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Numerical verification of a gap condition for a linearized nonlinear Schrödinger equation

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Abstract

We make a detailed numerical study of the spectrum of two Schrödinger operators $L_\pm$ arising from the linearization of the supercritical nonlinear Schrödinger equation (NLS) about the standing wave, in three dimensions. This study was motivated by a recent result of the second author on the conditional asymptotic stability of solitary waves in the case of a cubic nonlinearity. Underlying the validity of this result is a spectral condition on the operators $L_\pm$, namely that they have no eigenvalues nor resonances in the gap (a region of the positive real axis between zero and the continuous spectrum), which we call the gap property. The present numerical study verifies this spectral condition and shows further that the gap property holds for NLS exponents of the form $2\beta + 1$, as long as $\beta_* < \beta \leqslant 1$, where

$$\beta_* = 0.913\,958\,905 \pm 1e - 8.$$

Our strategy consists of rewriting the original eigenvalue problem via the Birman–Schwinger method. From a numerical analysis viewpoint, our main contribution is an efficient quadrature rule for the kernel $1/|x - y|$ in $\mathbb{R}^3$, i.e. proved spectrally accurate. As a result, we are able to give similar accuracy estimates for all our eigenvalue computations. We also propose an improvement in Petviashvili's iteration for the computation of standing wave profiles which automatically chooses the radial solution.

All our numerical experiments are reproducible. The Matlab code can be downloaded from http://www.acm.caltech.edu/~demanet/NLS/.

Mathematics Subject Classification: 35Q55, 65N25

1. Introduction

Suppose that $\psi(t,x) = e^{it\alpha^2}\phi(x)$ with $\alpha \neq 0$ and $x \in \mathbb{R}^d$ is a standing wave solution of the nonlinear Schrödinger equation (NLS)

$$i\partial_t \psi + \Delta\psi + |\psi|^{2\beta}\psi = 0, \tag{1}$$

where $0 < \beta < 2/(d-2)$ if $d \geqslant 3$ and $0 < \beta < \infty$ if $d = 1, 2$. Here we assume that $\phi = \phi(\cdot, \alpha)$ is a ground state, i.e.

$$\alpha^2\phi - \Delta\phi = \phi^{2\beta+1}, \qquad \phi > 0.$$

It is known that such ϕ exist and that they are radial, smooth and exponentially decaying; see Strauss [Str1], Berestycki and Lions [BerLio] and for uniqueness see Coffman [Cof], McLeod and Serrin [McS] and Kwong [Kwo]. In one dimension $d = 1$, these ground states are explicitly given as

$$\phi(x) = \frac{(\beta+1)^{1/2\beta}}{\cosh^{1/\beta}(\beta x)} \tag{2}$$

when $\alpha = 1$ (for other values of $\alpha \neq 0$ rescale), but in higher dimensions no explicit expression is known. From now on, we shall assume that $d = 3$.

A much studied question is the stability of these standing waves, both in the orbital (or Lyapunov) sense and the asymptotic sense. For the former, see for example Shatah [Sha], Shatah and Strauss [ShaStr], Grillakis *et al* [GriShaStr1, GriShaStr2], Weinstein [Wei1, Wei2], Grillakis [Gri] and for the latter see Soffer and Weinstein [SofWei1, SofWei2], Buslaev and Perelman [BusPer1, BusPer2] and Cuccagna [Cuc]. Reviews are in Strauss [Str2] and Sulem and Sulem [SulSul]. Also see Fröhlich *et al* [FroTsaYau, FroGusJonSig].

In order to study stability, one generally linearizes around the standing wave. This process leads to matrix Schrödinger operators of the form

$$\mathcal{H} = \mathcal{H}_0 + V = \begin{bmatrix} -\Delta + \alpha^2 & 0 \\ 0 & \Delta - \alpha^2 \end{bmatrix} + \begin{bmatrix} -V_1 & -V_2 \\ V_2 & V_1 \end{bmatrix}$$

on $L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$. Here $V_1 = (\beta+1)\phi^{2\beta}$ and $V_2 = \beta\phi^{2\beta}$.

Conjugating $\mathcal{H}$ by the matrix $\begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix}$ leads to the matrix operator

$$\begin{bmatrix} 0 & iL_- \\ -iL_+ & 0 \end{bmatrix}$$

with

$$L_- = -\Delta + \alpha^2 - \phi^{2\beta}$$
$$L_+ = -\Delta + \alpha^2 - (2\beta+1)\phi^{2\beta}.$$

The continuous spectrum of both L_- and L_+ equals $[\alpha^2, \infty)$. Since $L_-\phi = 0$ and $\phi > 0$, it follows that zero is a simple eigenvalue and the bottom of the spectrum of L_-. Moreover, $L_+\partial_j\phi = 0$ for $1 \leqslant j \leqslant 3$ so that $\ker(L_+) \subset \{\partial_j\phi : 1 \leqslant j \leqslant 3\}$. In fact, for monomial nonlinearities it is known that there is equality here (see Weinstein [Wei2][1]) and that there is a unique negative bound state of L_+.

It is known that $L_- \geqslant 0$ implies that the spectrum $\mathrm{spec}(\mathcal{H})$ satisfies $\mathrm{spec}(\mathcal{H}) \subset \mathbb{R} \cup i\mathbb{R}$ and that all points of the discrete spectrum other than zero are eigenvalues whose geometric and algebraic multiplicities coincide. On the other hand, the zero eigenvalue of $\mathcal{H}$ has

[1] In this paper a restriction $\beta \leqslant 1$ is imposed on $d = 3$, but using Kwong's results [Kwo] allows one to obtain the full range $\beta < 2$ by means of Weinstein's arguments.

geometric multiplicity four and algebraic multiplicity eight provided $\beta \neq \frac{2}{3}$, whereas for the L^2-critical case $\beta = \frac{2}{3}$ the algebraic multiplicity increases to ten. For this see [Wei1, BusPer1] or [RodSchSof1, CucPelVou, CucPel, ErdSch].

In order to carry out a meaningful asymptotic stability analysis it is essential to understand the discrete spectrum of $\mathcal{H}$. The root space at zero was completely described by Weinstein [Wei2]. Moreover, it is also well known that

$$\operatorname{spec}(\mathcal{H}) \subset \mathbb{R} \text{ iff } \beta \leqslant \tfrac{2}{3},$$

whereas in the range $\frac{2}{3} < \beta < 2$ there is a unique pair of simple complex-conjugate eigenvalues $\pm i\gamma$. This latter property reflects itself in the nonlinear theory in the following way: orbital stability holds iff $\beta < \frac{2}{3}$; see Berestycki and Cazenave [BerCaz], Weinstein [Wei2], Cazenave and Lions [CazLio] and [GriShaStr1, GriShaStr2].

In [Sch] the second author investigated the conditional asymptotic stability for the unstable case $\beta = 1$ (for related work on stable manifolds for PDE see Pillet and Wayne [PilWay], Gesztesy *et al* [GesJonLatSta] and Tsai and Yau [TsaYau]). This analysis depended on the fact that zero is the only eigenvalue of $\mathcal{H}$ in the interval $[-\alpha^2, \alpha^2]$ and that the edges $\pm\alpha^2$ are not resonances. The fact that $\pm\alpha^2$ are neither eigenvalues nor resonances is the same as requiring that the resolvent $(\mathcal{H} - z)^{-1}$ remains bounded on suitable weighted $L^2(\mathbb{R}^3)$ spaces for z close to $\pm\alpha^2$.

Using ideas of Perelman [Per2], it is shown in [Sch] that these properties can be deduced from the following properties of L_+, L_-: **neither L_+ nor L_- have any eigenvalues in the gap $(0, \alpha^2]$, and L_- has no resonance at α^2.**

In one dimension $d = 1$, the spectral properties of L_- and L_+ can be determined completely since the generalized eigenfunctions of these operators (more precisely, the Jost solutions) can be given explicitly in terms of certain hypergeometric functions (see Flügge [Flu], problem 39, p 94). This is due to the special form of ground state (2).

Unfortunately, it seems impossible to determine similar properties for the case of three dimensions by means of purely analytical methods. We therefore verify this gap property of $L_\pm$ numerically via the Birman–Schwinger method (see Reed and Simon [ReeSim4]). We will refer to the **gap property** as the fact that $L_\pm$ **have no eigenvalues in** $(0, \alpha^2]$ **and no resonance at** α^2**.** Our main result is as follows.

Claim 1. *There exists a number* $\beta_* = 0.913\,958\,905 \pm 1e-8$ *so that for all* $\beta_* < \beta \leqslant 1$ *the gap property holds.*

This statement can also be continued beyond $\beta = 1$. We only went up to 1 since $\beta = 1$ alone is needed in [Sch]. In the range $\beta < \beta_*$, our numerical analysis shows that the operator L_+ has eigenvalues in the gap $(0, 1]$. This is perhaps surprising, since it shows that the gap property does not hold for the entire $L^2(\mathbb{R}^3)$ super-critical range $\frac{2}{3} < \beta < 2$. However, it does hold at $\beta = 1$. In particular, the method of proof from [Sch] does not apply to all $\beta > \frac{2}{3}$ since it relies on the gap property. In contrast, in one dimension $d = 1$, Krieger and Schlag [KriSch] showed that this method does apply to the entire super-critical range $\beta > 2$. In fact, there the gap property does hold for all $\beta > 1$ (see [Flu]).

In the rest of the paper, we will be concerned with the description of the numerical method and will study its convergence properties. Our approach is naturally split into two halves. The first half addresses the accurate computation of the soliton. As the latter is the ground state solution of a nonlinear elliptic equation this is a nontrivial issue. For this purpose we rely on the iteration method of Petviashvili; see the recent work of Pelinovsky and Stepanyants [PelSte]. We modify the approach of these authors somewhat by introducing a corrective term which automatically re-centres the approximate soliton at each step of the iteration. In this way

we arrive at a positive solution which is radial and satisfies the defining semi-linear elliptic PDE to very good precision. Theorem 2 is the main statement concerning convergence of the Petviashvili iteration.

