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Analysis of periodic Schrödinger operators: Regularity and approximation of eigenfunctions

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Let V be a real valued potential that is smooth everywhere on $\mathbb{R}^3$, except at a periodic, discrete set $\mathcal{S}$ of points, where it has singularities of the Coulomb-type Z/r . We assume that the potential V is periodic with period lattice $\mathcal{L}$. We study the spectrum of the Schrödinger operator $H = -\Delta + V$ acting on the space of Bloch waves with arbitrary, but fixed, wavevector $\mathbf{k}$. Let $\mathbb{T} := \mathbb{R}^3/\mathcal{L}$. Let u be an eigenfunction of H with eigenvalue λ and let $\epsilon > 0$ be arbitrarily small. We show that the classical regularity of the eigenfunction u is $u \in H^{5/2-\epsilon}(\mathbb{T})$ in the usual Sobolev spaces, and $u \in \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ in the weighted Sobolev spaces. The regularity index m can be as large as desired, which is crucial for numerical methods. For any choice of the Bloch wavevector $\mathbf{k}$, we also show that H has compact resolvent and hence a complete eigenfunction expansion. The case of the hydrogen atom suggests that our regularity results are optimal. We present two applications to the numerical approximation of eigenvalues: using wave functions and using piecewise polynomials. © 2008 American Institute of Physics. [DOI: 10.1063/1.2957940]

I. INTRODUCTION AND STATEMENT OF MAIN RESULTS

Let V be a potential that is a smooth periodic function on $\mathbb{R}^3$ except at a discrete set $\mathcal{S}$, where it has Coulomb-type singularities, that is, for any $p \in \mathcal{S}$, the function $|x-p|V(x)$ is smooth in a neighborhood of p . We are interested in studying the spectrum of Schrödinger operators $H = -\Delta + V$ acting on the space of Bloch waves with Bloch wavevector $\mathbf{k}$ (see below). This question is interesting for the study of the nonrelativistic Born–Oppenheimer approximation of the Schrödinger operator for electrons moving in a lattice of atoms. Modeling electrons moving in a lattice of atoms is part of the implementation of the “density-functional theory” codes in quantum chemistry.^{1–7} We are especially interested in the regularity and approximability of the eigenfunctions u and eigenvalues λ of H .

Let $\mathcal{L} := \{n_1 \mathbf{v}_1 + n_2 \mathbf{v}_2 + n_3 \mathbf{v}_3\} \simeq \mathbb{Z}^3$ be the lattice of periods of V , where $(\mathbf{v}_j)$ is a basis of $\mathbb{R}^3$ and $n_j \in \mathbb{Z}$. Let $\mathbf{k} \in \mathbb{R}^3$. Let us denote by $\mathbf{v} \cdot \mathbf{w}$ the inner product of two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^3$. Then a Bloch wave with Bloch wavevector $\mathbf{k}$ is a measurable function $\psi_{\mathbf{k}}$ satisfying the twisted periodicity condition $\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{\mathbf{k}}(\mathbf{r})$ for all $\mathbf{R} \in \mathcal{L}$. Every Bloch wave $\psi_{\mathbf{k}}$ with Bloch wavevector $\mathbf{k}$ can be written in the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \quad (1)$$

where $u_{\mathbf{k}}$ is a truly periodic function with respect to the lattice $\mathcal{L}$ (so $u_{\mathbf{k}}$ is a Bloch wave with zero Bloch wavevector).

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The function $u_{\mathbf{k}}$ of Eq. (1) identifies with a function on the three dimensional torus $\mathbb{T} := \mathbb{R}^3/\mathcal{L}$, which in turn can be identified with the product $(S^1)^3$ of three circles S^1 . Let $\mathbf{k} = (k_1, k_2, k_3) \in \mathbb{R}^3$ and define

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

Then $H\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} H_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})$. This shows that the study of H on the space of Bloch waves with Bloch wavevector $\mathbf{k}$ is equivalent to the study of $H_{\mathbf{k}}$ on the space of periodic functions on $\mathbb{R}^3$ or, equivalently, to the study of $H_{\mathbf{k}}$ on suitable function spaces on $\mathbb{T}$.

Let us denote by $\mathcal{L}^* := \{\mathbf{w} \in \mathbb{R}^3, \mathbf{w} \cdot \mathbf{v} \in \mathbb{Z}, \forall \mathbf{v} \in \mathcal{L}\} \simeq \mathbb{Z}^3$ the *dual lattice of $\mathcal{L}$* . Then to find all eigenvalues and eigenfunctions for the Schrödinger operator H , it is enough to solve this problem for operators $H_{\mathbf{k}}$ corresponding to vectors $\mathbf{k}$ in a fundamental domain for $\mathcal{L}^*$, for instance, to the first Brillouin zone. However, this is not an essential point for our purposes in this paper.

Our results are formulated using both the usual Sobolev spaces $H^m(\mathbb{T})$ and the weighted Sobolev spaces $\mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S})$ of periodic functions. Let $m \in \mathbb{Z}_+ := \{0, 1, 2, \dots\}$. Then

$$H^m(\mathbb{T}) := \left\{ v: \mathbb{T} \rightarrow \mathbb{C}, \sum_{\xi} (1 + |\xi|)^{2m} |\hat{v}(\xi)|^2 < \infty \right\} = \{v, \partial^\alpha v \in L^2(\mathbb{T}), \forall |\alpha| \leq m\}, \quad (3)$$

where $\xi \in \mathcal{L}^*$ and $\hat{f}(\xi) = \int_{\mathbb{T}} e^{i\xi \cdot x} f(x) dx$ is the (unnormalized) Fourier transform. Note that we can extend this definition to all $m \in \mathbb{R}$ if we take $v \in C^\infty(\mathbb{T})'$, the space of distributions on $\mathbb{T}$.

Let us denote by $\mathcal{S}$ the set of points in $\mathbb{T} \simeq (S^1)^3$ where V has singularities. Let $a \in \mathbb{R}$ and $\rho: \mathbb{T} \rightarrow [0, 1)$ be a continuous function such that $\rho(x) = |x - p|$ for x close to $p \in \mathcal{S}$ and such that ρ is smooth and > 0 on $\mathbb{T} \setminus \mathcal{S}$. The function ρ will play an important role in what follows. We shall say that a function $F: \mathbb{T} \rightarrow \mathbb{R}$ is *smooth in polar coordinates* around $p \in \mathcal{S}$ if $F(\rho x')$ is a smooth function of $(\rho, x') \in [0, \infty) \times S^2$ in a generalized polar coordinate system (ρ, x') defined close to p . A basic condition that we shall impose on a potential V is that ρV be a smooth function in polar coordinates near each singular point $p \in \mathcal{S}$. A potential that satisfies this condition will be said to *satisfy Assumption 1*. A typical Coulomb potential will thus satisfy Assumption 1.

The function ρ is also needed in the definition of our weighted Sobolev spaces. Thus the m th *weighted Sobolev space with index a* of periodic functions on $\mathbb{R}^3$ is given by

$$\mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S}) := \{v: \mathbb{T} \setminus \mathcal{S} \rightarrow \mathbb{C}, \rho^{|\alpha| - a} \partial^\alpha v \in L^2(\mathbb{T}), \forall |\alpha| \leq m\}. \quad (4)$$

The difference between the two classes of Sobolev spaces is thus only the appearance of the weight function ρ , although this makes comparisons between the two spaces complicated, except when $m=0$. We discuss the relationship between these spaces further in Sec. V.

