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Quantum Bound States in Yang–Mills–Higgs Theory

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Abstract: We give rigorous proofs of the existence of infinitely many (non-BPS) bound states for two linear operators associated with the Yang–Mills–Higgs equations at vanishing Higgs self-coupling and for gauge group $SU(2)$: the operator obtained by linearising the Yang–Mills–Higgs equations around a charge one monopole and the Laplace operator on the Atiyah–Hitchin moduli space of centred charge two monopoles. For the linearised system we use the Riesz–Galerkin approximation to compute upper bounds on the lowest 20 eigenvalues. We discuss the similarities in the spectrum of the linearised system and the Laplace operator, and interpret them in the light of electric–magnetic duality conjectures.

1. Introduction

Developments in mathematical physics over the past decades have amply demonstrated that, in order to fully understand a quantum field theory, one also needs to study the corresponding classical field theory and its solutions. The simplest case, where one quantises and studies fluctuations about the vacuum, turns out to be a rather special one; in general there are other sectors where the vacuum is replaced by non-trivial classical field configurations, often characterised by the non-vanishing of a topological invariant.

This is particularly true for gauge theories like Yang–Mills and Yang–Mills–Higgs (YMH) theories. In the latter, the non-trivial classical field configurations are non-abelian monopoles. They satisfy the non-linear YMH field equations and carry non-vanishing winding numbers which physically manifest themselves as magnetic charges.

In this paper we are interested in two spectral problems which arise in the study of fluctuations around monopole fields but which, *a priori*, are not related in any obvious way.

One of them is obtained by linearising the YMH equations around a static monopole solution. The second has its origin in a more subtle and intricate feature of the YMH system in the so-called BPS limit, where the Higgs self-coupling vanishes. In that limit there exists a whole manifold of solutions, called the moduli space, which inherits a Riemannian metric from the YMH kinetic energy functional [1]. Associated to this metric there are naturally defined linear operators like the Laplace–Beltrami, Laplace–de Rham and Dirac operators on the moduli space, with interesting spectral properties.

Examples of both sorts of problem have been studied in the physics literature, for example in the papers [2,9,21] for the YMH system linearised about a single monopole and in [10,14,22] for the Laplace–Beltrami operator on the moduli space of two centred monopoles, also called the Atiyah–Hitchin manifold. A combination of analytical and numerical methods has revealed a host of interesting spectral phenomena, including infinitely many Coulomb-like bound states and Feshbach resonances, but there are very few mathematically rigorous results in this respect.

The primary purpose of this paper is to begin to fill this gap by applying techniques of spectral analysis to the linearised YMH equation and the Atiyah–Hitchin Laplacian. We prove the existence of infinitely many bound states in both systems and give upper bounds on the eigenvalues for the linearised YMH equations. In this way we also hope to introduce two interesting problems to the spectral analysis community and, conversely, useful analytical techniques to the community of theoretical physicists interested in magnetic monopoles.

A further motivation of this paper is to exhibit the striking similarity in the spectra of two operators which superficially look very different: the linearised YMH equation is defined on Euclidean three-space while the Atiyah–Hitchin Laplacian is defined on a non-compact Riemannian four-manifold. The similarities in their spectra are probably related to electric–magnetic duality conjectures in YMH quantum field theory, but the details are far from clear. We end this extended introduction with a summary of relevant background on duality conjectures.

YMH theory involves an $SU(2)$ gauge field and a Higgs field in the adjoint representation. The symmetry is spontaneously broken to $U(1)$ either via a boundary condition on the Higgs field (in the BPS limit) or by a Higgs potential (at generic coupling). In the BPS limit and in suitable units, the perturbative particle spectrum after symmetry breaking consists of a photon, a massless Higgs scalar, and massive W-bosons with equal and opposite electric charges $n = \pm 1$.

In addition to the perturbative particles, the theory contains solitonic magnetic monopoles [18,25], labelled by an integer magnetic charge m. When allowed to evolve in time, classical magnetic monopoles may acquire electric charge, thus becoming dyons (particles with both magnetic and electric charge). After quantisation, the electric charge is characterised by another integer n so that states in quantum YMH theory fall into different sectors labelled by a pair of integer charges (m, n). A magnetic monopole belongs to the sector $(1, 0)$, a W-boson to the sector $(0, 1)$ or $(0, -1)$, the simplest dyon to the sector $(1, 1)$ and so on.

Electric–magnetic duality conjectures relate the properties of sectors with different magnetic and electric charges. In the simplest version, due to Montonen and Olive [15], a sector with label (m, n) is conjectured to be equivalent, in a suitable sense, to the sector $(n, -m)$, with electric and magnetic charge being exchanged. In the more general S-duality conjecture [24], sectors related by an $SL(2, \mathbb{Z})$ action are conjectured to be equivalent. This applies in particular to the $SL(2, \mathbb{Z})$ orbit of the W-boson sector $(0, 1)$, which includes all sectors (m, n) with co-prime integers m and n.

For various reasons, S-duality can, at best, hold in supersymmetric versions of YMH quantum field theory [17]. The evidence to support the conjecture has therefore mostly come from the consideration of BPS quantum states, whose energy can be computed exactly even with semiclassical or perturbative methods since higher order corrections vanish on account of the supersymmetry [24].

Returning to the linear spectral problems addressed in the current paper, we note that both the linear fluctuations around a monopole and eigenmodes of the Laplace operator on the moduli space are, in fact, semi-classical approximations of dyonic states in quantum YMH theory. In particular, after quantisation of an angular collective coordinate which we review in Sect. 3.1, fluctuations around a single monopole ($m = 1$) may describe states with arbitrary electric charge $n \in \mathbb{Z}$. Eigenstates of the Laplace operator on the moduli space of two monopoles ($m = 2$) may have arbitrary electric charge $n \in \mathbb{Z}$. Since $(1, n), n \in \mathbb{Z}$ and $(2, n)$, n odd, all lie on the $SL(2, \mathbb{Z})$-orbit consisting of co-prime pairs (m, n), the corresponding sectors of YMH theory are related by S-duality.

Since we are not working in an explicitly supersymmetric setting and are looking at bound states which are not of the BPS-type, we do not expect the spectra in these sectors to be related in any simple way. Nonetheless, we find striking qualitative similarities. At the end of this paper, we will discuss them in the light of duality conjectures.

The paper is organised as follows. In Sect. 2 we establish general results on a self-adjoint extension and the number of bound states of a class of second order differential operators on the half-line $0 \leq \rho < \infty$. The class of Schrödinger operators we consider contains a Calogero $(1/\rho^2)$ potential near $\rho = 0$ and a Coulombic $(1/\rho)$ tail for $\rho \to \infty$. The technical assumptions we make are designed to cover the radial operators obtained from the linearised YMH equations and the Laplace operator on the Atiyah–Hitchin manifold after separation of variables, and require a generalisation of results available in the literature. In Sect. 3 we apply our results to a channel of the linearised YMH equations previously studied in [21] and [2], and prove the existence of infinitely many bound states. By means of suitable trial functions, we give numerical upper bounds for the lowest 20 eigenvalues. In Sect. 4 we turn to the Laplace operator on the Atiyah–Hitchin manifold. Following [14] and [22] to separate radial and angular variables, we focus on three single channels of the Laplace operator. We prove the existence of infinitely many bound states in each of them, compute the eigenvalues numerically, and compare with previous numerical results in the literature. Section 5 contains a discussion of our results and our conclusions.

2. Coulombic Bound States on the Half-Line

Our strategy for showing that the linearised YMH equations around the BPS monopole and the Laplace operator on the Atiyah–Hitchin manifold have infinitely many eigenvalues is to find an orthonormal family of states with energy below the bottom of the essential spectrum. In both cases the associated Hamiltonians reduce to one-dimensional Schrödinger operators on the half-line whose potentials have, as leading terms, a combination of a Calogero and a Coulombic potential.

Schrödinger operators on the half-line have been studied extensively in the literature since they arise as the radial part of Schrödinger operators in two- or three-dimensional Euclidean space, see for example [19, Appendix to X.I]. Denoting the radial coordinate by ρ (the more conventional r is reserved for a different radial coordinate below), the identity

$$-\frac{1}{\nu^2}\partial_\rho \nu^2 \partial_\rho = \frac{1}{\nu}\left(-\partial_\rho^2 + \frac{\nu''}{\nu}\right)\nu, \tag{1}$$

for an arbitrary non-vanishing and differentiable function ν of ρ, implies that, in any dimension, one can bring the radial derivative appearing in the Laplace operator on

Euclidean space into the 'flat' form ∂_ρ^2 at the expense of introducing the effective potential ν''/ν. In the most familiar three-dimensional case, $\nu(\rho) = \rho$, and the effective potential vanishes. In two dimensions, however, $\nu(\rho) = \sqrt{\rho}$, and so the effective potential is the attractive Calogero potential $-1/4\rho^2$.

The unusual feature of the potentials we encounter in this paper is that they combine small ρ behaviour which is typical of two-dimensional problems (involving attractive Calogero potentials) with large ρ behaviour which is characteristic of three dimensions (for example a $1/\rho$ Coulombic potential and a repulsive or 'centrifugal' Calogero potential). In this section we establish the framework for studying the selfadjointness and the spectrum of Hamiltonians of this type.

We write

$$\langle f, g\rangle = \int_0^\infty f(\rho)\overline{g(\rho)}\mathrm{d}\rho$$

for the inner product of the space $L^2(0, \infty)$ and

$$\|f\| = \sqrt{\langle f, f\rangle}$$

for the corresponding norm. We are interested in potentials on the open half-line which are real continuous and have the following behaviour near 0 and ∞:

$$V(\rho) = \begin{cases} \frac{c_2}{\rho^2} + \mathrm{O}(1), & \rho \to 0, \\ C_0 + \frac{C_1}{\rho} + \mathrm{o}\left(\frac{1}{\rho}\right), & \rho \to \infty, \end{cases} \tag{2}$$

for a constant $c_2 \in \mathbb{R}$ characterising the asymptotics for small ρ and constants $C_0, C_1 \in \mathbb{R}$ characterising the asymptotics for large ρ.