The second half of this paper deals with the numerical implementation of the Birman–Schwinger method. This requires a suitable discretization of the corresponding Birman–Schwinger operator. As we will see, this problem can be reduced to the accurate computation of Δ^{-1}, the inverse Laplacian on $\mathbb{R}^3$. We introduce new quadrature weights for the free-space Green's function $1/(4\pi|x-y|)$, which makes the computation of the integral exact on bandlimited functions. The formula is based on the sine-integral special function and should be of indepedent interest to numerical analysts. Theorem 3 is our main result concerning the super-algebraic (near-exponential) convergence of the proposed discretization of the Birman–Schwinger operator. Corollary 10 translates this convergence result into accuracy bounds for the eigenvalues.

All our results assume exact arithmetic. It is natural to ask whether rigorous bounds can be obtained in the presence of round-off errors. Results of this nature could be obtained in the context of interval arithmetic but would go beyond the scope and ambition of this paper. In all our experiments truncation errors always appear to dominate round-off errors.

Finally, we would like to mention that our code appears to be very robust and therefore should also apply to many other problems of a related nature. The *Matlab* source can be downloaded from the website of the first author.

2. Description of the numerical method

2.1. The Birman–Schwinger method

A direct numerical computation of the eigenvalues of $L_\pm$ would be problematic near α^2, the edge of the continuous spectrum. For example, it is unclear if a perceived numerical eigenvalue at $0.99\,\alpha^2$ belongs to the gap or if it has escaped from the continuous spectrum due to numerical approximation. Decay of the corresponding eigenfunction might help in making a decision, but this criterion is unacceptable over a truncated computational domain. Instead, we will reformulate the problem by the Birman–Schwinger method, which we now recall.

Let $H = -\Delta - V$, where $V > 0$ is a bounded potential that decays at infinity. In our case, this is $H = L_\pm - \alpha^2 I$. We would like to filter out positive eigenvalues, so we assume $Hf = -\lambda^2 f$ where $\lambda > 0$ and $f \in L^2$. Then $g = Uf$, where $U = \sqrt{V}$, satisfies

$$g = U(-\Delta + \lambda^2)^{-1} U g.$$

In other words, $g \in L^2$ is an eigenfunction of

$$K(\lambda) = U(-\Delta + \lambda^2)^{-1} U$$

with eigenvalue one. Note that $K(\lambda)$ is a compact, positive operator. Conversely, if $g \in L^2$ satisfies $K(\lambda)g = g$ then

$$f := U^{-1} g = (-\Delta + \lambda^2)^{-1} U g \in L^2$$

and $Hf = -\lambda^2 f$. Moreover, the eigenvalues of $K(\lambda)$ are strictly increasing as $\lambda \to 0$. Hence, we conclude that

$$\#\{\lambda : \ker(H + \lambda^2) \neq \{0\}\} = \#\{E > 1 : \ker(K(0) - E) \neq \{0\}\},$$

counted with multiplicity.

Finally, recall the symmetric resolvent identity:

$$(H - z)^{-1} = (-\Delta - z)^{-1} + (-\Delta - z)^{-1} U [I - U(-\Delta - z)^{-1} U]^{-1} U (-\Delta - z)^{-1}.$$

This shows that the Laurent expansion of $(H - z)^{-1}$ around $z = 0$ does not involve negative powers of z iff $I + U(-\Delta - z)^{-1}U$ is invertible at $z = 0$ which is the same as requiring that

$$\ker\{I - U(-\Delta)^{-1}U\} = \{0\}$$

because of the Fredholm alternative (assuming that V decays sufficiently fast at infinity to insure compactness). In other words, if H has no resonance or eigenvalue at the origin then $K(0)$ will not show an eigenvalue $E = 1$, and conversely.

Let us count the eigenvalues $\{\lambda_j\}_{j=1}^{\infty}$ of $K(0) = U(-\Delta)^{-1}U$ (which are all non-negative) in decreasing order. Then we arrive at the following conclusion: let N be a positive integer. **Then the operator H has exactly N negative eigenvalues and neither an eigenvalue nor a resonance at zero iff $\lambda_1 \geqslant \cdots \geqslant \lambda_N > 1$ and $\lambda_{N+1} < 1$.**

Note that the spectrum of the self-adjoint, compact Birman–Schwinger operator $K(0)$ is discrete and robust to numerical perturbations near $E = 1$, which is the desired numerical effect. Since $K(0)$ is compact, eigenvalues cannot accumulate at $E = 1$ from below. This is in contrast to any naive discretization attempt of the original spectral problem, which would lead to such an accumulation by way of the continuous spectrum of H. This is the reason why only the Birman–Schwinger method is successful here.

In view of the preceding argument, we therefore need to show the following to justify [Sch]: for $\beta = 1$, the second largest eigenvalue of[2]

$$K_-(x, y) = \frac{\phi^\beta(x)\phi^\beta(y)}{4\pi|x - y|}$$

is below one and the fifth largest eigenvalue of

$$K_+(x, y) = (2\beta + 1)\frac{\phi^\beta(x)\phi^\beta(y)}{4\pi|x - y|}$$

is below one. These properties will then imply the gap property, i.e. $L_\pm$ have no eigenvalues in $(0, 1]$ and no resonance at 1.

2.2. The modified Petviashvili's iteration

The first step of the numerical method is to find the soliton $\phi(x)$, which is the unique positive, radial decaying solution of

$$-\Delta\phi + \phi = |\phi|^{2\beta}\phi, \tag{3}$$

unique up to translation. As mentioned earlier, $\phi(x)$ is in fact exponentially decaying. A naive approach would be to solve a descent equation such as

$$\frac{\partial u}{\partial t} = \Delta u - u + |u|^{2\beta}u,$$

but, as shown in [BerLioPel], this equation is unstable near the fixed manifold of interest. Instead, we will solve the *modified Petviashvili's iteration* which reads

$$\phi_{n+1} = M_n^\gamma(I - \Delta)^{-1}(|\phi_n|^{2\beta}\phi_n) + \delta\sum_{j=1}^{3} R_{n,j}\frac{\partial\phi_n}{\partial x_j}. \tag{4}$$

[2] Note that due to the scaling $x \mapsto \alpha x$ and $\phi(x, \alpha) = \alpha^{1/\beta}\phi(\alpha x)$ we may assume that $\alpha = 1$. From now on we set $\phi(x) = \phi(x, 1)$.

The initial guess ϕ_0 can, for example, be taken as a Gaussian. The choice of constants M_n, $R_{n,j}$, γ and δ is crucial for convergence of the iteration and is given by[3]

$$M_n = \frac{\int (1+|\xi|^2)(\widehat{\phi_n})^2 \, \mathrm{d}\xi}{\int \widehat{\phi_n}(\widehat{|\phi_n|^{2\beta}\phi_n}) \, \mathrm{d}\xi}, \tag{5}$$

$$R_{n,j} = \frac{\int (1+|\xi|^2)\widehat{\phi_n}\,\widehat{\partial_j \phi_n} \, \mathrm{d}\xi}{\int \widehat{\partial_j \phi_n}[\partial_j(|\phi_n|^{2\beta}\phi_n)]^\wedge \, \mathrm{d}\xi}, \tag{6}$$

$$\gamma = \frac{2\beta+1}{2\beta}, \tag{7}$$

$$\delta = -1/2, \tag{8}$$

where $\partial_j = \partial/\partial x_j$, and the hat denotes Fourier transformations. It is important that no complex conjugates be taken in these Fourier integrals. This iteration, without the second term, was introduced by Petviashvili in 1976 and convergence was proved recently in [PelSte]. The addition of the second term is a minor increment whose purpose is to fix a potential source of instability due to numerical discretization and to force the iteration to choose the radial soliton (centred at the origin). This will be explained and justified in section 3.

Numerically, $(I-\Delta)^{-1}$ is realized in the Fourier domain, and Fourier transformations are implemented via the fast Fourier transform (FFT). Discretization issues are addressed in the next section. In practice, the iteration is accelerated via Aitken's method applied pointwise, i.e.

$$\phi_n^A(x) = \phi_n(x) - \frac{(\phi_{n+1}(x)-\phi_n(x))^2}{\phi_{n+2}(x) - 2\phi_{n+1}(x) + \phi_n(x)}.$$

The iteration is stopped when the Euler–Lagrange equation (3) is satisfied up to some very small tolerance in L^2. The resulting approximation of the soliton will be denoted by $\tilde{\phi}$.

2.3. Truncation and discretization

We now take up the task of computing the eigenvalues of the Birman–Schwinger operators as defined in section 2.1. The first step is to truncate the three-dimensional computational domain to a cube of sidelength L centred at the origin and to discretize functions $f(x)$ by evaluating them on the regular grid

$$x_j = (j_1, j_2, j_3)\frac{L}{N}, \tag{9}$$

with j_1, j_2, j_3 integers obeying $-N/2 \leqslant j_k \leqslant N/2-1$. Operators are, in turn, discretized as matrices acting on 'vectors' of function samples $f(x_j)$. Tools of numerical linear algebra can then be invoked to compute the eigenvalues of these matrices.

Typical values of L and N for which discretizing $K_\pm$ is expected to be reasonably accurate are $L \simeq 20$ and $N \simeq 100$. In this context, several vectors of $N^3 \simeq 10^6$ function samples can comfortably be stored simultaneously in the memory of a 2005-era computer, but we cannot yet afford to manipulate matrices containing $N^6 \simeq 10^{12}$ elements. This rules out the possibility of using popular approaches such as the QR algorithm, which compute eigenvalues by operating directly on the matrix entries.