In this first paper of a series, we investigate the immediate consequences of the theory of singular functions and totally characteristic differential operators for the study of $H_{\mathbf{k}}$. In spite of the obvious connections between singular functions and totally characteristic differential operators on one side and Schrödinger operators of the form $H_{\mathbf{k}}$ on the other side, this approach seems not to have been pursued before. The first results of this paper are a pair of regularity estimates. The first theorem is a regularity result for the eigenfunctions of $H_{\mathbf{k}}$ itself.

Theorem 1.1: *Let us assume that ρV is a smooth function of ρ and $x' \in S^2$ in polar coordinates near each singular point $p \in \mathcal{S}$, that is, V satisfies Assumption 1. Let us fix $\mathbf{k} \in \mathbb{R}^3$, $m \in \mathbb{Z}_+$, and $\epsilon > 0$. Let $H_{\mathbf{k}} u = \lambda u$, $u \in L^2(\mathbb{T})$, be an eigenvalue of $H_{\mathbf{k}}$. Then*

$$u \in H^{5/2 - \epsilon}(\mathbb{T}) \cap \mathcal{K}_{3/2 - \epsilon}^m(\mathbb{T} \setminus \mathcal{S}). \quad (5)$$

Moreover, for any $p \in \mathcal{S}$, the eigenfunction u has a complete Taylor-type expansion in ρ near p with coefficients in smooth functions on the 2-sphere S^2 , where the degree zero term ϕ_0 is a constant function. More precisely,

$$u(p + \rho x') - \sum_{k=0}^N \rho^k \phi_k(x') \in \mathcal{K}_{5/2-N-\epsilon}^\infty(V_p \setminus \mathcal{S}) \subset H^{5/2+N-\epsilon}(V_p) \quad (6)$$

in a small neighborhood V_p of p , for suitable $\phi_k \in C^\infty(S^2)$; that is, u is smooth in polar coordinates (ρ, x') near each p .

Let H' be the hydrogen atom Schrödinger operator. Then the ground state u_0 of H' is given by $u_0 = Ce^{-c\rho}$ for suitable constants C and c . Consequently, $u_0 \in H^{5/2-\epsilon}(\mathbb{R}^3) \cap \mathcal{K}_{3/2-\epsilon}^m(\mathbb{R}^3)$ for any $\epsilon > 0$, but $u_0 \notin H^{5/2}(\mathbb{R}^3)$ and $u_0 \notin \mathcal{K}_{3/2}^m(\mathbb{R}^3)$. This suggests that our results are optimal. The above theorem can also be used to rigorously justify the usual expansion of the eigenfunctions of the hydrogen atom in terms of spherical harmonics. It is the generalization of this expansion in terms of spherical harmonics for more general potentials that are not radially symmetric. We anticipate that this result can be used to obtain a generalization of Kato's "cusp theorem".⁸

In practice, to estimate the eigenvalues and their eigenfunctions for many electron atoms or molecules numerically, it is common to use the Hartree–Fock method or the density-functional method.⁹ The Hartree–Fock method involves some recursively defined potentials in equations similar to those considered in Theorem I.1. However, the recursively defined potentials are not as regular as the potential in the original equation. Our second regularity result concerns eigenfunctions of Schrödinger operators with these slightly less regular potentials arising in the iterations of the Hartree–Fock and density-functional methods. Before we can state it, we need to make some definitions.

Let us denote by

$$W^{\infty}(\mathbb{T} \setminus \mathcal{S}) := \{v \in C^\infty(\mathbb{T} \setminus \mathcal{S}), \rho^{|\alpha|} \partial^\alpha v \in L^\infty(\mathbb{T} \setminus \mathcal{S}), \forall \alpha \in \mathbb{Z}_+^3\}, \quad (7)$$

where $\mathcal{S} \subset \mathbb{T}$ is the set of points where the potential V may have singularities, as before. Note that Coulomb-type potentials satisfy $\rho V \in W^{\infty}(\mathbb{T} \setminus \mathcal{S})$. This property of V is referred to in this paper by saying that V satisfies Assumption 2. Clearly, a potential satisfying Assumption 1 will also satisfy Assumption 2.

Now we can state our regularity results for the eigenfunctions of Schrödinger operators as above, but with Coulomb-type potentials instead of the more regular potentials considered in Theorem I.1. The next theorem also guarantees that the potentials that arise in the Hartree–Fock method are always of this form.

Theorem I.2: *Let us assume that $\rho V \in W^{\infty}(\mathbb{T} \setminus \mathcal{S})$, that is, the potential V satisfies Assumption 2. Let us fix $\mathbf{k} \in \mathbb{R}^3$, $m \in \mathbb{Z}_+$, and $\epsilon > 0$. Let $H_{\mathbf{k}} u = \lambda u$, $u \in L^2(\mathbb{T})$, be an eigenvalue of $H_{\mathbf{k}}$. Then*

$$u \in H^2(\mathbb{T}) \cap \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S}) \cap W^{\infty}(\mathbb{T} \setminus \mathcal{S}). \quad (8)$$

Further, for any such u , $\Delta^{-1}|u|^2 \in W^{\infty}(\mathbb{T} \setminus \mathcal{S})$.

Again, in the case of the hydrogen Schrödinger operator on $\mathbb{R}^3$, the fact that the domain is H^2 and that eigenfunctions have $H^{5/2-\epsilon}$ regularity are well known (see Ref. 10, for example).

Note that in the Hartree–Fock and density-functional methods, one constructs iteratively a sequence of potentials V_n as follows. We first find the first occupied energy levels and eigenfunctions corresponding to the potential V_n . Then, to the Coulomb potential, we add all terms of the form $\Delta^{-1}|u|^2$, with u ranging through the determined set of eigenfunctions of the Schrödinger operator for V_n . If $\rho V_n \in W^{\infty}(\mathbb{T} \setminus \mathcal{S})$, then Theorem I.2 guarantees that V_{n+1} will satisfy the same assumption. By induction, all potentials appearing the Hartree–Fock and density-functional methods will satisfy this assumption. The same theorem then gives that all the eigenvalues of these operators satisfy the regularity assumption $u \in H^2(\mathbb{T}) \cap \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ needed in our first approximation result. At this point, we have only that the original eigenfunctions, that is, those for potentials satisfying Assumption 1 below, will have the regularity required for our second approximation result.

In the proof of the above two theorems, we use the following lemma, which implies that the operators $H_{\mathbf{k}}$ have many eigenvalues.

Theorem I.3: Assume that $\rho V \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$. Then the Hamiltonians $H_{\mathbf{k}}$ define unbounded, self-adjoint operators on $L^2(\mathbb{T})$ with domain $H^2(\mathbb{T})$ and with compact resolvent. In particular, $L^2(\mathbb{T})$ has an orthonormal basis consisting of eigenfunctions of $H_{\mathbf{k}}$.

Our second set of main results is a pair of approximation theorems which, by Theorems I.1 and I.2, apply to the eigenfunctions we want to compute. Theorem I.1 provides *a priori* estimates for the eigenfunctions of $H_{\mathbf{k}}$, which can then be used to approximate them using one of the standard discretization techniques.^{11–15} The fact that in the usual Sobolev spaces we obtain limited regularity [only $H^{5/2-\epsilon}(\mathbb{T})$] is a bad thing for the standard finite element approximation.^{16,17} In particular, we expect to obtain pollution effects when quadratic elements on quasiuniform meshes are used. This is also likely to slow down any implementation using plane waves (or trigonometric polynomials).