Let the differential expression corresponding to the Hamiltonian be given by

$$\tilde{H} = -\frac{d^2}{d\rho^2} + V(\rho), \tag{3}$$

with domain $C_0^\infty(0, \infty)$. Then $\tilde{H}$ is a densely defined symmetric operator acting on $L^2(0, \infty)$. Below we will fix a specific selfadjoint extension of $\tilde{H}$. We begin by determining conditions on V which are sufficient to ensure that $\tilde{H}$ is semi-bounded.

Lemma 1. *Suppose the potential V in (3) can be written as $V(\rho) = \frac{c_2}{\rho^2} + W(\rho)$ where $c_2 \geq -\frac{1}{4}$ and the function $W : [0, \infty) \to \mathbb{R}$ is bounded. Then the symmetric operator $\tilde{H}$ is semi-bounded below.*

Proof. Let

$$c_{\min} = \inf_{0 \leq \rho < \infty} W(\rho) > -\infty.$$

so that

$$V(\rho) \geq \frac{c_2}{\rho^2} + c_{\min} \qquad \forall \rho > 0.$$

Consider $u \in C_0^\infty(0, \infty)$. By virtue of Hardy's inequality [4, Lemma 5.3.1], we deduce

$$\langle (\tilde{H} - c_{\min})u, u\rangle \geq \int_0^\infty \left(|u'(\rho)|^2 - \frac{|u(\rho)|^2}{4\rho^2} \right) d\rho + \int_0^\infty \frac{|u(\rho)|^2}{\rho^2} \left(\frac{1}{4} + c_2 \right) d\rho$$
$$\geq \int_0^\infty \frac{|u(\rho)|^2}{\rho^2} \left(\frac{1}{4} + c_2 \right) d\rho.$$

The condition $c_2 \geq -\frac{1}{4}$ ensures that the right hand side is non-negative. □

Remark 2. If the potential V in (3) can be written in the slightly more general form

$$V(\rho) = \frac{c_2}{\rho^2} + \frac{c_1}{\rho} + W(\rho), \qquad c_1, c_2 \in \mathbb{R},$$

with W as in Lemma 1, then the corresponding operator $\tilde{H}$ is also semi-bounded below if either $c_2 > -1/4$ and $-\infty < c_1 < \infty$ or $c_2 = -1/4$ and $c_1 \geq 0$. As we will only be concerned with the case $c_1 = 0$ in our applications below, we omit the proof of this statement, which is an elementary extension of the proof given for Lemma 1.

Let us now turn to the question of selfadjoint extensions of $\tilde{H}$. We follow [3], [11, §7.2.3], [8] and [5]. We will identify and fix such a selfadjoint extension which, depending on the parameters occurring in V particularly on c_2, may or may not be unique. Throughout we suppose that the potential satisfies the following.

Assumption 3. The potential $V : (0, \infty) \to \mathbb{R}$ can be written in terms of a continuous and bounded function $W : [0, \infty) \to \mathbb{R}$ as

$$V(\rho) = \frac{c_2}{\rho^2} + W(\rho),$$

for some constant $c_2 \geq -\frac{1}{4}$, where

1. the limit $\lim_{\rho\to\infty} W(\rho) =: C_0$ exists and
2. $\int_1^\infty (W(\rho) - C_0)^2 d\rho < \infty$.

We now set

$$c_2 = m^2 - \frac{1}{4}, \quad m \geq 0, \tag{4}$$

and denote the Hamiltonian which comprises the leading term of $\tilde{H}$ for small ρ by

$$\tilde{H}_0 = -\frac{d^2}{d\rho^2} + \frac{m^2 - \frac{1}{4}}{\rho^2}, \quad m \geq 0,$$

in the same domain $C_0^\infty(0, \infty)$. Then, $\tilde{H}_0$ is essentially selfadjoint for $m \geq 1$ and has deficiency indices $(1, 1)$ for $0 \leq m < 1$. We briefly review the reason for this and explain why one of the extensions for $0 \leq m < 1$ is natural in the present context.

As already mentioned after (1), the differential operator $\tilde{H}_0$ arises as the radial part of the Laplacian on the two-dimensional Euclidean space $\mathbb{R}^2$. For Cartesian coordinates

(x_1, x_2), and polar coordinates $\rho = \sqrt{x_1^2 + x_2^2} \in (0, \infty)$ and $\varphi \in [0, 2\pi)$, we explicitly have

$$\Delta = \frac{\partial_1^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} = \frac{1}{\rho}\partial_\rho \rho \partial_\rho + \frac{1}{\rho^2}\partial_\varphi^2.$$

Therefore, solving $-\Delta\psi = 0$ with the ansatz

$$\psi = u(\rho)e^{im\varphi} \tag{5}$$

leads to the radial equation

$$-\frac{1}{\rho}\left(\rho u'\right)' + \frac{m^2}{\rho^2}u = 0.$$

Here m has to be an integer for (5) to be a single-valued function, but this does not affect the essence of the following argument and we will continue to assume that m is a non-negative real number. The identity (1) shows that the new radial function

$$\eta(\rho) = \sqrt{\rho}u(\rho) \tag{6}$$

then satisfies

$$\tilde{H}_0\eta = 0.$$

A basis of solutions for this equation is given by

$$\begin{aligned} \eta_1(\rho) = \rho^{\frac{1}{2}},\ \eta_2(\rho) = \rho^{\frac{1}{2}}\ln(\rho) \qquad &\text{if} \quad m = 0, \\ \eta_1(\rho) = \rho^{\frac{1}{2}+m},\ \eta_2(\rho) = \rho^{\frac{1}{2}-m} \qquad &\text{if} \quad m > 0. \end{aligned} \tag{7}$$

When $m \geq 1$ only one of these solutions is square integrable with respect to $d\rho$ near $\rho = 0$, and so $\rho = 0$ is a limit point for $\tilde{H}_0$ in that case.

When $0 \leq m < 1$, however, both η_1 and η_2 are square integrable with respect to $d\rho$ near $\rho = 0$, so that $\rho = 0$ is a limit circle for the differential expression $\tilde{H}_0$, and an additional boundary condition is required. Both functions u obtained from the fundamental solutions (7) via (6) in this case are square integrable with respect to the radial measure $\rho d\rho$ on $\mathbb{R}^2$, but $u_2(\rho) = \eta_2(\rho)/\sqrt{\rho}$ is singular at $\rho = 0$ and does not lie in the domain of the Laplacian. Thus, the requirement that solutions are in the domain of Δ naturally provides the boundary condition that we set below.

Due to the asymptotic behaviour of the potential, $\rho = \infty$ is a limit point for all values of m. We thus fix a selfadjoint extension of $\tilde{H}_0$ as follows. Let $\zeta \in C^\infty([0, \infty))$ be such that $\zeta(\rho) = 1$ for $\rho \leq 1$ and $\zeta(\rho) = 0$ for $\rho \geq 2$ and set $\zeta_m(\rho) = \zeta(\rho)\rho^{\frac{1}{2}+m}$. Let $\overline{\tilde{H}_0}$ be the closure of the operator $\tilde{H}_0$, the minimal operator associated to $\tilde{H}_0$, and let

$$\mathscr{D} = \mathrm{D}\left(\overline{\tilde{H}_0}\right) + \mathbb{C}\zeta_m. \tag{8}$$

We define H_0 to be the extension of $\tilde{H}_0$ with domain $\mathrm{D}(H_0) = \mathscr{D}$. By virtue of [3, Prop. 4.17], H_0 is selfadjoint. Moreover $\mathrm{D}(H_0) = \mathrm{D}\left(\overline{\tilde{H}_0}\right)$ if and only if $m \geq 1$, and in this case $\tilde{H}_0$ is essentially selfadjoint.

Lemma 4. *Suppose the potential V satisfies the conditions of the Assumption 3. Then the potential $W(\rho) - C_0$ is relatively compact with respect to H_0.*

Proof. Let

$$J_m(\rho) = \sum_{j=0}^{\infty} \frac{(-1)^j (\rho/2)^{2j+m}}{j!\Gamma(j+m+1)}$$

be the Bessel function of the first kind. Let

$$I_m(\rho) = i^{-m} J_m(i\rho),$$
$$K_m(\rho) = \begin{cases} \frac{\pi}{2} \frac{I_{-m}(\rho) - I_m(\rho)}{\sin(m\pi)}, & m \neq 0, 1, \dots \\ \frac{(-1)^{m-1}}{2} \left(\frac{\partial I_\nu(\rho)}{\partial \nu}\Big|_{\nu=m} + \frac{\partial I_\nu(\rho)}{\partial \nu}\Big|_{\nu=-m} \right), & m = 0, 1, \dots \end{cases}$$

be the modified Bessel functions. Then the resolvent $(H_0 + 1)^{-1}$ is given by the Green's function [3, §4.2]

$$G_m(\rho, \sigma) = \sqrt{\rho\sigma}\, I_m(\min\{\rho, \sigma\}) K_m(\max\{\rho, \sigma\}).$$

Decompose

$$G_m(\rho, \sigma) = \sum_{k=1}^{4} G_m^k(\rho, \sigma),$$

where

$$G_m^1(\rho, \sigma) = G_m(\rho, \sigma) \mathbb{1}_{(0,1]}(\rho) \mathbb{1}_{(0,1]}(\sigma),$$
$$G_m^2(\rho, \sigma) = G_m(\rho, \sigma) \mathbb{1}_{(0,1]}(\rho) \mathbb{1}_{(1,\infty)}(\sigma),$$
$$G_m^3(\rho, \sigma) = G_m(\rho, \sigma) \mathbb{1}_{(1,\infty)}(\rho) \mathbb{1}_{(0,1]}(\sigma),$$
$$G_m^4(\rho, \sigma) = G_m(\rho, \sigma) \mathbb{1}_{(1,\infty)}(\rho) \mathbb{1}_{(1,\infty)}(\sigma).$$

Then [3, (4.10)]

$$|G_m^1(\rho, \sigma)| \leq \begin{cases} a_{10} (\min\{\rho, \sigma\})^{\frac{1}{2}} |\ln(\max\{\rho, \sigma\})|, & m = 0, \\ a_{1m} (\min\{\rho, \sigma\})^{\frac{1}{2}+m} (\max\{\rho, \sigma\})^{\frac{1}{2}-m}, & m > 0, \end{cases}$$
$$|G_m^2(\rho, \sigma)| \leq a_{2m} \rho^{\frac{1}{2}+m} e^{-\sigma} \mathbb{1}_{(0,1]}(\rho) \mathbb{1}_{(1,\infty)}(\sigma),$$
$$|G_m^3(\rho, \sigma)| \leq a_{3m} e^{-\rho} \sigma^{\frac{1}{2}+m} \mathbb{1}_{(1,\infty)}(\rho) \mathbb{1}_{(0,1]}(\sigma),$$
$$|G_m^4(\rho, \sigma)| \leq a_{4m} e^{-|\rho-\sigma|} \mathbb{1}_{(1,\infty)}(\rho) \mathbb{1}_{(1,\infty)}(\sigma),$$

where $a_{im} > 0$ are constants depending on m.

