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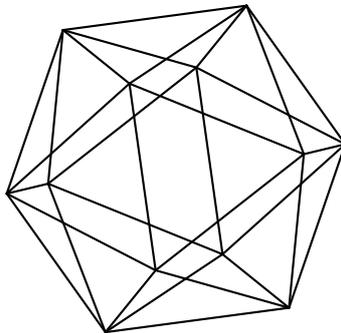
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ANALYSIS OF SCHRÖDINGER OPERATORS WITH INVERSE SQUARE POTENTIALS I (REGULARITY RESULTS IN 3D)

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ABSTRACT. Let V be a potential on $\mathbb{R}^3$ that is smooth everywhere except at a discrete set $\mathcal{S}$ of points, where it has singularities of the form Z/ρ^2, with $\rho(x) = |x - p|$ for x close to p and Z continuous on $\mathbb{R}^3$ with $Z(p) > -1/4$ for $p \in \mathcal{S}$. Also assume that ρ and Z are smooth outside $\mathcal{S}$ and Z is smooth in polar coordinates around each singular point. We either assume that V is periodic or that the set $\mathcal{S}$ is finite and V extends to a smooth function on the radial compactification of $\mathbb{R}^3$ that is bounded outside a compact set containing $\mathcal{S}$. In the periodic case, we let Λ be the periodicity lattice and define $\mathbb{T} := \mathbb{R}^3/\Lambda$. We obtain regularity results in weighted Sobolev space for the eigenfunctions of the Schrödinger-type operator $H = -\Delta + V$ acting on $L^2(\mathbb{T})$, as well as for the induced $\mathbf{k}$–Hamiltonians $H_{\mathbf{k}}$ obtained by resticting the action of H to Bloch waves. Under some additional assumptions, we extend these regularity and solvability results to the non-periodic case. We sketch some applications to approximation of eigenfunctions and eigenvalues that will be studied in more detail in a second paper.

CONTENTS

1. INTRODUCTION AND STATEMENT OF MAIN RESULTS

We study in this paper regularity and decay properties of the eigenfunctions of Schrödinger type operators with inverse-square singularities. We either assume that the potential is periodic or that it has a nice behaviour at infinity and only finitely many singularities. In order to explain our assumptions and results in more detail, we organize our Introduction in subsections, concentrating on the case of periodic

potentials, the non-periodic case being similar, but simpler. We first introduce the operators $H_{\mathbf{k}}$ obtained from the Hamiltonian $-\Delta + V$ acting on Bloch waves. In the second subsection of the Introduction, we explain our assumptions on the potential V. Finally, we state our main results and we summarize the contents of the paper.

This paper is written to put on a solid foundations the numerical methods developped in [21]. We have thus written this paper with an eye to the numerical analyst. More theoretical results on Hamiltonians with inverse square potentials in arbitrary dimensions will be included in the third part of this paper.

See [5, 8, 36, 42, 43] for other papers studying Hamiltonians with inverse square potentials, both from the point of view of physical and numerical applications. See also [9, 10, 11, 13, 12, 14, 18, 20, 40, 41, 44] for some related results.

1.1. The Hamiltonian $H_{\mathbf{k}}$.

Let V be a periodic potential on $\mathbb{R}^3$ with Bravais lattice (of translational symmetries) $\Lambda \cong \mathbb{Z}^3$. Assume that V is smooth except at a set of points $\mathcal{S}$, which is thus necessarily also periodic with with respect to the lattice Λ. We assume that there are only finitely many elements of $\mathcal{S}$ in any fundamental domain $\mathbb{P}$ of Λ. Let $p \in \mathcal{S}$ be a singular point and $\rho(x) = |x - p|$ for x close to p and ρ smooth outside $\mathcal{S}$. We assume that around p the potential V has a singularity of the form Z/ρ^2, where Z is continuous across p and smooth in polar coordinates around p. We shall study numerically Hamiltonian operators of the form

$$(1) \qquad\qquad H := -\Delta + V.$$

Systems with such potentials have been studied as theoretical models both from the viewpoint of classical mechanics and from the quantum mechanical viewpoint. In addition, they arise in a variety of physical contexts, such as in relativistic quantum mechanics from the square of the Dirac operator coupled with an interaction potential, or from the interaction of a polar molecule with an electron [36].

A standard method for studying these operators is through their action on Bloch waves. For any $\mathbf{k} \in \mathbb{R}^3$, the Bloch waves of H with wave vector $\mathbf{k}$ are elements of $L^2_{loc}(\mathbb{R}^3)$ that satisfy the semi-periodicity condition that, for all $X \in \Lambda$,

$$(2) \qquad\qquad \psi_{\mathbf{k}}(x + X) = e^{i\mathbf{k}\cdot X}\psi_{\mathbf{k}}(x).$$

(It is enough to consider $\mathbf{k}$ in the first Brillouin zone $\mathbb{P}_*$ of the reciprocal lattice to Λ. Also, the equality is that of two L^2_{loc} functions, and hence it holds only almost everywhere in x.) A Bloch wave with wavevector $\mathbf{k}$ can be written as

$$(3) \qquad\qquad \psi_{\mathbf{k}}(x) = e^{i\mathbf{k}\cdot x}u_{\mathbf{k}}(x)$$

for a function $u_{\mathbf{k}}$ that is truly periodic with respect to Λ_t and thus can be considered as living on the three-torus $\mathbb{T} := \mathbb{R}^3/\Lambda \simeq (S^1)^3$ (obtained by identifying points in $\mathbb{R}^3$ that are equivalent under the action of the lattice Λ by translations). Note that the periodicity condition that a Bloch wave satisfies prevents it from being in $L^2(\mathbb{R}^3)$, thus a nontrivial Bloch wave that satisfies the equation

$$(4) \qquad\qquad H\psi_{\mathbf{k}} = \lambda\psi_{\mathbf{k}}$$

is not, properly speaking, an eigenfunction of the Hamiltonian operator H. Rather, it is a generalized eigenfunction, corresponding to a value in the continuous spectrum of H. If $\psi_{\mathbf{k}}$ is a Bloch wave that is a generalized eigenfunction of H with generalized eigenvalue λ, then the function $u_{\mathbf{k}} := e^{-i\mathbf{k}\cdot x}\psi_{\mathbf{k}}(x)$ will then be an actual λ-eigenfunction of the $\mathbf{k}$–Hamiltonian $H_{\mathbf{k}}$ on $L^2(\mathbb{T})$ defined by

$$(5) \qquad H_{\mathbf{k}} := -\sum_{j=1}^{3}(\partial_j + ik_j)^2 + V.$$

Indeed, this follows from the equation

$$(6) \qquad H(e^{i\mathbf{k}\cdot x}u_{\mathbf{k}}(x)) = e^{i\mathbf{k}\cdot x}H_{\mathbf{k}}u_{\mathbf{k}}(x).$$

Thus, it is useful to understand the regularity of eigenfunctions $u_{\mathbf{k}}$ for the operators $H_{\mathbf{k}}$, as well as to arrive at theoretical estimates for the accuracy of various schemes to estimate them and their associated eigenvalues.

1.2. **Assumptions on the potential V.** In this paper, we extend and test the results of [23] to deal with the more singular potentials that have inverse-square singularities. More precisely, we extend the results of the aforementioned paper from potentials where ρV is smooth in polar coordinates to potentials where $\rho^2 V$ is smooth in polar coordinates and continuous on $\mathbb{T}$. (Recall that ρ is a function that locally gives the distance to the singular point). In particular, we obtain regularity results in weighted Sobolev spaces that will then permit us to derive estimates for the accuracy of two approximation schemes that we design and which are studied in detail in the forthcoming second part of this paper. The first scheme is a finite element method with a mesh graded towards the singular points as in [23, 7]. The second scheme is an augmented plane-wave method, similar to a "muffin-tin" method [32].