On the other hand, the fact that we get unlimited regularity in the weighted Sobolev spaces $\mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ means that, for $3/2-\epsilon > 1$, we can use the standard techniques developed in Refs. 18–23 to define a sequence of meshes that is graded toward the singular points to recover the optimal approximation property. Our first approximation theorem uses such an approach.

For any mesh (or tetrahedralization) $\mathcal{T}$ of $\mathbb{T}$, let us denote by $S(\mathcal{T}, m)$ the usual finite element space based on polynomials of order m . More precisely, $S(\mathcal{T}, m)$ will consist of those continuous functions on $\mathbb{T}$ that on each tetrahedron T of $\mathcal{T}$ coincide with a polynomial of degree m . For any fixed mesh $\mathcal{T}$, we shall denote by $u_{I,\mathcal{T},m} \in S(\mathcal{T}, m)$ the degree m Lagrange interpolant of u . We shall construct a sequence of meshes (or tetrahedralizations) $\mathcal{T}_n$ with the following quasioptimal approximation property with respect to the spaces $S_n = S(\mathcal{T}_n, m)$.

Theorem I.4: Let us assume that $\rho V \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$. Let $u \in \mathcal{K}_{3/2-\epsilon}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \cap H^2(\mathbb{T})$, where $\epsilon \in (0, \frac{1}{2})$ is fixed. Then there exists sequence $\mathcal{T}_n$ of tetrahedralizations of $\mathbb{T}$,

$$\|u - u_{I,\mathcal{T}_n,m}\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} (\|u\|_{\mathcal{K}_{3/2-\epsilon}^{m+1}(\mathbb{T} \setminus \mathcal{S})} + \max_{p \in \mathcal{S}} |u(p)|), \quad (9)$$

where m is the degree of polynomials we used in the approximation and $S_n = S(\mathcal{T}_n, m)$ is an increasing sequence of spaces of dimensions $\sim 2^{3n}$.

Another approach, closer to physical intuition, is to approximate using elements of spaces generated by plane waves. To implement this, first, let S_N be the vector space generated by the wave functions $e^{i\xi \cdot \mathbf{r}}$ satisfying $\xi \in \mathcal{L}^*$ and $|\xi| \leq N$. Then $\dim S_N \sim N^3$. The first result in our second approximation theorem uses these spaces. However, we can improve the exponent in the theorem if we enlarge the space by including “orbital functions.”²⁴ This method is analogous to that of including singular functions in the finite element spaces on polygons.¹⁶

To do this, first we need some notation. Let r_p be the distance function to $p \in \mathcal{S}$. (So $\rho = r_p$ close to p .) Let $\mathcal{Y}_{N,a}$ be the space spanned by spherical harmonics corresponding to eigenvalues λ of the Laplace operator on S^2 satisfying $|\lambda| \leq N^a$, $a > 0$. Finally, let χ_p be a smooth cutoff function that is equal to 1 in a neighborhood of p but is equal to 0 in a neighborhood of any other point $p \in \mathcal{S}$. The orbital functions with which we will enrich our space S_N will be of the form $w = \sum_{p,j,k} r_p^j Y_k \chi_p$ for $Y \in \mathcal{Y}_{N,a}$ and $1 \leq j \leq l$, and will form a space denoted W_s . So define $S'_{N,a,l}$ to be the vector space of functions of the form $v + w$, where $v \in S_N$ and $w \in W_s$ is as above. By Weyl’s theorem for S^2 , we have that the number of eigenvalues (with multiplicity) less than λ is asymptotically given by $C\lambda$. For this reason, we will choose to work with $a \leq 3$ here so that for sufficiently large N , we get $\dim(S'_{N,a,l}) \leq CN^3$, which is the same estimate we get for $\dim(S_N)$.

Theorem I.5: Assume that ρV is a smooth function of ρ and $x' \in S^2$ in the neighborhood of each point $p \in \mathcal{S}$ (that is, V satisfies Assumption 1). Let u be an eigenfunction of $H_{\mathbf{k}}$. Also, let $P_N u$ and $P'_{N,3,l} u$ denote the projections of u onto S_N and $S'_{N,3,l}$, respectively, in the $H^1(\mathbb{T})$ -norm. Then there exists $C > 0$ such that

$$\|u - P_N u\|_{H^1(\mathbb{T})} \leq C \dim(S_N)^{-(3-2\epsilon)/6} \|u\|_{H^{5/2-\epsilon}(\mathbb{T})},$$

but, in general, no exponent less than $-\frac{1}{2}$ will satisfy this relation. On the other hand, there exists a continuous norm p on $\mathcal{A}^E(\mathbb{T} \setminus \mathcal{S}) \cap H^{5/2-\epsilon}(\mathbb{T})$ such that, for $a \leq 3$,

$$\|u - P'_N u\|_{H^1(\mathbb{T})} \leq C_a \dim(S'_{N,a,l})^{-(l+3/2-\epsilon)/3} p(u).$$

The space $\mathcal{A}^E(\mathbb{T} \setminus \mathcal{S})$ here consists of functions with good expansions near $\mathcal{S}$, and the norm p will be described in the proof later. A complete discussion of this result would take us too far afield from the contents of this paper, so below we will prove only the case when $l=1$. Further results along these lines will be included in a future paper.

A different kind of attempt to improve the approximation properties of the eigenvalues, using finite differences and elementary methods, was made by Modine *et al.*²⁵ Many authors have studied the regularity properties of the eigenfunctions of Schrödinger operators, including Refs. 8 and 26–28.

Let us describe now the contents of the paper. In Sec. II we review the necessary results on the regularity of the Laplace operator in weighted Sobolev spaces. Our approach is based on the algebra of b -pseudodifferential operators. In Sec. III we prove Theorems I.1 and I.3, as well as the necessary mapping and Fredholm properties of H_k and of other related operators. In Sec. VI, we prove Theorem I.2 and we give an application to the Hartree–Fock method. Finally, in Sec. V we introduce our sequence of meshes and prove Theorems I.4 and I.5, including the necessary intermediate approximation results.

We hope to implement the results of this paper into currently used DFT codes.⁶

II. PRELIMINARIES ON DIFFERENTIAL OPERATORS

We have found it convenient in this paper to use the b -calculus of pseudodifferential operators developed by Melrose²⁹ in his book. (See also Refs. 30–32 and the references therein. See also Ref. 33 for another application to a problem inspired from physics.) The b -calculus can be used to provide a rigorous mathematical foundation to the study of differential equations containing terms of the forms $\rho \partial_\rho$ and $\rho^2 \partial_\rho^2$, which are well known to occur in the determination of the eigenfunctions of the Schrödinger operator associated with the hydrogen atom. (Generalizations can be handled as well.) Thus in this section we will summarize the definitions and results from this theory that we will use to prove our analytic results and refer the reader to that excellent book for further details. We will use the theory to prove most of Theorem I.1. Since applying the theory in this case is essentially the same as applying it in the case of the Laplace operator, we will also take the opportunity to formulate the needed consequences for the Laplace operator.