Let

$$\mathscr{I}_k = \int_0^\infty \int_0^\infty |(W(\rho) - C_0) G_m^k(\rho, \sigma)|^2 d\rho d\sigma,$$

so that

$$\int_0^\infty \int_0^\infty |(W(\rho) - C_0)G_m(\rho, \sigma)|^2 d\rho d\sigma = \sum_{k=1}^{4} \mathscr{I}_k.$$

Then

$$\mathscr{I}_2 \le a_{2m}^2 \int_0^1 |W(\rho) - C_0|^2 \rho^{1+2m} d\rho \int_1^\infty e^{-2\sigma} d\sigma < \infty,$$

since W is continuous on $[0, \infty)$. The square integrability of $W - C_0$ on $[1, \infty)$ ensures that

$$\mathscr{I}_3 \le a_{3m}^2 \int_0^1 \sigma^{1+2m} d\sigma \int_1^\infty |W(\rho) - C_0|^2 e^{-2\rho} d\rho < \infty,$$

and

$$\begin{aligned}
\mathscr{I}_4 &\le a_{4m}^2 \int_1^\infty \int_1^\infty |W(\rho) - C_0|^2 e^{-2|\rho-\sigma|} d\sigma d\rho \\
&= a_{4m}^2 \int_1^\infty |W(\rho) - C_0|^2 \left(e^{-2\rho} \int_1^\rho e^{2\sigma} d\sigma + e^{2\rho} \int_\rho^\infty e^{-2\sigma} d\sigma \right) d\rho \\
&\le a_{4m}^2 \int_1^\infty |W(\rho) - C_0|^2 d\rho < \infty.
\end{aligned}$$

Finally, using $|W(\rho) - C_0|^2 < B$ for $\rho \in [0, 1]$ and some positive real number B, we consider the term for $k = 1$. If $m > 0$ we have

$$\begin{aligned}
\mathscr{I}_1 &\le a_{1m}^2 \int_0^1 |W(\rho) - C_0|^2 \left(\rho^{1-2m} \int_0^\rho \sigma^{1+2m} d\sigma + \rho^{1+2m} \int_\rho^1 \sigma^{1-2m} d\sigma \right) d\rho \\
&\le a_{1m}^2 B \int_0^1 \left(\rho^{1-2m} \int_0^\rho \sigma^{1+2m} d\sigma + \rho^{1+2m} \int_\rho^1 \sigma^{1-2m} d\sigma \right) d\rho \\
&= \frac{a_{1m}^2 B}{4(m+1)}.
\end{aligned}$$

The computation of the integral in the last step is elementary, but has to be carried out separately for the case $m = 1$. However, the answer agrees with the general formula given above. If $m = 0$ we have

$$\begin{aligned}
\mathscr{I}_1 &\le a_{10}^2 \int_0^1 |W(\rho) - C_0|^2 \left(\ln^2(\rho) \int_0^\rho \sigma d\sigma + \rho \int_\rho^1 \ln^2(\sigma) d\sigma \right) d\rho \\
&\le a_{10}^2 B \int_0^1 \left(-\frac{1}{2}\rho^2 \ln^2(\rho) + 2\rho^2 \ln(\rho) + 2\rho - 2\rho^2 \right) d\rho \\
&= \frac{2a_{10}^2 B}{27},
\end{aligned}$$

where we have again omitted steps in an elementary integration.

Summing up, for $m \geq 0$ we have $\mathscr{I}_k < \infty$ under the assumptions of the lemma. Therefore, the operator

$$(W - C_0)(H_0 + 1)^{-1}$$

is Hilbert–Schmidt and hence compact. This ensures that indeed $W - C_0$ is relatively compact with respect to H_0. □

Definition 5. With $\tilde{H}$ of the form (3) and V satisfying the Assumption 3, we denote by H the extension of the operator $\tilde{H}$ to the domain $\mathrm{D}(H) = \mathscr{D}$ defined in (8).

By virtue of [20, Corollary 2 to Theorem XIII.14], H is always selfadjoint. Moreover, H is semi-bounded below and

$$\sigma_{\mathrm{ess}}(H) = [C_0, \infty).$$

We now establish conditions for H to have infinitely many bound states.

Theorem 6. *If Assumption 3 is satisfied, and moreover V has the asymptotic expansion*

$$V(\rho) = C_0 + \frac{C_1}{\rho} + o\left(\frac{1}{\rho}\right), \quad \textit{for} \quad \rho \to \infty,$$

with $C_1 < 0$, then H has infinitely many eigenvalues below C_0.

Proof. We use a similar argument to the one considered in [12, § 8.3]. By assumption, we can write the potential as

$$V(\rho) = C_0 + \frac{C_1 + f(\rho)}{\rho},$$

in terms of a continuous function f on $(0, \infty)$ satisfying

$$\lim_{\rho \to \infty} f(\rho) = 0.$$

We pick a $u \in C_0^\infty(0, \infty)$, such that $\mathrm{supp}(u) \subset (1, 2)$ and $\|u\| = 1$, and set

$$u_n(\rho) = 2^{-n/2} u(2^{-n}\rho), \qquad n = 0, 1, \ldots .$$

Then the u_n have non-overlapping support and satisfy the orthonormality condition

$$\langle u_n, u_m \rangle = \delta_{mn}.$$

Changing variables to $\sigma = 2^{-n}\rho$, we calculate

$$\begin{aligned} \langle (H - C_0) u_n, u_n \rangle &= \int_{2^n}^{2^{n+1}} \left(\left| \frac{du_n}{d\rho}(\rho) \right|^2 + \frac{C_1 + f(\rho)}{\rho} |u_n(\rho)|^2 \right) d\rho \\ &= 2^{-2n} \int_1^2 |u'(\sigma)|^2 d\sigma + 2^{-n} \int_1^2 \frac{C_1 + f(2^n\sigma)}{\sigma} |u(\sigma)|^2 d\sigma. \end{aligned} \tag{9}$$

Now we can pick n_0 so that, for all $\sigma \in [1, 2]$ and $n > n_0$, we have $|f(2^n\sigma)| < C_1$. If $C_1 < 0$, it follows that

$$\int_1^2 \frac{C_1 + f(2^n\sigma)}{\sigma}|u(\sigma)|^2 d\sigma < 0 \quad \text{for } n > n_0.$$

Thus, the last line of (9) is a sum of a positive and a negative term when $C_1 < 0$, $n > n_0$. Since the positive term decreases with n faster than the negative term, we can make the sum negative by choosing n big enough. Then $\langle (H - C_0)u_n, u_n\rangle < 0$ and therefore $\langle Hu_n, u_n\rangle$ lies below the essential spectrum for sufficiently large n. This is enough to ensure that we have an infinite number of negative eigenvalues as a consequence of the Rayleigh–Ritz principle, cf. [12, §8.3]. □

3. Bound States in the Linearised YMH Equations

3.1. BPS monopoles and dyons. The first example of a Schrödinger operator on the half-line to which we apply the results of the previous section arises in YMH theory in 3+1 dimensional Minkowski space. Our main reference for the derivation of this Schrödinger operator is the paper [21], to which we refer for details and background.

The YMH model consists of a non-abelian gauge potential $A = A_0 dt + A_1 dx_1 + A_2 dx_2 + A_3 dx_3$ coupled to a Higgs field ϕ, both taking values in the Lie algebra $su(2)$. Writing $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$, and $\partial_i = \partial/\partial x_i$, $i = 1, 2, 3$, we only require the spatial covariant derivatives $D_i = \partial_i + e[A_i, \cdot]$ and the spatial components of the Yang–Mills field strength tensor $F_{ij} = \partial_i A_j - \partial_j A_i + e\left[A_i, A_j\right]$, where $[\cdot, \cdot]$ is the Lie algebra commutator, e is the Yang–Mills coupling constant and $i, j = 1, 2, 3$.

In the following we set the coupling constant e to one and consider a particular limit of the theory, called the BPS limit, where the self-coupling of the Higgs field vanishes. In that limit, the second order static YMH equations are implied by the first order BPS equations

$$D_i\phi = \frac{1}{2}\epsilon_{ijk}F_{jk},$$

where $i, j, k = 1, 2, 3$ and repeated indices are summed over.