Instead, we will resort to a modification of the power method, known as the implicitly restarted Arnoldi iteration, which is implemented in Matlab's *eigs* command [Eigs]. This method has the advantage of only requiring applications of the operator to diagonalize, i.e.

[3] The notation $[\ldots]^\wedge$ means the Fourier transform of the quantity in the brackets.

matrix-vector products. For well-conditioned problems, such as the one we are addressing, *eigs* computes the top eigenvalues of the finite matrix up to machine precision, i.e. about 15 decimal digits in Matlab.

The only remaining issue is then to find a good discretization $\tilde{K}_\pm$ of the Birman–Schwinger operators $K_\pm$, and to quantify the accuracy. Multiplication by $\phi(x)$ to some power will be done sample-wise on the grid x_j. Inverting minus the Laplacian in a space of decaying functions over $\mathbb{R}^3$, or equivalently convolving with the fundamental solution $G(x) = 1/4\pi|x|$, is a bit more complicated. Discretizing $G(x)$ by sampling at x_j is quite inaccurate and is problematic if $x = 0$ belongs to the grid x_j. Dividing by $|\xi|^2$ in frequency poses similar difficulties. Instead, for reasons which will be explained in section 3, we use the following discretization,

$$\tilde{G}(x_j) = \begin{cases} \dfrac{1}{2\pi^2|x_j|}\left(\dfrac{L}{N}\right)^3 \operatorname{Si}\left(\dfrac{\pi N|x_j|}{L}\right) & \text{if } x_j \neq 0, \\ \dfrac{1}{2\pi}\left(\dfrac{L}{N}\right)^2 & \text{if } x_j = 0, \end{cases} \tag{10}$$

where $\operatorname{Si}(x) = \int_0^x (\sin t/t)\,\mathrm{d}t$. The discrete (circular) convolution of $\tilde{G}(x_j)$ with a vector $f(x_j)$ is computed efficiently as the multiplication $\widehat{\tilde{G}(x_j)}\,\widehat{f(x_j)}$ of their respective FFT, followed by an inverse FFT.

In this context, applying the full Birman–Schwinger operator, say K_-, to a vector of samples $f(x_j)$ consists of the obvious sequence of steps: (1) multiply $f(x_j)$ by $\tilde{U}(x_j) = \tilde{\phi}(x_j)^\beta$, (2) perform an FFT, (3) multiply the result by $\widehat{\tilde{G}(x_j)}$, (4) perform an inverse FFT and finally (5) multiply the result by $\tilde{U}(x_j)$ again.

Since the complexity of a one-dimensional FFT in Matlab is $O(N \log N)$ operations for most values of N (not necessarily a power of two), one application of $\tilde{K}_\pm$ will require $O(N^3 \log N)$ operations. This is a substantial improvement over the naive matrix-vector product which would require $O(N^6)$ operations.

3. Convergence analysis

3.1. The modified Petviashvili's iteration

In this section we discuss convergence of the iteration (4). The first result in this direction, in the case $\delta = 0$, can be found in [PelSte]. To make this discussion self-contained, we recall their argument and apply it to our specific problem.

Theorem 2 (Pelinovsky and Stepanyants). *Let $\phi(x)$ be the unique radial solution of (3) and let $H^1_r(\mathbb{R}^3)$ denote the subset of all radial functions in $H^1(\mathbb{R}^3)$. Consider the iteration (4) with M_n and γ given by equation (5), but $\delta = 0$. Then there exists an open neighbourhood $\mathcal{N}$ of ϕ in $H^1_r(\mathbb{R}^3)$, in which ϕ is the unique fixed point and (4) converges to ϕ. The iteration is strictly stable in the sense that, for all $\phi_0 \in \mathcal{N}$,*

$$\|\phi_{n+1} - \phi\|_1 \leqslant (1 - C)\|\phi_n - \phi\|_1, \qquad 0 < C \leqslant 1, \tag{11}$$

where $\|\cdot\|_1$ is the norm in the Sobolev space $H^1(\mathbb{R}^3)$.

Proof. Put $p = 2\beta + 1$. Let us first write down the linearized iteration, about the fixed point ϕ, for the perturbation $w_n = \phi_n - \phi$. It reads[4]

$$\hat{w}_{n+1} = (1-p)\gamma a_n \hat{\phi} + p\frac{\widehat{\phi^{p-1}} * \hat{w}_n}{1+|\xi|^2}, \tag{12}$$

where $*$ denotes convolution, a_n comes from the linearization of M_n and is given by

$$a_n = \frac{\int w_n \phi^p \, \mathrm{d}x}{\int \phi^{p+1} \, \mathrm{d}x}.$$

(Up to higher-order terms, we have the asymptotic relation $1+(1-p)a_n \sim M_n$.) This formula suggests that ϕ plays a special role in the stability of the linearized iteration. Indeed, we claim that we can actually expand w_n as

$$w_n = a_n \phi + q_n, \tag{13}$$

where a_n is exactly as defined above and q_n is a remainder. In order to see this, let us introduce the operator $A = (I-\Delta)^{-1}\mathcal{H}$, where $\mathcal{H} = I - \Delta - p\phi^{p-1}$. It is easy to check that it is bounded and self-adjoint with respect to the H^1 inner product,

$$(f, g) \equiv \langle f, (I-\Delta)g \rangle.$$

The operator A therefore provides a spectral decomposition of $L^2(\mathbb{R})$, orthogonal with respect to the inner product $(\cdot,\cdot)$. It was noticed in [PelSte] (or by a straightforward extension of their argument), that the spectra of A and $\mathcal{H}$ obey

$$\dim(\mathrm{neg}(A)) = \dim(\mathrm{neg}(\mathcal{H})) = 1,$$

$$\mathrm{null}(A) = \mathrm{null}(\mathcal{H}) = 3.$$

The first four eigenfunctions of A are precisely ϕ and $\partial_i \phi$, with eigenvalues $1-p < 0$ and 0, respectively. Equation (13) is just the expansion of w_n in this orthogonal system. Since the iterates ϕ_n are all radial, the components along $\partial_i \phi$ are zero. The remainder q_n belongs to the space Y_p defined by

$$Y_p = \{u \in L^2(\mathbb{R}^3) : \langle u, \phi^p \rangle = \langle u, \partial_i \phi^p \rangle = 0\}.$$

In the space Y_p, the spectrum of A is strictly positive, bounded from below by the fifth eigenvalue[5] $\lambda_5 > 0$ and from above by

$$\lambda_M = \sup_u \frac{(u, Au)}{(u,u)} = 1 - p \inf_u \frac{\langle u, \phi^{p-1} u \rangle}{(u,u)} = 1.$$

For the last equality we have used the fact that $\phi(x) > 0$ and $\phi(x) \to 0$ as $|x| \to \infty$.

The recurrence equations for a_n and q_n can be found from equation (12),

$$a_{n+1} = (p - \gamma(p-1))a_n,$$

$$q_{n+1} = (I - A)q_n.$$

The choice we made for γ ensures that the component along ϕ is immediately put to zero (in the linearized iteration.) It is also clear that we have $\|q_{n+1}\|_1 \leqslant (1-\lambda_5)\|q_n\|_1$ in $H^1(\mathbb{R}^3)$. In the scope of the linearized iteration, equation (11) follows with $C = \lambda_5$.

[4] Throughout this paper, we use the following convention for the Fourier transform:

$$\hat{f}(\xi) = \int \mathrm{e}^{-\mathrm{i}x\cdot\xi} f(x) \, \mathrm{d}x, \qquad f(x) = \frac{1}{(2\pi)^3} \int \mathrm{e}^{\mathrm{i}x\cdot\xi} \hat{f}(\xi) \, \mathrm{d}\xi.$$

[5] It always exists by lemma 2.5 in [PelSte].

Call $\mathcal{P}$ the nonlinear operator for the Petviashvili iteration in the case $\delta = 0$, so that (4) is written as $\phi_{n+1} = \mathcal{P}(\phi_n)$. We follow [PelSte] and apply the contraction mapping theorem in a neighbourhood of the fixed point ϕ, within the closed subspace $H^1_r(\mathbb{R}^3)$. We have already computed the Fréchet derivative of $\mathcal{P}$ at ϕ,

$$\mathcal{P}'(\phi)w = (I - A)P_{Y_p}w, \tag{14}$$

where P_{Y_p} is the projection onto Y_p, orthogonal in H^1. Let $0 < \epsilon < \lambda_5$. By continuity of $\mathcal{P}'(u)$ as a function of u, in the operator H^1 norm, we can assert that there exists a small open neighbourhood $\mathcal{N}$ of ϕ in which

$$\|\mathcal{P}'(u)\|_{1\to 1} < 1 - \lambda_5 + \epsilon.$$

By a standard application of the contraction mapping theorem (see [HutPym] p 126), the fixed point is unique in $\mathcal{N}$ and we have the estimate

$$\|\phi_{n+1} - \phi\|_1 \leqslant (1 - \lambda_5 + \epsilon)\|\phi_n - \phi\|_1.$$

This concludes the proof. □

Let us now examine how the above argument generalizes to the case $\delta \neq 0$. The purpose of the second term in equation (4) is precisely to put to zero the components along the three basis functions $\partial_i\phi$ should the initial condition not be radial. This is also useful in the context of the numerical realization of $\mathcal{P}$, since numerical round-off errors do not correspond in general to radial perturbations. To be precise, the linearized iteration (12) becomes

$$\hat{w}_{n+1} = (1 - p)\gamma a_n\hat{\phi} + 2\delta \sum_{j=1,2,3} b_{n,j}\widehat{\partial_j\phi} + p\frac{\widehat{\phi^{p-1}} * \hat{w}_n}{1 + |\xi|^2},$$

with a_n as previously and

$$b_{n,i} = \frac{\int w_n\partial_i\phi^p \,\mathrm{d}x}{\int \partial_i\phi\partial_i\phi^p \,\mathrm{d}x}$$

is the component of w_n along $\partial_i\phi$, in the natural H^1 inner product. Asymptotically, note that $R_{n,i} \sim 2b_{n,i}$. In order to obtain the above formula for $b_{n,i}$ we have linearized $\phi_n = \phi + w_n$, used the PDE $(I - \Delta)\phi = \phi^p$ and applied Parseval's theorem. So we have

$$w_n = a_n\phi + \sum_j b_{n,j}\partial_j\phi + q_n,$$

and the recurrence relation for $b_{n,i}$ is

$$b_{n+1,i} = (1 + 2\delta)b_{n,i}.$$

Choosing $\delta = -1/2$ as advocated previously will put to zero the components along $\partial_i\phi$.