A. Definition of b -differential operators

Let $\bar{M}$ be a smooth manifold with boundary $\partial \bar{M}$. We shall denote by $M := \bar{M} \setminus \partial \bar{M}$ its interior. Let ρ be a smooth function on $\bar{M}$ on M that in a neighborhood of the boundary equals the distance to $\partial \bar{M}$ and such that $\rho > 0$ on M . We start by being more specific about the types of differential equations that the b -calculus is designed to study. These involve a specific class of differential operators on the interior M of $\bar{M}$ called b -differential operators.

Definition II.1: Let $\bar{M}$ be a smooth manifold with boundary. A b -differential operator of degree m on the interior M of $\bar{M}$ is a differential operator of degree m on M that, near $\partial \bar{M}$, has the form

$$P = \sum_{j=0}^m A_j(\rho) (\rho \partial_\rho)^j, \quad (10)$$

where $A_j(\rho)$ is a differential operator on $\partial \bar{M}$ of degree $\leq (m-j)$ for all ρ , and this family is smooth up to $\rho=0$, i.e., up to $\partial \bar{M}$.

B. Examples

An example closely related to our applications is $\bar{M} = \{|x| \leq 1\}$, the closed *unit ball* in $\mathbb{R}^3$. If r denotes the distance function to the origin, then we choose $\rho = 1 - r$ close to the boundary and we smooth it near the origin. Yet another example, even more closely related to our work, is when $M = \mathbb{R}^3 \setminus \{0\}$, that is, the space with one point removed such that $\bar{M} = [0, \infty) \times S^2$, with $\{0\} \times S^2$ covering the origin. In this second example, we take the same function ρ as we considered in Sec. I. Let ∂_j , $j=1,2,3$, be the three partial derivatives on $\mathbb{R}^3$, which we restrict to $M := \mathbb{R}^3 \setminus \{0\}$.

Recall that we have introduced the three dimensional torus $T = \mathbb{R}^3 / \mathcal{L}$, where $\mathcal{L} := \{n_1 \mathbf{v}_1 + n_2 \mathbf{v}_2 + n_3 \mathbf{v}_3\}$ is the lattice of orbits of the potential V . Also, recall that $S \subset T$ is the set of points where V may have singularities. There are two ways we can complete the open manifold $T \setminus S$ to a compact manifold. One, clearly, is by putting back the set S to recover T . In this paper, instead of this, we will add a spherical boundary around each point of S , thus “stretching out” these punctures. We call the resulting manifold with boundary $\bar{M}_S$, where the boundary $\partial \bar{M}_S$ is a disjoint set of 2-spheres, one around each point in S . Formally, this space is the disjoint union

$$\bar{M}_S := (T \setminus S) \cup (S^2 \times S). \quad (11)$$

Close to the boundary, our manifold $\bar{M}_S$ is defined to be isometric to the product $S^2 \times [0, \epsilon)$, $\epsilon > 0$. Essentially, the construction of the manifold $\bar{M}_S$ corresponds to taking spherical coordinates around each of the singular points. So again, we may use for ρ in the b -calculus the function ρ defined in Sec. I, that is, a smoothed distance to the set of singular points S .

When we change the coordinates from rectangular coordinates x_i with weighted rectangular differentials $\rho \partial_j$ to spherical coordinates and spherical differentials, we obtain exactly the coordinates ρ , θ , and ϕ standard for spherical coordinates, and the differentials $\rho \partial_\rho$, ∂_θ , and ∂_ϕ , which are the building blocks of the set of b -differential operators on $\bar{M}_S$. Thus, for instance, we can restate our definitions of $W^{\infty, \infty}(T \setminus S)$ and $\mathcal{K}_a^m(T \setminus S)$, $a \in \mathbb{N}$, to involve b -differential operators of degree a rather than strings of differentials $\rho^{|\alpha|} \partial^\alpha$, where $|\alpha| = a$.

Let $P = \sum_{|\alpha| \leq m} a_\alpha(x) \partial^\alpha$, $\partial^\alpha := \prod_j \partial_j^{\alpha_j}$, $a_\alpha \in C^\infty(\mathbb{R}^n)$ be a differential operator of order m on $\mathbb{R}^n$. Here we use the notation $|\alpha| = \sum_{j=1}^n \alpha_j$ for $\alpha \in \mathbb{Z}_+^n$. Recall that the principal symbol of P is the smooth function

$$\sigma(P)(\xi) = \sum_{|\alpha| \leq m} \prod_j \xi_j^{\alpha_j}. \quad (12)$$

The definition of the principal symbol extends to an arbitrary differential operator P on a smooth manifold M , so that the principal symbol $\sigma(P)$ becomes a smooth function on T^*M , the cotangent bundle of M . A b -differential operator $P = \sum_{j=0}^m A_j(\rho) (\rho \partial_\rho)^j$ is called b -elliptic if, and only if, the principal symbol of the related operator

$$P' = \sum_{j=0}^m A_j(\rho) \partial_\rho^j$$

is elliptic up to $\rho=0$.

Let us now see how the Laplace operator fits into this setting. The differentials $\partial_j := \partial / \partial x_j$ descend to differentials on the quotient $T := \mathbb{R}^3 / \mathcal{L}$. Let $\rho: T \rightarrow [0, 1]$ be equal to the distance to p , close to $p \in S$, and be smooth and strictly positive otherwise (that is, ρ is a version of the smoothed distance to S that we also used earlier). Then operators $\rho^m \partial^\alpha$ are typical examples of b -differential operators on $\bar{M}_S$, provided that $|\alpha| \leq m$. These are the main examples of b -differential operators that will concern us. The following result is well known.

Lemma II.2: $D := -\rho^2 \Delta$ is a b -differential operator.

Proof: Let Δ_{S^2} denote the (negative definite) Laplace operator (or, more precisely, the

Laplace–Beltrami operator) on the round 2-sphere. Then, in polar coordinates near one of the singular points $p \in \mathcal{S}$, we have

$$\Delta = \rho^{-2}((\rho\partial_\rho)^2 + \rho\partial_\rho + \Delta_{S^2}). \quad (13)$$

This completes the proof. $\square$

C. Indicial family and regularity results

A very important invariant associated with a b -differential operator P is its *indicial family* $\hat{P}(\tau)$ defined by

$$\hat{P}(\tau) := \sum_{j=0}^m A_j(0)\tau^j \quad \text{if} \quad P = \sum_{j=0}^m A_j(\rho)(\rho\partial_\rho)^j. \quad (14)$$

The operator $\hat{P}(\tau)$ is the Mellin transform of $\sum_{j=0}^m A_j(0)(\rho\partial_\rho)^j$. The Mellin transform $\mathcal{M}(f)(s) = \int_0^\infty x^{-s-1}f(x)dx$ is a generalization of the Fourier transform, which justifies the notation $\hat{P}(\tau)$ for the indicial family of P . For example,

$$-\hat{D}(\tau) = \tau^2 + \tau + \Delta_{S^2}. \quad (15)$$

Note that in some texts τ is replaced with $i\tau$ in the definition of indicial operators.

With the help of the indicial family of a b -differential operator P , we can study the Fredholm and regularity properties of P with respect to the weighted b -Sobolev spaces defined by the following.