In terms of the a basis t_1, t_2, t_3 of the $su(2)$ Lie algebra satisfying $[t_i, t_j] = \epsilon_{ijk}t_k$, a particular solution of the BPS equations is the spherically symmetric BPS monopole:

$$A_i(\mathbf{x}) = \left(\frac{1}{r^2} - \frac{1}{r\sinh(r)}\right)(\mathbf{x} \times \mathbf{t})_i, \quad \phi(\mathbf{x}) = \frac{1 - r\coth(r)}{r^2}\mathbf{x} \cdot \mathbf{t}, \tag{10}$$

where $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$ and we have denoted Euclidean vectors by bold letters. The invariance of the BPS equations under Euclidean symmetries implies that translating this solution in space gives an $\mathbb{R}^3$ worth of solutions. Gauge invariance of the equations means that $SU(2)$ gauge transformations map solutions to solutions. In gauge theories, solutions related by gauge transformations which are the identity at infinity are generally considered equivalent, but gauge transformations which are non-trivial at infinity may have a physical significance. Such gauge transformations are often called 'large', and will play a role in the interpretation of our results. We therefore review them briefly.

As discussed and explained in [10], for monopoles in $SU(2)$ YMH theory, there is essentially a circle of large gauge transformations, generated by the Higgs field itself and parameterised by an angle $\chi \in [0, 2\pi)$:

$$g_\chi(\mathbf{x}) = \exp(\chi\phi(\mathbf{x})). \tag{11}$$

Note that, for large r, $\phi(\mathbf{x}) \approx -\hat{\mathbf{x}}$, so that $g_\chi(\mathbf{x})$ is asymptotically a rotation about $\mathbf{x}$. Acting with translations and the large gauge transformations (11), and dividing out by small gauge transformations yields the moduli space of monopoles of magnetic charge one:

$$M_1 = \mathbb{R}^3 \times S^1. \tag{12}$$

The physical significance of the angular variable χ on S^1 becomes manifest when it varies in time. The monopole then acquires an electric charge proportional to the angular speed $\dot{\chi}$, thus turning into a dyon. Quantum states are given by wave functions on the moduli space [10]. A wave function of the form $\exp(in\chi)$, with $n \in \mathbb{Z}$ describes a dyon of electric charge n.

3.2. Linearising around the BPS monopole. The Schrödinger operator we would like to study is obtained by linearising the general, time-dependent YMH equations around the static configuration (10). The stationary ansatz

$$A_i(t, \mathbf{x}) = A_i(\mathbf{x}) + a_i(\mathbf{x})e^{i\omega t}, \qquad \phi(t, \mathbf{x}) = \phi(\mathbf{x}) + \varphi(\mathbf{x})e^{i\omega t},$$

considered in [21], leads to the following coupled partial differential equations on Euclidean $\mathbb{R}^3$:

$$\begin{aligned} &D_i D_i \varphi + [a_i, D_i\phi] + D_i [a_i, \phi] = -\omega^2\varphi, \\ &D_i D_i a_j - D_i D_j a_i + [a_i, F_{ij}] = [\phi, D_j\varphi] + [\varphi, D_j\phi] + [\phi, [a_j, \phi]] - \omega^2 a_j. \end{aligned}$$

Exploiting the (suitably defined) rotational symmetry of the BPS monopole and focusing on the vanishing total angular momentum, the ansatz

$$\varphi(\mathbf{x}) = 0, \quad a_i(\mathbf{x}) = \frac{1}{r}\left(v(r)((\hat{\mathbf{x}} \cdot \mathbf{t})\hat{x}_i - t_i) + \sqrt{2}\alpha(r)(\hat{\mathbf{x}} \cdot \mathbf{t})\hat{x}_i\right), \tag{13}$$

involving two unknown functions of the radial coordinate r, leads to the following set of ordinary differential equations

$$\begin{aligned} \left(-\frac{d^2}{dr^2} + \frac{3}{\sinh^2(r)} - \frac{2\coth(r)}{r} + \coth^2(r)\right) v + \frac{2\sqrt{2}\coth(r)}{\sinh(r)}\alpha = \omega^2 v, \\ \left(-\frac{d^2}{dr^2} + \frac{2}{\sinh^2(r)} + \frac{2}{r^2}\right)\alpha + \frac{2\sqrt{2}\coth(r)}{\sinh(r)} v = \omega^2\alpha. \end{aligned} \tag{14}$$

As explained in [21], this system of equations can be decoupled when $\omega \neq 0$, and brought into the form

$$\left(-\frac{d^2}{dr^2}+\frac{1}{\sinh^2(r)}+\frac{2}{r^2}-\frac{2\coth(r)}{r}+\coth^2(r)\right)\xi=\omega^2\xi,$$
$$\left(-\frac{d^2}{dr^2}+\frac{2}{\sinh^2(r)}\right)\zeta=\omega^2\zeta, \tag{15}$$

via the (invertible) transformation

$$\omega\alpha=\frac{d\zeta}{dr}-\frac{\zeta}{r}+\frac{\sqrt{2}}{\sinh(r)}\xi,$$
$$\omega v=-\frac{d\xi}{dr}-\frac{1-r\coth(r)}{r}\xi-\frac{\sqrt{2}}{\sinh(r)}\zeta, \tag{16}$$

provided $\omega\neq 0$. We note that the equations (14) also have a zero-energy solution which can easily be given explicitly, see e.g. [21]. Since $\omega=0$ for this solution, it cannot be obtained from solutions of the system (15) which we study here.

As also explained in [21], the equation for ζ does not have bound states, and moreover gauge invariance requires that $\zeta=0$. Therefore, we focus on the equation for ξ, which is a Sturm–Liouville problem for the Schrödinger operator

$$\tilde{H}_{\text{YMH}}=-\frac{d^2}{dr^2}+V_{\text{YMH}} \tag{17}$$

with the potential

$$V_{\text{YMH}}(r)=\frac{1}{\sinh^2(r)}+\frac{2}{r^2}-\frac{2\coth(r)}{r}+\coth^2(r).$$

This potential has the asymptotic expansion

$$V_{\text{YMH}}(r)=\begin{cases}\frac{2}{r^2}+\mathrm{O}(1), & r\to 0,\\ 1-\frac{2}{r}+\frac{2}{r^2}+\mathrm{O}\left(\frac{1}{r^3}\right), & r\to\infty,\end{cases}$$

so, in particular, is of the form (2) with $c_2=2$, $C_0=1$ and $C_1=-2$. It is easy to check that it satisfies the assumptions of Theorem 6 (and *a fortiori* those of Lemmas 1 and 4). As $m=3/2>1$ in (4), we have the following result.

Corollary 7. *The closure H_{YMH} of $\tilde{H}_{\text{YMH}}$ acting on $L^2(0,\infty)$ is selfadjoint, its essential spectrum is the segment* $[1,\infty)$ *and it has infinitely many eigenvalues below* 1.

The infinitely many eigenstates of the Schrödinger operator (17) define radially symmetric fluctuations around the BPS monopole via substitution into the equations (16) and (13). They therefore belong to the sector with magnetic change $m=1$. However, as explained in [21], the fluctuations do not have well defined electric charge.

To obtain eigenstates of the electric charge operators, one needs to include the collective angular coordinate χ for large gauge transformations (11) in the discussion. These gauge transformations act on the underlying BPS monopoles (10) but also, by conjugation, on the fluctuations (13), rotating them to $\varphi(\mathbf{x})_\chi=0$ and

$$a_i(\mathbf{x})_\chi = \left(\frac{v(r)+\sqrt{2}\alpha(r)}{r}\right)(\hat{\mathbf{x}}\cdot\mathbf{t})\hat{x}_i + \cos(\chi|\phi|(\hat{\mathbf{x}}))\left(\frac{v(r)}{r}\right)((\hat{\mathbf{x}}\cdot\mathbf{t})\hat{x}_i - t_i)$$
$$+ \sin(\chi|\phi(\hat{\mathbf{x}})|)(\mathbf{t}\times\hat{\mathbf{x}})_i.$$

Quantum states of definite electric charge are obtained by taking superpositions of these states, weighted with the dyonic wave function $\exp(in\chi)$. This is essentially a Fourier transform from the angular variable χ to the integer label n, and entirely analogous to the standard interpretation of the moduli space wave functions, which describe superpositions of BPS monopoles. The electric charge n is arbitrary, so we replicate the infinitely many eigenstates of the Schrödinger operator (17) in each of the dyonic sectors $(1, n)$, $n \in \mathbb{Z}$.

3.3. Upper bounds on the eigenvalues. Having shown that H_{YMH} has infinitely many negative eigenvalues we would like to find good numerical approximations to the first few of them, improving on previous numerical work in [2] and [21] which relied on shooting methods. For this purpose, we employ the Riesz–Galerkin method with a basis which exploits the fact that the potential V_{YMH} approaches at infinity the potential

$$V_C(r) = \frac{\alpha}{r} + \frac{l(l+1)}{r^2} + 1,$$

which combines a Coulomb potential with a centrifugal potential for orbital angular momentum quantum number l. In order to match the asymptotic form of V_{YMH} we pick $\alpha = -2$ and $l = 1$, so that

$$V_{\text{YMH}}(r) = V_C(r) + \left(\frac{1+\cosh^2(r)}{\sinh^2(r)} + \frac{2-2\coth(r)}{r}\right).$$

The eigenfunctions of the radial Coulomb Hamiltonian with differential expression

$$H_C = -\frac{d^2}{dr^2} + V_C$$

are well-known. They are defined in terms of the associated Laguerre polynomial $L_k^N(r)$

$$L_k^N(r) = (-1)^N \frac{d^N}{dr^N} L_{k+N}(r)$$

where $L_k(r) = e^r \frac{d^k}{dr^k}\left(r^k e^{-r}\right)$ is the k-th Laguerre polynomial. The eigenfunctions of H_C with $l = 1$ and $\alpha = -2$, satisfying

$$H_C\xi_n = E_n\xi_n, \qquad E_n = -\frac{1}{n^2}, \tag{18}$$

are

$$\xi_n(r) = N_n^{-1/2} r^2 e^{-\frac{r}{n}} L_{n-2}^3\left(\frac{2r}{n}\right).$$

Here N_n is a normalisation constant ensuring $\|\xi_n\| = 1$ and the principal quantum number takes the values $n = 2, 3, \ldots$.

