the interval $[-\lambda, \lambda]$ is 0.

**Remark 2.1.** For the 3D monomial NLS equation, the structure of the discrete spectrum away from the essential spectrum has been verified numerically in [12] for a range of supercritical exponents. Verification of their findings regarding the spectral gap is a consequence of theorem 2.

**Remark 2.2.** In [26], using arguments derived from [23], it is shown that the discrete spectrum for the Hamiltonian $\mathcal{H}$, as in (1.4), associated with supercritical monomial nonlinearities is determined by the discrete spectrum of $L_{\pm}$. A slightly stronger version of the theorem, with minimal changes to the proof, applies to linearizations about a minimal mass soliton, $R = R_{\text{min}}$, of saturated nonlinearities.

Let us review the generalized kernel of a Hamiltonian resulting from linearizing about a soliton. Studying JL and following [36], we see by direct calculation that the vectors

$$\begin{pmatrix} 0 \\ R_j \\ 0 \end{pmatrix} \quad (\partial_\lambda R)_{\lambda=0} = \begin{pmatrix} R_j \\ 0 \\ 0 \end{pmatrix}$$

for all $j = 1, \ldots, d$ are contained in ker (JL). Differentiating (1.2) with respect to $\lambda$, we have by a simple calculation that $L_+ \partial_\lambda R = -R$. Differentiating with respect to $x$, $L_- (x R) = -2 \nabla R$. Hence, the vectors

$$\begin{pmatrix} 0 \\ x_j R \end{pmatrix}, \quad \begin{pmatrix} (\partial_\lambda R)_{\lambda=0} \\ 0 \end{pmatrix}$$

lie in the generalized null space. So far we have constructed at $2d + 2$ dimensional generalized null space. For power nonlinearities, $g(s) = s^\sigma$,

$$\left(\partial_\lambda R\right)_{\lambda=0} = \frac{1}{2} \begin{pmatrix} 1 \\ R \cdot x \cdot \nabla R \end{pmatrix}.$$ 

We use this explicit form in our calculations. See in [18, 26, 36] for a nice analytic description of the discrete spectrum.
2.2. Natural orthogonality conditions

As noted in definition 1.6, even if the spectral property holds, it only implies the absence of embedded eigenvalues on a subspace of \( \mathcal{U} \subset L^2 \times L^2 \). That we must limit ourselves to a subspace will become clear in section 3.2, where we demonstrate that the operators \( \mathcal{L}_\pm \) have negative eigenvalues.

This subspace will be defined as the orthogonal complement to the span of a set of vectors. If this collection of vectors is not chosen properly, we may find that the spectral property holds though the operator still has embedded eigenvalues. Thus the constraints on the set of vectors whose orthogonal complement will define \( \mathcal{U} \) are:

1. They must be orthogonal to eigenstates of embedded eigenvalues,
2. Orthogonality with respect to them should induce positivity of \( \mathcal{L} \) on \( \mathcal{U} \).

A way of satisfying both requirements is to use the discrete spectrum of the adjoint problem. To that end, we rely on the following simple results.

**Lemma 2.3.** If \((\lambda, \vec{u})\) is an eigenvalue, eigenvector pair for \( J_L \) and \((\sigma, \vec{v})\) is an eigenvalue, eigenvector pair for \((J_L)^*\), then

\[
(\lambda - \sigma^*) \langle \vec{u}, \vec{v} \rangle = 0.
\]

Thus, if \( \lambda - \sigma^* \neq 0 \), the states are orthogonal.

**Corollary 2.4.** An eigenstate of \( J_L \) associated with a purely imaginary eigenvalue, \( i\tau \neq 0 \), is orthogonal to \( \ker_g((J_L)^*) \).

**Corollary 2.5.** Let \((i\tau \neq 0, \vec{\psi})\) and \((\lambda > 0, \vec{\phi})\) be eigenvalue, eigenvector pairs of \( J_L \). Then

\[
\langle \psi_1, \phi_2 \rangle = 0,
\]

\[
\langle \psi_2, \phi_1 \rangle = 0.
\]

**Proof.** By the Hamiltonian symmetry of the problem, \(-\lambda, (\phi_2, \phi_1)^T\) and \(\lambda, (-\phi_2, -\phi_1)^T\) are eigenvalue pairs of the adjoint, \((J_L)^*\). Therefore,

\[
\langle \psi_1, \phi_2 \rangle - \langle \psi_2, \phi_1 \rangle = 0,
\]

\[
-\langle \psi_1, \phi_2 \rangle - \langle \psi_2, \phi_1 \rangle = 0.
\]

Adding and subtracting these equations give the result. \(\square\)

These observations motivate using the known spectrum of the adjoint system in constructing the orthogonal subspace. For the 3D cubic problem, we can thus use the eigenstates at the origin and the two off axis real eigenvalues.

3. Bilinear forms and the spectral property

In this section we shall prove the positivity of the bilinear form in definition 1.6 on an appropriate subspace. With this spectral property in hand, we will conclude there are no embedded eigenvalues.

In the following subsections, we establish the following:

**Theorem 6.** The generalized spectral property holds for the 3D cubic problem for \((f, g)^T \in \mathcal{U} \subset L^2 \times L^2\) specified by the following orthogonality conditions:

\[
\langle f, R \rangle = 0, \quad \langle g, R + x \cdot \nabla R \rangle = 0, \quad \langle f, \phi_2 \rangle = 0, \quad \langle f, x_j R \rangle = 0 \quad \text{for } j = 1, \ldots, d,
\]

where \( \vec{\phi} = (\phi_1, \phi_2)^T \) is the eigenstate associated with the positive eigenvalue \( \sigma > 0 \).

The orthogonal subspace in theorem 6 is motivated by the observation in section 2.2, as all of the elements arise from the spectrum of the adjoint problem. This unstable eigenstate exists as the solitons of the 3D cubic problem are well known to be linearly unstable [32, chapter 4].

Remark 3.1. Henceforward, we assume the unstable eigenfunction of the 3D cubic problem is radial. This claim is substantiated by direct integration in our numerical results section, as well as the fact that the spectral decomposition for the critical problem remains valid under the assumption of radial symmetry, hence the multiplicity of radial eigenfunctions must be at least 4. Since $R, \partial R, R$ are the only radial components of the kernel, the unstable eigenmode must also be radial.

Following [15], we computationally verify the spectral property in the following steps:

- First, the bilinear form is decomposed by spherical harmonics into

$$B(z, z) = B_+(f, f) + B_-(g, g) = \sum_{k=0}^{\infty} \sum_{l=0}^{L_k} B_+(f^{(k,l)}, f^{(k,l)}) + \sum_{k=0}^{\infty} \sum_{l=0}^{L_k} B_-(g^{(k,l)}, g^{(k,l)}), \quad (3.1)$$

where $z = (f, g)^T$, and $f^{(k,l)}$ and $g^{(k,l)}$ are the components of $f$ and $g$ in the $k$th spherical harmonic with angular component $l$. Since $L_{\pm}$ are radially symmetric operators, they are independent of $l$.

- We then identify the dimension of the subspace of negative eigenvalues for $L_{\pm}^{(k)}$. Although at first this would appear to require an infinite number of computations, a monotonicity property of these operators with respect to $k$ limits this to a finite number of harmonics.

- Finally, we show that our orthogonality conditions are sufficient to point us away from the negative directions, allowing us to prove our result.

### 3.1. The index of an operator

For a bilinear form $B$ on a vector space $V$, the index of $B$ with respect to $V$ is given by

$$\text{ind}_V(B) \equiv \max \{ k \in \mathbb{N} \mid \text{there exists a subspace } P \text{ of codimension } k \text{ such that } B|_P \text{ is positive} \}.$$  

Our results rely on the following generalization of theorem XIII.8 of [24], which is itself a generalization of the Sturm oscillation theorem (section XIII.7 of [24]):

**Theorem 7.** Let $U^{(k)}$ be the solution to

$$L^{(k)} U^{(k)} = -\frac{d^2}{dr^2} U^{(k)} - \frac{d}{r} \frac{d}{dr} U^{(k)} + V(r) U^{(k)} + \frac{k(k + d - 1)}{r^2} U^{(k)} = 0$$

with initial conditions given by the limits

$$\lim_{r \to 0} \frac{U^{(k)}(r)}{r^k} = 1, \quad \lim_{r \to 0} \frac{d U^{(k)}(r)}{r^k} = 0,$$

where $V$ is sufficiently smooth and rapidly decaying. Then, the number $N(U^{(k)})$ of zeros of $U^{(k)}$ is finite and

$$\text{ind}_{H_1} (B^{(0)}) = N(U^{(0)}),$$

$$\text{ind}_{H_1} (B^{(k)}) = N(U^{(k)}), \quad k \geq 1,$$

where $B^{(k)}$ is the bilinear form associated with $L^{(k)}$. 
The space $H^1_{\text{rad}}$ is the set of radially symmetric $H^1(\mathbb{R}^d)$ functions. The space $H^1_{\text{rad}+}$ is the subset of $H^1_{\text{rad}}$ for which
\[ \int |f|^2 |x|^{-2} dx < \infty. \]

We will omit the subscript notation in our subsequent index computations. It will be $H^1_{\text{rad}}$ for $k = 0$ and $H^1_{\text{rad}+}$ for $k \geq 1$.

If one wishes to remove the limits from the statement of the initial conditions, let $U^{(k)}(r) = r^k \tilde{U}^{(k)}(r)$. Then the operator becomes
\[ \tilde{L}^{(k)} = -\frac{d^2}{dr^2} - \frac{d - 1 + 2k}{r} \frac{d}{dr} + V \]
and the initial conditions become $\tilde{U}^{(k)}(0) = 1$ and $(d/dr)\tilde{U}^{(k)}(0) = 0$. Indeed, we use precisely this change of variables when making our numerical computations; see appendix C.1. The proof of theorem 7 can be adapted from the proof of theorem XIII.8 in [24].

**Corollary 3.2.** The index is monotonic with respect to $k$,
\[ \text{ind}(B^{(k+1)}) \leq \text{ind}(B^{(k)}). \]
This has the useful consequence that once we find a value $k$ for which $\text{ind}(B^{(k)}) = 0$, we can immediately conclude that $B^{(k')} \geq 0$ for all $k' \geq k$.