Definition II.3: If M is the interior of a manifold $\bar{M}$ with boundary and if ρ measures distance to the boundary, we define

$$H^m(M) = H_b^m(\bar{M}) = \left\{ u: M \rightarrow \mathbb{C}, \int_M |Pu|^2 d\text{vol}_b < \infty \right\}, \quad (16)$$

for all b -differential operators P of degree $\leq m$, where near ∂M , $d\text{vol}_b = (d\rho/\rho)d\text{vol}_{\partial\bar{M}}$ and, away from $\partial\bar{M}$, $d\text{vol}_b$ is any smooth volume form. Then the weighted b -Sobolev spaces are the spaces

$$\rho^\gamma H_b^m(\bar{M}) = \{u: M \rightarrow \mathbb{C}, u = \rho^\gamma v, v \in H_b^m(M)\}. \quad (17)$$

We will use later the obvious fact that multiplication by ρ^α is an isomorphism from $\rho^\gamma H_b^m(\bar{M})$ to $\rho^{\gamma+\alpha} H_b^m(\bar{M})$. We endow the space $\rho^\gamma H_b^m(M)$ with the metric $\|\rho^\gamma u\|_{\rho^\gamma H_b^m(M)} = \|u\|_{H_b^m(M)}$. It is then known, but not obvious, that the b -Sobolev spaces defined above can be identified with the Sobolev spaces defined in Sec. I by

$$\mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S}) = \rho^{a-3/2} H_b^m(\mathbb{T} \setminus \mathcal{S}). \quad (18)$$

It is important to have available both definitions of these weighted Sobolev spaces, as some of their properties are easier to prove in one formulation, whereas others are easier to prove in the other formulation.

These weighted Sobolev spaces have a number of other well known nice properties, which can be found in Melrose's²⁹ book (see also Refs. 34–37). The first lemma states that b -differential operators define bounded maps between the weighted b -Sobolev spaces $\rho^\gamma H_b^s(M)$.

Lemma II.4: If P is a b -differential operator of degree m , then $P: \rho^\gamma H_b^s(M) \rightarrow \rho^\gamma H_b^{s-m}(M)$ is a bounded map for all γ and a .

The next lemma gives the Sobolev embedding and Rellich compactness properties for maps between these Sobolev spaces.

Lemma II.5: The inclusion map $\rho^\alpha H_b^s(M) \rightarrow \rho^\gamma H_b^r(M)$ is continuous if $\alpha \geq \gamma$ and $s \geq r$. It is

compact if $\alpha > \gamma$ and $s > r$.

The Fredholm and mapping properties for a b -elliptic, b -differential operator P are studied by constructing various sorts of parametrices for P acting between weighted spaces. The first “small parametrix” Q that is constructed corresponds essentially to the properly supported parametrix coming from the standard theory of pseudodifferential operators such as in Refs. 38 and 39. Without entering further into technical details, let us just note that Q is a pseudodifferential operator whose symbol is the inverse of that of P .

Theorem II.6: *If P is an order m b -elliptic, b -differential operator on a manifold M that is the interior of a manifold with boundary $\bar{M}$, then there exists an operator Q on M with the following properties.*

- (1) *The map $Q: \rho^\gamma H_b^s(M) \rightarrow \rho^\gamma H_b^{s+m}(M)$ is bounded for all $s, \gamma \in \mathbb{R}$.*
- (2) *The remainder maps, $R_1 = 1 - QP$ and $R_2 = 1 - PQ$, are bounded and smoothing, i.e., for all a and γ the maps $R_i: \rho^\gamma H_b^a(M) \rightarrow \rho^\gamma H_b^s(M)$ are well defined and continuous for all $a, s, \gamma \in \mathbb{R}$.*

Fredholm and more refined regularity results for a b -elliptic operator P as in Eq. (10) are determined by a subset $\text{Spec}_b(P) \subset \mathbb{C} \times \mathbb{Z}_+$ defined by

$$\text{Spec}_b(P) = \{(z, k) \in \mathbb{C} \times \mathbb{Z}_+, \hat{P}(\tau)^{-1} \text{ has a pole of order } k+1 \text{ at } z\}. \quad (19)$$

For the Laplace operator we have the following.

Lemma II.7: *Taking $D = -\rho^2 \Delta$ as before, we obtain $\text{Spec}_b(D) = \mathbb{Z} \times \{0\}$.*

Proof: The eigenvalues of $-\Delta_{S^2}$ are of the form $l(l+1)$, $l \in \mathbb{Z}_+$. Let ϕ_l be an eigenfunction with eigenvalue $-l(l+1)$. Then we know that $\hat{D}(z) = (-z^2 - z - \Delta_{S^2})$. We have that $\hat{D}(z)$ is not invertible if and only if $z(z+1) = l(l+1)$ for some $l \in \mathbb{Z}_+$, which implies either $z = l$ or $z = -l - 1$. Moreover, the roots are simple. This gives the desired result. $\square$

Now again considering a general elliptic b -differential operator P , define

$$\text{spec}_b(P) = \{z \in \mathbb{C}, (z, k) \in \text{Spec}_b(P) \text{ for some } k \in \mathbb{Z}_+\}. \quad (20)$$

In particular,

$$\text{spec}_b(\rho^2 \Delta) = \mathbb{Z}. \quad (21)$$

In terms of this set, the b -calculus tells us the following.

Theorem II.8: *An elliptic b -differential operator $P: \rho^\gamma H_b^{k+m}(M) \rightarrow \rho^\gamma H_b^k(M)$ is Fredholm if and only if $\gamma + ic \notin \text{spec}_b(P)$ for all $c \in \mathbb{R}$. That is, in this case, there exists a continuous operator $Q_\gamma: \rho^\gamma H_b^k(M) \rightarrow \rho^\gamma H_b^{k+m}(M)$ such that $1 - PQ_\gamma$ and $1 - Q_\gamma P$ are compact operators on their respective spaces.*

Note that the operator Q_γ as above is a true parametrix, as opposed to the “small parametrix” Q from Theorem II.6, which inverts P on these spaces only up to bounded smoothing operators, which are not compact on a noncompact manifold such as $\mathbb{T} \setminus S$. The operators Q_γ all can be taken to play the role of Q in Theorem II.6, but they cannot be chosen to be independent of γ . The theory of the b -calculus, in fact, provides a much stronger regularity result than implied by Theorem II.6. It is stated in terms of two more definitions.

Definition II.9: *An index set is a subset $E \subset \mathbb{C} \times \mathbb{Z}_+$ with the following three properties.*

- (1) *$E \cap \{\alpha \leq \text{Re}(z)\} \times \mathbb{Z}_+$ is finite for any $\alpha \in \mathbb{R}$.*
- (2) *If $(z, n) \in E$ then so is (z, k) for all $0 \leq k \leq n$.*
- (3) *If $(z, n) \in E$ then so is $(z+k, n)$ for all $k \in \mathbb{Z}_+$.*

Then for a manifold M that is the interior of a manifold $\bar{M}$ with boundary, we say that a function $f: M \rightarrow \mathbb{C}$ is polyhomogeneous with index set E near $\partial \bar{M}$ if for each $(z, n) \in E$ there exist $a_{z,n} \in C^\infty(\partial \bar{M})$ such that for all N ,

$$g_N := f - \sum_{\substack{(z,n) \in E \\ \operatorname{Re}(z) \leq N}} \rho^z (\log \rho)^n a_{z,n} \in \rho^N \mathcal{C}^N(\bar{M}), \quad (22)$$

that is, g_N is N times continuously differentiable on $\bar{M}$ and vanishes at $\partial\bar{M}$ with all derivatives up to order N . The space of all polyhomogeneous functions on M with index set E on $\partial\bar{M}$ is denoted by $\mathcal{A}^E(M)$.