Table 1. The values of λ_n for $\mathfrak{d} = 20$, the extrapolated values for $\mathfrak{d} = 1000$ and the approximation based on (18)

n	λ_n for basis $\mathfrak{d} = 20$	Extrapolated value of λ_n for $\mathfrak{d} = 1000$	Coulomb approximation of $1 - \frac{1}{(n+1)^2}$
1	0.773243	0.772215	0.750000
2	0.897117	0.896315	0.888889
3	0.941347	0.940714	0.937500
4	0.962124	0.961609	0.960000
5	0.973529	0.973099	0.972222
6	0.980458	0.980094	0.979592
7	0.984983	0.984669	0.984375
8	0.988100	0.987825	0.987654
9	0.990179	0.990096	0.990000
10	0.990339	0.991761	0.991736
11	0.993265	0.993174	0.993056

The set $\{\xi_n\}_{n=2}^{\infty}$ is an orthonormal basis for $L^2(0,\infty)$. In order to implement the Riesz–Galerkin method, we pick a finite-dimensional subspace

$$\mathrm{Span}\{\tilde{b}_n\}_{n=1}^{\mathfrak{d}} \subset \mathrm{D}(H)$$

of dimension $\mathfrak{d}$, where

$$\tilde{b}_n(r) = N_{n+1}^{1/2}\xi_{n+1}(r) = \left(\sum_{p=0}^{n-1} d_p^{n+1} r^{p+2}\right) e^{-\frac{r}{n+1}} \tag{19}$$

for suitable coefficients $d_p^{n+1} \in \mathbb{R}$. We then compute the mass matrix

$$M = [M(i,j)]_{i,j=1}^{\mathfrak{d}} = \mathrm{diag}(N_2, \ldots, N_{\mathfrak{d}}), \qquad M(i,j) = \int_0^\infty \tilde{b}_i(r)\tilde{b}_j(r)dr,$$

and the stiffness matrix

$$S = [S(i,j)]_{i,j=1}^{\mathfrak{d}}, \qquad S(i,j) = \int_0^\infty H_{\text{YMH}}\tilde{b}_i(r)\tilde{b}_j(r)dr. \tag{20}$$

According to the Rayleigh–Ritz principle, the kth negative eigenvalue of $S\underline{u} = \nu M\underline{u}$ is an upper bound for the kth negative eigenvalue of H_{YMH}. Further details on the computation of the entries of S are given in "Appendix" A.

For a basis of dimension $\mathfrak{d} = 20$ we obtain the results shown in Table 1 for the first eleven eigenvalues. We saw convergence of our computations up to single precision as we increased the size of $\mathfrak{d}$ from 1 to 20. Additionally, we have the extrapolated results obtained for the first eleven eigenvalues for a basis of dimension $\mathfrak{d} = 1000$ via linear interpolation. In [21], approximation to these eigenvalues were found via a shooting method and they appear to be below those found in Table 1. There is no guarantee that the former are above the true eigenvalues of H_{YMH}, whereas the latter certainly are, due to the Rayleigh–Ritz principle.

4. The Laplace Operator on the Moduli Space of Two Monopoles

4.1. The Atiyah–Hitchin metric and its asymptotic forms. The BPS monopole (10) and the moduli space (12) of charge one magnetic monopoles have remarkable generalisations for higher magnetic charges. Following the discovery of the charge one solution, there was rapid progress in constructing various solutions of higher magnetic charge. It is now well-understood that, for given magnetic charge k, there is in fact a $4k$-dimensional family of static monopole solutions which constitute the so-called moduli space of charge k monopoles [1].

The basic, physical reason for the existence of so many static solutions is that, in the BPS limit, monopoles do not exert any forces on each other so that they can be 'superimposed' with arbitrary values of the individual positions and phases. The interpretation of the $4k$ parameters in the moduli space as giving the positions and phases of k monopoles works well for well-separated monopoles. However, when the monopoles are close together they deform each other and become bound states with a rich and complicated geometry. All of this is captured by the moduli spaces.

The moduli spaces inherit a Riemannian metric from the kinetic energy functional of YMH theory. It was first argued by Manton in [13] that geodesic motion on the moduli space, equipped with this metric, is a good approximation to the dynamics of monopoles, provided they are moving sufficiently slowly. This is essentially an adiabatic approximation, where the time evolution is via a sequence of static equilibrium configurations. It was subsequently shown by Atiyah and Hitchin [1] that the moduli space metric is hyperkähler. Combined with symmetry considerations, this is sufficient to determine the moduli space metric for monopoles of charge two. In that case, the moduli space is eight dimensional, and has the form

$$M_2 = \mathbb{R}^3 \times \frac{M_2^0 \times S^1}{\mathbb{Z}_2}. \tag{21}$$

The $\mathbb{R}^3$- and S^1- factors describe the centre-of-mass motion of the two monopoles and carry flat metrics. The manifold M_2^0 describes the interesting, relative motion of the two monopoles, and we refer to it as the Atiyah–Hitchin manifold in the following. However, the reader should be aware that some authors reserve this name for the quotient $M_2^0/\mathbb{Z}_2$. The manifold M_2^0 is simply-connected and homotopic to a 2-sphere. The metric on M_2^0 is also hyperkähler. In four dimensions, the hyperkähler property is equivalent to self-duality of the Riemann tensor so that the Atiyah–Hitchin manifold is an example of a gravitational instanton.

The group $SO(3)$ of spatial rotations is a symmetry group of YMH theory and acts isometrically on the Atiyah–Hitchin manifold. Therefore, it is convenient to parametrise the Atiyah–Hitchin manifold in terms of this $SO(3)$ action and one transverse radial or 'shape' coordinate. The latter parametrises a 1-parameter family of two-monopole configurations which includes two well-separated monopoles where the shape parameter is simply the distance between the two monopoles. However, when the two monopoles get close, they deform each other until they coalesce to a doughnut-shaped configuration. The $SO(3)$ orbits are generically isomorphic to $SO(3)/\mathbb{Z}_2$, but the orbit of the doughnut-shaped configuration is exceptional and isomorphic to S^2, called the core in the following.

The metric on the Atiyah–Hitchin manifold M_2^0 is most conveniently written in terms of left-invariant 1-forms σ_1, σ_2 and σ_3 on $SO(3)$, see [10] for details. Denoting the transverse coordinate by r, the metric takes the Bianchi IX form

$$ds^2 = f^2 dr^2 + a^2\sigma_1^2 + b^2\sigma_2^2 + c^2\sigma_3^2,$$

where f, a, b and c are functions of r. The self-duality of the metric implies

$$\frac{2bc}{f}\frac{da}{dr} = (b-c)^2 - a^2, \tag{22}$$

and two other related equations obtained by cyclic permutation of a, b, c. The function f can be chosen to fix the radial coordinate r. Following [10], we pick

$$f = -\frac{b}{r}.$$

The initial conditions for the coefficient functions are

$$a(\pi) = 0, \quad b(\pi) = \pi, \quad c(\pi) = -\pi.$$

The unique solution with these initial conditions can be written in terms of elliptic functions as follows. Let

$$r = 2K\left(\sin\frac{\beta}{2}\right), \qquad 0 \le \beta \le \pi, \tag{23}$$

where K is the elliptic integral

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{d\tau}{\sqrt{1-k^2\sin^2\tau}}.$$

With

$$w_1 = bc, \quad w_2 = ca, \quad w_3 = ab, \tag{24}$$

the solution is then given by

$$\begin{aligned} w_1(r) &= -\sin\beta\, r\frac{dr}{d\beta} - \frac{1}{2}(1+\cos\beta)r^2, \\ w_2(r) &= -\sin\beta\, r\frac{dr}{d\beta}, \\ w_3(r) &= -\sin\beta\, r\frac{dr}{d\beta} + \frac{1}{2}(1-\cos\beta)r^2. \end{aligned} \tag{25}$$

It turns out that $b > a > 0$ away from the core, and that c is negative (in fact, $c < -2$). Defining a proper radial distance coordinate R via

$$R(r) = \int_\pi^r -f(\rho)\,d\rho = \int_\pi^r \frac{b(\rho)}{\rho}\,d\rho, \tag{26}$$

we have the following behaviour near the core

$$R = (r-\pi) + \mathrm{O}\left((r-\pi)^2\right).$$

This allows us to deduce expansions for the coefficient functions of the Atiyah–Hitchin metric [10,22]:

$$a(r(R)) = 2R + \mathrm{O}\left(R^2\right), \quad b(r(R)) = \pi + \frac{1}{2}R + \mathrm{O}\left(R^2\right), \quad c(r(R)) = -\pi + \frac{1}{2}R + \mathrm{O}\left(R^2\right). \tag{27}$$

For large r, the coefficient functions a, b and c can be approximated by the functions a_{TN}, b_{TN} and c_{TN} given by

$$a_{\text{TN}}(r) = b_{\text{TN}}(r) = r\sqrt{1 - \frac{2}{r}}, \qquad c_{\text{TN}}(r) = -\frac{2}{\sqrt{1 - \frac{2}{r}}}. \tag{28}$$

Theses functions are exact solutions of the self-duality equations (22), and give rise to another hyperkähler metric, called the Taub-NUT metric with negative 'mass' parameter. This metric has $U(2)$ rather than $SO(3)$ symmetry. In the form given above, the metric is degenerate at $r = 2$ and changes signature form $(+, +, +, +)$ to $(-, -, -, -)$ as one crosses from $r > 2$ to $r < 2$. For later use, we note that, as explained in [10], it follows from (24) and (25) that

$$\begin{aligned} a(r) &= a_{\text{TN}}(r) + \mathrm{O}\left(r^2 e^{-r}\right), \\ b(r) &= b_{\text{TN}}(r) + \mathrm{O}\left(r^2 e^{-r}\right), \\ c(r) &= c_{\text{TN}}(r) + \mathrm{O}\left(e^{-2r} p(r)\right), \end{aligned} \tag{29}$$

where p is an algebraic function of r.