The coefficients $b_{n,j}$ are not directly available in practice, which is why $R_{n,i}$ is defined solely in terms of the current iterate ϕ_n. It is easy to check that any radial ϕ_n yields $R_{n,i} = 0$ but that a small translation by a vector of length ϵ would make $R_{n,i}$ proportional to ϵ. So the constant $R_{n,j}$ measures the departure from radialness, and the purpose of the correction term is precisely to keep $R_{n,j}$ close to zero. This property is useful in the context of the numerical realization of the operator $\mathcal{P}$, since numerical round-off errors do not correspond in general to radial perturbations. In practice this modification works very well (see section 4).

As we observe, the analysis of the linearized iteration does not pose any difficulty. However, we leave the extension of the argument of theorem 2 to the full *nonlinear* iteration as an open problem. The difficulty is that the operator $\mathcal{P}$ is in general not defined on H^1 because the constants $R_{n,i}$ involve 3/2 derivatives of ϕ_n in L^2. *A fortiori*, $\mathcal{P}$ is not Frechet-differentiable

for functions in H^1. Note that the contraction argument needs to be modified, since the soliton ϕ is not unique in $H^1(\mathbb{R}^3)$—it is unique up to a translation. The question of stability of the modified Petviashvili's iteration in the nonradial case is possibly related to the problem of proving uniqueness of the radial soliton, which, in itself, is not trivial.

3.2. Truncation and discretization

In this section we prove *spectral convergence* of the proposed discretization of the Birman–Schwinger operator, which is numerical analysis jargon for almost-exponential or super-algebraic convergence with respect to the large discretization parameters L and N/L. We study the numerical algorithm exactly as implemented in the code, without any simplification, except for the assumption of exact arithmetic.

Recall that we denote by $x_j = (j_1, j_2, j_3)L/N$, $j \in \mathbb{Z}^3$ the nodes of a cubic grid with spacing L/N in all three directions, not necessarily bounded in some of the arguments that follow. Obviously, we take $L \leqslant N$. Unless otherwise specified, we consider the operator K_-, since $K_+ = (2\beta + 1)K_-$.

We now formulate our main result. Most of the rest of this section is devoted to its justification. We will use the notation $\langle x \rangle = \sqrt{1 + |x|^2}$.

Theorem 3. *Let K be the Birman–Schwinger operator as above and $\tilde{K}$ its numerical realization, extended to functions of continuous x by sampling and interpolation (see below for details). Let $\tau > 0$ be the decay rate of $U(x) = \phi(x)^\beta$, $|U(x)| \leqslant C \cdot \mathrm{e}^{-\tau|x|}$. Assume that Petviashvili's method gives an accurate approximation $\tilde{\phi}$ of the soliton in the sense that, for some $\epsilon > 0$, and denoting $\tilde{U} = \tilde{\phi}^\beta$,*

$$|U(x_j) - \tilde{U}(x_j)| \leqslant C \cdot \min\left(\frac{\epsilon}{\langle x_j \rangle}, \mathrm{e}^{-\tau|x_j|}\right). \tag{15}$$

Then we have, for all $s > 3/2$ and $f \in H^s(\mathbb{R}^3)$, in exact arithmetic

$$\|(K - \tilde{K})f\|_{L^2} \leqslant C_s \cdot \left[\epsilon + L\mathrm{e}^{-\tau L/4} + \left(\frac{N}{L}\right)^{-s}\right] \cdot \|f\|_{H^s}, \tag{16}$$

for some constant $C_s > 0$ depending on s.

Discretization is error-free in the context of the Shannon sampling theorem. Let us introduce $B_{N/L}(\mathbb{R}^3)$, the space of band-limited square-integrable functions,

$$B_{N/L}(\mathbb{R}^3) = \{u \in L^2(\mathbb{R}^3) : \hat{u}(\xi) = 0,\ |\xi| > \pi N/L\}.$$

The hat denotes Fourier transformation. We can then define the *sampling* operator S and *interpolation* operator T as

$$S : B_{N/L}(\mathbb{R}^3) \to \ell^2, \qquad f(x) \mapsto \{f(x_j)\},$$
$$T : \ell^2 \to B_{N/L}(\mathbb{R}^3), \qquad \{f(x_j)\} \mapsto \sum_{j \in \mathbb{Z}^3} h(x - x_j) f(x_j).$$

Here $h(x)$ is the interpolating kernel defined by $\hat{h}(\xi) = (L/N)^3$ if $|\xi| \leqslant \pi N/L$, and zero otherwise. The content of Shannon's sampling theory is that S is an isometry from $B_{N/L}(\mathbb{R}^3)$ to ℓ^2 and T in that context is both the adjoint and a left inverse for S on its range (hence the interpolation property of h.) Note that the properly normalized ℓ^2 norm is

$$\|\{f(x_j)\}_j\|_{\ell^2} = \sqrt{\left(\frac{L}{N}\right)^3 \sum_j |f(x_j)|^2}.$$

With a slight abuse of notation, let us denote by $\tilde{G}$ the operator of discrete convolution by $\tilde{G}(x_j)$, with

$$\tilde{G}(x_j) = \begin{cases} \dfrac{1}{2\pi^2|x_j|}\left(\dfrac{L}{N}\right)^3 \mathrm{Si}\left(\dfrac{\pi N|x_j|}{L}\right) & \text{if } x_j \neq 0, \\ \dfrac{1}{2\pi}\left(\dfrac{L}{N}\right)^2 & \text{if } x_j = 0. \end{cases} \tag{17}$$

Recall that x_j are the points of a Cartesian grid. This particular expression for the weights $\tilde{G}(x_j)$ is chosen so that the inversion of the Laplacian is *exact* on decaying functions, bandlimited in the space $B_{N/L}(\mathbb{R}^3)$. By 'decaying', we mean a member of some weighted L^2 space. More generally, let us introduce weighted Sobolev spaces as

$$H^s_m(\mathbb{R}^3) = \{u : \langle x\rangle^m u(x) \in H^s(\mathbb{R}^3)\}$$

and equipped with the norm

$$\|u\|_{s,m} = \|\langle x\rangle^m u\|_s.$$

Of course, $L^2_m = H^0_m$.

Lemma 4. *We have*

$$(T\tilde{G}Sf)(x) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{1}{|x-y|} f(y)\,\mathrm{d}y,$$

for all $f \in B_{N/L}(\mathbb{R}^3) \cap L^2_1(\mathbb{R}^3)$.

Proof. The restriction $f \in L^2_1$ is simply chosen so that the integral makes sense. Since $f \in B_{N/L}(\mathbb{R}^3)$, we can express it as

$$f(x) = \sum_j h(x - x_j) f(x_j).$$

Substituting in the integral, we get

$$\begin{aligned}(-\Delta)^{-1} f(x_j) &= \sum_{k\in\mathbb{Z}^3} \frac{1}{4\pi}\int \frac{1}{|x_j - y|} h(y - x_k)\,\mathrm{d}y\, f(x_k) \\ &= \sum_{k\in\mathbb{Z}^3} w(j,k) f(x_k).\end{aligned}$$

The quadrature weights $w(j,k)$ can be computed explicitly. By Parseval,

$$w(j,k) = \frac{1}{(2\pi)^3}\int \frac{1}{|\xi|^2} \mathrm{e}^{-\mathrm{i}(x_j - x_k)\cdot\xi} \hat{h}(\xi)\,\mathrm{d}\xi.$$

In the event $x_j \neq x_k$, we can express this integral in a spherical coordinate frame whose z-axis is aligned with $x_j - x_k$. It becomes

$$\begin{aligned} w(j,k) &= \frac{1}{(2\pi)^2}\left(\frac{L}{N}\right)^3 \int_0^{\pi N/L} r^2\,\mathrm{d}r \int_0^{\pi} \sin\theta\,\mathrm{d}\theta \frac{1}{r^2} \mathrm{e}^{-\mathrm{i}|x_j - x_k| r\cos\theta}, \\ &= \left(\frac{L}{N}\right)^3 \frac{1}{(2\pi)^2} \int_0^{\pi N/L} \mathrm{d}r \int_{-1}^{1} \mathrm{e}^{\mathrm{i}|x_j - x_k| r x}\,\mathrm{d}x, \\ &= \left(\frac{L}{N}\right)^3 \frac{1}{(2\pi)^2} 2\int_0^{\pi N/L} \frac{\sin|x_j - x_k| r}{|x_j - x_k| r}\,\mathrm{d}r, \\ &= \left(\frac{L}{N}\right)^3 \frac{1}{2\pi^2}\frac{1}{|x_j - x_k|}\mathrm{Si}\left(\frac{\pi N|x_j - x_k|}{L}\right). \end{aligned}$$

$\mathrm{Si}(x)$ is the special function $\int_0^x \sin t/t \, \mathrm{d}t$. Thus we have $w(j,k) = \tilde{G}(x_j - x_k)$, as in equation (10). The special case $x_j = x_k$ can be handled separately in a similar fashion, and one can check that it corresponds to the limit $x_j - x_k \to 0$ in the general expression.