Each of the functions $\rho^z (\log \rho)^n a_{z,n}$ is called a *singular function* of u and Eq. (22) is called the *singular function expansion* of u . The singular function corresponding to $\operatorname{Re}(z)$ minimal is called the *first singular function* of u .

Now we can state the refined regularity result for b -elliptic operators.

Theorem II.10: *Let P be a b -elliptic operator on functions over M , and suppose that $u \in \rho^\alpha H_b^\infty(M)$ satisfies $Pu=0$. Then u is polyhomogeneous with index set E^α , the smallest index set containing all $(z,n) \in \operatorname{Spec}_b(P)$ with $\operatorname{Re}(z) \geq \alpha$.*

An alternative approach to Theorem II.10, called the theory of “singular functions,” was developed by Kondratiev⁴⁰ in the framework of boundary value problems (see also Refs. 35 and 41). Singular functions have a long history of applications in physics and engineering.

Corollary II. 11: *The only possible index sets for $D=-\rho^2\Delta$ are the sets of the form $E^s := \{(n,0), n \in \mathbb{Z}, n \geq s\}$.*

Proof: This follows from Lemma II.7 and from the definition of index sets. $\square$

III. MAPPING AND FREDHOLM PROPERTIES: PROOFS OF THEOREMS I.1 AND I.3

We now want to apply the tools from Sec. II to the Schrödinger operator

$$H_{\mathbf{k}} := - \sum_{j=1}^3 (\partial_j + ik_j)^2 + V \quad (23)$$

defined in Sec. I by Eq. (2).

Recall that the compact manifold with boundary $\bar{M}_S = (\mathbb{T} \setminus S) \cup (S \times S^2)$ was introduced in Eq. (11). Its interior identifies with $\mathbb{T} \setminus S$ and its boundary are a disjoint union of 2-spheres. The assumptions on the potential V for the two main regularity theorems stated in Sec. I are as follows.

Assumption 1. *We have $\rho V \in \mathcal{C}^\infty(\bar{M}_S)$.*

That is, the function ρV extends to a smooth function on the manifold with boundary $\bar{M}_S$ introduced in Eq. (11).

Assumption 2. *We have $\rho V \in W^{\infty,\infty}(\mathbb{T} \setminus S)$.*

If V satisfies Assumption 1, then it also satisfies Assumption 2. This is simply because $\mathcal{C}^\infty(\bar{M}_S) \subset W^{\infty,\infty}(\mathbb{T} \setminus S)$. In most applications, V has a Coulomb-type singularity, in which case we have $\rho V \in \mathcal{C}^\infty(\mathbb{T}) \subset \mathcal{C}^\infty(\bar{M}_S)$ and hence V satisfies Assumption 1 (the stronger assumption). As mentioned in Sec. I, we need the weaker Assumption 2 for an application to the Hartree–Fock method.

At a first reading, one may assume in this section that V satisfies Assumption 1, which is the one needed for Theorem I.1. However, with an eye on the proof of Theorem I.2 in Sec. IV, we show how some of our results generalize to the weaker case when V satisfies only Assumption 2.

The proofs in either case (Assumption 1 or Assumption 2) come from the fact that our operators $H_{\mathbf{k}}$ are perturbations of the Laplacian. In Sec. II, we saw how to obtain regularity results using the b -calculus by considering the operator $D=-\rho^2\Delta$. Let us therefore introduce the perturbation operators $B_{\mathbf{k},V,\lambda}$ by

$$\rho B_{\mathbf{k},V,\lambda} := \rho^2(H_{\mathbf{k}} - \lambda) - D = \rho^2 \left(\sum_{j=1}^3 (-2ik_j \partial_j + k_j^2) + V - \lambda \right). \quad (24)$$

In the proofs of both Theorems I.1 and I.2 we will use the fact that $H_{\mathbf{k}} - \lambda$ is a “small” perturbation of the Laplacian, in which it is a relatively compact perturbation. Since the Laplacian Δ is self-adjoint on $L^2(\mathbb{T})$ and has domain $H^2(\mathbb{T})$, this will imply (see Theorem I.3) that $H_{\mathbf{k}}$ is also self-adjoint on $L^2(\mathbb{T})$ with domain $H^2(\mathbb{T})$. This in turn implies that under either assumption on V , all eigenfunctions of $H_{\mathbf{k}}$ will lie in $H^2(\mathbb{T})$.

In the proof of Theorem I.1, we will also use that the perturbation $\rho B_{\mathbf{k},V,\lambda}$ of D is small in the b -calculus sense, that is, that it has order less than the order of D and adding it to D results in a new b -differential operator with the same indicial family [see (iii) of Lemma III.1]. We will thus be able to get all the same regularity properties for $H_{\mathbf{k}} - \lambda$ as for Δ when V satisfies Assumption 1.

To prove Theorem I.2, we will no longer be able to use the b -calculus because in this situation, $H_{\mathbf{k}} - \lambda$ is no longer a b -differential operator. We will still be able to use Theorem I.3, but this is not sufficient to give the regularity needed for the Hartree–Fock method. Thus in addition we will use a refined regularity result.

A. Proof of Theorem I.1

In this subsection, we will give the proof of Theorem I.1 modulo the proof of Theorem I.3. Then we will prove a series of lemmas that culminate in the proof of this theorem as a corollary.

When V satisfies Assumption 1, it is not difficult to see that $H_{\mathbf{k}} - \lambda$ is a b -differential operator.

Lemma III.1: Assume that the potential V satisfies Assumption 1. Then

- (1) the operator $B_{\mathbf{k},V,\lambda}$ of Eq. (24) is a b -differential operator of order 1,
- (2) $\rho^2(H_{\mathbf{k}} - \lambda)$ is an elliptic b -differential operator of order 2, and,
- (3) The indicial family of $\rho^2(H_{\mathbf{k}} - \lambda)$ is the same as that of $D = -\rho^2\Delta$.

Proof: Since V satisfies Assumption 1, (i) follows from the fact that a smooth function on $\bar{M}_S$ is a b -differential operator of order zero on $\bar{M}_S$ and $\rho\partial_j$ is a b -differential of order one on $\bar{M}_S$. (ii) follows from (i) using also Eq. (24) and the fact that $\rho^2\Delta$ is an elliptic b -differential operator of order 2 on $\bar{M}_S$. (It has the same principal symbol as the Laplacian of a smooth metric on $\bar{M}_S$.) (iii) follows from the fact that the indicial family of $\rho B_{\mathbf{k},V,\lambda}$ is zero and from Eq. (24) defining $B_{\mathbf{k},V,\lambda}$. $\square$

Equipped with this, we can now give the proof of Theorem I.1. We first prove an apparently weaker form of the theorem, under the additional assumption that $u \in H^2(\mathbb{T})$, using the concepts introduced in Sec. II. Then in Theorem I.3, which we give at the end of this section, we show the additional assumption that $u \in H^2(\mathbb{T})$ is automatically satisfied.