In order to state our results, we first need to set some notation and introduce our assumptions on the potential V. Let $\mathcal{S} \subset \mathbb{T} := \mathbb{R}^3/\Lambda$ be the finite set of points where V has singularities. By abuse of notation, we shall denote by $|x - y|$ the induced distance between two points $x, y \in \mathbb{T}$. Let then $\rho : \mathbb{T} \to [0, 1]$ be a nonnegative continuous function smooth outside $\mathcal{S}$ such that

$$(7) \qquad \rho(x) = |x - p| \ \text{ for } x \text{ close to } p \in \mathcal{S},$$

as before, and further assume also that $\rho(x) = 1$ for x far from $\mathcal{S}$.

Our first assumption on V is that $\rho^2 V$ be smooth in polar coordinates up to $\rho = 0$ near each singularity. Let us explain this in more detail. We first replace each singular point $p \in \mathcal{S}$ with a 2-sphere in a smooth way, thus obtaining a space denoted $\overline{\mathbb{T} \smallsetminus \mathcal{S}}$. This is the usual procedure of blowing up the singularities. We think of stretching out the holes where the singularities of V are and compactifying the result using boundary spheres. It would be possible to carry out analysis similar to the calculations in this paper with only the assumption that $\rho^2 V$ be smooth on $\overline{\mathbb{T} \smallsetminus \mathcal{S}}$. To simplify some calculations and to obtain closed form results, however, we will further require the resulting function Z to be constant on the blow up of

each point in $\mathcal{S}$, which can be reformulated as saying that $\rho^2 V$ is also *continuous* on $\mathbb{T}$. Our first assumption on the potential V is therefore

(8)   **Assumption 1** : $Z := \rho^2 V \in \mathcal{C}^\infty(\overline{\mathbb{T} \smallsetminus \mathcal{S}}) \cap \mathcal{C}(\mathbb{T})$.

Assumption 1, more precisely the continuity of Z at $\mathcal{S}$, allows us to formulate our second assumption. Namely,

(9)   **Assumption 2** : $\eta_0 := \min_{p \in \mathcal{S}} Z(p) > -1/4$.

Thefore, the constant

(10) $\eta := \sqrt{1/4 + \eta_0},$

which will play an important role in this paper, is a *positive real number*. This constant will appear in many results below. We will use Assumptions 1 and 2 throughout the paper, except in Section 2, where we prove more general forms of our results, not requiring Assumption 2.

1.3. **Regularity and approximation results.** The domains of all the Hamiltonian operators considered in this paper will be contained in weighted Sobolev spaces on $\mathbb{T} \smallsetminus \mathcal{S}$. We define these spaces by:

(11) $\mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S}) := \{v : \mathbb{T} \smallsetminus \mathcal{S} \to \mathbb{C}, \ \rho^{|\beta|-a} \partial^\beta v \in L^2(\mathbb{T}), \ \forall \ |\beta| \le m\}.$

These spaces have been considered in many other papers, most notably in Kondratiev's groundbreaking paper [26]. They can be identified with the b-Sobolev spaces of [33] (associated to a manifold with boundary), but with a different indexing and notation. These spaces were generalized in [3] to more general manifolds with corners with additional structure (Lie manifolds).

To formulate the stronger regularity for eigenvalues, we shall need the following notation. For each point $p \in \mathcal{S}$, let

(12) $\nu_0(p) = \begin{cases} 2 & Z(p) \ge \frac{3}{4} \\ 1 + \sqrt{1/4 + Z(p)} & Z(p) \in (-\frac{1}{4}, \frac{3}{4}) \\ 1 & Z(p) \le -\frac{1}{4}, \end{cases}$

and

(13) $\nu_0 = \min_{p \in \mathcal{S}} \nu_0(p).$

For each point $p \in \mathcal{S}$ for which $Z(p) \in (-1/4, 3/4]$, define a smooth cutoff function χ_p that is equal to 1 in a small neighborhood of p and is zero outside another small neighborhood of p, so that all the functions χ_p have disjoint supports. Define the space W_s to be the complex linear span:

(14) $W_s = \sum_{Z(p) \in (-1/4, 3/4]} \mathbb{C} \chi_p \rho^{\sqrt{1/4 + Z(p)} - 1/2}.$

Using also the notation introduced in the previous subsection, we then have the following result, whose proof follows from the proof of Theorem 2.3 below.

Theorem 1.1. *Consider a potential V satisfying Assumptions 1 and 2. Then the Hamiltonian operator $H_{\mathbf{k}}$ acting as an unbounded operator on $L^2(\mathbb{T})$ has a distinguished self-adjoint extension with domain*

$$\mathcal{D}(H_{\mathbf{k}}) = \mathcal{K}_2^2(\mathbb{T} \smallsetminus \mathcal{S}) + W_s \subset \mathcal{K}_\nu^2(\mathbb{T} \smallsetminus \mathcal{S}), \quad \nu < \nu_0 = \min_{p \in \mathcal{S}} \nu_0(p) \in (0, 2].$$

In particular, if $\eta_0 := \eta_0 := \min_{p \in \mathcal{S}} Z(p) \geq 3/4$, then $H_{\mathbf{k}}$ is in fact essentially self-adjoint and, if $\eta_0 > 3/4$, then $\mathcal{D}(H_{\mathbf{k}}) = \mathcal{K}_2^2(\mathbb{T} \smallsetminus \mathcal{S})$.

The importance of the above theorem is the following corollary, which says that under Assumptions 1 and 2, the Hamiltonian operators $H_{\mathbf{k}} = -\sum_{j=1}^3 (\partial_j + i k_j)^2 + V$ acting on $L^2(\mathbb{T})$ can be completely understood through their eigenfunctions and eigenvalues.

Corollary 1.2. *Under the assumptions of Theorem 1.1, there exists a complete orthonormal basis of $L^2(\mathbb{T})$ consisting of eigenfunctions of $H_{\mathbf{k}}$.*

We can now state a regularity theorem for the eigenfunctions of $H_{\mathbf{k}}$ near a point $p \in \mathcal{S}$, or equivalently, for Bloch waves associated to the wavevector $\mathbf{k}$. Recall the functions χ_p supported near points of $\mathcal{S}$ and used to define the spaces W_s.

Theorem 1.3. *Assume that V satisfies Assumptions 1 and 2. Let $H_{\mathbf{k}} u = \lambda u$, where $u \in \mathcal{D}(H_{\mathbf{k}})$, $u \neq 0$. Then, for any $m \in \mathbb{Z}_+$,*

$$u \in \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S}), \quad \forall a < \eta := \min_{p \in \mathcal{S}} \sqrt{1/4 + Z(p)}.$$

Moreover, we can find constants $a_p \in \mathbb{R}$ such that

$$u - \sum_{p \in \mathcal{S}} \chi_p \rho^{\sqrt{1/4 + Z(p)} - 1/2} \in \mathcal{K}_{a'+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S}), \quad \forall a' < \min_{p \in \mathcal{S}} \sqrt{9/4 + Z(p)}.$$

The next result, which is the last we will mention in this introduction, will permit us to construct approximation schemes for the solutions of equations of the form $(\lambda + H_{\mathbf{k}}) u = f$.

Theorem 1.4. *Let us use the notation of Theorem 1.1 and both Assumptions 1 and 2. Then there exists $C_0 > 0$ such that $\lambda + H_{\mathbf{k}} : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S}) \to \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \smallsetminus \mathcal{S})$ is an isomorphism for all $m \in \mathbb{Z}_{\geq 0}$, all $|a| < \eta$, and all $\lambda > C_0$. In particular, H_k is symmetric and bounded below, thus has a Friedrichs extension, which is equal to the closed extension considered in Theorem 1.1 above.*

From now on, we shall write $H_{\mathbf{k}}$ for the Friedrichs extension of the original operator defined in Equation (6) and $\mathcal{D}(H_{\mathbf{k}})$ for its domain.