In our study of the spectrum of the Laplace operator on the Atiyah–Hitchin manifold we need the asymptotics of a, b and c both as a function of r and as a function of the proper radial distance R. Substituting the asymptotic expressions (28) into the definition (26) one finds (see also [22]) that

$$R(r) = r + \ln r + \mathrm{O}(1). \tag{30}$$

4.2. The Laplace operator on the Atiyah–Hitchin manifold. One may approximate the quantum mechanics of k interacting monopoles at low energy by solving the Schrödinger equation on the moduli space of charge k monopoles, taking the covariant Laplace operator associated to the Riemannian metric as the Hamiltonian. For details of this programme we refer the reader to [10], where it is explained and applied to the asymptotic form of the manifold M_2^0, and to [22] where bound states and scattering states on M_2^0 are discussed in detail, using a combination of numerical and semiclassical techniques.

The wave function for a two-monopole quantum state is a $\mathbb{C}$-valued function on the moduli space (21). However, assuming without loss of generality that we work in the centre-of-mass frame of the two monopoles we can neglect the dependence on $\mathbb{R}^3$. Introducing an angular coordinate $\chi \in [0, 2\pi)$ on S^1, the Hamiltonian is then

$$H = -\frac{\hbar^2}{16\pi}\frac{\partial^2}{\partial \chi^2} - \frac{\hbar^2}{4\pi}\Delta_{\text{AH}},$$

where Δ_{AH} is the covariant Laplace operator on M_2^0. It can be written in terms of the left-invariant (and right-generated) vector fields ξ_1, ξ_2 and ξ_3 on $SO(3)$ which are dual to the forms σ_1, σ_2 and σ_3 (see again [10] for details). Then

$$\Delta_{\text{AH}} = \frac{1}{abcf}\frac{\partial}{\partial r}\left(\frac{abc}{f}\frac{\partial}{\partial r}\right) + \frac{\xi_1^2}{a^2} + \frac{\xi_2^2}{b^2} + \frac{\xi_3^2}{c^2}.$$

Assuming without loss of generality a harmonic dependence of the wave function on the angular coordinate χ, the stationary Schrödinger equation is

$$H(e^{iS\chi}\Phi) = Ee^{iS\chi}\Phi$$

for a function $\Phi : M_2^0 \to \mathbb{C}$. This is equivalent to

$$-\frac{1}{abcf}\frac{\partial}{\partial r}\left(\frac{abc}{f}\frac{\partial \Phi}{\partial r}\right) + \left(\frac{\xi_1^2}{a^2} + \frac{\xi_2^2}{b^2} + \frac{\xi_3^2}{c^2}\right)\Phi = \epsilon\Phi, \tag{31}$$

where $\epsilon = \frac{4\pi E}{\hbar^2} - \frac{S^2}{4}$. The quantum number S is necessarily an integer and characterises the total electric charge of the quantum state [10].

We will now derive and study spectral problems for functions on the half-line which can be obtained from (31) by separating the dependence of the function Φ on the angular coordinates and the radial coordinate r. For details about the separation of variables we refer the reader to [10] and [22]. Here we only give enough background to help the reader appreciate the interpretation of the bound states which we will encounter in terms of magnetic monopoles.

The vector fields ξ_1, ξ_2 and ξ_3 generate rotations of a two-monopole configuration about body-fixed orthogonal axes. The sum of squares $\xi_1^2 + \xi_2^2 + \xi_3^2$ commutes with the Laplace operator on M_2^0 and represents the total angular momentum of the two-monopole configuration. As usual in quantum theory, it has eigenvalues $-j(j+1)$, for an integer $j \geq 0$.

The operator ξ_3 does not commute with the Laplace operators on M_2^0, but does commute with its asymptotic form where a, b, and c are replaced by a_{TN}, b_{TN} and c_{TN}. For well-separated monopoles, ξ_3 generates the rotation about the line joining the monopoles and an eigenvalue s of $-i\xi_3$ characterises the relative electric charge of the two monopoles. The metamorphosis of body-fixed relative angular into electric charge is one of the interesting and subtle aspects of the theory of non-abelian monopoles. Again we refer the reader to [10] for details. Finally, note that, as a consequence of the $\mathbb{Z}_2$-division in (21), the relative electric charge s and the total electric charge S have to have an even sum. This essentially reflects the fact that the individual electric charges (only defined asymptotically) are both integers.

To study the spectrum of (31), we separate variables in terms of Wigner functions D^j_{sm} for the dependence on $SO(3)$. Referring to [10,22] for details, the conservation of the total angular momentum but not of the relative electric charge means that one may fix j but needs to consider linear combinations of Wigner functions with all allowed values of s, with coefficient functions u_{js} of the radial coordinate. This leads to systems of coupled ordinary differential equations, increasing in size with j, whose structure is described in [22]. It turns out that, because of parity considerations, only a single radial equation needs to be considered for $j = 0$ (where necessarily $s = 0$) and also for $(j, s) = (1, 1), (2, 1)$ or $(3, 2)$. In the case $j = 0$ there are no bound states (albeit very interesting scattering, see [22]), but the other three single channels support bound states, which we now discuss. The radial equation takes the form

$$-\frac{1}{abcf}\frac{d}{dr}\left(\frac{abc}{f}\frac{du_{js}}{dr}\right) + V_{js}u_{js} = \epsilon u_{js}, \tag{32}$$

where the potentials V_{js} are given in Table 2.

Table 2. The potentials for the three single channels with bound states in terms of a, b and c

(j, s)	V_{js}
(1, 1)	$\frac{1}{b^2} + \frac{1}{c^2}$
(2, 1)	$\frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}$
(3, 2)	$\frac{4}{a^2} + \frac{4}{b^2} + \frac{4}{c^2}$

Bound state energies for the channels $(j, s) = (1, 1)$ and $(j, s) = (2, 1)$ were computed numerically in [14] using a shooting method applied to (32). The bound states in the channel $(j, s) = (3, 2)$ were missed in [14] but pointed out in [23], where their bound state energies were also computed using a shooting method. The results in [13,23] are not rigorous. Our goal is to use our results from Sect. 2 to prove that infinitely many bounds states do indeed exist in each of these three channels, and to provide lower bounds for the eigenvalues.

In order to apply the results from Sect. 2, we need to 'flatten' the radial derivative using equation (1). To do this, we first change coordinates to the proper radial distance coordinate R, defined in (26), which satisfies $dR = -f\,dr$. With

$$\nu = \sqrt{-abc},$$

the radial derivative becomes

$$-\frac{1}{abcf}\frac{d}{dr}\frac{abc}{f}\frac{d}{dr} = -\frac{1}{\nu^2}\frac{d}{dR}\nu^2\frac{d}{dR}.$$

Defining

$$\eta = \nu u$$

and substituting $u = \frac{\eta}{\nu}$ into (32) we obtain

$$H_{js}\eta = \epsilon\eta, \tag{33}$$

where

$$H_{js} = -\frac{d^2}{dR^2} + V_{js}^{\text{eff}}, \qquad V_{js}^{\text{eff}} = \frac{1}{\nu}\frac{d^2\nu}{dR^2} + V_{js}. \tag{34}$$

This is the promised reduction of the Atiyah–Hitchin Laplacian to a standard Schrödinger operator on the half-line.

4.3. Bound states of the Atiyah–Hitchin Laplacian. The Sturm–Liouville problem (33) has the form required to apply the result of Sect. 2. The potentials V_{js}^{eff} are analytic on $(0, \infty)$ since they are implicitly defined in terms of elliptic functions. With R related to r via an integral, and a, b, c being determined in terms of r via the relations (23), (24) and (25), we have not been able to express V_{js}^{eff} in terms of R explicitly. However, we can determine the asymptotic information near $R = 0$ and $R = \infty$ required to establish the existence of infinitely many bound states with the result of Sect. 2, and to give numerical estimates for the eigenvalues.

Near the core of the Atiyah–Hitchin manifold, we can use (27) to determine leading terms in V_{js}^{eff} in the limit $R \to 0$. We find $\nu = \sqrt{R} + \mathrm{O}(R)$ and therefore

$$\frac{1}{\nu}\frac{d^2\nu}{dR^2} = -\frac{1}{4R^2} + \mathrm{O}(1).$$

Table 3. The asymptotic forms of the potentials V_{js}^{eff} for small and large R

(j, s)	V_{js}^{eff} **near** $R = 0$	V_{js}^{eff} **for** $R \to \infty$	c_2	C_0	C_1
(1,1)	$-\frac{1}{4R^2} + \frac{2}{\pi^2} + \mathrm{O}(R)$	$\frac{1}{4} - \frac{1}{2R} + \mathrm{o}\left(\frac{1}{R}\right)$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{2}$
(2, 1)	$\frac{3}{4R^2} + \frac{2}{\pi^2} + \mathrm{O}(R)$	$\frac{1}{4} - \frac{1}{2R} + \mathrm{o}\left(\frac{1}{R}\right)$	$\frac{3}{4}$	$\frac{1}{4}$	$-\frac{1}{2}$
(3, 2)	$\frac{3}{4R^2} + \frac{8}{\pi^2} + \mathrm{O}(R)$	$1 - \frac{2}{R} + \mathrm{o}\left(\frac{1}{R}\right)$	$\frac{3}{4}$	1	-2

Collecting leading terms in V_{js}^{eff} for $R \to 0$, we arrive at the second column of Table 3.