Theorem III.2: Assume that V satisfies Assumption 1 and fix $\mathbf{k} \in \mathbb{R}^3$ and $m \in \mathbb{Z}_+$. Let $H_{\mathbf{k}}u = \lambda u$, $u \in H^2(\mathbb{T})$, be an eigenfunction of $H_{\mathbf{k}}$. Then, in the neighborhood of each singular point $p \in \mathcal{S}$, u is polyhomogeneous with index set $E = \mathbb{Z}_+ \times \{0\}$ and its first singular function (the one corresponding to ρ^0) is constant. In particular $u \in \mathcal{A}^E(\mathbb{T} \setminus \mathcal{S}) \cap H^{5/2-\epsilon}(\mathbb{T}) \cap \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$, for any $\epsilon > 0$.

Proof: By elliptic regularity away from the singular set $\mathcal{S}$, we know that any eigenfunction u of $H_{\mathbf{k}}$ is smooth on $\mathbb{T} \setminus \mathcal{S}$. Now we use the regularity theory from the b -calculus. We have from Lemma III.1 that $\rho^2 H_{\mathbf{k}}$ is a b -differential operator whose indicial set is the same as the index set of D , namely, $E^s = \{(n, 0), n \geq s\}$, by Corollary II.11. Theorem II.10 then gives that, for each element $p \in \mathcal{S}$, there exist smooth functions $\phi_k(\theta) \in C^\infty(S^2)$ with the following property. In a small neighborhood $\mathcal{V}_p$ of p , u has an asymptotic expansion of the form

$$u \sim \sum_{k=-1}^{\infty} \rho^k \phi_k(\theta).$$

Recall that this means that for all N ,

$$h_N(\rho, \theta) := u - \sum_{k=-1}^N \rho^k \phi_k(\theta) \in \dot{C}^N(\bar{M}_S \cap \mathcal{V}_p),$$

where $\dot{C}^N(\bar{M}_S \cap \mathcal{V}_p)$ is the space of all functions on $\bar{M}_S \cap \mathcal{V}_p$, which are N times differentiable and which vanish together with all N derivatives up to order N at $\partial\bar{M}_S$. Thus we can also say that $h(\rho, \theta) \in \dot{C}^N(\mathcal{V}_p)$, that is, each such h is N -times differentiable near $p \in S$ and vanishes with all of its derivatives up to order N at p .

Now we also know by Theorem I.3 that $u \in H^2(\mathbb{T})$. Thus we see that, in fact, the -1 term of this series must vanish or $\partial_\rho u$ would not be in $L^2(\mathbb{T})$. Further, we know that $(H_{\mathbf{k}} - \lambda)u = 0$ since u is an eigenfunction of $H_{\mathbf{k}}$. Write

$$u = \phi_0(\theta) + \rho \phi_1(\theta) + \rho^2 \phi_2(\theta) + h_2(\rho, \theta)$$

and apply $(H_{\mathbf{k}} - \lambda)$ to this. Then the leading order term in ρ must in particular vanish (since the whole thing vanishes). This term is $-\rho^{-2} \Delta_{S^2} \phi_0$, so we find further that ϕ_0 must be a constant function.

It is standard that in $\mathbb{R}^3$, a function of the form $\rho^k \phi_k(\theta)$ is in $H^{k+3/2-\epsilon}(B(0;1))$ (proven by a combination of direct calculation and interpolation). Thus consider

$$h_N(\rho, \theta) = u - \sum_{k=0}^N \rho^k \phi_k(\theta) = \rho^{N+1} \phi_{N+1} + \rho^{N+2} \phi_{N+2} + \rho^{N+3} \phi_{N+3} + h_{N+3}(\rho, \theta).$$

Since $h_{N+3}(\rho, \theta) \in \dot{C}^{N+3}(\bar{M}_S \cap \mathcal{V}_p) \subset H^{N+5/2-\epsilon}(\mathcal{V}_p)$, and each $\rho^{N+k} \phi_{N+k} \in H^{N+k+3/2-\epsilon}(B(0;1))$, we have the better regularity $h_N(\rho, \theta) \in H^{N+5/2-\epsilon}(\mathcal{V}_p)$. Finally, since $\phi_0(\theta)$ is constant, it is, in fact, in $C^\infty(\mathcal{V}_p)$. Thus overall we may conclude that $u \in H^{5/2-\epsilon}(\mathcal{V}_p)$ around each $p \in S$, and $u \in C^\infty(\mathbb{T} \setminus S)$, so $u \in H^{5/2-\epsilon}(\mathbb{T})$. $\square$

Now we need to prove Theorem I.3. We start with several lemmas.

Lemma III.3: For any $f \in W^{\infty, \infty}(\mathbb{T} \setminus S)$, the multiplication map

$$\mathcal{K}_a^m(\mathbb{T} \setminus S) \ni u \rightarrow fu \in \mathcal{K}_a^m(\mathbb{T} \setminus S) = \rho^{a-3/2} H_b^m(\mathbb{T} \setminus S) \quad (25)$$

is continuous for all $m \in \mathbb{Z}_+$ and all $a \in \mathbb{R}$.

Proof: Recall that $\mathcal{K}_a^m(\mathbb{T} \setminus S) = \rho^{a-3/2} H_b^m(\mathbb{T} \setminus S)$. Let us write $D_\rho^\alpha = (\rho \partial_\rho)^{\alpha_1} \partial^{\alpha'}$. Then the well known formula $\partial^\alpha(fu) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} \partial^\beta f \partial^{\alpha-\beta} u$ extends to $D_\rho^\alpha(fu) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} D_\rho^\beta f D_\rho^{\alpha-\beta} u$. The result then follows from the fact that $D_\rho^\beta f \in L^\infty(\bar{M}_S)$, whereas $D_\rho^\beta u \in L^2(\mathbb{T} \setminus S)$, by definitions. $\square$

Lemma III.4. Assume that the potential V satisfies Assumption 2. Let $m, a \in \mathbb{R}$. Then

- (i) the operator $H_{\mathbf{k}} - \lambda$ maps $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S)$ to $\mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S)$ continuously,
- (ii) the operator $\rho^{-1} B_{\mathbf{k}, V, \lambda}$ maps $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S)$ to $\mathcal{K}_a^m(\mathbb{T} \setminus S)$ continuously, and
- (iii) $\rho^{-1} B_{\mathbf{k}, V, \lambda} : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S)$ is compact.

Proof: First consider the case that V satisfies Assumption 1. Then (i) follows from Lemma III.1 (i) and (ii) using also Lemma II.4. Next, we have $\rho^2(H_{\mathbf{k}} - \lambda + \Delta) = \rho B_{\mathbf{k}, V, \lambda}$. Thus (ii) follows from Lemma III.1 (i) and Lemma II.4. (iii) follows from (ii) and the compactness of the embedding $\mathcal{K}_a^m(\mathbb{T} \setminus S) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S)$ (see Lemma II.5).

To prove that properties (i)–(iii) remain valid if V satisfies only Assumption 2, let us write $\rho^2(H_{\mathbf{k}} - \lambda + \Delta) = \rho B_{\mathbf{k}, 0, \lambda} + \rho(\rho V)$. Then we use the results already proven for $V=0$ and Lemma III.3, which states that multiplication by ρV is bounded on all spaces $\mathcal{K}_a^m(\mathbb{T} \setminus S)$. $\square$

This gives us the following corollary.

Corollary III.5. Let V satisfy Assumption 2; then the map $B_{\mathbf{k}, V, \lambda} : \mathcal{K}_a^m(\mathbb{T} \setminus S) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S)$ is bounded for all m and a .