We observe additionally that with the exception of Corollary 1.2, all of the results above extend to Hamiltonian operators on $\mathbb{R}^3$ associated to a non-periodic potential with a finite number of inverse square singularities satisfying Assumptions 1 and 2 and radial limits at infinity. This is because the techniques employed to obtain the results are local, and a Hamiltonian operator over $\mathbb{R}^3$ with a smooth potential that has radial limits at infinity is always essentially self-adjoint. Of course, in this situation, there are only isolated eigenvalues below the continuous spectrum, and the bulk of the spectrum is continuous.

The paper is organized as follows. In Section 2 we prove Theorem 1.1 identifying a closed self-adjoint extension of the operator H_k, and Theorem 1.3 giving regularity results for eigenfunctions of this closure. Some of the results of this section do not rely on Assumption 2. Beginning with Section 3, however, we shall require that Assumption 2 be satisfied. In that section, we prove that for $\eta > -1/4$, H_k is bounded from below, and we can thus identify the closure from Section 2 as the Friedrichs extension of $H_{\mathbf{k}}$. In Section 4 we discuss how our results extend to the the nonperiodic case and how to use them in numerical methods.

2. Regularity and singular values

The regularity analysis of the operators $H_{\mathbf{k}}$ is done locally in the neighborhood of each $p \in \mathcal{S}$. Let us recall that $Z := \rho^2 V \in \mathcal{C}^\infty(\overline{\mathbb{T} \smallsetminus \mathcal{S}}) \cap \mathcal{C}(\mathbb{T})$, which is our Assumption 1, which we will require to hold true throughout this paper. In this section, we shall mention explicitly when Assumption 2 is used, since some of the results hold in greater generality.

For simplicity of the notation, we shall assume that $\mathcal{S}$ consists of a single point p. The results for potentials with several singularities with different values of $Z(p)$ can then be pieced together from local versions of the result in the one singularity case. The proofs of Theorems 1.1 and Theorem 1.3 (which we prove in this section in more general forms not requiring Assumption 2), rely on the pseudodifferential operator techniques of the b-calculus and b-operators [4, 33, 30, 39]. A review of these basic tools is contained in [23], so we will not go into detail about them again here. Throughout this paper, we will refer to b-operators and the b-calculus, although the properties can be equivalently described in terms of cone operators and the cone calculus, and in fact, in some of the references in this section, they are referred to in this way. For a discussion of the equivalence of the b- and cone calculi, see [29].

2.1. **The boundary spectral set.** In order to use the b-calculus, we study the associated b-differential operators

$$P_{\mathbf{k},\lambda} := -\rho^2(H_{\mathbf{k}} - \lambda).$$

We can write such an operator in polar coordinates around $p \in \mathcal{S}$ as

(15) $$P_{\mathbf{k},\lambda} = (\rho\partial_\rho)^2 + \rho\partial_\rho + \Delta_{S^{n-1}} - \rho^2 V - \rho B_{\mathbf{k},\lambda},$$

where

$$B_{\mathbf{k},\lambda} := \rho \left(\sum_{j=1}^n (-2i\partial_j + k_j^2) - \lambda \right)$$

is a first order b-operator.

The operator $P_{\mathbf{k},\lambda}$ is an elliptic b-operator on $\overline{\mathbb{T} \smallsetminus \mathcal{S}}$. We calculate the indicial family of $P_{\mathbf{k},\lambda}$ at a point $p \in \mathcal{S}$, denoted $(\widehat{P_{\mathbf{k},\lambda}})_p(\tau)$, by replacing $\rho \partial_\rho$ with τ in Equation (15), and by replacing the coefficients with their values at $\rho = 0$. Doing this, we find that the indicial families for $P_{\mathbf{k},\lambda}$ at $p \in \mathcal{S}$ are, in fact, independent of λ and $\mathbf{k}$, since the dependence on $\mathbf{k}$ and λ affects only $B_{\mathbf{k},\lambda}$, and ρ vanishes at the singular points. We summarize this discussion in the following lemma.

Lemma 2.1. *Let $P := P_{0,0}$. Then the indicial family of $P_{\mathbf{k},\lambda}$ at $p \in \mathcal{S}$ is given by*

$$(16) \qquad (\widehat{P_{\mathbf{k},\lambda}})_p(\tau) = \hat{P}_p(\tau) = \tau^2 + \tau + \Delta_{S^2} - Z(p).$$

Lemma 2.1 allows us to calculate the boundary spectral set $\mathrm{Spec}_b(P_p)$ for $P_{\mathbf{k},\lambda}$ at a given p. The *boundary spectral set* for $P_{\mathbf{k}}$ is then defined by ([33])

$$\mathrm{Spec}_b(P_p) := \{(\tau, n) \mid \hat{P}_p(\tau)^{-1} \text{ has a pole of order } n+1 \text{ at } \tau\}.$$

By Lemma 2.1, the set $\mathrm{Spec}_b(P_p)$ will also be independent of $\mathbf{k}$ and λ. To calculate the spectral set $\mathrm{Spec}_b(P_p)$ explicitly, recall that the eigenvalues of Δ_{S^2} are $-l(l+1)$, for $l \in \mathbb{Z}_{\geq 0}$, and define

$$(17) \qquad \beta_{l,p} := \frac{\sqrt{(1+2l)^2 + 4Z(p)} - 1}{2}, \quad l \in \mathbb{Z}_{\geq 0}$$

$$(18) \qquad \alpha_{l,p} := \frac{-\sqrt{(1+2l)^2 + 4Z(p)} - 1}{2}, \quad l \in \mathbb{Z}_{\geq 0}.$$

By an abuse of notation, we take $\sqrt{(1+2l)^2 + 4Z(p)}$ to denote the positive imaginary root when the quantity under the root is negative. Our discussion gives the following.

Lemma 2.2. *If $Z(p) \notin \{-(1/2 + l)^2\}_{l=0}^{\infty}$, we have*

$$(19) \qquad Spec_b(P_p) = \bigcup_{l \in \mathbb{Z}_{\geq 0}} \{(\beta_{l,p}, 0), (\alpha_{l,p}, 0)\},$$

and, if $Z(p) = -(1/2 + l_p)^2$, for some $l_p \geq 0$, $l_p \in \mathbb{Z}$, then

$$(20) \qquad Spec_b(P_p) = \{(-1/2, 1)\} \cup \bigcup_{l \in \mathbb{Z}_{\geq 0}} \{(\beta_{l,p}, 0), (\alpha_{l,p}, 0)\}.$$

When $Z(p) < -1/4$, a finite number of these values of α and β will be complex with real part equal to $-1/2$. This is one of the reasons why we have introduced Assumption 2, which states that $Z(p) > -1/4$ for all $p \in \mathcal{S}$. Of course, if Assumption 2 is satisfied, $\mathrm{Spec}_b(P_p)$ is given only by Equation (19). The case when $Z(p)$ is close to $-1/4$ is important because it gives to some interesting numerical phenomena and also because in various applications, it has an interesting interpretation, see for instance [36].

The machinery of the b-calculus now gives us information about closed self-adjoint extensions of $H_{\mathbf{k}}$ (see [30, 17, 16, 38] for details). Note that in this setting, we are considering extensions of our operator acting on the core consisting of smooth functions supported away from the points of $\mathcal{S}$. For $Z(p) < 3/4$, there will

be several possible self-adjoint extensions. Compare this to the case of extending the Laplacian operator on $\mathbb{T}$ from acting on the core consisting of all smooth functions. In this case, there is a unique self-adjoint extension. This is because the core is larger than in our case. The extension obtained using the larger core is one of the possible extensions obtained using the smaller core, but it is not the only one. This is why one does not see the issue of choosing a self-adjoint extension arising when the potential is of the form $Z\rho^\alpha$ for $\alpha > -2$, for instance, in the Coulomb case considered in [23].

With the above lemmas in place, we can now prove Theorem 1.1. In fact, we shall prove a stronger result that does not require Assumption 2.