We have just proved that $\tilde{G}Sf = S(-\Delta^{-1})f$. Now the output $(-\Delta)^{-1}f$ is not in general square-integrable (see also lemma 8 below), but it is still band-limited. The interpolation operator T is still the inverse of sampling for band-limited functions with some growth, so we obtain the desired conclusion. □

Remark. It is interesting to note that the choice we made for $\hat{h}$, the indicator of a ball, as a model for bandlimited functions is not standard. The most natural frequency window associated with a Cartesian grid is the indicator of the cube $[-\pi N/L, \pi N/L]^3$. Choosing a cubic window for the definition of $B^{\mathrm{std}}_{N/L}$, the space of L^2 band-limited functions, would have made the sampling operator S not only an isometry but a *unitary* map from $B^{\mathrm{std}}_{N/L}$ *onto* ℓ^2. In our context, with the spherical window, S is only unitary from $B_{N/L}$ to a *subset* of ℓ^2, namely the range $SB_{N/L}$. However, in the context of Poisson's equation, spherical windows are better suited as a model for bandlimited functions since they allow us to formulate a closed-form expression for the weights $\tilde{G}(x_j)$.

Remark. The introduction of balls instead of cubes to define bandlimited functions is merely a convenient characterization of the set of functions for which the numerical quadrature is exact. Theorem 3, however, does not make any assumption on functions being band-limited inside a ball. In fact, the functions we have to discretize, such as the soliton $\phi(x)$, are not band-limited. The price to pay is a small truncation error, which we now quantify in a sequence of lemmata.

The following elementary lemma establishes the fact that the smoother the function, the more accurate its sampling.

Lemma 5. *For all $s > 3/2$ and $f \in H^s(\mathbb{R}^3)$,*

$$\|f - TSf\|_{L^2} \leqslant C_s \left(\frac{N}{L}\right)^{-s} \|f\|_s.$$

The constant C_s is a decreasing function of $s \in (3/2, \infty)$.

Proof. Sampling in x corresponds to periodizing in ξ, so the Fourier transform of $TSf - f$ is

$$F(\xi) = \sum_{m \in \mathbb{Z}^3} \hat{f}(\xi - 2\pi m N/L)\chi_{|\xi| \leqslant \pi N/L}(\xi) - \hat{f}(\xi).$$

We get two contributions, call them (I) and (II), in

$$\|F\|_2^2 = \int_{|\xi| \leqslant \pi N/L} |\sum_{m \neq 0} \hat{f}(\xi - 2\pi m N/L)|^2 \, \mathrm{d}\xi$$

$$+ \int_{|\xi| > \pi N/L} |\hat{f}(\xi)|^2 \, \mathrm{d}\xi.$$

The second integral (II) is easily bounded by

$$(II) \leqslant \sup_{|\xi| > \pi N/L} \langle \xi \rangle^{-2s} \cdot \|f\|_s^2 \leqslant \pi^{-2s} \left(\frac{N}{L}\right)^{-2s} \|f\|_s^2.$$

The first integral (I) can be expressed as

$$(I) = \sum_{m \neq 0} \sum_{m' \neq 0} I_{m,m'},$$

where

$$I_{m,m'} = \int_{B_0(\pi N/L)} \left| \hat{f}\left(\xi - 2\pi m \frac{N}{L}\right) \hat{f}\left(\xi - 2\pi m' \frac{N}{L}\right) \right|,$$

$$\leqslant \sup_{|\xi| \leqslant \pi N/L} \langle \xi - 2\pi m N/L \rangle^{-s} \cdot \sup_{|\xi| \leqslant \pi N/L} \langle \xi - 2\pi m' N/L \rangle^{-s}$$

$$\times \int_{B_0(\pi N/L)} |\hat{f}(\xi - 2\pi m N/L)| \langle \xi - 2\pi m N/L \rangle^{s}$$

$$\cdot |\hat{f}(\xi - 2\pi m' N/L)| \langle \xi - 2\pi m' N/L \rangle^{s} \, \mathrm{d}\xi.$$

Obviously $\sup_{|\xi| \leqslant \pi N/L} \langle \xi - 2\pi m N/L \rangle^{-s} \leqslant C \cdot (|m| N/L)^{-s}$ and the integral can be bounded by Cauchy–Schwarz. We have thus separated

$$I_{m,m'} \leqslant C \cdot J_m J_{m'} \cdot \left(\frac{N}{L}\right)^{-2s},$$

where

$$J_m = |m|^{-s} \sqrt{\int_{|\xi + 2\pi m \frac{N}{L}| \leqslant \pi N/L} |\hat{f}(\xi)|^2 \langle \xi \rangle^{2s} \, \mathrm{d}\xi}.$$

Each point ξ in the frequency domain is covered by at most one ball $B_{2\pi m(N/L)}(\pi N/L)$. Consequently, Cauchy–Schwarz for sequences gives

$$\sum_{m \neq 0} J_m \leqslant C \cdot \sqrt{\sum_{m \neq 0} |m|^{-2s}} \cdot \sqrt{\int_{\mathbb{R}^3} |\hat{f}(\xi)|^2 \langle \xi \rangle^{2s} \, \mathrm{d}\xi}.$$

The sum over m converges only when $s > 3/2$ in three dimensions. This governs the dependence of the constant C_s on s. Each J_m gives one factor $\|f\|_s$, which completes the argument. □

Note that the above result is sharp with respect to the range of s for which it is valid. The Sobolev embedding from H^s into continuous functions is only valid when $s > 3/2$ in three dimensions, and it does not in general make sense to sample a discontinuous function.

Let us note in passing that lemma 5 generalizes without difficulty to weighted norms.

Lemma 6. *For all $s > 3/2$, $m \in \mathbb{Z}$ and $f \in H^s_m(\mathbb{R}^3)$,*

$$\|f - TSf\|_{L^2_m} \leqslant C_s \left(\frac{N}{L}\right)^{-s} \|f\|_{s,m}.$$

Proof. It is sufficient to exhibit a bandlimited multiplier $\xi_m(x)$ equivalent to $\langle x \rangle^m$ in the sense that

$$C_1 \langle x \rangle^m \leqslant \xi_m(x) \leqslant C_2 \langle x \rangle^m,$$

for then weighted norms can be expressed with ξ_m instead and

$$\xi_m(f - TSf) = (Id - TS)\xi_m f.$$

Then the conclusion would follow from an application of lemma 5 to $\xi_m f$.

Such a function $\xi_m(x)$ can be constructed by convolving $\langle x \rangle^m$ by some appropriate nonnegative, band-limited kernel. For example,

$$\xi_m(x) = \langle x \rangle^m * \prod_{j=1}^{3} \left(\mathrm{sinc}\left(\frac{x_j}{a}\right)\right)^{2|m|+4}$$

will do for $m \neq 0$, provided $a > 0$ is chosen so that the band limit of the kernel is compatible with the sampling of S. □

We will frequently need to switch from discrete to continuous norms, using the following result.

Corollary 7. *Let $f \in H^s(\mathbb{R}^3)$, for $s > 3/2$. Then*

$$\|f(x_j)\|_{\ell^2} \leqslant C_s \cdot \|f\|_{H^s}.$$

Proof. Decompose TSf as $f + (TSf - f)$ and estimate in L^2. By lemma 5 and the sampling theorem,

$$\|f(x_j)\|_{\ell^2} \leqslant \|f\|_{L^2} + C_s \cdot \left(\frac{N}{L}\right)^{-s} \|f\|_{H_s} \leqslant C \cdot \|f\|_{H^s}. \qquad \square$$

Let us collect some more background results. We have already hinted at the fact that $(-\Delta)^{-1}$, defined as the convolution with $G(x)$, is not bounded on L^2 or on any H^s for that matter. But it is bounded between *weighted* Sobolev spaces. Let us recall the following classical result from [JenKat].

Lemma 8. ***(Jensen and Kato)*** *The kernel $G(x - y) = 1/(4\pi|x - y|)$ maps boundedly $H^{-1}_m(\mathbb{R}^3)$ to $H^1_{-m'}(\mathbb{R}^3)$ and is in addition Hilbert–Schmidt from L^2_m to $L^2_{-m'}$, provided*

$$m, m' > \tfrac{1}{2} \qquad \text{and} \qquad m + m' > 2.$$

A similar property holds for the discretized kernel $\tilde{G}$. Weighted discrete ℓ^2 spaces, relative to the grid x_j, are defined as

$$\ell^2_m = \{u_j : \langle x_j\rangle^m u_j \in \ell^2\}.$$

Lemma 9. *The kernel $\tilde{G}(x_j - x_k)$ defined in equation (10) maps boundedly ℓ^2_m to $\ell^2_{-m'}$ provided*

$$m, m' > \tfrac{1}{2} \qquad \text{and} \qquad m + m' > 2.$$

The operator norm of $\tilde{G}$ is uniform in $N/L \geqslant 1$.