For large r, we need to combine the behaviour of the Atiyah–Hitchin metric coefficients with respect to r given in (29) with the relation (30) between r and the proper radial distance R to derive the asymptotic behaviour of $V_{js}^{\text{eff}}(R)$. The basic method is to compute asymptotics with respect to r and then deduce from (30) that, for example,

$$\lim_{R\to\infty} \frac{R}{r^2} = 0,$$

and so, by definition,

$$\frac{1}{r^2} = \mathrm{o}\left(\frac{1}{R}\right) \quad \text{for} \quad R \to \infty.$$

One then finds, for example,

$$\frac{1}{a_{\text{TN}}^2} = \frac{1}{r^2} + \mathrm{O}\left(\frac{1}{r^3}\right), \qquad \frac{1}{c_{\text{TN}}^2} = \frac{1}{4} - \frac{1}{2r},$$

and therefore in particular

$$\frac{1}{a^2} = \mathrm{o}\left(\frac{1}{R}\right), \quad \frac{1}{c^2} = \frac{1}{4} - \frac{1}{2R} + \mathrm{o}\left(\frac{1}{R}\right).$$

Similarly,

$$\nu = \sqrt{2}r - 1 - \frac{3}{4r} + \mathrm{O}\left(\frac{1}{r^2}\right),$$

implies

$$\frac{1}{\nu}\frac{d^2}{dR^2}\nu = \mathrm{o}\left(\frac{1}{R}\right).$$

We collect the resulting asymptotic terms in the potentials V_{js}^{eff} in the third column of Table 3.

By virtue of the results of Sect. 2, we arrive at the following.

Corollary 8. *The radial Hamiltonians $H_{js} : \mathscr{D} \longrightarrow L^2(0, \infty)$ defined in (34) are selfadjoint. Their essential spectrum is the segment $[C_0, \infty)$, where C_0 is given in Table 3. Each of these Hamiltonians has infinitely many eigenvalues below C_0.*

Table 4. The computed eigenvalues of H_{js} for three channels

$(j, s) = (1, 1)$	$(j, s) = (2, 1)$	$(j, s) = (3, 2)$
0.23151604	0.24264773	0.92838765
0.24250546	0.24597017	0.95655735
0.24605425	0.24745446	0.97063593
0.24898588	0.24836885	0.97876253
	0.24942162	0.98390049
		0.98736886

4.4. Numerical approximation of the eigenvalues. Having established the existence of infinitely many eigenvalues, we would like to produce numerical approximations for them, in analogy with our treatment of the linearised YMH equations in Sect. 2. There we were able to exploit the asymptotic agreement between the radial YMH Hamiltonian (17) and the radial Coulomb Hamiltonian. A natural exactly solvable approximation to the Laplace operator on the Atiyah–Hitchin manifold is provided by the Laplace operator on the (negative mass) Taub-NUT space.

As explained in [10,22], replacing the Atiyah–Hitchin radial functions a, b, c by their Taub-NUT counterparts (28) (with $f = -b/r$ similarly replaced) in the eigenvalue equation (31), and separating variables leads to an exactly solvable radial problem on the half-line $(0, \infty)$. The additional $U(1)$ symmetry of the Taub-NUT metric means that ξ_3 commutes with the Laplace operator, so that separating variables into Wigner functions of the angular coordinates and a radial function u_{js}, yields decoupled radial equations. Writing $u_{js}(r) = h_{js}(r)/r$, the radial equations derived in [10] are

$$\left(\frac{d^2}{dr^2} - \frac{j(j+1)}{r^2} - \frac{s^2}{4}\left(1 - \frac{4}{r}\right) + \epsilon\left(1 - \frac{2}{r}\right)\right) h_{js}(r) = 0.$$

Remarkably, the singularity in Taub-NUT at $r = 2$ is not visible in this radial equation, which can be solved exactly in terms of confluent hypergeometric functions. The relevant eigenvalues are

$$\epsilon_{(s,n)} = \frac{1}{2}\sqrt{n^2 - s^2}\left(n - \sqrt{n^2 - s^2}\right), \qquad |s| \leq j, \qquad n = j+1, j+2 \ldots. \tag{35}$$

One might think that the exact solutions of the Taub-NUT radial equation could be used as trial wavefunctions for the radial Atiyah–Hitchin equation (33), in analogy with our use of the Coulomb wavefunctions in the YMH radial problem. However, there are theoretical and practical problems to overcome. The Atiyah–Hitchin and Taub-NUT manifolds are different manifolds (even topologically), and identifying radial coordinates on the two spaces is arbitrary. Pragmatically, one might identify, for example, the proper radial distance coordinate R on the Atiyah–Hitchin space with the radial coordinate r on the Taub-NUT space because they have the same range, and the Taub-NUT problem is most easily solved in terms of r. However, even with this choice, the numerical computation of the potential V_{js}^{eff} in (33) as a function of R with control over numerical errors is very difficult because it involves, amongst others, the inversion of the elliptic function arising in (23). We were therefore not able to construct useful trial wavefunctions for the Atiyah–Hitchin Laplacian from the Taub-NUT eigenfunctions by following this idea. Instead we consider a more pedestrian approach.

In Table 4 we show the numerically computed lowest four to six eigenvalues in each of the channels listed by means of the Matlab routine Chebfun, [7]. These calculations are

Table 5. The Taub-NUT approximation to the first eigenvalues from (35) and agreement with the eigenvalues from Table 4

$(j, s) = (1, 1)$	Agreement (%)	$(j, s) = (2, 1)$	Agreement (%)	$(j, s) = (3, 2)$	Agreement (%)
0.23205081	+ 99.77	0.24264069	− 99.99(7)	0.92820323	− 99.98
0.24264069	+ 99.94	0.24596669	− 99.99(9)	0.95643924	− 99.99
0.24596669	− 99.96	0.24744871	− 99.99(7)	0.97056275	− 99.99
0.24744871	− 99.38	0.24823935	− 99.95	0.97871376	− 99.99(5)
		0.24744871	− 99.20	0.98386677	− 99.99(7)
				0.98733975	− 99.99(7)

The signs displayed correspond to whether the Taub-NUT eigenvalue is above (+) or below (−) the Atiyah–Hitchin eigenvalue

expected to be more accurate than those in [14,23]. We use the radial Atiyah–Hitchin Hamiltonian in the form (32). The equations (22) for the coefficient functions (with $f = -b/r$) are used to express derivatives of a, b and c, in terms of a, b and c. For each integration of (32), the coefficient functions a, b and c are obtained from (22), starting with initial data $a = 2h$, $b = \pi + h$ and $c = -\pi + h$ where $h = 0.001$.

We have listed the corresponding Taub-NUT eigenvalues from (35) in Table 5. For the channel $(j, s) = (1, 1)$, the lowest four energies occur when $n = 2, 3, 4, 5$, for $(j, s) = (2, 1)$ they occur when $n = 3, 4, 5, 6, 7$ and for $(j, s) = (3, 2)$ they occur when $n = 4, 5, 6, 7, 8, 9$. Our calculations confirm the remarkable agreement between numerically computed eigenvalues for the Atiyah–Hitchin Hamiltonian and the Taub-NUT eigenvalues. This agreement was pointed out and discussed in [14] for the three lowest lying eigenvalue in the channels $(j, s) = (1, 1)$ and $(j, s) = (2, 1)$, and also in [23] for $(j, s) = (3, 2)$.

Note that the Taub-NUT approximation is slightly below our numerically computed eigenvalues for the Atiyah–Hitchin Laplacian for all but two (the lowest when $(j, s) = (1, 1)$ and $n = 2, 3$).

5. Conclusion

In this paper we rigorously established the existence of infinitely many eigenstates of operators which arise in linearisations of the $SU(2)$ YMH equations in the BPS limit and in symmetry reductions of the Laplace operator on the moduli space of two monopoles. We have also provided sharp numerical estimates of the eigenvalues in some cases. As promised in the Introduction, we would now like to look at the physical interpretations of these eigenstates in YMH theory, with a particular emphasis on their significance for electric–magnetic duality conjectures.

As discussed in Sect. 3.2, suitable quantum superpositions of the eigenstates of the Schrödinger operator (17) define fluctuations around the BPS monopole of definite electric charge $n \in \mathbb{Z}$. The eigenstates we found therefore give rise to an infinite tower of Coulombic bound states in each of the dyonic sectors $(1, n)$, $n \in \mathbb{Z}$. These Coulombic bound states are covered by an essential spectrum arising from other sectors, see [21] for details.

The eigenstates of the Atiyah–Hitchin Laplacian discussed in Sects. 4.3 and 4.4 describe quantum states of magnetic monopoles of charge $m = 2$ and relative electric charge $s = 1$ (with angular momentum $j = 1$ or $j = 2$) or $s = 2$ (with angular momentum $j = 3$). The total electric charge has to be odd when $s = 1$ and even when $s = 2$, but is otherwise arbitrary. We thus have two families of dyonic sectors, with each

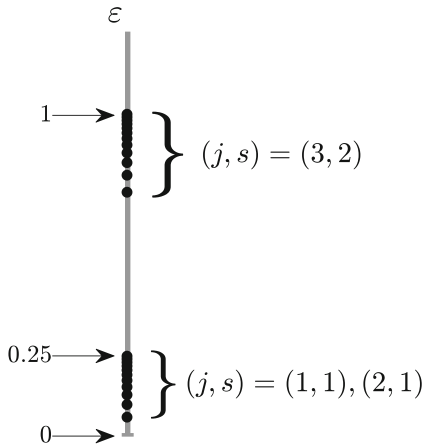

Fig. 1. The qualitative nature of the spectrum of the Laplace operator (acting on differential forms) on the Atiyah–Hitchin manifold: the special eigenvalue $\varepsilon = 0$ for the Sen (or BPS) state is also the lower bound of the essential spectrum. The Coulombic bound states studied here are all embedded in the essential spectrum. The spectrum of the linearised YMH operator has the same qualitative form

sector containing infinitely many Coulombic bound states: one family labelled by $(2, n)$, n odd, and one by $(2, n)$ with n even. The bound states are also covered by an essential spectrum arising from other channels.