Theorem 2.3. *Consider a potential V satisfying Assumption 1 and assume that $\mathcal{S}$ consists of just one point p. Then the Hamiltonian operator $H_\mathbf{k}$ acting as an unbounded operator on $L^2(\mathbb{T})$ has distinguished self-adjoint extension with domain $\mathcal{D}(H_\mathbf{k}) \subset \mathcal{K}^2_\nu(\mathbb{T} \smallsetminus \mathcal{S})$ for all $\nu < \nu_0 \in (0, 2]$. In particular, if $Z(p) \geq 3/4$, then $H_\mathbf{k}$ is in fact essentially self-adjoint and, if $Z(p) > 3/4$, then $\mathcal{D}(H_\mathbf{k}) = \mathcal{K}^2_2(\mathbb{T} \smallsetminus \mathcal{S})$. If Assumption 2 is satisfied, we also have*

$$\mathcal{D}(H_\mathbf{k}) = \mathcal{K}^2_2(\mathbb{T} \smallsetminus \mathcal{S}) + \mathbb{C}\chi\rho^{\eta - 1/2}, \quad \eta = \sqrt{1/4 + Z(p)}.$$

where χ is a cutoff function that is zero outside some neighborhood of p and equals 1 close to p.

Proof. For each $\mathbf{k}$ and λ, the operator $H_\mathbf{k} - \lambda$ is a symmetric, unbounded b-operator on $L^2(\mathbb{T})$ (see [33, 30, 17]). Define the operator $A = \rho^{1/2} H_\mathbf{k} \rho^{-1/2}$. Then A is a symmetric unbounded b-operator on $\rho^{-1} L^2_b(\mathbb{T} \smallsetminus \mathcal{S}) = \mathcal{K}^0_{1/2}(\mathbb{T} \smallsetminus \mathcal{S})$. The self-adjoint extensions of A correspond exactly to those of $H_\mathbf{k} - \lambda$ with domains shifted by weight $\rho^{1/2}$, so we will study the self-adjoint extensions of A as the calculations are somewhat easier in this case.

By Lemma 2.1, the indicial roots of A are the roots of $H_\mathbf{k}$ shifted by $1/2$. So we let

(21) $$\tilde{\beta}_l = \sqrt{(l + 1/2)^2 + Z(p)} \quad \text{and} \quad \tilde{\alpha}_l = -\tilde{\beta}_l.$$

Note that $0 \neq \tilde{\beta}_l \in \mathbb{R}$ if $Z(p) > -(l + \frac{1}{2})^2$, there is a double root at $\tilde{\beta}_l = 0$ if $Z(p) = -(l + \frac{1}{2})^2$, and $0 \neq \tilde{\beta}_l \in i\mathbb{R}$ if $Z(p) < -(l + \frac{1}{2})^2$. The critical strip for self-adjointness of unbounded operators on $\rho^{-1} L^2_b(\mathbb{T} \smallsetminus \mathcal{S})$ is $(-1, 1)$, that is, an operator is essentially self-adjoint if and only if it has no indicial roots with real part in this interval (see [30, 17]). Recalling that $l \in \mathbb{Z}_{\geq 0}$, we see that for $Z(p) \geq \frac{3}{4}$, there are no roots in the critical strip so the operator is essentially self-adjoint. If further $Z(p) > \frac{3}{4}$ we get the somewhat stronger result that $\mathcal{D}(H_\mathbf{k}) = \mathcal{K}^2_2(\mathbb{T} \smallsetminus \mathcal{S})$. For $Z(p) \in \left(-\frac{1}{4}, \frac{3}{4}\right)$ we get two real roots in the critical strip corresponding to $l = 0$, for $Z(p) = -\frac{1}{4}$, we get a double root at 0 in the critical strip corresponding to $l = 0$, and for $Z(p) < -\frac{1}{4}$, we get a finite number of complex conjugate imaginary root pairs and possibly two real roots or a double root at 0 in the critical strip corresponding to some finite set of l.

By the theory in [17], the space $\mathcal{E} := \mathrm{Dom}(A_{\max})/\mathrm{Dom}(A_{\min})$ is finite dimensional and spanned by functions local around p of the form:

$$(22) \qquad \bigcup_{|\Re(\tilde{\beta}_l)|\in(0,1)} \bigcup_{m=-l}^{l} \{w\rho^{\tilde{\beta}_l}\psi_l^m, w\rho^{-\tilde{\beta}_l}\psi_l^m\} \cup \bigcup_{\tilde{\beta}_l=0} \bigcup_{m=-l}^{l} \{w\psi_l^m, w\ln\rho\psi_l^m\},$$

where w is a local cutoff function that equals 1 near p and 0 for ρ large, and where the ψ_l^m are an orthonormal basis for spherical harmonics with eigenvalue $l(l+1)$. Further, the operator A with domain $\mathcal{D} := \mathrm{Dom}(A_{\min}) + \mathrm{span}(u_1, \ldots, u_n)$ is self adjoint if, and only if, linear combinations of these basis functions form a maximal set on which the pairing, $[u,v]_A$ is trivial, where

$$(23) \qquad [u,v]_A := \frac{1}{2\pi} \oint_\gamma \hat{A}\hat{u}(\sigma) \cdot_{S^2} \overline{\hat{v}(\overline{\sigma})}\, d\sigma.$$

Here γ is a simple closed loop around the indicial roots of A in the critical strip, $\hat{}$ represents the Mellin transform and $\cdot_{S^2}$ denotes the standard L^2 paring on S^2. Since the ψ_l^m are orthonormal, this pairing reduces to a sum of loop integrals of the form:

$$(24) \qquad [u_l, v_l]_A = -\frac{1}{2\pi} \oint_\gamma (\sigma^2 + \tilde{\beta}_l^2)\hat{u}_l(\sigma)\overline{\hat{v}_l(\overline{\sigma})}\, d\sigma,$$

where $u_l = u_+ w\rho^{\tilde{\beta}_l} + u_- w\rho^{-\tilde{\beta}_l}$ and $v_l = v_+ w\rho^{\tilde{\beta}_l} + v_- w\rho^{-\tilde{\beta}_l}$ if $\tilde{\beta}_l \neq 0$ and $u_l = u_+ w + u_- w \log(\rho)$ and $v_l = v_+ w + v_- w \log(\rho)$ if $\tilde{\beta}_l = 0$.

We can consider three cases: $\tilde{\beta}_l > 0$, $\tilde{\beta}_l = 0$ and $\tilde{\beta}_l \in i\mathbb{R}$. First, as in [17], define

$$\Phi(\sigma) = \widehat{-\rho\partial_\rho w}(\sigma) := -\int_0^\infty \rho^{-i\sigma}w'(\rho)d\rho.$$

Then we get: $\overline{\hat{\Phi}(\overline{\sigma})} = \hat{\Phi}(-\sigma)$ and $\Phi(0) = 1$. Also, using the properties of the Mellin transform, we find that for any $\sigma \in \mathbb{C}$,

$$\widehat{w\rho^{\pm\tilde{\beta}_l}}(\sigma) = \frac{\Phi(\sigma \pm i\tilde{\beta}_l)}{\sigma \pm i\tilde{\beta}_l}.$$

Now consider the case $\tilde{\beta}_l > 0$. Carrying out the loop integral by evaluating residues, we arrive at the equation

$$[u_l, v_l]_A = k(u_+\bar{v}_- - u_-\bar{v}_+)$$

for a constant $k \neq 0$. If we set $[u_l, u_l] = 0$, this reduces to $\arg(u_+) = \arg(u_-)$. Thus to get a self-adjoint boundary condition at p for A we can fix any ratio of $|u_+|$ to $|u_-|$. We will choose to enlarge the minimal domain by the set with $|u_-| = 0$, so spanned by $\{w\rho^{\tilde{\beta}_l}\psi_l^m\}_{m=-l}^l$. Note that if $Z(p) > -\frac{1}{4}$, we have $l = 0$, so to create a self-adjoint extension of $A = \rho^{1/2}H_{\mathbf{k}}\rho^{-1/2}$, we only need to expand the minimal domain by the span of $w\rho^\eta = w\rho^{\sqrt{1/4+Z(p)}}$.