### 3.2. Numerical estimates of the index

To compute the indices of the operators, we proceed as follows. First, we solve the initial value problems
\[ \mathcal{L}^{(0)}_+ U^{(0)} = 0, \quad U^{(0)}(0) = 1, \quad \frac{d}{dr} U^{(0)}(0) = 0, \quad (3.2a) \]
\[ \mathcal{L}^{(0)}_- Z^{(0)} = 0, \quad Z^{(0)}(0) = 1, \quad \frac{d}{dr} Z^{(0)}(0) = 0 \quad (3.2b) \]
for radially symmetric functions $U^{(0)}$ and $Z^{(0)}$. For higher harmonics, $k = 1, 2, \ldots$, we solve the initial value problems
\[ \mathcal{L}^{(k)}_+ U^{(k)} = 0, \quad U^{(k)}(0) = 0, \quad \lim_{r \to 0} r^{-k} U^{(k)}(r) = 1, \quad (3.3a) \]
\[ \mathcal{L}^{(k)}_- Z^{(k)} = 0, \quad Z^{(k)}(0) = 0, \quad \lim_{r \to 0} r^{-k} Z^{(k)}(r) = 1 \quad (3.3b) \]
for radially symmetric functions $U^{(k)}$ and $Z^{(k)}$.

**Proposition 3.3.** The indices of 3D Cubic NLS are
\[ \text{ind}\mathcal{L}^{(0)}_+ = 1, \quad \text{ind}\mathcal{L}^{(1)}_+ = 1, \quad \text{ind}\mathcal{L}^{(2)}_+ = 0, \]
\[ \text{ind}\mathcal{L}^{(0)}_- = 1, \quad \text{ind}\mathcal{L}^{(1)}_- = 0. \]

Once this proposition is established, corollary 3.2 immediately gives us

**Corollary 3.4.** For 3D Cubic NLS,
\[ \text{ind}\mathcal{B}^{(k)}_+ = 0 \quad \text{for } k > 2, \]
\[ \text{ind}\mathcal{B}^{(k)}_- = 0 \quad \text{for } k > 1, \]
where $\mathcal{B}^{(k)}_\pm$ is the bilinear form associated with $\mathcal{L}^{(k)}_\pm$. 

Figure 2. Index computations for 3D Cubic NLS. The number of zero crossings (other than \(r = 0\)) determines the codimension of the subspace on which the operator \(L^{(k)}_{\pm}\) is positive.

Using the method discussed in section C, we compute \(U^{(k)}\) and \(Z^{(k)}\) for each problem, \(k = 0, 1, 2\). The profiles appear in figures 2, 3 and 4. All were computed with the tolerance setting \(10^{-13}\).

As a consistency check on the numerics, we note that asymptotically, the potential vanishes, and

\[
L^{(k)}_{\pm} \approx -\frac{d^2}{dr^2} - \frac{d - 1}{r} U^{(k)} + \frac{k(k + d - 2)}{r^2}.
\]  

(3.4)

In the region where \(r \gg 1\), and the equations are essentially free and the solutions must behave as

\[
U^{(k)}(r) \approx C_0^{(k)} r^k + C_1^{(k)} r^{2-d-k}, \tag{3.5a}
\]

\[
Z^{(k)}(r) \approx D_0^{(k)} r^k + D_1^{(k)} r^{2-d-k}. \tag{3.5b}
\]

Estimating these constants from the numerics, we see that they have the ‘correct’ signs. For instance in figure 2(a), \(U^{(0)}\) clearly has one zero crossing. For sufficiently large \(r\), the function appears to be increasing past a local minimum. However, since the constants appear to have stabilized, we contend we have entered the free region; the signs and magnitudes of the constants thus forbid another zero.

**Proposition 3.5.** For the operators in proposition 3.3 and corollary 3.4 there exists a universal \(\delta_0 > 0\), sufficiently small, such that for the perturbed operators

\[
\overline{L}^{(k)}_{\pm} = L^{(k)}_{\pm} - \delta_0 e^{-|x|}
\]

the associated bilinear forms are stable:

\[
\text{ind}(\overline{B}^{(k)}_{\pm}) = \text{ind}(B^{(k)}_{\pm}).
\]

**Proof.** The proof follows from the definition of the index of \(B\); the form \(B\) is positive on some subspace of the operator of the indicated codimension. Let \(\delta_0\) be a sufficiently small value that it holds for \(L^{(k)}_{\pm}\) for \(k = 0, 1, 2\) and \(\overline{L}^{(k)}_{\pm}\) for \(k = 0, 1\). This \(\delta_0\) now holds for all higher values of \(k\) by a monotonicity argument. For example, for \(k > 2\),

\[
\overline{B}^{(k)}_{\pm}(f, f) = B^{(2)}_{\pm}(f, f) + \int \frac{(k + 4)(k - 2)}{|x|^2} |f|^2 \, dx \geq 0.
\]

Since the last term is positive, these indices of zero are stable to perturbation. \(\square\)
3.3. Invertibility of operators

In conjunction with the results on the indices of operators, we need to compute a number of inner products of the form $\langle Lu, u \rangle$, where $L$ is one of our operators and $u$ solves $Lu = f$. These are computed numerically, but we can rigorously justify the existence and uniqueness of these solutions, $u$, for the problems under consideration.

**Proposition 3.6 (Numerically verified for 3D problems).** Let $f$ be a smooth, radially symmetric, localized function satisfying the bound $|f(r)| \leq Ce^{-\kappa r}$ for some positive constants $C$ and $\kappa$. There exists a unique radially symmetric solution

$$(1 + r^{k+1})u \in L^\infty([0, \infty)) \cap C^2([0, \infty))$$

to

$$Lu = f,$$

where $L = L^{(k)}_\pm$ for one of the 3D problems.
Proof. This is proposition 2 and 4 of [15], along with our computations of the indices in proposition 3.3. See appendix B for a proof in 1D.

\[ \square \]

Corollary 3.7. The solutions to the problems of proposition 3.6 are smooth and decay at a rate proportional to \( r^{-1-k} \) as \( r \to \infty \).

### 3.4. Estimates of inner products

In order to prove the spectral property for each of these NLS equations, we need to approximate the bilinear forms associated with \( L_{\pm}^{(k)} \) on certain functions. These particular functions are, generically, of the form \( L u = f \), where \( f \) is from one of the orthogonality conditions.

Proposition 3.8 (Numerical approximation of inner products). For the 3D cubic problem, let \( U_1^{(0)}, U_2^{(0)}, U_1^{(1)} \) and \( Z_1^{(0)} \) solve

\[
\begin{align*}
L_+^{(0)} U_1^{(0)} &= R, & (1 + r)U_1^{(0)} &\in L^\infty, \\
L_+^{(0)} U_2^{(0)} &= \phi_2, & (1 + r)U_2^{(0)} &\in L^\infty, \\
L_+^{(1)} U_1^{(1)} &= r R, & (1 + r^2)U_1^{(0)} &\in L^\infty, \\
L_-^{(0)} Z_1^{(0)} &= R + r R', & (1 + r)Z_1^{(0)} &\in L^\infty,
\end{align*}
\]

where \( \phi_2 \) is the eigenstate associated with the positive real eigenvalue of \( J L \). Then,

\[
\begin{align*}
K_1^{(0)} &= \left( L_+^{(0)} U_1^{(0)}, U_1^{(0)} \right) = 1.04846, \\
K_2^{(0)} &= \left( L_+^{(0)} U_2^{(0)}, U_2^{(0)} \right) = 0.00215981, \\
K_3^{(0)} &= \left( L_+^{(0)} U_1^{(0)}, U_2^{(0)} \right) = -0.116369, \\
K_1^{(1)} &= \left( L_+^{(1)} U_1^{(1)}, U_1^{(1)} \right) = -0.581854, \\
J_1^{(0)} &= \left( L_-^{(0)} Z_1^{(0)}, Z_1^{(0)} \right) = -0.662038.
\end{align*}
\]

Proof. These results follow from direct computation. \( \square \)

Finally, we state the following

Proposition 3.9. For each of the inner products in proposition 3.8, there exists a \( \delta_0 \) sufficiently small such that inner products associated with \( \overline{L} \) can be made arbitrarily close to those of \( L \); they are stable. These perturbed values will be denoted with overlines.

Proof. This follows immediately from the invertibility of the operator and continuity. \( \square \)

### 3.5. Proof of the spectral property

We are now ready to prove the spectral property. Closely following steps 1 and 3 of section 2.4 of [15], we prove positivity of \( \overline{B}_+^{(0)} \). The other cases are similar.

Since \( K_1^{(0)} \) and \( K_2^{(0)} > 0 \), orthogonality to \( R \) and \( \phi_2 \) will not give positivity. However, if \( f \) is orthogonal to both of these, then it is also orthogonal to

\[
q = R - \frac{K_1^{(0)}}{K_2^{(0)}} \phi_2
\]
and

\[
\langle L_0^{(0)} q, q \rangle = K_1^{(0)} - 2 \frac{K_3^{(0)}}{K_2^{(0)}} K_3^{(0)} + \left( \frac{K_1^{(0)}}{K_2^{(0)}} \right)^2 K_2^{(0)}
\]

\[
= -\frac{1}{K_2^{(0)}} \left( (K_3^{(0)})^2 - K_1^{(0)} K_2^{(0)} \right)
\]

\[
= -5.22138.
\]

By proposition 3.9, we can take \( \delta_0 \) sufficiently small such that

\[
-\frac{1}{K_2^{(0)}} \left( (K_3^{(0)})^2 - K_1^{(0)} K_2^{(0)} \right) < 0.
\]

We proceed with this value of \( \delta_0 \).

Let \( \bar{Q} \) solve

\[
L_0^{(0)} \bar{Q} = q.
\]

Obviously,

\[
Q = \bar{U}_1^{(0)} - \frac{K_3^{(0)}}{K_2^{(0)}} \bar{U}_2^{(0)}
\]

and

\[
\mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) < 0.
\]

First, we give a heuristic argument for positivity. For a moment, suppose \( \bar{Q} \in H^1_{rad} \), which it is not since it decays too slowly to be in \( L^2 \). We could then imagine decomposing \( H^1_{rad} \) into \( \text{span}\{Q\} \) and its orthogonal complement, where the orthogonalization is done with respect to the \( \mathcal{B}_+^{(0)} \) quadratic form. Since \( \mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) < 0 \), the form is non-degenerate and this decomposition is well defined. Because \( \text{ind}\mathcal{B}_+^{(0)} = 1 \), \( \mathcal{B}_+^{(0)} \geq 0 \) on \( \text{span}\{\bar{Q}\} \). To prove this claim, we argue by contradiction. Suppose there were an element, \( Z \in \text{span}\{\bar{Q}\} \) for which \( \mathcal{B}_+^{(0)}(Z, Z) < 0 \). Then, because of our decomposition, \( \mathcal{B}_+^{(0)} < 0 \) on \( \text{span}\{Z, \bar{Q}\} \), a space of dimension two. This contradicts our index calculation, proving the claim.