Proof. The Hilbert–Schmidt norm of $\tilde{G}$ between ℓ^2_m and $\ell^2_{-m'}$ is

$$\|\tilde{G}\|^2_{HS} = \sum_{j,k} |\tilde{G}(x_j - x_k)|^2 \langle x_j\rangle^{-2m'} \langle x_k\rangle^{-2m}.$$

The diagonal part D of the sum, for $j = k$, is

$$D = \frac{1}{(2\pi)^2} \left(\frac{L}{N}\right)^4 \sum_j \left(1 + \left|j\frac{L}{N}\right|^2\right)^{-(m+m')}$$

and can be compared with the integral

$$D \leqslant C \cdot \frac{L}{N} \int_{\mathbb{R}^3} (1 + |x|^2)^{-(m+m')}\, \mathrm{d}x,$$

which converges when $m + m' > 3/2$. The off-diagonal part OD, for $j \neq k$, is bounded by

$$OD \leqslant \left(\frac{L}{N}\right)^6 \sum_{j,k:j\neq k} \frac{1}{|j(L/N) - k(L/N)|^2} \left(1 + \left|j\frac{L}{N}\right|^2\right)^{-m'} \left(1 + \left|k\frac{L}{N}\right|^2\right)^{-m}$$

(because $|Si(x)| < 2$). Its continuous counterpart is

$$OD \leqslant C \cdot \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{1}{|x-y|^2} (1+|x|^2)^{-m} (1+|y|^2)^{-m'} \, \mathrm{d}x \, \mathrm{d}y.$$

The double integral is the Hilbert–Schmidt norm of G, squared, between L^2_m and $L^2_{-m'}$, and is bounded by lemma 8. □

We can now turn to the proof of the main result, theorem 3. The Birman–Schwinger operator is defined as

$$K = U(x)(-\Delta^{-1})U(x), \qquad U(x) = \phi(x)^{\beta}.$$

The approximation $\tilde{K}$ is defined as

$$\tilde{K} = T\tilde{U}(x_j)\tilde{G}_c\tilde{U}(x_j)S,$$

where the subscript c in $\tilde{G}_c$ indicates that the convolution is not over the whole infinite grid $L/N \times \mathbb{Z}^3$ but is a circular convolution over the finite cubic array $(-L/2 : L/N : (L/2 - L/N))^3$ (in the Matlab notation.) Let us denote this bounded grid by $\square_N$.

Proof of theorem 3. Let us divide the proof into four successive approximation steps, using the triangle inequality.

(i) Let us first show that

$$(I) = \|T\tilde{U}(x_j)(\tilde{G}_c - \tilde{G})(\tilde{U}(x_j)Sf)\|_{L^2}$$

is adequately small in the sense of theorem 3. By Shannon's sampling theorem (ST is the orthogonal projector onto Ran S), we can rewrite

$$(I) \leqslant \|\tilde{U}(x_j)(\tilde{G}_c - \tilde{G})(\tilde{U}(x_j)f(x_j))\|_{\ell^2}.$$

We denote the operation of folding back a grid point by periodicity onto the grid $\square_N$ as follows:

$$\lfloor x_j \rceil \equiv \left(x_j + (1,1,1)\frac{L}{2} \right) \bmod L - (1,1,1)\frac{L}{2}.$$

The discrepancy between the two types of convolution is

$$(\tilde{G}_c - \tilde{G})g(x_j) = \sum_{k \in \mathbb{Z}^3} g(x_k)\tilde{G}(x_j - x_k) - \sum_{x_k \in \square_N} g(x_k)\tilde{G}(\lfloor x_j - x_k \rceil).$$

Let us introduce the intermediate quantity

$$\tilde{G}_b g(x_j) = \sum_{x_k \in \square_N} g(x_k)\tilde{G}(x_j - x_k),$$

where the subscript b stands for 'bounded convolution'. The first contribution is

$$\begin{aligned}(I_A) &= \|\tilde{U}(x_j)(\tilde{G}_b - \tilde{G})(\tilde{U}(x_j)f(x_j))\|_{\ell^2} \\ &= \|\tilde{U}(x_j) \sum_{x_k \notin \square_{S_N}} \tilde{G}(x_j - x_k)\tilde{U}(x_k)f(x_k)\|_{\ell^2} \\ &\leqslant \sup_j |\tilde{U}(x_j)\langle x_j\rangle^2| \cdot \|\tilde{G}\|_{\ell^2_1 \to \ell^2_{-2}} \cdot \sup_{x_j \notin \square_N} |\tilde{U}(x_j)\langle x_j\rangle| \cdot \|f(x_j)\|_{\ell^2}.\end{aligned}$$

The first factor is obviously bounded by equation (15); the second factor is bounded by lemma 9; the third factor is less than $\epsilon + C \cdot Le^{-\tau L}$ by equation (15) and the fourth factor is less than $C \cdot \|f\|_{H^s}$ by corollary 7.

The second contribution is

$$(I_B) = \|\tilde{U}(x_j)(\tilde{G}_c - \tilde{G}_b)(\tilde{U}(x_j)f(x_j))\|_{\ell^2}.$$

The kernels $\tilde{G}_c$ and $\tilde{G}_b$ differ only when $x_j \notin \square_N$ and in that case we have the estimate

$$|\tilde{G}(x_j) - \tilde{G}(\lfloor x_j \rceil)| \leqslant \frac{1}{L}\chi_{x_j \notin \square_N}(j,k).$$

Therefore

$$(I_B) \leqslant \frac{1}{L}\left\| \tilde{U}(x_j) \sum_{\substack{x_k \in \square_N \\ x_k \notin x_j + \square_N}} \tilde{U}(x_k) f(x_k) \right\|_{\ell^2}$$

$$\leqslant \frac{1}{L}\left\| \tilde{U}(x_j) \cdot \sqrt{\left(\frac{L}{N}\right)^3 \sum_{\substack{x_k \in \square_N \\ x_k \notin x_j + \square_N}} |\tilde{U}(x_k)|^2} \right\|_{\ell^2} \cdot \|f(x_j)\|_{\ell^2}.$$

The quantity underneath the square root can be bounded, up to a multiplicative constant, by

$$\int_{x \notin B_{x_j}(L/2)} \mathrm{e}^{-2\tau|x|}\,\mathrm{d}x \leqslant \int_{x \notin B_0(L/2-|x_j|)} \mathrm{e}^{-2\tau|x|}\,\mathrm{d}x.$$

$$\leqslant C \cdot \left\langle \frac{L}{2} - |x_j| \right\rangle^2 \mathrm{e}^{-2\tau((L/2)-|x_j|)}.$$

With this bound, (I_B) becomes

$$(I_B) \leqslant \frac{C}{L}\sqrt{\left(\frac{L}{N}\right)^3 \sum_{x_j \in \square_N} \mathrm{e}^{-\tau|x_j|}\left\langle \frac{L}{2} - |x_j| \right\rangle \mathrm{e}^{-\tau((L/2)-|x_j|)}} \cdot \|f(x_j)\|_{\ell^2}$$

$$\leqslant \frac{C}{L}\sqrt{\int_{B_0(L)} \mathrm{e}^{-\tau|x|}\left\langle \frac{L}{2} - |x| \right\rangle \mathrm{e}^{-\tau((L/2)-|x|)}\,\mathrm{d}x} \cdot \|f(x_j)\|_{\ell^2}$$

$$\leqslant CL\mathrm{e}^{-\tau L/4}\|f(x_j)\|_{\ell^2}.$$

As before, the ℓ^2 norm of $f(x_j)$ can be bounded, up to a constant, by the H^s norm of f (corollary 7). This shows that (I_A) and (I_B) are both within the bounds of equation (16).

(ii) Let us now study the difference

$$(II) = \|T\tilde{U}(x_j)\tilde{G}(\tilde{U}(x_j)Sf - SU(x)f)\|_{L^2}.$$

We have already observed that $T\tilde{U}(x_j)$ is bounded between ℓ^2_{-2} and L^2. We also know from lemma 9 that $\tilde{G}$ is bounded from ℓ^2_1 to ℓ^2_{-2}. Hence, it suffices to show that the following quantity is adequately small:

$$\|(\tilde{U}(x_j)S - SU(x))f\|^2_{\ell^2_1} = \left(\frac{L}{N}\right)^3 \sum_j \langle x_j\rangle^2 |\tilde{U}(x_j) - U(x_j)|^2 |f(x_j)|^2.$$

By equation (15) and corollary 7, we can bound this expression by $C\epsilon^2\|f\|^2_{H^s}$.

(iii) The third contribution

$$(III) = \|(T\tilde{U}(x_j) - U(x)T)\tilde{G}SU(x)f\|_{L^2}$$

can be bounded analogously. We know that SU maps ℓ^2 to ℓ^2_2 boundedly and $\tilde{G}$ maps ℓ^2_2 to ℓ^2_{-1} boundedly. It remains to show that

$$\|(T\tilde{U}(x_j) - U(x)T)g\|_{L^2}$$

is small in proportion to $g \in \ell^2_{-1}$. By the sampling theorem, this is also

$$\|(\tilde{U}(x_j) - SU(x)T)g(x_j)\|_{\ell^2} = \|(\tilde{U}(x_j) - U(x_j))g(x_j)\|_{\ell^2}.$$

Again, equation (15) allows to bound this quantity by $C\epsilon\|g(x_j)\|_{\ell^2_{-1}}$.

(iv) The last, and perhaps most important contribution, is

$$(IV) = \|U(T\tilde{G}S + \Delta^{-1})Uf\|_{L^2}.$$

Obviously, multiplication by $U(x)$ is bounded from H^s to H^s_2, as well as from H^s_{-2} to H^s, for all $s \geqslant 0$. So it suffices to show that

$$\|(T\tilde{G}S + \Delta^{-1})g\|_{L^2_{-2}} \leqslant C_s \cdot \left(\frac{N}{L}\right)^{-s} \cdot \|g\|_{H^s_2},$$

for all $s > 3/2$. It is important to note that

$$T\tilde{G}Sg = -\Delta^{-1}TSg,$$

which follows from applying lemma 4 to TSg. Since by lemma 8, Δ^{-1} is bounded between L^2_2 and L^2_{-2}, it is enough to check that

$$\|TSg - g\|_{L^2_2} \leqslant C_s \cdot \left(\frac{N}{L}\right)^{-s} \cdot \|g\|_{H^s_2}.$$

This is precisely the content of lemma 6. The proof is complete. □

It is likely that theorem 3 could actually be formulated with exponential decay in N/L, but we leave this as a challenge to the reader. In order to do so, it would be necessary to prove the analyticity of the soliton $\phi(x)$, which we believe is still an open problem in three dimensions. Our numerical experiments strongly support the analyticity conjecture (see section 4).