Next consider the case when $\tilde{\beta}_l = 0$. In this case we get

$$\hat{w}(\sigma) = \frac{\Phi(\sigma)}{\sigma} \quad \text{and} \quad \widehat{w\log\rho} = \frac{\Phi(\sigma)}{\sigma^2} - \frac{\Phi'(\sigma)}{\sigma}.$$

Carrying out the loop integral in this case, we arrive at the equation

$$[u_l, v_l]_A = k(u_+ \bar{v}_- + u_- \bar{v}_+).$$

Again setting $[u_l, u_l]_A = 0$, we arrive this time at the condition $u_+ \bar{u}_- \in i\mathbb{R}$. So we may this time again choose to fix $u_- = 0$ and enlarge the minimal domain by the set spanned by $\{w\psi_l^m\}_{m=-l}^l$.

Finally, consider the case when $\tilde{\beta}_l = ia$. This time we get the equation

$$[u_l, v_l]_A = k(u_+ \bar{v}_+ - u_- \bar{v}_-).$$

Setting $[u_l, u_l] = 0$ we arrive at the condition $|u_+| = |u_-|$. We can choose $u_+ = 1$ and $u_- = -1$ to get a self-adjoint condition by enlarging the minimal domain by the set spanned by $\{w \cos(a \log \rho)\psi_l^m\}_{m=-l}^l$.

In order to get back to the corresponding choice of self-adjoint extension of $H_\mathbf{k} - \lambda$, we multiply each basis element by $\rho^{-1/2}$. Since each of these basis functions is in $\rho^\mu L^2(\mathbb{T})$ for all $\mu < 1$, overall we find that $\mathcal{D}(H) \subset \rho^\mu L^2(\mathbb{T})$ for all $\mu < 1$. This completes the proof of Theorem 1.1. $\qquad\square$

2.2. Some corollaries.

We now prove some consequences of Theorem 2.3. First, its proof implies the following stronger result:

Corollary 2.4. *If $\eta_0 > 0$, then $\mathcal{D}(H_\mathbf{k}) \subset H^2(\mathbb{T}) \cap \rho^\epsilon C^0(\mathbb{T})$, for some $\epsilon > 0$.*

We now deduce Corollary 1.2 from Theorem 1.1 and its proof. This corollary is specific to the periodic case.

Proof. (of Corollary 1.2). The extension of $H_\mathbf{k}$ is self-adjoint, hence has real spectrum, so we get that for $\lambda \notin \mathbb{R}$, the operator

$$\lambda - H_\mathbf{k} : \mathcal{D}(H_\mathbf{k}) \to L^2(\mathbb{T})$$

is a bounded invertible operator with bounded inverse $Q_{\mathbf{k},\lambda}$, which is the resolvent of $H_\mathbf{k}$ at λ. By Theorem 1.1, by the definition of the weighted Sobolev spaces $\mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S})$, and by the b-Rellich lemma [3, 33], we have for some $\epsilon > 0$ that

$$\mathcal{D}(H_\mathbf{k}) \subset \mathcal{K}_\epsilon^2(\mathbb{T} \smallsetminus \mathcal{S}) \Subset L^2(\mathbb{T}).$$

(Recall that $\Subset$ means "compactly embedded".) Thus for $\lambda \notin \mathbb{R}$, the resolvent of $H_\mathbf{k}$,

$$\mathcal{R}_\lambda(H_\mathbf{k}) : L^2(\mathbb{T}) \to L^2(\mathbb{T})$$

is a compact operator. By standard results of functional analysis, if a self-adjoint operator has compact resolvent, then L^2 has a complete orthonormal basis consisting of eigenfunctions for this operator. $\qquad\square$

2.3. Singular functions expansion.

To prove Theorem 1.3, we again use results of the b-calculus, this time primarily from [33]. Again, we prove a more general statement that does not require the Assumption 2. Let ν_0 be as in Equation (12).

Theorem 2.5. *Assume $\mathcal{S} = \{p\}$ and $Z := \rho^2 V$ satisfies Assumption 1. Assume $H_{\mathbf{k}} u = \lambda u$ where $u \in \mathcal{D}(H_{\mathbf{k}})$. Then for any $m \in \mathbb{Z}_+$ and any $\nu < \nu_0$,*

$$u \in \mathcal{K}_\nu^m(\mathbb{T} \smallsetminus \mathcal{S}).$$

Further, near each $p \in \mathcal{S}$, where $Z(p) \neq (l + 1/2)^2$ for any $l \geq 0$, u has a complete (though not unique) expansion of the form:

$$(25) \qquad u = u_0 + \sum \rho^\gamma g_\gamma, \quad \gamma \in \mathcal{I}_{Z(p)}, \ \Re(\gamma) > -1/2,$$

where the formula for $\mathcal{I}_{Z(p)}$ is given in Equation (27) below, u_0 is smooth up to $\rho = 0$ in polar coordinates and vanishes to all orders there, hence is in fact smooth on $\mathbb{T}$ and vanishes to all orders at p, and the coefficient functions g_γ are smooth functions on S^2. Under the additional Assumption 2, when $Z(p) > -1/4$, the first coefficient $g_{\eta-1/2}$ is a constant function.

Proof. Any eigenfunction u of $H_{\mathbf{k}}$ must be in its domain, thus in $\mathcal{K}_\nu^2(\mathbb{T} \smallsetminus \mathcal{S})$ for all $\nu < \nu_0$. Our first goal is to improve the degree of smoothness from 2 to m for $m \in \mathbb{N}$. To do this, we use the fact that any $\lambda \in \mathbb{C}$, the operator $H_{\mathbf{k}} - \lambda$ is Fredholm as a map between weighted Sobolev spaces:

$$(26) \qquad H_{\mathbf{k}} - \lambda : \mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S}) \to \mathcal{K}_{a-2}^{m-2}(\mathbb{T} \smallsetminus \mathcal{S})$$

for all $a \in \mathbb{R}$ such that $a \notin \cup_{l \in \mathbb{Z}_{\geq 0}} \{\beta_{l,p} + \frac{3}{2}, \alpha_{l,p} + \frac{3}{2}\} = \mathrm{Spec}_b(H_{\mathbf{k}}) + 3/2$. By general b-calculus theory, the set $\mathrm{Spec}_b(H_{\mathbf{k}})$ is a discrete subset of $\mathbb{C}$ and furthermore, for any γ_0 and η, it has only a finite number of elements in the strip $\gamma_0 \leq \Re(z) \leq \eta$. Thus for any ν_0, there exist arbitrarily close $\nu < \nu_0$ such that the condition on a is satisfied for $a = \nu + 2s$, where $s \in \mathbb{N}$. Together with standard bootstrapping arguments, this allow us to improve the regularity of eigenfunctions of $H_{\mathbf{k}}$ in terms of weighted Sobolev spaces to $\mathcal{K}_\nu^m(\mathbb{T} \smallsetminus \mathcal{S})$ for all m and $\nu < \nu_0$.