Continuing, if \( u \in H^1_{rad} \), \( u \perp q \) (with respect to \( L^2 \)), then using the hypothetical orthogonal decomposition, we may write

\[
u = c \bar{Q} + u^+,
\]

\[
\mathcal{B}_+^{(0)}(u^+, \bar{Q}) = 0.
\]

If \( c = 0 \), then \( u \) lies in a subspace of \( H^1_{rad} \) on which \( \mathcal{B}_+^{(0)} \geq 0 \). Indeed, the orthogonality condition, \( u \perp q \), is sufficient to ensure \( u \) is orthogonal to \( \bar{Q} \) with respect to the \( \mathcal{B}_+^{(0)} \) quadratic form. Taking the \( L^2 \) inner product of \( u \) with \( q \),

\[
0 = c \langle \bar{Q}, q \rangle + \langle u^+, q \rangle = c \mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) + \langle u^+, \mathcal{L}_+^{(0)} \bar{Q} \rangle
\]

\[
= c \mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) + \mathcal{B}_+^{(0)}(u^+, \bar{Q}) = c \mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) + 0.
\]

Since \( \mathcal{B}_+^{(0)}(\bar{Q}, \bar{Q}) \neq 0 \), we conclude \( c = 0 \).

Unfortunately, the above argument does yet not work because \( \bar{Q} \) is not in \( L^2 \). To get positivity of \( \mathcal{B}_+^{(0)} \), we regularize the problem and follow the above scheme. First, we introduce the smooth cutoff function \( \chi_A(r) = \chi(r/A) \), defined such that

\[
\chi(r) = \begin{cases} 
1 & r < 1, \\
0 & r \geq 2
\end{cases}
\]
and the norm
\[ \| f \|_2 = \| \nabla f \|_2^2 + \int |\nabla \| f \|)^2. \]

Let \( \overline{Q}_A(r) = \overline{Q}(r) \chi_A(r) \). Next, we observe that

\[ \lim_{A \to +\infty} \| \overline{Q}_A - \overline{Q} \|_\star + |\mathcal{B}_\star^{(0)}(\overline{Q}, \overline{Q}) - \mathcal{B}_\star^{(0)}(\overline{Q}_A, \overline{Q}_A)| = 0. \tag{3.9} \]

Since \( \mathcal{B}_\star^{(0)}(\overline{Q}, \overline{Q}) < 0 \), for sufficiently large \( A \), \( \mathcal{B}_\star^{(0)}(\overline{Q}_A, \overline{Q}_A) < 0 \) too. Thus, we can legitimately decompose \( H_{\text{rad}}^1 \) as

\[ H_{\text{rad}}^1 = \text{span} \{ \overline{Q}_A \} \oplus \text{span} \{ \overline{Q}_A \}^\perp \tag{3.10} \]

with the orthogonal decomposition done with respect to \( \mathcal{B}_\star^{(0)} \).

Finally, let \( u \in H_{\text{rad}}^1 \), \( u \perp R \) and \( u \perp \phi_2 \). Then \( u \perp q \). With \( A \) sufficiently large to make the above decomposition valid,

\[ u = c(A) \overline{Q}_A + u_A^\perp. \tag{3.11} \]

As in the heuristic argument \( \mathcal{B}_\star^{(0)}(u_A^\perp, u_A^\perp) \geq 0 \). Thus,

\[ \mathcal{B}_\star^{(0)}(u, u) = c(A)^2 \mathcal{B}_\star^{(0)}(\overline{Q}_A, \overline{Q}_A) + \mathcal{B}_\star^{(0)}(u_A^\perp, u_A^\perp) \geq c(A)^2 \mathcal{B}_\star^{(0)}(\overline{Q}_A, \overline{Q}_A). \]

We will have our result if \( c(A) \to 0 \) as \( A \to +\infty \).

Since \( \langle u, q \rangle = 0 \),

\[ c(A) \langle \overline{U}_A^\perp, q \rangle = -\langle u_A^\perp, q \rangle \]
\[ = -\langle u_A^\perp, \overline{Z}_\star^{(0)} \overline{Q} \rangle \]
\[ = -\langle u_A^\perp, \overline{Z}_\star^{(0)} (\overline{Q} - \overline{Q}_A) \rangle. \]

Therefore,

\[ |c(A)| = \left| \frac{\langle u_A^\perp, \overline{Z}_\star^{(0)} (\overline{Q} - \overline{Q}_A) \rangle}{\langle \overline{U}_A^\perp, q \rangle} \right| \leq \frac{\| u_A^\perp \|_\star \| \overline{Q} - \overline{Q}_A \|_\star}{\| \overline{U}_A^\perp, q \|}. \]

Also,

\[ |\langle \overline{U}_A^\perp, q \rangle - (\overline{Q}, q) \rangle| = |\langle \overline{U}_A^\perp - \overline{Q}_A, \overline{Z}_\star^{(0)} \overline{Q} \rangle| \leq \| \overline{U}_A^\perp - \overline{Q}_A \|_\star \| \overline{Q} \|_\star. \]

Since this vanishes as \( A \to +\infty \), we have that for all \( A \) sufficiently large,

\[ |c(A)| \leq C \| u_A^\perp \|_\star \| \overline{Q} - \overline{Q}_A \|_\star \]

for a constant \( C \) independent of \( A \).

By construction,

\[ \| u_A^\perp \|_\star \leq C \left( \| u \|_\star + c(A) \| \overline{U}_A \|_\star \right) \leq C \left( \| u \|_\star + c(A) \| \overline{U}_A - \overline{Q}_A \|_\star + \| \overline{Q}_A \|_\star \right). \]

Substituting into our previous estimate on \( c(A) \),

\[ |c(A)| \leq C \left( \| u \|_\star + c(A) \| \overline{U}_A - \overline{Q}_A \|_\star + \| \overline{Q}_A \|_\star \right) \| \overline{Q} - \overline{Q}_A \|_\star. \]

We can clearly see that as \( A \to +\infty \), \( c(A) \to +0 \). We conclude

\[ \mathcal{B}_\star^{(0)}(u, u) \geq 0 \]
for \( u \in H^1_{\text{rad}} \) and \( u \perp R \) and \( u \perp \phi_2 \). This yields the estimate

\[
B^{(0)}_+(u, u) \geq \delta_0 \int e^{-|x|/2} |u|^2 \, dx.
\]

Following the same analysis for \( \mathcal{L}_- \), we conclude

\[
B^{(0)}_-(g, g) \geq \delta_0 \int e^{-|x|/2} |g|^2 \, dx
\]

for \( g \in H^1_{\text{rad}} \) and \( g \perp R + rR' \) since \( J^{(0)}_1 < 0 \). Repeating this again for \( f \in H^1_{\text{rad}(1)} \), \( f \perp rR \), we get

\[
B^{(1)}_-(f, f) \geq \delta_0 \int e^{-|x|/2} |f|^2 \, dx
\]

because \( K^{(1)}_1 < 0 \).

Let us assume that \( \delta_0 \) has been taken sufficiently small such that:

- The indices of all operators are stable, as in proposition 3.5,
- The above arguments on the positivity of \( B^{(k)}_+ \) for \( k = 0, 1 \) and \( B^{(0)}_- \) hold.

Then for \( z = (f, g)^T \) satisfying the orthogonality conditions,

\[
\mathcal{B}(z, z) = \mathcal{B}_+(f, f) + \mathcal{B}_-(g, g)
\]

\[
= \sum_{k=0}^{L_k} \sum_{l=0}^{L_k} B^{(k)}_+(f^{(k,l)}, f^{(k,l)}) + \sum_{k=0}^{L_k} \sum_{l=0}^{L_k} B^{(k)}_-(g^{(k,l)}, g^{(k,l)})
\]

\[
= \sum_{k=0}^{L_k} \sum_{l=0}^{L_k} B^{(k)}_+(f^{(k,l)}, f^{(k,l)}) + \sum_{k=0}^{L_k} \sum_{l=0}^{L_k} B^{(k)}_-(g^{(k,l)}, g^{(k,l)}) - \delta_0 \int e^{-|x|} \left( |f|^2 + |g|^2 \right) \, dx
\]

\[
= B(z, z) - \delta_0 \int e^{-|x|/2} |z|^2 \, dx \geq 0.
\]

We almost have the expression in definition 1.6. To complete the proof, note that for any \( \theta \in (0, 1) \),

\[
(1 + \theta) \mathcal{B}(z, z) \geq \theta \left( \int |\nabla z|^2 \, dx + \int V_+ |f|^2 + \int V_- |g|^2 \) + \delta_0 \int e^{-|x|/2} |z|^2 \, dx.
\]

We can take \( \theta = \theta_* \) sufficiently small such that

\[
\theta_* \left( \int V_+ |f|^2 + \int V_- |g|^2 \right) + \delta_0 \int e^{-|x|/2} |z|^2 \, dx \geq \frac{\delta_0}{2} \int e^{-|x|/2} |z|^2 \, dx.
\]

The above step holds because \( |V_\pm| \lesssim e^{-2r} \) as \( r \to \infty \). This reveals the degree of flexibility we have in choosing the perturbation \( \delta_0 e^{-r} \). Continuing, we have

\[
\mathcal{B}(z, z) \geq \frac{\theta_*}{1 + \theta_*} \int |\nabla z|^2 \, dx + \frac{\delta_0}{2(1 + \theta_*)} \int e^{-|x|/2} |z|^2 \, dx.
\]

Shrinking \( \delta_0 \) again, so that it is smaller than

\[
\min \left\{ \frac{\theta_*}{1 + \theta_*}, \frac{\delta_0}{2(1 + \theta_*)} \right\}
\]

gives us the spectral property. \( \Box \)
4. Other problems

In principle, this scheme can be applied to any linearized NLS. One finds the indices of the operators, picks an appropriate subspace to project away from, and computes the necessary inner products. However, our experiments show that the algorithm is not as universal as might be hoped. In this section we exhibit computations for several 1D NLS equations,

$$i\psi_t + \psi_{xx} + |\psi|^2\psi = 0.$$  \hfill (4.1)

Sometimes our approach works, ruling out embedded eigenvalues in a range of supercritical cases, while in others it fails, leaving a large range of interesting problems unresolved using our techniques.