3.3. Accuracy of eigenvalues

Let us remark that the accuracy of the discretization depends crucially on the smoothness of the function to which the operator is applied. This follows not only from sampling issues but also from the choice of quadrature weigths $\tilde{G}(x_j)$ used to invert the laplacian. As a consequence, only the eigenvalues of K corresponding to very smooth eigenfunctions will be computed to high accuracy.

Since K is compact and self-adjoint on $L^2(\mathbb{R}^3)$, let us write its spectral decomposition as

$$Ke_j = \lambda_j e_j, \qquad \langle e_j, e_k\rangle = \delta_{jk}.$$

Its discrete counterpart $\tilde{K}$ is also self-adjoint and compact (of finite rank) but only on the space $B_{N/L}$. We have

$$\tilde{K}\tilde{e}_j = \tilde{\lambda}_j\tilde{e}_j, \qquad \langle \tilde{e}_j, \tilde{e}_k\rangle = \delta_{jk}.$$

Any $f \in B_{N/L}$ can therefore be expanded as $f = \sum_j \langle f, \tilde{e}_j\rangle \tilde{e}_j$.

The following result about accuracy of eigenvalues is mostly a consequence of theorem 3. Let $\epsilon_{L,N}$ denote the small factor on the right-hand side of equation (16), namely

$$\epsilon_{L,N} = C_s \cdot \left[\epsilon + L\mathrm{e}^{-\tau L/4} + \left(\frac{N}{L}\right)^{-s}\right].$$

Corollary 10. *If λ_j is simple then*

$$|\lambda_j - \tilde{\lambda}_j| \leqslant \frac{\epsilon_{L,N}\|e_j\|_{H^s}}{|\langle e_j, \tilde{e}_j\rangle|}, \tag{18}$$

and, for $\epsilon_{L,N}$ sufficiently small,

$$\|e_j - \tilde{e}_j\|_{L^2} \leqslant 2\frac{\epsilon_{L,N}\|\tilde{e}_j\|_{H^s}}{d_j},$$

where $d_j = \min_{k\neq j}|\lambda_j - \lambda_k|$.

If λ_j has multiplicity $p > 1$, denote by Π_j the orthoprojector onto the jth eigenspace, and by $\tilde{\Pi}_j$ its numerical counterpart. Then, for all $1 \leqslant m \leqslant p$,

$$|\lambda_j - \tilde{\lambda}_{j,m}| \leqslant \frac{\epsilon_{L,N}\sqrt{\sum_{n=1}^{p}\|e_{j,n}\|_{H^s}^2}}{\|\Pi_j \tilde{e}_{j,m}\|_{L^2}}, \tag{19}$$

and, for $\epsilon_{L,N}$ sufficiently small,

$$\|\Pi_j - \tilde{\Pi}_j\|_{HS} \leqslant 2\frac{\epsilon_{L,N}\sqrt{\sum_{n=1}^{p}\|\tilde{e}_{j,n}\|_{H^s}^2}}{d_j}.$$

The above norm is the Hilbert–Schmidt (HS) norm.

Proof. The proof is loosely related to the argument behind Gershgorin's circle theorem.

• Take λ_j simple. Let $\Pi = TS$ be the orthogonal projection from L^2 to $B_{N/L}$. We can then expand

$$\Pi e_j = \sum_k \theta_{j,k}\tilde{e}_k, \qquad \theta_{j,k} = \langle e_j, \tilde{e}_k\rangle.$$

Consider the relation

$$\tilde{K}e_j = \lambda_j e_j + r_j, \tag{20}$$

where by theorem 3 the remainder $r_j = (\tilde{K} - K)e_j$ obeys

$$\|r_j\|_{L^2} \leqslant \epsilon_{L,N}\|e_j\|_{H^s}. \tag{21}$$

We can project equation (20) onto $B_{N/L}$ and expand it on the basis $\tilde{e}_k$, which gives

$$\theta_{j,k}\tilde{\lambda}_k = \theta_{j,k}\lambda_j + \langle r_j, \tilde{e}_k\rangle. \tag{22}$$

For $k = j$, we can bound

$$|\lambda_j - \tilde{\lambda}_j| \leqslant \frac{|\langle r_j, \tilde{e}_j\rangle|}{|\theta_{j,j}|},$$

which is exactly (18) after using the estimate (21) on r_j.

In order to obtain the estimate for the eigenfunctions, we should instead consider

$$K\tilde{e}_j = \tilde{\lambda}_j\tilde{e}_j + \tilde{r}_j,$$

with $\|\tilde{r}_j\|_{L^2} \leqslant \epsilon_{L,N}\|\tilde{e}_j\|_{H^s}$, and this time expand it on the basis e_k,

$$\theta_{j,k}\lambda_k = \theta_{j,k}\tilde{\lambda}_j + \langle \tilde{r}_j, e_k\rangle. \tag{23}$$

For $k = j$, it would give the same estimate as (18) but with $\tilde{e}_j$ substituted for e_j. For $k \neq j$, we can rewrite equation (23) as

$$|\theta_{j,k}| \leqslant \frac{|\langle \tilde{r}_j, e_k\rangle|}{|\tilde{\lambda}_j - \lambda_k|}. \tag{24}$$

We are not quite finished since the eigenvalue gap, at the denominator, is measured with $\tilde{\lambda_j}$ instead of λ_j. Put $\delta_j = |\lambda_j - \tilde{\lambda}_j|$. Let us also introduce $\tilde{d}_j = \min_{k\neq j} |\tilde{\lambda}_j - \lambda_k|$ and observe that $\tilde{d}_j \geqslant d_j - \delta_j$. Then, squaring (24) and summing over $k \neq j$, we get

$$\sum_{k\neq j} |\theta_{j,k}|^2 \leqslant \frac{\|\tilde{r}_j\|_{L^2}^2}{\tilde{d}_j^2}$$

and, as a result,

$$|\theta_{j,j}|^2 \geqslant 1 - \frac{\|\tilde{r}_j\|_{L^2}^2}{\tilde{d}_j^2}. \tag{25}$$

Our estimate for δ_j, equation (18), can therefore be improved to

$$\delta_j^2 \leqslant \frac{\epsilon_{L,N}^2 \|e_j\|_{H^s}^2}{1 - ((\epsilon_{L,N}^2 \|\tilde{e}_j\|_{H^s}^2)/(d_j - \delta_j)^2)}.$$

It is not hard to see that, as $\epsilon_{L,N}$ gets small, δ_j, defined here implicitly, decreases to zero. Take L, N and $1/\epsilon$ sufficiently large so that $\delta_j \leqslant d_j/4$. Going back to equation (25), we obtain

$$|\theta_{j,j}|^2 \geqslant 1 - 2\frac{\|\tilde{r}_j\|_{L^2}^2}{d_j^2}.$$

The estimate for eigenvectors follows since

$$\|e_j - \tilde{e}_j\|^2 = 2 - 2\theta_{jj} \leqslant 2 - 2\theta_{jj}^2.$$

• Assume now that λ_j has multiplicity $p > 1$. The previous argument goes through, with the following modifications. The change of basis coefficients are now $\theta_{jn,k} = \langle e_{jn}, \tilde{e}_k \rangle$, where $n = 1, \ldots, p$. Equation (22) becomes

$$\theta_{jn,k}\tilde{\lambda}_k = \theta_{jn,k}\lambda_j + \langle r_{j,n}, \tilde{e}_k \rangle. \tag{26}$$

Let us study the discrepancy between λ_j and $\tilde{\lambda}_{jm}$, for some m. We need to take a linear combination of equation (26) with the weights

$$\alpha_n = \frac{\theta_{jn,jm}}{\sqrt{\sum_n |\theta_{jn,jm}|^2}}.$$

We then obtain the inequality

$$|\lambda_j - \tilde{\lambda}_{jm}| \leqslant \frac{\sum_n \alpha_n |\langle r_{j,n}, \tilde{e}_{jm} \rangle|}{\sqrt{\sum_n |\theta_{jn,jm}|^2}}.$$

Observe that $\|\Pi_j \tilde{e}_{jm}\|_{L^2} = \sqrt{\sum_n |\theta_{jn,jm}|^2}$ and the numerator can be bounded by Cauchy–Schwarz (in n) to yield (19).

As for the eigenfunctions, Hilbert–Schmidt norms and trace inner products are to be substituted for their L^2 scalar counterpart. More precisely,

$$\begin{aligned} \|\Pi_j - \tilde{\Pi}_j\|_{HS}^2 &= \mathrm{Tr}(\Pi_j - \tilde{\Pi}_j)^2 \\ &= \mathrm{Tr}\Pi_j + \mathrm{Tr}\tilde{\Pi}_j - 2\mathrm{Tr}\Pi_j\tilde{\Pi}_j \\ &= 2p - 2\mathrm{Tr}\Pi_j\tilde{\Pi}_j, \end{aligned}$$

so we need to find a bound on the latter quantity. Observe first that

$$\mathrm{Tr}\Pi_j\tilde{\Pi}_j = \sum_n \sum_{m=1}^{p} |\theta_{jn,jm}|^2.$$

The change of basis coefficients are normalized in the sense that, for all $n = 1, \ldots, p$,

$$1 = \sum_k |\theta_{jn,k}|^2 = \sum_m |\theta_{jn,jm}|^2 + \sum_{k \neq j} |\theta_{jn,k}|^2.$$

Summing over n, we get

$$p = \mathrm{Tr}\Pi_j \tilde{\Pi}_j + \sum_n \sum_{k \neq j} |\theta_{jn,k}|^2. \tag{27}$$

The bound on $\theta_{jn,k}$ for $k \neq j$ can be obtained as above and is

$$|\theta_{jn,k}| \leqslant \frac{|\langle \tilde{r}_{jn}, e_k \rangle|}{|\tilde{\lambda}_{jn} - \lambda_k|}. \tag{28}$$