Next, to obtain the expansion in 1.3 we use a general result in the b-calculus literature, see eg [33], that implies that any $u \in \cup_{m,a} \mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S})$ which is an eigenfunction for $H_{\mathbf{k}}$ in some weighted $L^2(\mathbb{T})$ in fact has much stronger regularity: it polyhomogeneous in ρ near each $p \in \mathcal{S}$ with index set $\mathcal{I}_{Z(p)}$. If $Z(p) \notin \{-(l + \frac{1}{2})^2\}_{l=0}^\infty$ (for instance if $Z(p) > -1/4$), then the index set is simply a set of complex numbers that is finite in any strip $\gamma_0 \leq \Re(z) \leq \eta$:

$$(27) \qquad \mathcal{I}_{Z(p)} = \bigcup_{n=0}^\infty \{\beta_{l,p} + n, \alpha_{l,p} + n\}_{l \in \mathbb{Z}_{\geq 0}}.$$

This means that around each $p \in \mathcal{S}$, there exist smooth coefficient functions $g_\gamma \in \mathcal{C}^\infty(S^2)$ such that for all N,

$$(28) \qquad u_N := u - \sum \rho^\gamma g_\gamma \in \rho^N \mathcal{C}^N(\overline{\mathbb{T} \smallsetminus \mathcal{S}}), \quad \gamma \in \mathcal{I}_{Z(p)} \Re(\gamma) \leq N$$

that is, u_N is N times continuously differentiable up to $\rho = 0$ in polar coordinates at p and in these coordinates, vanishes with all of its derivatives up to order ρ^N there. We take the limit in the topology of the smallest $\mathcal{K}_a^m$ to which u belongs.

If $Z(p) \neq -(l+\frac{1}{2})^2$ for any $l \geq 0$ and if $u \in L^2(\mathbb{T})$, when we let $N \to \infty$, we find that

$$u = u_0 + \sum \rho^\gamma g_\gamma, \quad \gamma \in \mathcal{I}, \Re(\gamma) > -1/2,$$

where u_0 is smooth up to $\rho = 0$ in polar coordinates and vanishes to all orders there, hence is in fact smooth on $\mathbb{T}$ and vanishes to all orders at p.

Since the set of γ that appear in this expansion is discrete in $\mathbb{R}$, we get that the smallest exponent that appears will in fact be somewhat better than $-3/2$. This first exponent will be ν_0 if $Z(p) \leq 3/4$. If $Z(p) > 3/4$, then eigenfunctions will in fact be in a space with higher weight than $\mathcal{K}_2^2(\mathbb{T} \smallsetminus \mathcal{S})$: the weight will be $1 + \sqrt{Z(p) + 1/4}$.

Finally, we can note that the terms of the expansion of an eigenfunction for $H_{\mathbf{k}}$ that are not in $\mathcal{K}_2^2(\mathbb{T} \smallsetminus \mathcal{S})$ will be of the forms determined in the proof of Theorem 1.1 (see, eg [19] for a proof). So, for instance, if $Z(p) \geq -1/4$, the leading term of any eigenfunction u will be constant in S^2, and u minus its leading term will vanish at p. Further, if $Z(p) \geq -1/4$, then the exponents γ will all be real numbers. Thus we obtain:

$$(29) \qquad u = u_0 + \rho^{\eta - \frac{1}{2}} g_{\eta - 1/2} + \sum \rho^\gamma g_\gamma, \quad \gamma \in \mathcal{I}_{Z(p)} \gamma > \eta - 1/2,$$

where $g_{\eta - 1/2}$ a constant. This completes the proof of Theorem 1.3. $\qquad \square$

3. INVERTIBILITY

In this section we prove the boundedness and invertibility result in Theorem 1.4. From now on, we require both Assumptions 1 and 2 to be satisfied by our potential V.

3.1. **Preliminary results.** We begin with a few standard results lemma.

Lemma 3.1. *Let $m, a \in \mathbb{R}$. Then*

(i) For any $f \in \mathcal{C}^\infty(\overline{\mathbb{T} \smallsetminus \mathcal{S}})$, the multiplication map

$$\mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S}) \ni u \to fu \in \mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S}) = \rho^{a-3/2} H_b^m(\mathbb{T} \smallsetminus \mathcal{S})$$

is continuous for all $m \in \mathbb{Z}_+$ and all $a \in \mathbb{R}$.
(ii) The operator $H_{\mathbf{k}} - \lambda$ maps $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S})$ to $\mathcal{K}_{a-1}^{m-1}(\mathbb{T} \smallsetminus \mathcal{S})$ continuously.
(iii) The operator $\rho^{-1} B_{\mathbf{k}, \lambda}$ maps $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S})$ to $\mathcal{K}_a^m(\mathbb{T} \smallsetminus \mathcal{S})$ continuously.
(iv) $\rho^{-1} B_{\mathbf{k}, \lambda} : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S}) \to \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \smallsetminus \mathcal{S})$ is compact.

Proof. The simple proofs of these results are the same as that of the analogous results in [23], and follow directly from properties of b-operators [3, 33, 30]. $\qquad \square$

We also need the following standard lemma (again, see [23] for its proof).

Lemma 3.2. *Let $a \in \mathbb{R}$ be arbitrary and assume that $u \in \mathcal{K}_{1+a}^2(\mathbb{T} \smallsetminus \mathcal{S})$ and that $v \in \mathcal{K}_{1-a}^2(\mathbb{T} \smallsetminus \mathcal{S})$. Then $(\Delta u, v) + (\nabla u, \nabla v) = 0$.*

We shall also need the following consequence of the general properties of the b-calculus [33, 39].

Proposition 3.3. *Let us fix $\lambda \in \mathbb{C}$ and $a \notin \{\tilde{\beta}_{l,p}, \tilde{\alpha}_{l,p}\} = \cup_{l \in \mathbb{Z}_{\geq 0}}\{\beta_{l,p} + \frac{1}{2}, \alpha_{l,p} + \frac{1}{2}\}$. Let N be the number of elements in the set $\{\tilde{\beta}_{l,p}, \tilde{\alpha}_{l,p}\}$ that are between 0 and a, counted with multiplicity. Then the operator $H_{\mathbf{k}} - \lambda$ is Fredholm as a map between weighted Sobolev spaces:*

$$H_{\mathbf{k}} - \lambda : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \smallsetminus \mathcal{S}) \to \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \smallsetminus \mathcal{S})$$

and has index $-N$ if $a > 0$, respectively N if $a < 0$.

Proof. We consider again the operator $P_{0,0} = \rho(H_{\mathbf{k}} - \lambda)\rho$, which is a b-differential operator. It is unitarily equivalent to $\rho^{1/2}P_{0,0}\rho^{-1/2}$ acting on b-Sobolev spaces (see the proof of Theorem 2.3), which has $\{\tilde{\beta}_{l,p}, \tilde{\alpha}_{l,p}\}$ as a b-spectrum. The result then follows from the characterization of Fredholm b-differential operators [33, 27, 28].

It remains to determine the index of $H_{\mathbf{k}} - \lambda$. Let m_a be the index of the operator for a fixed value of a. Then it is a standard result that $m_a - m_b$ is given by the number of singular functions with exponent between a and b [27, 33, 39, 35]. This is enough to complete the proof. $\square$

See [22] for an extension of this result and for more details.

Now recall the Hardy inequality, which states that

$$(30) \qquad \int_{\mathbb{R}^N} r^{-2}|u(x)|^2 dx \leq (2/(N-2))^2 \int_{\mathbb{R}^N} |\nabla u(x)|^2 dx$$

for any $u \in H^1(\mathbb{R}^N)$, $N \geq 3$, where r is the distance to the origin [15]. We can use this to prove the following important lemma. To simplify notation, after the lemma statement, we shall let $(u,v) := (u,v)_{L^2(\mathbb{T})}$.