4.1. Numerical estimates of the index

As in the 3D problem, we first compute the indices of the operators $L_{\pm}$ to identify the number of ‘bad’ directions. In contrast to the multidimensional problems where there are an arbitrarily high, but finite, number of harmonics which must be examined, 1D problems only require us to study the operators restricted to even and odd functions. This requires the following results, whose proofs are quite similar to that of theorem 7:

**Corollary 4.1.** Let $U$ be the even solution to

$$\begin{aligned}
LU &= -U'' + V(r)U = 0, \\
U(0) &= 1, \\
U'(0) &= 0,
\end{aligned}$$

where $V$ is sufficiently smooth and rapidly decaying. Then, the number $N(U)$ of zeros of $U$ is finite and

$$\text{ind}_{H^1_e}(B) = N(U),$$

where $B$ is the bilinear form associated with $L$.

**Corollary 4.2.** Let $U$ be the odd solution to

$$\begin{aligned}
LU &= -U'' - \frac{d-1}{r}U' + V(r)U = 0, \\
U(0) &= 0, \\
U'(0) &= 1,
\end{aligned}$$

where $V$ is sufficiently smooth and rapidly decaying. Then, the number $N(U)$ of zeros of $U$ is finite and

$$\text{ind}_{H^1_o}(B) = N(U),$$

where $B$ is the bilinear form associated with $L$.

$H^1_e$ and $H^1_o$ are the subspaces of $H^1(\mathbb{R})$ restricted to even and odd functions. In what follows, we shall omit them in the subscripts of the indices.

To proceed, we numerically solve the initial value problems

$$\begin{aligned}
L_+^{(e)}U^{(e)} &= 0, & U^{(e)}(0) &= 1, & \frac{d}{dx}U^{(e)}(0) &= 0, \\
L_-^{(e)}Z^{(e)} &= 0, & Z^{(e)}(0) &= 1, & \frac{d}{dx}Z^{(e)}(0) &= 0
\end{aligned} \hfill (4.2a)$$

for even functions $U^{(e)}$ and $Z^{(e)}$. We then solve

$$\begin{aligned}
L_+^{(o)}U^{(o)} &= 0, & U^{(o)}(0) &= 0, & \frac{d}{dx}U^{(o)}(0) &= 1, \\
L_-^{(o)}Z^{(o)} &= 0, & Z^{(o)}(0) &= 0, & \frac{d}{dx}Z^{(o)}(0) &= 1
\end{aligned} \hfill (4.3a)$$
Figure 5. Index computations for 1D NLS. The number of zero crossings (other than \( x = 0 \)) determines the codimension of the subspace on which the operator \( L_{\pm}^{(e/o)} \) is positive.

for odd functions \( U^{(o)} \) and \( Z^{(o)} \). \( L_{\pm} \) have the same definitions as before; the Laplacian is now one dimensional.

**Proposition 4.3 (Numerically verified).** The indices for the 1D NLS equation with \( \sigma = 2, 2.1, 2.5, 3 \) are

\[
\begin{align*}
\text{ind} L_{\pm}^{(e)} &= 1, & \text{ind} L_{\pm}^{(o)} &= 1, \\
\text{ind} L_{\pm}^{(e)} &= 1, & \text{ind} L_{\pm}^{(o)} &= 0.
\end{align*}
\]

**Proof.** Using the method discussed in section C, we compute \( U^{(\alpha)} \) and \( Z^{(\alpha)} \) for each problem, \( \alpha = e, o \). The profiles appear in figure 5. All are computed with a relative tolerance of \( 10^{-10} \) and an absolute tolerance of \( 10^{-12} \) using MATLAB. The consistency checks on the asymptotic constants for these functions appear in figures 7 and 8 in the appendix.

Proposition 3.5 applies to these 1D problems too. As in the 3D case, we ultimately use a perturbed bilinear form in the proof of the spectral property.

### 4.2. Estimates of the inner products

We now compute a series of inner products and show that in some cases the natural orthogonality conditions are sufficient to yield a spectral property. Rigorously, these results require the following proposition on the invertibility of the \( L_{\pm}^{(e/o)} \) operators:

**Proposition 4.4 (Numerically verified).** Let \( f \) be a smooth, localized function satisfying the bound \( |f(x)| \leq Ce^{-\kappa|x|} \) for some positive constants \( C \) and \( \kappa \). If \( f \) is even/odd, there exists a unique even/odd solution \( u \in L^\infty(\mathbb{R}) \cap C^2(\mathbb{R}) \) to

\[
Lu = f, \tag{4.4}
\]

where \( L = L_{\pm}^{(e/o)} \) for a 1D problem.

**Proof.** See appendix B. \( \square \)
Proposition 4.5 (Numerical). Let \( U_1^{(e)} \), \( Z_1^{(e)} \) and \( U_1^{(o)} \), all elements of \( L^\infty(\mathbb{R}) \), solve the following boundary value problems:

\[
\mathcal{L}_+^{(e)} U_1^{(e)} = R, \quad \frac{d}{dx} U_1^{(e)}(0) = 0, \tag{4.5a}
\]

\[
\mathcal{L}_-^{(e)} Z_1^{(e)} = \frac{1}{\sigma} R + x R', \quad \frac{d}{dx} Z_1^{(e)}(0) = 0, \tag{4.5b}
\]

\[
\mathcal{L}_+^{(o)} U_1^{(o)} = R', \quad U_1^{(o)}(0) = 0. \tag{4.5c}
\]

Let

\[
K_1^{(e)} \equiv \mathcal{B}_s^{(e)} (U_1^{(e)}) = \left\langle \mathcal{L}_+^{(e)} U_1^{(e)}, U_1^{(e)} \right\rangle, \tag{4.6a}
\]

\[
J_1^{(e)} \equiv \mathcal{B}_s^{(e)} (Z_1^{(e)}) = \left\langle \mathcal{L}_-^{(e)} Z_1^{(e)}, Z_1^{(e)} \right\rangle, \tag{4.6b}
\]

\[
K_1^{(o)} \equiv \mathcal{B}_s^{(o)} (U_1^{(o)}) = \left\langle \mathcal{L}_+^{(o)} U_1^{(o)}, U_1^{(o)} \right\rangle. \tag{4.6c}
\]

Then,

\[
\begin{array}{cccc}
\sigma & K_1^{(e)} & J_1^{(e)} & K_1^{(o)} \\
2.0 & -0.557768 & 0.292551 & -1.30410 \\
2.1 & -0.496932 & 0.216284 & -1.21364 \\
2.5 & -0.297841 & -0.0216292 & -0.924662 \\
3.0 & -0.122559 & -0.218499 & -0.671783 \\
\end{array}
\]

4.2.1. Proof of the spectral property for some supercritical cases. We restrict our attention to the 1D supercritical problems \( \sigma = 2.5 \) and \( \sigma = 3 \). Repeating the procedure of section 3.5, for \( z = (f, g)^T \), the orthogonality of \( f \) to \( R \) and \( x R \) gives us \( Z_+ \geq 0 \) and the orthogonality of \( g \) to \((1/\sigma)R + x R' \) gives us \( Z_- \geq 0 \). This proves the spectral property on the restricted subspace. Since these orthogonality conditions are consistent with those formulated in section 2.2, we conclude that there are no non-zero purely imaginary eigenvalues.

4.2.2. An inconclusive supercritical case. In the case of \( \sigma = 2.1 \), we have that \( J_1^{(e)} > 0 \), which means that orthogonality of \( g \) with respect to \((1/\sigma)R + x R' \), is insufficient to guarantee positivity of \( \mathcal{L}_- \). It is possible that if we extend our scope, as in the 3D cubic problem, to include orthogonality to the eigenstate associated with the unstable eigenvalue we will be able to prove the spectral property for this problem. However, we do not pursue that here; rather we wish to highlight the failure of our algorithm at a seemingly arbitrary supercritical nonlinearity.

4.2.3. The critical case. The critical 1D problem, with \( \sigma = 2 \), is also inconclusive. As in the supercritical problems we will look at the inner products against \( R \) and \( \frac{1}{\sigma} R + x R' \). We also employ inner products arising from the rest of the generalized kernel, \( x^2 R \) and \( \rho \), where \( \rho \) solves

\[
L_+ \rho = -x^2 R.
\]

See [36] for details. This motivates the following numerical result:

Proposition 4.6 (Numerical). Let \( Z_2^{(e)} \) solve

\[
\mathcal{L}_-^{(e)} Z_2^{(e)} = \rho, \quad \frac{d}{dx} Z_2^{(e)}(0) = 0. \tag{4.7}
\]
Then
\[
J_2^{(\ell)} \equiv B^{(\ell)}(Z_2^{(\ell)}, Z_2^{(\ell)}) = \left\langle c^{(\ell)} Z_2^{(\ell)}, Z_2^{(\ell)} \right\rangle = 3.779 \, 15. \tag{4.8a}
\]
\[
J_3^{(\ell)} \equiv B^{(\ell)}(Z_3^{(\ell)}, Z_3^{(\ell)}) = \left\langle c^{(\ell)} Z_3^{(\ell)}, Z_3^{(\ell)} \right\rangle = 0.864 \, 273. \tag{4.8b}
\]

Since \( K_1^{(\ell)} < 0 \), we may conclude that \( \mathcal{L}_+ \geq 0 \), when the operator is restricted to even functions that are orthogonal to \( R \). However, orthogonality to neither \( \frac{1}{2} R + x R' \) nor \( \rho \) is, individually, sufficient to gain positivity of \( \mathcal{L}_+^{(\ell)} \). We are thus motivated to consider orthogonality to the subspace \( \text{span}[\frac{1}{2} R + x R', \rho] \), as in the proof of the 3D cubic problem. We examine the quantity
\[
- \frac{1}{J_2^{(\ell)}} \left( (J_1^{(\ell)})^2 - J_1^{(\ell)} J_2^{(\ell)} \right) = 0.094 \, 8958. \tag{4.9}
\]
However, we need this to be negative. Thus, we have no set of natural orthogonality conditions which yield a spectral property.

4.2.4. The critical case with other orthogonality conditions. If we had instead used the orthogonality condition, \( g \perp R \), and then solved the boundary value problem \( \mathcal{L}_+^{(\ell)} \hat{Z}_3^{(\ell)} = R \), the inner product,
\[
\hat{J}_1^{(\ell)} \equiv \left\langle \mathcal{L}_+^{(\ell)} \hat{Z}_1^{(\ell)}, \hat{Z}_1^{(\ell)} \right\rangle = -3.770 \, 731.
\]
This would give us a spectral property, but it is not a convenient subspace.