The families of charge sectors $(1, n)$, $n \in \mathbb{Z}$ and $(2, n)$, n odd, have both featured prominently in studies of S-duality since they are related by the $SL(2, \mathbb{Z})$ action reviewed in the Introduction. The fact that both contain so-called quantum BPS states was one of the first pieces of strong evidence for S-duality. In the language of this paper, BPS quantum states are bound states with energy equal to the lower bound of the essential spectrum.

Here, we did not consider BPS states, but we can indicate briefly how they fit into our discussion, referring to [6] where the N = 4 supersymmetric theory is studied in notation similar to the one used here. The BPS states in the $(1, n)$ sectors correspond to zero-energy solutions of the coupled system (14) which, as already pointed out, cannot be obtained via the transformation (16) used here. In the $(2, n)$ sectors (n odd), the BPS state is the famous Sen form. It is a zero-energy eigenstate of the Atiyah–Hitchin Laplacian acting on differential forms. As explained in [6], all eigenfunctions (zero-forms) of the Laplace operator are part of a supersymmetry multiplet of differential eigenforms of the Laplacian. However, the zero-energy eigenstates are special, and the corresponding supersymmetric multiplet does not contain ordinary functions on the Atiyah–Hitchin space. As a result, we do not see them in our analysis. However, Fig. 1 illustrates the relation of the BPS state to the essential spectrum of Laplace operator acting on forms and to the eigenvalues studied here.

The Coulombic families of bound states we found both for $(1, n)$, $n \in \mathbb{Z}$ and $(2, n)$, n odd, provide further evidence for the similarities between these two families of charge sectors, and possibly further evidence for S-duality. The latter would not require the spectra in these sectors to be equal, since it also involves a change in the Yang–Mills coupling constant. It would, however, suggest that the tower of Coulombic states found for the linearised YMH equations and for the $s = 1$ channels of the Atiyah–Hitchin

Laplacian represent different approximations, valid for different values of the Yang–Mills coupling constant, to the same physical system of bound states.

The Coulombic bound states in the $(j, s) = (3, 2)$ channel of the Atiyah–Hitchin Laplacian are physically the most surprising of the bound states studied here. They describe bound states of dyons with charges (1, 1) and (1, −1) and were overlooked in [14] since one might expect dyons of equal and opposite electric charges to exchange their electric charge and turn into pure monopoles. As pointed out in [23], this does not happen because the bosonic nature of pure monopoles does not allow them to be in a state of orbital angular momentum $j = 3$. Applying S-duality to these states leads to surprising predictions. A pair of dyons with charges (1, 1) and (1, −1) is S-dual to a pair with charges (−1, 1) and (1, 1). The Coulombic bound states we found would therefore be dual to bound states in a system consisting of a monopole and an anti-monopole, both carrying one unit of electric charge (breather states).

To end, we remark that the study of bound states in single channels arising in the linearised YMH equations and the Atiyah–Hitchin Laplacian are merely the first steps in a full exploration of these spectral problems. Both contain interesting scattering processes with strikingly similar qualitative features [21,22]. For higher angular momenta, both yield infinitely many multi-channel problems, with both bound states and scattering processes. Our analysis suggests that all of these warrant careful further study.

A. Detailed Evaluation of the Stiffness Matrices for the Linearised YMH Equations

To compute the stiffness matrix in (20) we first split the Hamiltonian H_{YMH} into two parts

$$H_{\text{YMH}} = H_1 + H_2,$$

where

$$H_1 = -\frac{d^2}{dr^2} + \frac{2}{r^2} - \frac{2}{r},$$
$$H_2 = \frac{1 + \cosh^2(r)}{\sinh^2(r)} + \frac{2}{r}(1 - \coth(r)).$$

Now defining

$$S_k(i, j) = \int_0^\infty H_k \tilde{b_i}(r)\tilde{b_j}(r)dr, \qquad k = 1, 2,$$

one finds that $S_1(i, j)$ is straightforward to calculate, but that the evaluation of $S_2(i, j)$ is rather involved. To organise it, we write the basis functions (19) as

$$\tilde{b_i}(r) = r\left(\sum_{p=1}^{i} d_{p-1}^{i+1} r^p\right) e^{-\left(\frac{1}{i+1}\right)r},$$

and introduce the notation $\hat{d}_p^{ij} \in \mathbb{R}$ for the coefficients of the product

$$\tilde{b_i}(r)\tilde{b_j}(r) = r^2\left(\sum_{p=2}^{i+j} \hat{d}_p^{ij} r^p\right) e^{-\left(\frac{1}{i+1}+\frac{1}{j+1}\right)r}.$$

Then

$$S_2(i,j) = \int_0^\infty \frac{r^2\left(1+\cosh^2(r)+\frac{2}{r}\sinh^2(r)-\frac{2}{r}\sinh(r)\cosh(r)\right)}{\sinh^2(r)} \left(\sum_{p=2}^{i+j} \hat{d}_p^{ij} r^p\right) e^{-\left(\frac{1}{i+1}+\frac{1}{j+1}\right)r} dr$$
$$= \sum_{p=2}^{i+j} \hat{d}_p^{ij} \int_0^\infty \frac{r^2}{\sinh^2(r)} \left(\frac{3}{2}+\frac{e^{2r}}{4}+\frac{e^{-2r}}{4}-\frac{1}{r}+\frac{e^{-2r}}{r}\right) r^p e^{-\left(\frac{1}{i+1}+\frac{1}{j+1}\right)r} dr$$
$$= \sum_{p=2}^{i+j} \hat{d}_p^{ij} \left(\frac{3}{2}\mathscr{L}\left(\frac{r^{2+p}}{\sinh^2(r)}\right)\left(\frac{1}{i+1}+\frac{1}{j+1}\right)+\frac{1}{4}\mathscr{L}\left(\frac{r^{2+p}}{\sinh^2(r)}\right) \times \left(\frac{1}{i+1}+\frac{1}{j+1}-2\right) + \frac{1}{4}\mathscr{L}\left(\frac{r^{2+p}}{\sinh^2(r)}\right)\left(\frac{1}{i+1}+\frac{1}{j+1}+2\right) - 2\mathscr{L}\left(\frac{r^{1+p}}{\sinh(r)}\right) \times \left(\frac{1}{i+1}+\frac{1}{j+1}+1\right)\right), \tag{36}$$

where $\mathscr{L}(f(t))(s)$ is the Laplace transform of $f(t)$ and we used the exponential definitions of the hyperbolic functions. Using [16, 25.11.25] we see that

$$\mathscr{L}\left(\frac{r}{\sinh(r)}\right)(s) = \int_0^\infty \frac{2e^{-sr}r}{e^r-e^{-r}}dr = \frac{1}{2}\int_0^\infty \frac{e^{-\frac{sx}{2}}x}{e^{\frac{x}{2}}-e^{-\frac{x}{2}}}dx = \frac{1}{2}\int_0^\infty \frac{e^{-\left(\frac{s+1}{2}\right)x}x}{1-e^{-x}}dx = \frac{1}{2}\Gamma(2)\xi\left(2,\frac{s+1}{2}\right),$$

where $\Gamma(t)$ is the Gamma function , $\xi(q,w)$ is the Hurwitz zeta function and we have made the substitution $2r = x$. This evaluates the last term in (36). To simplify the other terms, we start by defining the function

$$K(a,s) = \mathscr{L}\left(\frac{r^a}{\sinh^2(r)}\right)(s), \quad a = 2, 3, \ldots.$$

Taking the derivative of $K(2,s)$ with respect to s we have

$$\partial_s K(2,s) = \partial_s \mathscr{L}\left(\frac{r^2}{\sinh^2(r)}\right)(s) = \int_0^\infty \frac{r^2}{\sinh^2(r)}\partial_s e^{-sr}dr$$

$$
\begin{aligned}
&= -\int_0^\infty \frac{r^3}{\sinh^2(r)} e^{-sr} dr \\
&= -K(3, s).
\end{aligned}
$$

By induction we have the relation

$$
K(a+1, s) = (-\partial_s)^{(a-1)} K(2, s), \quad a = 2, 3, ... \tag{37}
$$

Using [16, 25.11.25, 25.11.12] we can write

$$
\begin{aligned}
K(2, s) &= \mathscr{L}\left(\frac{r^2}{\sinh^2(r)}\right)(s) \\
&= \int_0^\infty \frac{4r^2 e^{-sr}}{(e^r - e^{-r})^2} dr \\
&= \frac{1}{2}\int_0^\infty \frac{x^2 e^{-\left(\frac{s+2}{2}\right)x}}{(1 - e^{-x})^2} dx \\
&= \frac{1}{2}\int_0^\infty e^{-\frac{sx}{2}} x^2 \frac{d}{dx}\left(\frac{-1}{1 - e^{-x}}\right) dx \\
&= \int_0^\infty \frac{x e^{-\frac{sx}{2}}}{1 - e^{-x}} dx - \frac{s}{4}\int_0^\infty \frac{x^2 e^{-\frac{sx}{2}}}{1 - e^{-x}} dx \\
&= \Gamma(2)\xi\left(2, \frac{s}{2}\right) - \frac{2}{4}\Gamma(3)\xi\left(3, \frac{s}{2}\right) \\
&= \Phi'\left(\frac{s}{2}\right) + \frac{s}{4}\Phi''\left(\frac{s}{2}\right),
\end{aligned} \tag{38}
$$

where $\Phi(z)$ is the Digamma function and we have made the substitution $2r = x$. Substituting (38) into (37) gives

$$
K(a+1, s) = (-\partial_s)^{(a+1)}\left(\Phi'\left(\frac{s}{2}\right) + \frac{s}{4}\Phi''\left(\frac{s}{2}\right)\right).
$$

This can now be used to evaluate the expression for $S_2(i, j)$ in (36) in terms of the Digamma function.

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