Lemma 3.4. *There are constants $C, \gamma > 0$ such that for any $u \in \mathcal{K}_1^1(\mathbb{T} \smallsetminus \mathcal{S})$,*

$$(H_{\mathbf{k}}u, u)_{L^2(\mathbb{T})} + C(u,u)_{L^2(\mathbb{T})} \geq \gamma(u,u)_{\mathcal{K}_1^1(\mathbb{T}\smallsetminus\mathcal{S})} := \gamma \int_{\mathbb{T}} \left(\rho^{-2}|u(x)|^2 + |\nabla u(x)|^2\right)dx.$$

Proof. For an operator $T : \mathcal{K}_1^1(\mathbb{T} \smallsetminus \mathcal{S}) \to \mathcal{K}_{-1}^{-1}(\mathbb{T} \smallsetminus \mathcal{S})$, we shall write $T \geq 0$ if $(Tu, u) \geq 0$ for all $u \in \mathcal{K}_1^1(\mathbb{T} \smallsetminus \mathcal{S})$. Now let $\phi \geq 0$ be a smooth functionon $\mathbb{T}$ that is equal to 1 in a small neighborhood of $\mathcal{S}$ and has support on the set where $\rho(x)$ is given by the distance to $\mathcal{S}$ and let $V_0(x) = Z(p)\phi(x)\rho^{-2}(x)$ for x in the support of ϕ and close to $p \in \mathcal{S}$. Outside the support of ϕ, we let $V_0 = 0$. Then Hardy's inequality applied to $\phi^{1/2}u$, which we can think of as living now on $\mathbb{R}^3$ rather than $\mathbb{T}$, gives

$$(31) \qquad \left(\phi^{1/2}(-\Delta + zV_0)\phi^{1/2}u, u\right) \geq 0 \quad \text{and} \quad \left(\phi^{1/2}(-\Delta)\phi^{1/2}u, u\right) \geq 0.$$

We can think of this as saying that the most singular part of the operator $H_{\mathbf{k}}$, that is, $T = \phi^{1/2}(-\Delta + zV_0)\phi^{1/2}$, satisfies $T \geq 0$. We will prove Lemma 3.4 by decomposing the operator $H_{\mathbf{k}} + C$ as a sum of four operators

$$H_{\mathbf{k}} = T_1 + T_2 + T_{3,C} + T_{4,C},$$

which we will show are all bounded from below for sufficiently large C.

Recall we can write

$$H_{\mathbf{k}} = -\Delta + V_0 + V_1 + \rho^{-1}B_{\mathbf{k},0},$$

where $V_1 := V - V_0$ satisfies $\rho V_1 \in C(\mathbb{T})$ and $\rho^{-1}B_{k.0}$ is a first order differential operator over $\mathbb{T}$ with smooth coefficients.

Assumption 2 and Equation (31) imply that for $\epsilon < 1$, the operator

$$(32) \qquad\qquad T_1 := (1 - \epsilon)T \geq 0.$$

Fix any suitable value for $\epsilon > 0$. Then we can write $H_{\mathbf{k}} + C$ in terms of T_1 by decomposing in terms of the multiplication operators $\phi^{1/2}$ and $(1 - \phi^{1/2})$:

$$(33) \qquad H_{\mathbf{k}} + C = \epsilon T + T_1 - \psi^{1/2}\Delta\psi^{1/2} - (1 - \phi^{1/2})\Delta(1 - \phi^{1/2}) + V_1 + R_1,$$

where R_1 is a first order differential operator with smooth coefficients and $\psi = 2\phi^{1/2}(1 - \phi^{1/2})$.

Let $T_2 := -\psi^{1/2}\Delta\psi^{1/2} - (1 - \phi^{1/2})\Delta(1 - \phi^{1/2})$. Then $T_2 \geq 0$ by the Hardy equality applied to $\psi^{1/2}u$ and to $(1 - \phi^{1/2})u$. Define $T_3 := -\epsilon\Delta + R_1 + C/2$ and $T_4 = \epsilon\phi\rho^{-2} + V_1 + C/2$. We claim that for C large enough, $T_3 \geq 0$ and $T_4 \geq 0$, which will prove the result.

The proof that $T_4 \geq 0$ for $C >> 0$ follows from a straightforward calculation minimising the function $\epsilon\phi\rho^{-2} + V_1$. The proof that $T_3 \geq 0$ for $C >> 0$ is basically the same as the proof that a Schrödinger operator with periodic Coulumb type potential is bounded below. This is proved, for example, in [23]. $\qquad\square$

Note that the above lemma implies that $H_{\mathbf{k}}$ is bounded from below as an operator $\mathcal{K}_1^1(\mathbb{T}\setminus\mathcal{S}) \to \mathcal{K}_{-1}^{-1}(\mathbb{T}\setminus\mathcal{S})$, which is the special case of Theorem 1.4 when $m = a = 0$. In addition, if we define the form $\alpha(u,v) := ((H_{\mathbf{k}} + C)u, v)$, where the right-hand side is the natural pairing between elements of $\mathcal{K}_{-1}^{-1}$ and $\mathcal{K}_1^1$, then this lemma implies that $\alpha(u,v)$ satisfies the assumptions of the Lax-Milgram lemma for the vector space $V = \mathcal{K}_1^1(\mathbb{T}\setminus\mathcal{S})$. This and Céa's lemma imply that for any element $u \in \mathcal{K}_1^1(\mathbb{T}\setminus\mathcal{S})$ and any finite dimensional subspace $V \subset \mathcal{K}_1^1(\mathbb{T}\setminus\mathcal{S})$ we can construct a unique (Galerkin) approximation $u_V \in V$ for u that, up to a multiple independent of u, is the best approximation for u in V.

If we could also use the $\mathcal{K}_1^1$ norm in our approximation results, we would now have the necessary tools to prove it. However, we need to use the slightly smaller space $\mathcal{K}_{a+1}^1$ instead. Thus we the stronger result, Theorem 1.4 to ensure the Lax-Milgram theorem and Céa's lemma apply to the analogous form on these spaces.

We shall also need the following regularity result.

Proposition 3.5. *Let $a, \lambda \in \mathbb{R}$, $m \in \mathbb{Z}_+$. There exists a constant $C > 0$ such if $u \in \mathcal{K}_{a+1}^1(\mathbb{T}\setminus\mathcal{S})$ and $(\lambda + H_{\mathbf{k}})u \in \mathcal{K}_{a-1}^{m-1}(\mathbb{T}\setminus\mathcal{S})$ then $u \in \mathcal{K}_{a+1}^{m+1}(\mathbb{T}\setminus\mathcal{S})$ and*

$$\|u\|_{\mathcal{K}_{a+1}^{m+1}} \leq C\big(\|(\lambda + H_{\mathbf{k}})u\|_{\mathcal{K}_{a+1}^{m+1}} + \|u\|_{\mathcal{K}_{a+1}^1}\big).$$

Proof. We consider again the operator $P_{0,0} = \rho(H_{\mathbf{k}} - \lambda)\rho$, which is a b-differential operator. Our result then follows from the regularity for b-pseudodifferential operators [33, 3]. $\qquad\square$

We now complete the proof of Theorem 1.4 as follows.

Proof. (of Theorem 1.4). As in [31], by regularity for b-differential operators, if we prove our result for $m = 0$, then the regularity result of Proposition 3.5 implies it for all $m \geq 0$. We shall thus assume $m = 0$ and focus on extending Lemma 3.4, where $a = 0$, to the case when $|a| < \eta$.

Fix C as in Lemma 3.4. Let $D_a := C + H_{\mathbf{k}} : \mathcal{K}^1_{a+1}(\mathbb{T} \setminus \mathcal{S}) \to \mathcal{K}^{-1}_{a-1}(\mathbb{T} \setminus \mathcal{S})$, that is to say, $C + H_{\mathbf{k}}$ with fixed domain and range. As usual, we may identify the dual of $\mathcal{K}^1_b(\mathbb{T} \setminus \mathcal{S})$ with the space $\mathcal{K}^{-1}_{-b}(\mathbb{T} \setminus \mathcal{S})$ using the L^2-inner product. Then using the symmetry of $H_{\mathbf{k}}$, we find that $D_a^* = D_{-a}$.

By Lemma 3.4, the operator D_0 is invertible. By basic results in b-calculus, D_a is Fredholm for $|a| < \eta$ since the weighted spaces in its domain and range do not correspond to an indicial root as calculated in the previous section (see Proposition 3.3). Hence, for such a, the family $\rho^a D_a \rho^{-a}$ is a continuous family of Fredholm operators between the same pair of spaces. Since index is constant over such families, we have that $\mathrm{ind}(D_a) = 0$ for all $0 \leq a < \eta$. We want to know these operators are all isomorphisms. By the index calculation, it now suffices to show they are all injective.