Suppose we use the orthogonality conditions of \([15]\), and let \( g \perp \Lambda R \) and \( g \perp \Lambda R' \). Then, we compute as follows: let \( \hat{Z}_1^{(\ell)} \) and \( \hat{Z}_2^{(\ell)} \) solve
\[
\mathcal{L}_-^{(\ell)} \hat{Z}_1^{(\ell)} = \Lambda R, \quad \frac{d}{dx} \hat{Z}_1^{(\ell)}(0) = 0, \tag{4.10a}
\]
\[
\mathcal{L}_-^{(\ell)} \hat{Z}_2^{(\ell)} = \Lambda R, \quad \frac{d}{dx} \hat{Z}_2^{(\ell)}(0) = 0. \tag{4.10b}
\]
Then,
\[
\hat{J}_1^{(\ell)} \equiv B^{(\ell)}(\hat{Z}_1^{(\ell)}, \hat{Z}_1^{(\ell)}) = \left\langle c^{(\ell)} \hat{Z}_1^{(\ell)}, \hat{Z}_1^{(\ell)} \right\rangle = 0.292 \, 551, \tag{4.11a}
\]
\[
\hat{J}_2^{(\ell)} \equiv B^{(\ell)}(\hat{Z}_2^{(\ell)}, \hat{Z}_2^{(\ell)}) = \left\langle c^{(\ell)} \hat{Z}_2^{(\ell)}, \hat{Z}_2^{(\ell)} \right\rangle = 2.576 \, 56, \tag{4.11b}
\]
\[
\hat{J}_3^{(\ell)} \equiv B^{(\ell)}(\hat{Z}_3^{(\ell)}, \hat{Z}_2^{(\ell)}) = \left\langle c^{(\ell)} \hat{Z}_3^{(\ell)}, \hat{Z}_2^{(\ell)} \right\rangle = -1.276 \, 57. \tag{4.11c}
\]
As one would hope, given that the 1D spectral property was established in [21],
\[
- \frac{1}{J_2^{(\ell)}} \left( (\hat{J}_3^{(\ell)})^2 - \hat{J}_1^{(\ell)} \hat{J}_2^{(\ell)} \right) = -0.339 \, 932. \tag{4.12}
\]
This sign ensures that projection away from those two directions is sufficient to point us away from the negative eigenvalue, rendering \( \mathcal{L}_-^{(\ell)} \geq 0 \).

5. Discussion

We have demonstrated a computer assisted algorithm for proving the positivity of a bilinear form, \( B \), on a subspace \( U \). Because of the relationship between \( B, \mathcal{L} \), and the linearized operator,
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Figure 6. For subcritical and critical solitons, the spectrum of $J_L$ typically takes the above form. The spectrum of $\mathcal{H}$ can be obtained by multiplying by $i$ (rotate the above figures by $90^\circ$).

JL, we infer that there are no embedded eigenvalues. We succeeded with this program in the case of the 3D cubic equation, and in two supercritical 1D problems. As suggested by Sulem, it is likely to also be successful for solitons (with $\lambda = 1$) of the 3D cubic-quintic equation (CQNLS),

$$i\psi_t + \Delta\psi + |\psi|^2\psi - \gamma|\psi|^4\psi = 0$$

for $\gamma$ sufficiently close to zero. In the forthcoming publication of Asad and Simpson [2], the methods presented here are used to assess the range of $\gamma$ for which the unstable solitons of 3D CQNLS lack embedded eigenvalues. They also explore the range of supercritical exponents in 1D for which the spectral property can be established. In addition, in Simpson and Zwiers [30] similar techniques are used to establish a necessary spectral property to prove stability of the vortex profile blow-up for 2D cubic NLS.

For subcritical and critical problems, a similar algorithm may succeed, though there is an additional subtlety. As seen in figure 6, many subcritical problems will have eigenvalues inside the gap. As noted, our approach cannot distinguish between embedded eigenvalues and gap eigenvalues on the subspace $U$, so it would be essential to project away from those states. Indeed, for subcritical problems, the unstable states that we employed in the supercritical problems are no more, and they cannot be used to define $U$. For critical problems, the multiplicity of the zero eigenvalue increases by two. This gives additional directions which may be useful in establishing a spectral property.

It remains to be seen how to extend our technique to other NLS/GP equations. Indeed, the failure in the 1D critical problem is curious. The success or failure of the approach is likely related to the choice of our operator $\Lambda = d/2 + x \cdot \nabla$. In [15], the authors proved the spectral property using this $\Lambda$, as it is generated by the scaling invariance of the mass critical problem. This results in the so-called ‘pseudoconformal invariant’ for critical NLS and has great implications for blow-up. See [21] and [32] for additional details.

Finally, recall that $\Lambda$ determines the operators $L_{\pm}$. These each have an index identifying the number of negative directions. We then choose orthogonality conditions that simultaneously
must satisfy the two properties:
(1) They must be orthogonal to any embedded eigenvalues,
(2) Orthogonality in $L^2$ with respect to these directions must imply orthogonality to the negative directions of $L_\pm$, with respect to the $B_\pm$ quadratic form.

The first requirement is satisfied by the vectors from the adjoint problem, as discussed in section 2.2. We appear to have little flexibility in altering these. Changing $/\Lambda_1$ will change $L_\pm$; in turn this changes the negative directions. Thus, a different skew adjoint operator may extend the applicability of the algorithm.

**Appendix A. Commutator estimates**

In this appendix we shall develop estimates that rule out arbitrarily large embedded eigenvalues.

**Appendix A.1. Large eigenvalues**

We first establish upper bounds on the magnitude of embedded $L^2$ eigenvalues of $JL$. In this analysis, we examine the fourth order equation that comes from squaring the operator; the eigenvalue problem becomes

$$L_+ L_- u = \mu^2 u. \tag{A.1}$$

The $L_\pm$ operators are as in the introduction. We assume $\mu \in \sigma_{\text{cont}}(JL) = (\lambda, \infty)$ so that it resides in the essential spectrum. As our proof applies to many NLS equations, we do not specify the potentials $V_\pm$.

From the properties of the soliton and the nonlinearity, we have that any solution to equation (A.1) is locally smooth via an iteration argument, as in [20]. Following [3], asymptotic analysis tells us the solution decays exponentially fast. As a result, the possible range of frequencies is limited by

$$\|\nabla u\|_{L^2} \leq \mu \|u\|_{L^2}. \tag{A.2}$$

See [34, 31] for references on microlocal analysis.

We prove

**Theorem 8.** There exists a $\mu_0 > \lambda$ such that for all $\mu \geq \mu_0$, the eigenvalue equation (A.1) has no non-trivial solution in $L^2$.

**Proof.** We begin by defining the Mourre commutator

$$M \equiv x \cdot \nabla + \nabla \cdot x. \tag{A.3}$$

Using the structure of these operators, we immediately have the identities

$$\langle [M, L_+] L_- u, u \rangle = 0, \quad \langle [L_+, L_- - \mu^2] u, u \rangle = 0. \tag{A.4}$$

Combining these two identities with the frequency bound of (A.2), we can rule out $L^2$ solutions for sufficiently large $\mu$. First, we compute

$$\langle (\Delta^2 - 2\Delta \Delta + \Delta(V_+(x)) + V_-(x) \Delta - \lambda V_+ + V_+ + (\lambda^2 - \mu^2) + V_- V_+\rangle u, u \rangle = 0. \tag{A.5}$$

Next, observe

$$ML_- L_+ - L_+ L_- M = [M, L_+] L_- + L_- [M, L_+] + [L_+, L_-] M,$$

$$[M, -\Delta] = 4\Delta, \quad [M, V_-] = 2x \cdot \nabla V_-.$$
Furthermore, this estimate combined and standard Sobolev embeddings implies
\( u \langle \Delta \rangle \Delta - 4(\nabla\cdot \nabla V_+ + 2(\nabla \cdot \nabla V_+)\Delta \nabla V_+) = 0. \) (A.6)

Hence, \( \int \sum \nabla (\Delta u) \cdot \nabla u \) for any \( k \); hence, \( u \) is smooth.

The system we assess is
\[
\int [-4(\Delta u)^2 - 4\lambda(V_+ + V_+)u^2 - 4(\mu^2 - \lambda^2)u^2] + 2(\lambda(u \cdot \Delta V_+ + x \cdot \nabla V_+) + \Delta(\lambda u \cdot \Delta V_+) - d(\Delta V_+ - \Delta V_+)^2 \leq \mu^2 \|u\|_{L^2}^2 + \|F\|_{L^\infty} \|u\|_{L^2}^2.
\]

where
\[
F = 4V_+ - 2(\lambda(x \cdot \nabla V_+ + x \cdot \nabla V_+) + 2(\lambda(x \cdot \nabla V_+)V_+ + \Delta(\lambda(x \cdot \nabla V_+ + x \cdot \nabla V_+) - x \cdot \nabla(\Delta V_+ - \Delta V_+)^2 - d(\Delta V_+ - \Delta V_+)^2)
\]

and \( C_j = C_j(V_+, V_+, \lambda, d) \) for \( j = 1, 2 \). Hence, for \( \mu \) large, we have that
\[
\int (-4(\Delta u)^2 - 4\lambda(V_+ + V_+)u^2 - C_3(\mu, \lambda, V_+, V_+)u^2) \leq 0,
\]

for \( C_3 > 0 \) and \( u \) a smooth function, hence \( u = 0. \)

Appendix A.2. Spherical harmonics

As our potentials are radially symmetric, we expand our functions in spherical harmonics. Separating the radial variable, \( r \), from the angular variables, \( \theta \), the expansion takes the form
\[
\sum_k u_k(r)\phi_k(\theta).
\]
where
\[ \Delta_S \phi_k(\theta) = (k^2 + (d - 1)d) \phi_k(\theta). \]

See [35] for a description of the eigenspaces of the spherical Laplacian, \( \Delta_S \). Then, we have the following ODE eigenvalue problem:
\[
\left[ \left( -\frac{\partial^2}{\partial r^2} - \frac{d-1}{r} \frac{\partial}{\partial r} + \frac{\alpha^2}{r^2} + \lambda - V_-(r) \right) \times \left( -\frac{\partial^2}{\partial r^2} - \frac{d-1}{r} \frac{\partial}{\partial r} + \frac{\alpha^2}{r^2} + \lambda - V_+(r) \right) - \mu^2 \right] u_k(r) = 0.
\]

where \( \alpha^2 = k^2 + (d - 1)d \) for \( k = 0, 1, 2, \ldots \).

We have the following theorem:

\textbf{Theorem 9.} There exists some \( \alpha_0 > 0 \) such that for all \( \alpha \geq \alpha_0 \), the eigenvalue equation (A.7) has only the trivial solution in \( L^2 \).