It is natural to define $\tilde{d}_j = \min_{k,n} |\tilde{\lambda}_{jn} - \lambda_k|$. The way to bound $\tilde{d}_j$ from below by, say, $3d_j/4$ is very analogous to the simple case and based on some adequate control of the size of the denominator in equation (19). This can be obtained from

$$1 = \|\Pi_j \tilde{e}_{jm}\|_2^2 + \sum_{k \neq jn} |\theta_{k,jm}|^2$$

and

$$\sum_{k \neq jn} |\theta_{k,jm}|^2 \leqslant \sum_{k \neq jn} \frac{|\langle r_k, \tilde{e}_{jm} \rangle|^2}{|\lambda_k - \tilde{\lambda}_{jm}|^2} = \sum_{k \neq jn} \frac{|\langle e_k, \tilde{r}_{jm} \rangle|^2}{|\lambda_k - \tilde{\lambda}_{jm}|^2} \leqslant \frac{\|\tilde{r}_{jm}\|_{L^2}^2}{\tilde{d}_j^2}.$$

(We have used $K = K^*$ and $\tilde{K} = \tilde{K}^*$ for band-limited functions.) Eventually, we use theorem (3) one more time to bound

$$\|\tilde{r}_{jn}\|_{L^2} \leqslant \epsilon_{L,N} \|\tilde{e}_{jn}\|_{H^s}. \tag{29}$$

The desired estimate is obtained by combining the intermediate inequalities (27)–(29). This concludes the proof. □

Note that, in the formulation of the corollary or in its justification, it is nowhere necessary to obtain bounds on errors in computing *other* eigenvalues $\lambda_k \neq \lambda_j$. This is the sense in which our argument is close to Gershgorin's theorem: we only need one row of the matrix $\langle e_j, \tilde{K} e_k \rangle$, namely, the jth row.

4. Numerical results and discussion

Our numerical approximation to the soliton $\phi(x)$, obtained by Petviashvili's iteration, is plotted in log-scale in figure 1. For this experiment, we have taken $\beta = 1$, a cube of sidelength $L = 20$ and a grid of size $N = 200$. Note the apparent exponential decay both in space and frequency. Figure 2 checks the convergence of Petviashvili's iteration, namely that $M_n \to 1$ and that $-\Delta\phi_n + \phi_n - \phi_n^{2\beta+1} \to 0$ as $n \to \infty$.

With the correction term for re-centring, Petviashvili's iteration yields an approximation to the soliton that is as radial as allowed by the grid. In this case the constants $R_{n,j}$ are kept at or below machine precision, 10^{-16}. Without the correction term, $R_{n,j}$ can still be monitored and can become as large as 10^{-4}, signalling a spurious translation of the same order of magnitude for the soliton. Numerically we prefer to be on the safe side and use the modified iteration, with the correction term.

In the above setting we observe nice convergence of the error, as measured by different indicators, to machine accuracy. This is not always the case. For values of L too big in comparison with N (typically, for L of the order of $N/4$ and above), the Petviashvili iteration possibly

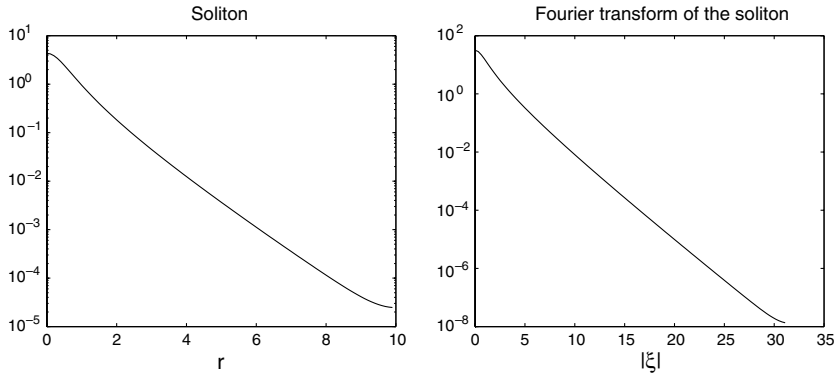

Figure 1. Left: the soliton $\phi(r)$ in space. Right: the soliton $\hat{\phi}(|\xi|)$ in frequency. Both depend only on the radial coordinate.

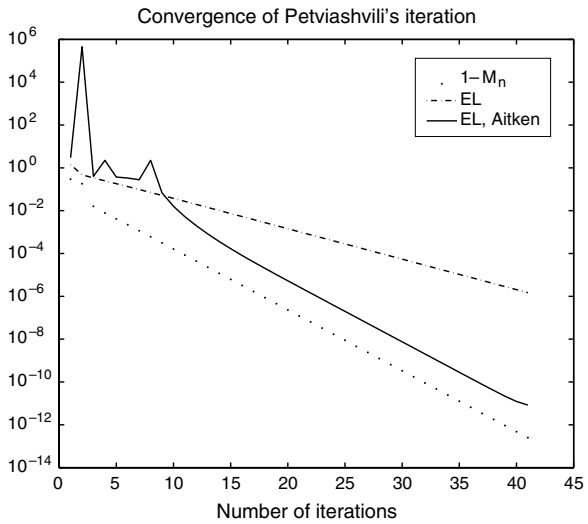

Figure 2. Convergence of Petviashvili's iteration. The x-axis is the number of iteration. Dotted line: $1 - M_n$, where M_n is the Petviashvili constant. (— · —) Euler–Lagrange remainder, $\| - \Delta\phi_n + \phi_n - \phi_n^{2\beta+1}\|/\|\phi_n\|$, with norms in L^2. (——) Same remainder but for the Aitken iterate ϕ_n^A.

reaches acceptable error levels but then diverges away from the fixed point. A careful inspection of the remainder $-\Delta\phi_n + \phi_n - |\phi_n^{2\beta}|\phi_n$ indicates that this might be due the fifth eigenvalue λ_5 of the linearized iteration operator A becoming negative, in the notation of section 3.1.

Next, we show a plot of the two, respectively, five largest eigenvalues of the Birman–Schwinger operator K_-, respectively, K_+, as a function of β in the range $[\frac{2}{3}, 1]$ (figure 3). As mentioned earlier, $\lambda_2(K_-)$ is less than 1 for all values of β, but there exists a number β_* below which $\lambda_5(K_+) > 1$. This is the signature of at least one eigenvalue in the gap of L_+, for $2/3 \leqslant \beta < \beta_*$ (inspection of λ_6 reveals that there is only one eigenvalue in the gap.) For this experiment, we used $L = 15$ and $N = 60$. Note that, in both cases, $\lambda_2 = \lambda_3 = \lambda_4$ is triple, and λ_5 is simple, so we only show at most three curves. Our numerical implementation correctly picks up the multiplicity, exactly (to all 16 digits), and in all the cases that we have tried.

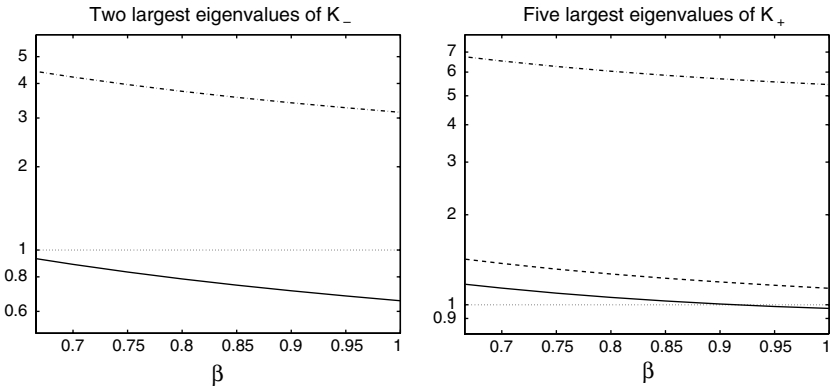

Figure 3. Left: largest eigenvalues of K_-, as a function of β in the range $[\frac{2}{3}, 1]$. The first eigenvalue is simple, and the second to fourth are identical (multiplicity 3). Right: five largest eigenvalues of K_+, as a function of β. The first eigenvalue is simple, the second to fourth eigenvalues are identical and the fifth eigenvalue is simple. In both cases, the value one is indicated by the dotted line.

Table 1. Fifth eigenvalue of K_+, as a function of β near β_*. Here $L = 25$ and $N = 200$. Each value took about one day to obtain. Cubic interpolation reveals $\beta_* \simeq 0.913\,95\,89\,05 \pm 1e-8$.

β	$\lambda_5(K_+)$
0.913 958 50	1.000 000 164 77
0.913 958 75	1.000 000 063 04
0.913 959 00	0.999 999 961 30
0.913 959 25	0.999 999 859 57

An accurate computation of the numerical value of the exceptional exponent β_* requires higher values of L and N. On a 2005 standard desktop, we have tried $L = 25$ and $N = 200$. We then obtain β_* by interpolation of $\lambda_5(K_+)$ for different closeby values of β (see table 1). The confidence on β_*, which we estimate to be about eight digits, is directly related to the level of accuracy of $\lambda_5(K_+)$. The latter is determined by inspection of convergence as L and N increase. So the bounds given in claim 1 would not qualify as a theorem but merely serve as an indication of how accurate we believe our computation is.

At this point the reader might wonder if, instead of a full three-dimensional simulation, there exists a computational strategy involving only the radial coordinate to compute both the soliton and the eigenvalues of the Birman–Schwinger operators. We believe the answer is positive but will involve significantly different ideas from the ones presented in this paper. In particular, spectral accuracy will be more difficult to obtain. We leave the problem of determining more digits of the constant β_*, likely through the use of a one-dimensional method, as a challenge to the interested reader.

Finally, the Matlab code we used to generate the figures and compute an estimation of β_* can be downloaded from http://www.acm.caltech.edu/~demanet/NLS/.

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