The inclusion $\mathcal{K}^1_{a+1}(\mathbb{T} \setminus \mathcal{S}) \subset \mathcal{K}^1_1(\mathbb{T} \setminus \mathcal{S})$ allows us to compute $(D_a u, u) = (\nabla u, \nabla u) + (u, u)$ for $u \in \mathcal{K}^1_{a+1}(\mathbb{T} \setminus \mathcal{S})$, by Lemma 3.2. Assume $D_a u = 0$, then $(D_a u, u) = 0$, and hence $u = 0$. This implies that the operator D_a is injective for $0 \leq a < \eta$. Since it is Fredholm of index zero, it is also an isomorphism. This proves our result for $0 \leq a < \eta$. To prove the result for $-\eta < a \leq 0$, we take adjoints and use $D_a = (D_{-a})^*$.

By the characterization in [17] of the Friedrichs extension of a b-operator which is bounded below, we can see that the extension we constructed in Theorem 1.1 is in fact the Friedrichs extension of $H_{\mathbf{k}}$. The proof of Theorem 1.4 is now complete. $\square$

The fact that the domain of the Friedrichs extension is $(C - H_{\mathbf{k}})^{-1}(L^2(\mathbb{T} \setminus \mathcal{S}))$ and the theorem we have just proved give us a second way to identify the domain of the Friedrichs extension of $H_{\mathbf{k}}$. Following the method of [23], we see that when $H_{\mathbf{k}}$ is Fredholm on $\mathcal{K}^2_2(\mathbb{T} \setminus \mathcal{S})$, the domain of the Friedrichs extension of $H_{\mathbf{k}}$ consists of the span of $\mathcal{K}^2_2(\mathbb{T} \setminus \mathcal{S})$ and of the singular functions that are in $\mathcal{K}^1_1(\mathbb{T} \setminus \mathcal{S})$ but are not in $\mathcal{K}^2_2(\mathbb{T} \setminus \mathcal{S})$. This can be used to obtain an alternative proof of Theorem 1.1 if V satisfies both Assumptions 1 and 2, as follows.

Proposition 3.6. *Let C_0 be as in Theorem 1.4 and W_s be as in Equation (14). Assume the set $\{\tilde{\beta}_{l,p}, \tilde{\alpha}_{l,p}\}$ does not contain 1. Then for $\lambda > C_0$, the map*

$$\lambda + H_{\mathbf{k}} : \mathcal{K}^{m+1}_2(\mathbb{T} \setminus \mathcal{S}) + W_s \to \mathcal{K}^{m-1}_0(\mathbb{T} \setminus \mathcal{S})$$

is an isomorphism.

Proof. Let $T := \lambda + H_{\mathbf{k}}$ with the indicated domain and codomain. Proposition 3.3 shows that T is Fredholm with index zero. Since

$$\mathcal{K}^{m+1}_2(\mathbb{T} \setminus \mathcal{S}) + W_s \subset \mathcal{K}^1_1(\mathbb{T} \setminus \mathcal{S}),$$

Theorem 1.4 shows that T is injective. Hence it is also surjective, hence an isomorphism. $\square$

4. Extensions and numerical tests

We now discuss the extension to the non-compact case and indicate some applications to numerical methods.

4.1. **The non-compact case.** Most of our results in the previous sections extend to the non-compact case. Let $\overline{\mathbb{R}^3}_{rad}$ be the radial compactification of $\mathbb{R}^3$. We assume that the set of singular points $\mathcal{S} \subset \mathbb{R}^3$ is finite and we replace each of the points in $\mathcal{S}$ with a two-sphere (that is, we blow up the singular points). Let $\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad}$ denote the resulting compact manifold with boundary. By ρ we denote a continuous function $\rho : \mathbb{R}^3 \to [0, 1]$ that is smooth outside $\mathcal{S}$, close to each $p \in \mathcal{S}$ it has the form $\rho(x) = |x - p|$, and it is constant equal to 1 outside a compact set. (Thus the difference with the function ρ considered in the periodic case is that now ρ is constant equal to 1 in a neighborhood of infinity.) Then in the non-compact case, our Assumption 1 on $Z := \rho^2 V$ is replaced with

(34)   **Assumption** $1'$: $Z := \rho^2 V \in \mathcal{C}^\infty(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad}) \cap \mathcal{C}(\mathbb{R}^3).$

Assumption 2 remains unchanged.

We consider now $H = -\Delta + V$ instead of the restrictions $H_\mathbf{k}$. Assumptions $1'$ and 2 allow us to extend to H all the results for $H_\mathbf{k}$ of the previous sections, except Corollary 1.2 and Proposition 3.3. The weighted Sobolev spaces $\mathcal{K}_a^m(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad})$ are defined in the same way (but using the new function ρ).

Let b_e the infimum of V on the sphere at infinity. Then Corollary 1.2 must be replaced with the following characterization of the essential spectrum $\sigma_e(H)$ of H:

(35) $\sigma_e(H) = [b_e, \infty).$

To prove this result, one needs also the Fredholm conditions for operators in the scattering or SG calculus [28, 34, 38, 37]. Then in Proposition 3.3 one has to take $\lambda < b_e$. Of course, in Theorem 1.4 one will have $C_0 > -b_e$.

However, in the non-compact case, for applications to numerical methods, our results on eigenvalues and eigenfunctions must be complemented by decay properties at infinity. The following is proved as in [2], Theorem 4.4. See also [1, 24, 25]. Let $r : \mathbb{R}^3 \to \mathbb{R}$ be a smooth function such $r(x) = |x|$ for x outside a compact set.

Theorem 4.1. *Let V be a potential satisfying Assumptions $1'$ and 2. Also, let $0 < \epsilon < V(x) - \lambda$ for x outside a compact set and be u an eigenvector of $H_\mathbf{k}$ corresponding to λ. Then $e^{\epsilon r} u \in \mathcal{K}_\nu^m(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad}).$*

Under Assumptions $1'$ and 2, a perturbation argument further yields following result on the decay properties of the eigenfunctions and the solutions of the equation $(C + H_\mathbf{k})u = f$.

Theorem 4.2. *Let us assume that $C + H_\mathbf{k} : \mathcal{K}_1^1(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad}) \to \mathcal{K}_{-1}^{-1}(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad})$ is invertible (which is the case if $C > C_0$, with C_0 as in Theorem 1.4), then for $|a|$ and $|\epsilon|$ small*

$$C + H_\mathbf{k} : e^{\epsilon r} \mathcal{K}_{a+1}^{m+1}(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad}) \to e^{\epsilon r} \mathcal{K}_{a-1}^{m-1}(\overline{(\mathbb{R}^3 \setminus \mathcal{S})}_{rad})$$

is again invertible.

Proof. The proof uses the same arguments used in the proof of Theorem 1.4, the continuity of the family $e^{\epsilon r} H_{\mathbf{k}} e^{-\epsilon r}$ in ϵ, and the regularity result 3.5. $\qquad\square$

4.2. **Applications and numerical tests.** Let u be an eigenvector of $H_{\mathbf{k}}$ or the solutions of equations of the form $(\lambda + H_{\mathbf{k}})u = f$, with f smooth enough. Our results give smoothness properties for u. They also give decay properties of u in the non-periodic case. These properties, in turn, can be used to obtain approximation properties of u. Standard numerical methods results (Cea's lemma or the results reviewed in [6]) then lead to error estimates in the Finite Element Method for the numerical solutions of the equation $(C + H_{\mathbf{k}})u = f$ or for the eigenfunctions of $H_{\mathbf{k}}$. We have tested these approximation results in the periodic case using, first, a graded mesh and, second, augmented plane waves. In both cases, the tests are in good agreement with our theoretical results. These numerical and the needed approximation results will be discussed in full detail in the second part of our paper [21].

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