\textbf{Proof.} Let us denote the radial inner product by
\[
\langle u, v \rangle_r = \int uvr^{d-1} \, dr,
\]
and the operators:
\[
\Delta_r = r^{1-d} \frac{\partial}{\partial r} \left( r^{d-1} \frac{\partial}{\partial r} \right),
\]
\[
P_r = d + 2r \frac{\partial}{\partial r}.
\]

Using the same commutator approach as in section A.1,
\[
\left\{ \left[ 4\Delta_r - \frac{4\alpha^2}{r^2} - 2r V_-(r) \right] \left[ -\Delta_r + \frac{\alpha^2}{r^2} + \lambda - V_+(r) \right] 
+ \left[ -\Delta_r + \frac{\alpha^2}{r^2} + \lambda - V_+(r) \right] \left[ 4\Delta_r - \frac{4\alpha^2}{r^2} - 2r V_+(r) \right] 
+ (V_- - V_+) \Delta_r - \Delta_r (V_- - V_+) \left[ d + 2r \frac{\partial}{\partial r} \right] u_k, u_k \right\}_r = 0.
\]

Thus,
\[
\left\{ \begin{array}{l}
-8(\Delta_r)^2 u + 16\Delta_r \left( \frac{\alpha^2}{r^2} u_k \right) + 8\lambda \Delta_r u_k - 4(V_- + V_+) \Delta_r u_k - \frac{8\alpha^4}{r^4} u_k \\
- \frac{8\lambda \alpha^2}{r^2} u_k + \frac{4\alpha^2}{r^2} (V_- + V_+) u_k + 2(r V'_-(r) + r V'_+(r)) \Delta_r u_k \\
-2\frac{\alpha^2}{r} (V'_-(r) + V'_+(r)) u_k - 2\lambda r (V'_-(r) + V'_+(r)) u_k \\
+ 2r V'_-(r) V_+(r) u_k + 2r V'_-(r) V'_+(r) u_k \\
+ \left( d + 2r \frac{\partial}{\partial r} \right) ((V_- - V_+) \Delta_r - \Delta_r (V_- - V_+)) u_k, u_k \end{array} \right\}_r = 0.
\]
This implies

\[ \int \left[ -8(\Delta r, u_k)^2 - \left( \frac{16\alpha^2}{r^2} + 8\lambda \right) ((u_k)_r)^2 - \left( \frac{8\alpha^2}{r^2} + \frac{8\lambda\alpha^2}{r^2} \right) u_k^2 \right] r^{d-1} \, dr \\
+ \int \left[ 4(V_++V_-)+2r(V_-)-6r(V_+_r)((u_k)_r)^2 r^{d-1} \, dr \\
+ \int \left[ \frac{4\alpha^2}{r^2}(V_++V_-)-\frac{(d-4)\alpha^2}{r^4} - \frac{d(d-1)+2\alpha^2}{r}(V_-)_r \\
+ \frac{(d-1)(d-2)-2\alpha^2}{r}((V_+_r)_r)-(d-2)(V_-)_rr+3d(V_+_rr) \\
+2r((V_+_r)(V_+)(V_+_rr)+2r(V_+_rrr)-2\lambda r((V_-)_r+(V_+_r)_r) \right] u_k^2 r^{d-1} \, dr \\
\leq 0. \]

In the preceding calculations, we integrated by parts several times above. To justify this, \( r = 0 \) must be a root of \( u_k \) of sufficiently high multiplicity to compensate for the singular terms. Fortunately, spherical harmonics result from eigenvalues of the spherical Laplacian. These take the values

\[ \nu_k = k^2 + (d-2)k, \]

and for each \( k \), the eigenfunctions (and hence the spherical harmonics) are traces of harmonic polynomials of degree \( k \). As a result, in order to give a smooth solution as guaranteed above, \( u_k(0) \) must be a zero of multiplicity \( k \). For \( k \geq \max\{0, 5-d\} \), the behaviour of \( u \) is sufficient to make the calculations rigorous. See [35], chapter 8 for a detailed description of eigenfunctions for the Laplacian on the sphere.

In the commutator expression, the parameter that must dominate is \( \alpha^4 \). Since \( V_+, V_- \) are smooth, exponentially decaying functions by assumption, all terms involving \( V_+, V_- \) and derivatives thereof are nicely bounded at 0 and exponentially decaying. Hence, for \( 0 \leq r \leq 1 \), all of the functions above are easily controlled by \( \alpha^4/r^4 \) for \( \alpha \) sufficiently large.

Similarly, for \( r > r_\star \), \( r_\star \) sufficiently large, the exponential decay of \( V_-, V_+ \) and their derivatives imply that any function above is dominated \( (\alpha^4/r^4) \) once \( \alpha \) is sufficiently. In the intermediate region, using the smoothness of the potential functions we can find \( \alpha \) large enough to bound the lower order terms. In order to determine \( \alpha \) exactly, a careful analysis must be done involving all of the extrema of \( V_-, V_+ \) and their derivatives. As these functions are uniformly bounded, there exists \( \alpha_0 \) such that for all \( \alpha \geq \alpha_0 \), the operator when conjugated by the radial Mourre operator gives a negative definite system. Hence, the result holds. \( \square \)

Remark A.1. Any embedded eigenvalue can be expressed purely as a finite sum of spherical harmonics with radial coefficients. Combining this with the result in section A.1 gives a limited range for the calculations one must do in order to determine whether or not an operator has no embedded eigenvalues.

Appendix B. Proof of the invertibility of the operators

In this section we give a full proof of proposition 4.4. This relies on our numerically computed indices, from proposition 3.3. This proof generalizes to the 3D problem, establishing proposition 3.6.
Following [15, 21], we first prove uniqueness and then existence. Before beginning the uniqueness part, we recall the following extension of the Levinson theorem [8, 19], from [13]:

**Theorem 10 (Eastham).** For the equation
\[ y^{(n)} + a_1(x)y^{(n-1)} + \cdots + a_n(x)y = 0, \]
assume
\[ \int_a^\infty x^{j-1}|a_j(x)|\,dx < \infty \]
for some \( a > 0 \) and \( j = 1, \ldots, n \). Then there exist \( n \) solutions, \( y_k(x) \), such that as \( x \to \infty \),
\[ y_k^{(i-1)}(x) \sim \frac{x^{k-i}}{(k-i)!}, \quad 1 \leq i \leq k, \]
\[ y_k^{(i-1)}(x) = o(x^{(k-i)}), \quad k+1 \leq i \leq k. \]

To prove uniqueness, let \( u \in L^\infty(\mathbb{R}) \) solve \( Lu = 0 \). We prove \( u = 0 \). The equation,
\[ -u'' + V(x)u = 0, \]

satisfies the hypotheses of the above theorem, so there exist two solutions, \( \rho_1(x) \) and \( \rho_2(x) \), such that as \( x \to +\infty \),
\[ \rho_1(x) \sim 1, \quad \rho_1'(x) = o(x^{-1}), \quad (B.1a) \]
\[ \rho_2(x) \sim x, \quad \rho_2'(x) = o(1). \quad (B.1b) \]

Due to the behaviour as \( x \to +\infty \), \( \rho_1 \) and \( \rho_2 \) are linearly independent. These can then be extended to all of \( \mathbb{R} \) by the classical theory of linear systems with smooth coefficients.

By the same argument, there exist \( \tilde{\rho}_1 \) and \( \tilde{\rho}_2 \) satisfying
\[ \tilde{\rho}_1(x) \sim 1, \quad \tilde{\rho}_1'(x) = o(x^{-1}), \quad (B.2a) \]
\[ \tilde{\rho}_2(x) \sim x, \quad \tilde{\rho}_2'(x) = o(1) \quad (B.2b) \]
as \( x \to -\infty \). These two are also linearly independent. We will make use of these two sets of functions in what follows. An important relation between them is that, by uniqueness, \( \tilde{\rho}_j(x) = \rho_j(-x) \) for \( j = 1, 2 \).

Given the values \( u(0) = u_0 \) and \( u'(0) = u'_0 \), we know from the existence and uniqueness of solutions to linear systems with smooth coefficients, that there exist two unique pairs of constants, \( \{c_1, c_2\} \) and \( \{\tilde{c}_1, \tilde{c}_2\} \) such that
\[ u(x) = c_1\rho_1(x) + c_2\rho_2(x) \]
\[ = \tilde{c}_1\tilde{\rho}_1(x) + \tilde{c}_2\tilde{\rho}_2(x). \]

As \( x \to +\infty \),
\[ u(x) \sim c_1 + c_2x. \]
Since \( u(x) \in L^\infty \), we conclude \( c_2 = 0 \). Since it is proportional to \( \rho_1(x) \), \( u'(x) \) vanishes as \( x \to +\infty \). An analogous argument ensures that \( u'(x) \) also vanishes as \( x \to -\infty \). Thus we have
\[ \lim_{|x| \to \infty} u'(x) = 0. \quad (B.3) \]

Since \( u \in C^2(\mathbb{R}) \) and its derivative vanishes, we conclude \( u' \in L^\infty(\mathbb{R}) \). Furthermore, we claim \( u' \in L^2(\mathbb{R}) \). Multiplying the equation by \( u \) and integrating by parts,
\[ \int_{-L}^L |u'|^2 \,dy - uu'_L^L + \int_{-L}^L Vu^2 \,dy = 0. \]

Sending \( L \to \infty \) proves the claim. In addition, this shows \( \langle Lu, u \rangle = 0 \).
Let $\chi_A(x)$ be the cutoff function

$$
\chi_A(x) = \begin{cases} 
1, & |x| \leq A, \\
2 \left( \frac{\log A}{\log |x|} - \frac{1}{2} \right), & A < |x| \leq A^2, \\
0, & A^2 < |x|.
\end{cases}
$$

(B.4)

and assume $A > 1$. Let $u_A(x) = \chi_A(x)u(x)$. We prove

$$
\lim_{A \to \infty} \langle \mathcal{L}u_A, u_A \rangle = \langle \mathcal{L}u, u \rangle = 0.
$$

(B.5)

which will be essential to the uniqueness proof. Trivially, the potential component, $\int V u^2_A$, converges to $\int V u^2$, since $V$ is highly localized. We now justify the convergence of the kinetic component,

$$
\int |u_A'|^2 \, dy = \int_{-A}^{-A^2} |\chi_A'|^2 u^2 \, dy + \int_{A^2}^A |\chi_A'|^2 u^2 \, dy + 2 \int_{A}^{A^2} \chi_A' u A' \, dy
$$

(B.6)

The integral $I_1$ converges to $\int |u'|^2$, the desired quantity. We must show the other two vanish.

First, we split $I_2$ into

$$
I_2 = \int_{-A}^{A^2} |\chi_A'|^2 u^2 \, dy = \int_{-A}^{A^2} |\chi_A'|^2 u^2 \, dy + \int_{A}^{A^2} |\chi_A'|^2 u^2 \, dy.
$$

Using our explicit characterization of the cutoff function,

$$
\chi_A'(x) = -\frac{2 \log A}{x(\log |x|)^2},
$$

$$
\int_{A}^{A^2} |\chi_A'|^2 u^2 \, dy \leq \|u\|_{L^2}^2 \int_{A}^{A^2} \frac{4(\log A)^2}{y^2(\log |y|)^4} \, dy.
$$

As $A \to +\infty$, the integral is $\sim 1/((\log(A^{-1}))^6 A)$, which vanishes as $A \to +\infty$. The integral over $(-A^2, -A)$ is treated similarly.

The other integral is

$$
I_3 = 2 \int_{-A}^{A} \chi_A u A'u \, dy + 2 \int_{A}^{A^2} \chi_A u A' \, dy.
$$

Again, using the explicit characterization of the cutoff function,

$$
\int_{A}^{A^2} \chi_A u A' \, dy \leq \|u\|_{L^\infty} \|u'\|_{L^{(A,A')}} \int_{A}^{A^2} \frac{2 \log A}{y(\log |y|)^2} \, dy
$$

$$
\leq \|u\|_{L^\infty} \|u'\|_{L^{(A,A')}}.
$$

Since the derivative vanishes as $x \to +\infty$, (B.3), this also vanishes. The other part of $I_3$ is treated analogously. This proves convergence of the bilinear form.

We now specialize to either even or odd functions. By our index computations in proposition 3.3, $\mathcal{L}_k^{(e/o)}$ each have index 1, except for $\mathcal{L}_k^{(o)}$ which has index 0. Without loss of generality, we assume $\mathcal{L}$ is an index 1 operator, and proceed. Let $\psi$ be the negative eigenvector with $\|\psi\|_{L^2} = 1$ for the relevant symmetry. Let $V_A = \text{span} \{ \psi, u_A \}$. We now show that $\mathcal{L} = \mathcal{L} - \delta_{0}e^{(0)}$ restricted to this subspace is negative definite, proving uniqueness by contradiction. By the index computations this will imply $u_A$ and $\psi$ are collinear, allowing us to conclude that $u = 0$ since $u_A$ has the same symmetry properties as $u$. 

Let $q$ be any element of $V_A$, 

$$ q = c_1 u_A + c_2 \psi. $$

Then,

$$ \langle L q, q \rangle = c_1^2 \langle L u_A, u_A \rangle + 2c_1c_2 \langle L u_A, q \rangle + c_2^2 \langle L \psi, \psi \rangle. $$

We claim this is negative, which shows $L$, restricted to $V_A$, is negative definite. Since the index of $L$ is stable to perturbation, there is only one negative eigenvalue. Thus, $\dim V_A = 1$, and we must have $u_A = c(A) \psi$. But then $-\lambda c(A) = \langle u_A, \lambda \psi \rangle = \langle u_A, L \psi \rangle = \langle L u_A, \psi \rangle$. Since the right-hand side vanishes as $A \to \infty$, we conclude that $c(A) = 0$; hence $u = 0$.

To prove the claim that the form is negative, it is equivalent to show

$$ \langle L u_A, \psi \rangle^2 < \langle L u_A, u_A \rangle \langle L \psi, \psi \rangle. \quad (B.7) $$

As $A \to \infty$,

$$ \langle L u_A, u_A \rangle \to -\delta_0 \int e^{-|y|} |u|^2, $$

$$ \langle L u_A, \psi \rangle \to -\delta_0 \int e^{-|y|} \lambda \psi $$

and

$$ \langle L \psi, \psi \rangle \leq \lambda < 0. $$

Thus, $(B.7)$ holds for $A$ sufficiently large and $\delta_0$ sufficiently small. Indeed, given $u \neq 0$, and $\psi$, let

$$ \delta_0 \leq \frac{1}{2} \int e^{-|y|} |u|^2 \frac{d}{d}.$$ 

Fixing this value of $\delta_0$, we can then find a value of $A$ sufficiently large such that the inequality holds.

For the operator $L^{(0)}$, the proof is simpler, as we need only observe that

$$ \langle L^{(0)} u_A, u_A \rangle < 0, $$

contradicting the positivity of the operator. This concludes our proof of uniqueness of the solutions.

We now prove existence. Again, this follows [15, 21]. We have the two fundamental sets of solutions $\{\rho_1, \rho_2\}$ and $\{\tilde{\rho}_1, \tilde{\rho}_2\}$. $\rho_1$ and $\tilde{\rho}_1$ are asymptotically constant at $\infty$ and $-\infty$, respectively. Note that these two must be linearly independent, for if they were collinear, we would have a solution in $L^\infty$, solving $Lu = 0$. Hence, there is a constant $K > 0$ such that

$$ |\rho_1(x)| \leq K |x| \quad \text{as } x \to -\infty, $$

$$ |\tilde{\rho}_1(x)| \leq K |x| \quad \text{as } x \to +\infty. $$

We construct a Green’s function from these two to get the solution

$$ u(x) = \tilde{\rho}_1(x) \int_x^\infty \frac{\rho_1(s) f(s)}{W(s)} ds + \rho_1(x) \int_{-\infty}^x \frac{\tilde{\rho}_1(s) f(s)}{W(s)} ds, $$

where $W = \tilde{\rho}_1 \rho'_1 - \rho_1 \tilde{\rho}_1'$ is the Wronskian. The integrals converge and have the appropriate decay due to the properties of $\rho_1$ and $\tilde{\rho}_1$, and our assumption that $f$ is highly localized.
Finally, if $f$ is even, consider
\[
 u(-x) = \tilde{\rho}_1(-x) \int_{-\infty}^{\infty} \frac{\rho_1(s)f(s)}{W(s)} \, ds + \rho_1(-x) \int_{-\infty}^{-x} \frac{\tilde{\rho}_1(s)f(s)}{W(s)} \, ds \\
= \tilde{\rho}_1(-x) \int_{-\infty}^{x} \frac{\rho_1(s)f(s)}{W(s)} \, ds + \rho_1(-x) \int_{x}^{\infty} \frac{\tilde{\rho}_1(s)f(s)}{W(s)} \, ds \\
= \rho_1(x) \int_{-\infty}^{x} \frac{\rho_1(s)f(s)}{W(s)} \, ds + \rho_1(x) \int_{x}^{\infty} \frac{\tilde{\rho}_1(s)f(s)}{W(s)} \, ds.
\]

Thus $u(x) = u(-x)$. An analogous proof holds for $f$ odd.

Appendix C. Numerical methods

The software tools we use in our computations are the MATLAB and Fortran 90/95 implementations of an adaptive nonlinear collocation algorithm discussed in [27–29]. Although they are quite similar, we found the Fortran implementation to be faster and more robust for solving the 3D problems which require us to compute the ground state. For the 1D problems, where we have an explicit formula for the ground state, the MATLAB algorithm bvp4c sufficed. We use these tools to solve for the soliton, compute the index functions, and solve the relevant boundary value problems and associated inner products.

The codes used to perform these computations are available at http://hdl.handle.net/1807/25174.

Appendix C.1. Singularities at the origin

A useful feature of this algorithm is that it can handle boundary value problems of the form
\[
 \frac{d}{dr} y = \frac{1}{r} Sy + f(r, y),
\]
where $S$ is some constant coefficient matrix. The $r^{-1}$ singularity naturally appears in the 3D problems. The higher harmonics introduce a $r^{-2}$ singularity which can be addressed by a change of variables. Let $\mathcal{L}^{(k)}$ denote one of the operators applied to the $k$th harmonic,
\[
\mathcal{L}^{(k)} = -\frac{d^2}{dr^2} - \frac{d - 1}{r} \frac{d}{dr} + \nabla + \frac{k(k + d - 2)}{r^2}.
\]
If $W$ solves $\mathcal{L}^{(k)} W = f$ and $W$ is non-singular at the origin, then
\[
\lim_{r \to 0} r^{-3} W(r) = \text{const} \neq 0.
\]
This motivates the change of variable $W(r) = r^k \tilde{W}(r)$. In terms of $\tilde{W}(r)$, the equation becomes
\[
r^k \mathcal{L}^{(k)} \tilde{W} = f,
\]
where
\[
\mathcal{L}^{(k)} = -\frac{d^2}{dr^2} - \frac{d - 1 + 2k}{r} \frac{d}{dr} + \nabla
\]
and $\tilde{W}$ satisfies the condition $\tilde{W}'(0) = 0$. We compute with $\mathcal{L}^{(k)}$ to get $\tilde{W}$ and then multiply by $r^k$. When we compute indices for these higher harmonic operators, the other initial condition becomes $\tilde{W}(0) = 1$. 

Appendix C.2. Verification of 1D index functions

As in the 3D cubic problem, we can verify *a posteriori* that our zero count of the index functions for the 1D NLS problems is accurate by checking limiting constants. Asymptotically, the 1D index functions $U^\alpha$ and $Z^\alpha$ satisfy

\[ U^\alpha(x) \approx C_0^\alpha + C_1^\alpha x, \]  
\[ Z^\alpha(x) \approx D_0^\alpha + D_1^\alpha x. \]  

As figures 7 and 8 show, the constants have settled down and have the appropriate signs to rule out any additional zeros.

Appendix C.3. Artificial boundary conditions

Another subtlety of the computations is the far field boundary conditions. The soliton, $R$, vanishes as $r \to +\infty$, but we only compute out to some finite value, $r_{\text{max}}$. For simplicity, we use the notation $r$ and $r_{\text{max}}$ for both 1D and 3D. To accommodate this, we introduce an artificial boundary condition at $r_{\text{max}}$, and then check, *a posteriori*, that it is consistent. First, we must do some asymptotic analysis.
We seek an asymptotic expansion for $R$, using (1.2)

$$(-\Delta + \lambda - f(R))R = 0.$$ 

As $r \to \infty$, we look for an expansion of the form

$$e^{-\sqrt{\lambda} r} \sum_{n=0}^{\infty} c_n r^{-n}.$$ (C.2)

To extract the leading order behaviour, we wish to find $\gamma$. We compute

$$\frac{\partial}{\partial r}(e^{-\sqrt{\lambda} r} r^{\gamma}) = -\sqrt{\lambda} e^{-\sqrt{\lambda} r} r^{\gamma} + \gamma e^{-\sqrt{\lambda} r} r^{\gamma-1},$$

$$\frac{\partial^2}{\partial r^2}(e^{-\sqrt{\lambda} r} r^{\gamma}) = \lambda e^{-\sqrt{\lambda} r} r^{\gamma} - 2\lambda \gamma e^{-\sqrt{\lambda} r} r^{\gamma-1} + \gamma(\gamma-1)e^{-\sqrt{\lambda} r} r^{\gamma-2}.$$ 

Plugging (C.2) into (1.2),

$$[(-\lambda + \lambda) + \frac{(2\sqrt{\lambda} \gamma + \sqrt{(d-1)} \lambda)}{r} + O(r^{-2})] = 0.$$ 

Hence, $\gamma = -(d-1)/2$ and the leading order behaviour is

$$r^{-(d-1)/2} e^{-\sqrt{\lambda} r}.$$ (C.3)
Figure 9. The numerically computed ground state for the different problems. Computed on the indicated domain, with a tolerance of $10^{-13}$ while assessing the indices of the operators restricted to even functions for $d = 1$ and the zeroth harmonic for $d = 3$. The computed solitons are monotonic and decay at the anticipated rate.

Figure 10. As $r \to \infty$, $R$ asymptotically satisfies $-\Delta R + \lambda R \sim 0$. The figures indicate that the relevant domain, which is different for different problems, is sufficiently large that artificial boundary conditions are good approximations. From the same computation as in figure 9.

As $r \to \infty$,

\[
R(r) \approx \begin{cases} 
R \ast e^{-\sqrt{\lambda} r} & d = 1, \\
\frac{1}{r} e^{-\sqrt{\lambda} r} & d = 3,
\end{cases}
\]  
(C.4)

From this, we develop the Robin boundary condition,

\[
\lim_{r \to \infty} \frac{R(r)}{R'(r)} = \begin{cases} 
\frac{1}{\sqrt{\lambda}} & d = 1, \\
\frac{1}{1 + \sqrt{\lambda} r} & d = 3,
\end{cases}
\]

which we formulate as

\[
R(r_{\text{max}}) + \frac{1}{\sqrt{\lambda}} R'(r_{\text{max}}) = 0 \quad \text{for } d = 1
\]  
(C.5a)
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Figure 11. The numerically computed ground state and the off axis unstable mode of 3D cubic NLS. Computed on the indicated domain, with a tolerance of $10^{-12}$.

Figure 12. Zooming in on the components of the numerically computed unstable mode, $\phi$, we see the periodic structure of the solution.

$R(r_{\text{max}}) + \frac{r_{\text{max}}}{1 + \sqrt{\lambda}r_{\text{max}}}R'(r_{\text{max}}) = 0$ for $d = 3$ (C.5b)

assuming we have taken $r_{\text{max}}$ sufficiently large. For our computations, aside from noting that the solver algorithm terminates without errors, we have two a posteriori checks available. First, we can see that we have computed the ground state. Plotting the computed $R$ on both a linear and a log scale in figure 9 we verify that $R$ is a hump shaped monotonically decaying function. It also has the anticipated $r^{-1}e^{-r}$ decay rate.

The second thing that can be checked is that the numerically computed $R$ satisfies, asymptotically, the artificial boundary condition (C.5b). To do this, we plot $R(r) + (r/(1 + \sqrt{\lambda}r))R'(r)$ and observe that it vanishes as $r \to \infty$, as can be seen in figure 10.

To compute the off axis eigenstates $\phi$ for the 3D cubic problem with eigenvalue $\sigma > 0$, we rely on the relationship

$L_+L_\phi = -\sigma^2 \phi_\phi.$
As $r \to \infty$, our functions satisfy the asymptotically satisfy the free, linear equations for the different parts of the 3D cubic problem. The figures indicate that the relevant domain, which is different for different problems, is sufficiently large that artificial boundary conditions are good approximations.

Asymptotically, this is the free equation

$$(-\Delta + 1)^{\frac{1}{2}} \phi_1 = -\sigma^2 \phi_1.$$  

Seeking a radially symmetric solution and using similar expansion techniques as in the case of the soliton, we will find that

$$\phi_1(r) \approx c_1 r^{-(d-1)/2} e^{-r \sqrt{1+i \sigma}} + c_2 r^{-(d-1)/2} e^{-r \sqrt{1-i \sigma}}$$  

as $r \to \infty$.

Let

$$\theta \equiv \frac{1}{2} \arctan(\sigma),$$  

$$\rho \equiv (1 + \sigma^2)^{1/4}.$$  

In 1D, we can construct an artificial boundary condition that, as $r \to r_{\text{max}}$,

$$\phi'_1 + \rho \cos(\theta) \phi_1 + \rho \sin(\theta) \phi_2 = 0,$$  

$$\phi'_2 + \rho \cos(\theta) \phi_2 - \rho \sin(\theta) \phi_1 = 0.$$  

Figure 13. As $r \to \infty$, our functions satisfy the asymptotically satisfy the free, linear equations for the different parts of the 3D cubic problem. The figures indicate that the relevant domain, which is different for different problems, is sufficiently large that artificial boundary conditions are good approximations.
Analogously, in 3D, as $r \to r_{\text{max}}$,
\[
\phi_1' + \rho \cos(\theta)\phi_1 + r^{-1}\phi_1 + \rho \sin(\theta)\phi_2 = 0, \quad (C.9a)
\]
\[
\phi_2' + \rho \cos(\theta)\phi_2 + r^{-1}\phi_2 - \rho \sin(\theta)\phi_1 = 0. \quad (C.9b)
\]
As in the case of the soliton, we can verify that the solutions have the appropriate shape, decay as expected, and satisfy the artificial boundary conditions. The shape and decay are plotted in figure 11. The functions rapidly reach machine precision. If we zoom in on the
As \( r \to \infty \), our functions asymptotically satisfy the free equations for the 1D critical problem with various orthogonality conditions. 

Unstable modes, as in figure 12, we can see the periodic structure. However, as is suggested by these figures, once the \( \phi_j \)’s are sufficiently small, \( \lesssim O(10^{-12}) \), this fine structure degrades. Fortunately, the numerical error is sufficiently small as to not impact our computations. The artificial boundary condition plot appears in figure 13.

Another place where we use artificial boundary conditions is in solving the various boundary value problems for \( U_j^{(k)} \) or \( Z_j^{(k)} \). The rapid decay of the soliton leads to the functions satisfying the free equation, for \( d > 1 \),

\[-\Delta q + k(k + d - 2)r^{d-2k}q = 0,\]

where \( q \) is one of these functions. In this region, the function must asymptotically be like \((3.5b)\). Of course, we work with the variables \( \tilde{U}_j^{(k)} \) and \( \tilde{Z}_j^{(k)} \). Since these vanish as \( r \to \infty \), they asymptotically behave as

\[ q \propto r^{2-d-2k}. \]
Figure 13 shows that these artificial boundary conditions are asymptotically satisfied. For our \( d = 1 \) computations, we have the artificial boundary conditions

\[
\frac{d}{dx} U_j^{(c/o)}(x_{\text{max}}) = 0, \quad \frac{d}{dx} Z_j^{(c/o)}(x_{\text{max}}) = 0.
\]

We can similarly check that the inner products are asymptotically constant and that our computed functions asymptotically satisfy the artificial boundary conditions. See figures 14 and 15.

The last place we make use of artificial boundary conditions is in solving \( L_{\varphi} \rho = -x^2 R \) for the critical problem in section 4.2.3. Using the same procedure as above, one will find that \( \rho \propto x^3 e^{-x} \) form which the artificial boundary condition

\[
\rho(x) + \left(1 - \frac{3}{x}\right) \rho(x) = 0
\]

(C.12)

can be constructed.
Appendix C.4. Computation of the indices

In computing the indices of operators $\mathcal{L}_{\pm}^{(k)}$ (from which we recover the indices of $\mathcal{L}_{\pm}^{(k)}$), we simultaneously solve the mixed boundary value problem/initial value problems

\[ -\Delta R + \lambda R - g(|R|^2)R = 0, \quad R'(0) = 0, \quad (C.5a) \text{ or (C.5b)}, \]

\[ \mathcal{L}_+^{(k)} \mathcal{U}^{(k)} = 0, \quad \mathcal{U}^{(k)}(0) = 1, \quad \frac{d}{dr} \mathcal{U}^{(k)}(0) = 0, \quad (C.14) \]

\[ \mathcal{L}_-^{(k)} \mathcal{Z}^{(k)} = 0, \quad \mathcal{Z}^{(k)}(0) = 1, \quad \frac{d}{dr} \mathcal{Z}^{(k)}(0) = 0. \quad (C.15) \]
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Figure 18. Inner products for the 1D critical problem with various orthogonality conditions.

(a) $L_{\pm}^{(c)}$ in the critical case with the natural orthogonality conditions.

(b) $L_{\pm}^{(o)}$ in the critical case.

(c) $L_{-}^{(c)}$ in the critical case with the alternative orthogonality condition.

(d) $L_{-}^{(o)}$ in the critical case with the FMR orthogonality conditions.

Figure 18. Inner products for the 1D critical problem with various orthogonality conditions.

For the 3D cubic equation, this is the complete set of equations; $\lambda = 1$ and $f(s) = s$. The analogous computations are made in $d = 1$. In addition to verifying that the soliton was adequately computed, we can check, a posteriori, that the index functions, $U^{(k)}$ and $Z^{(k)}$ asymptotically satisfy the free equation. This was shown in the index figures of sections 3.2 and 4.1, where we checked the constants.

Appendix C.5. Computation of the inner products

As in the computation of the indices, we similarly solve mixed boundary value/initial value problem for $R$, the $U_{i}^{(a)}$ and $Z_{j}^{(a)}$, and the inner products.

In computing the inner products, we introduce the dependent variables $\kappa_{j}^{(a)}(r)$ and $\gamma_{j}^{(a)}(r)$, where

$$
\frac{d}{dr} \kappa_{j}^{(a)}(r) = L_{+}^{(a)} U_{i}^{(a)} U_{i}^{(a)} r^{d-1}, \quad \kappa_{j}^{(a)}(0) = 0,
$$

(C.16)
\[
\frac{d}{dr} y_j^{(\alpha)}(r) = L^{(\alpha)} Z_j^{(\alpha)} Z_j^{(-\alpha)}, \quad y_j^{(\alpha)}(0) = 0 \tag{C.17}
\]
for \(\ell_1\) and \(\ell_2\) the appropriate indices. Clearly,
\[
\lim_{r \to \infty} \kappa_r^{(\alpha)}(r) = K_r^{(\alpha)}, \\
\lim_{r \to \infty} \gamma_r^{(\alpha)}(r) = J_r^{(\alpha)}.
\]
We approximate the inner products by computing to \(r_{\text{max}}\). As demonstrated in figures 16–18 these converge rapidly and are essentially constant in the region of the free equation. This is entirely consistent with the exponential decay of the soliton and functions related to it, such as its derivative.

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