Proof: Assume $V=0$ first. Then the result follows since $B_{\mathbf{k}, 0, \lambda}$ is a b -differential operator of order 1. In general, the result follows from the decomposition $B_{\mathbf{k}, V, \lambda} = B_{\mathbf{k}, 0, \lambda} + \rho V$ and Lemma III.3,

which says that multiplication by $\rho V \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$ is bounded on all spaces $\mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S})$. $\square$

Next, using the Fredholm results in Theorem II.8, we get the following.

Lemma III.6: *Let V satisfy Assumption 2. The map $H_{\mathbf{k}} - \lambda : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})$ is Fredholm if and only if $a - \frac{1}{2} \notin \mathbb{Z}$.*

Proof: Lemma III.4 (iii) states that $\rho^{-1}B_{\mathbf{k},V,\lambda} = (H_{\mathbf{k}} - \lambda) - \rho^{-2}D$ is compact. Since the property of being Fredholm is preserved by adding a compact operator, it suffices to prove this theorem for $\mathbf{k}=0$, $\lambda=0$, and $V=0$, that is, for $-\Delta$. Let $D := -\rho^2\Delta$, as before. Thus

$$\text{spec}_b(P_\lambda) = \text{spec}_b(\rho^2\Delta) = \mathbb{Z}, \quad (26)$$

as determined in Sec. II [Eq. (21)].

Note that this is independent of which point in $\mathcal{S}$ we expand around. Thus this is the correct set for all the boundary components of $\mathbb{T} \setminus \mathcal{S}$. So we have that D is Fredholm for all $\gamma \notin \mathbb{Z}$. Multiplying by $-\rho^{-2}$ to get Δ and rewriting in terms of the spaces introduced in Sec. I using Eq. (18), we thus obtain the desired result for Δ , and the full result follows when we add a compact operator to get $H_{\mathbf{k}} - \lambda$. Note that the shift of $\frac{1}{2}$ in weights is due to the factor $\rho^{a-3/2}$ in Eq. (18). $\square$

We shall need the following standard result, which we state for further use.

Lemma III.7: *Let $a \in \mathbb{R}$ be arbitrary and assume that $u \in \mathcal{K}_{1+a}^2(\mathbb{T} \setminus \mathcal{S})$ and that $v \in \mathcal{K}_{1-a}^2(\mathbb{T} \setminus \mathcal{S})$. Then $(\Delta u, v) + (\nabla u, \nabla v) = 0$.*

Proof: Let $C(u, v) := (\Delta u, v) + (\nabla u, \nabla v)$. Then it is known that $C=0$ if $u, v \in \mathcal{C}_c^\infty(\mathbb{T} \setminus \mathcal{S})$, simply by integration by parts (no boundary appears in our lemma). The result follows from the continuity of C on the indicated spaces and from the density of $\mathcal{C}_c^\infty(\mathbb{T} \setminus \mathcal{S})$ in $\mathcal{K}_b^2(\mathbb{T} \setminus \mathcal{S})$, $b \in \mathbb{R}$. $\square$

This gives the following proposition, which is of independent interest.

Proposition III.8: *The operator $1 - \Delta : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})$ is an isomorphism for all $|a| < 1/2$.*

Proof: By regularity, we can assume $m=0$. Let $D_a = 1 - \Delta : \mathcal{K}_{a+1}^1(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{-1}(\mathbb{T} \setminus \mathcal{S})$, that is to say, $1 - \Delta$ with fixed domain and range. Then $D_a^* = D_{-a}$.

By Lemma III.6, D_a is Fredholm for $|a| < 1/2$. Since D_0 is self-adjoint it has index zero. Further, 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 the index is constant over such families, we have that $\text{ind}(D_a) = 0$ for all $|a| < \frac{1}{2}$.

Let $\frac{1}{2} > a \geq 0$. The inclusion $\mathcal{K}_{a+1}^1(\mathbb{T} \setminus \mathcal{S}) \subset \mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})$ 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 III.7. Assume $D_a u = 0$, then $(D_a u, u) = 0$, and hence $u = 0$. This implies that the operator $1 - \Delta : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})$ is injective for $0 \leq a < \frac{1}{2}$. Since it is Fredholm of index zero, it is also an isomorphism. This proves our result for $0 \leq a < \frac{1}{2}$.

For $-\frac{1}{2} < a \leq 0$, we take adjoints and use $D_a = (D_{-a})^*$. The proof is now complete. $\square$

Although we do not use this to prove Theorem I.3, it is useful to note here the following result, which will be needed for the proof of Theorem I.2.

Corollary III.9: *We have $H^2(\mathbb{T}) \subset \mathcal{K}_{3/2-\epsilon}^2(\mathbb{T} \setminus \mathcal{S})$ for all $\epsilon > 0$.*

Proof: If the result is true for ϵ , it will be true for all $\epsilon' > \epsilon$. We can therefore assume $\epsilon \in (0, \frac{1}{2})$. We have $L^2(\mathbb{T}) = \mathcal{K}_0^0(\mathbb{T} \setminus \mathcal{S})$ and hence

$$H^2(\mathbb{T}) = (1 - \Delta)^{-1} L^2(\mathbb{T}) \subset (1 - \Delta)^{-1} \mathcal{K}_{-1/2-\epsilon}^0(\mathbb{T} \setminus \mathcal{S}) \subset \mathcal{K}_{3/2-\epsilon}^0(\mathbb{T} \setminus \mathcal{S}), \quad (27)$$

where for the last result we have used Proposition III.8 for $a = \frac{1}{2} - \epsilon \in (0, 1/2)$. $\square$

Now we have the tools needed to prove that V is a relatively compact perturbation of Δ .

Lemma III.10: *Using the notation of Eq. (24), we have that the operator*

$$\rho^{-1}B_{\mathbf{k},V,0}(1 - \Delta)^{-1} : L^2(\mathbb{T}) \rightarrow L^2(\mathbb{T})$$

is well defined and is compact for all V satisfying Assumption 2.

Proof: We have $L^2(\mathbb{T}) = \mathcal{K}_0^0(\mathbb{T} \setminus \mathcal{S}) \subset \mathcal{K}_{-1/2-\epsilon}^0(\mathbb{T} \setminus \mathcal{S})$. Next we use Corollary III.5 and Proposition III.8 for $\epsilon \in (0, 1/2)$ to conclude that the maps

$$(1 - \Delta)^{-1} : \mathcal{K}_{-1/2-\epsilon}^0(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{3/2-\epsilon}^2(\mathbb{T} \setminus \mathcal{S}),$$

$$\rho^{-1}B_{\mathbf{k},V,0}:\mathcal{K}_{3/2-\epsilon}^2(\mathbb{T}\setminus\mathcal{S})\rightarrow\mathcal{K}_{1/2-\epsilon}^1(\mathbb{T}\setminus\mathcal{S})$$

are well defined and bounded. The result then follows from the compactness of $\mathcal{K}_{1/2-\epsilon}^1(\mathbb{T}\setminus\mathcal{S})\rightarrow\mathcal{K}_0^0(\mathbb{T}\setminus\mathcal{S})=L^2(\mathbb{T})$ (Lemma II.5). $\square$

Finally, using standard results as in Refs. 42 and 43 we can complete the proof of Theorem I.3.

Proof: (Proof of Theorem I.3) We have that $1+H_{\mathbf{k}}=(1-\Delta)+\rho^{-1}B_{\mathbf{k},V,0}$. The proof is then obtained from Lemma III.10 because Δ is self-adjoint with domain $H^2(\mathbb{T})$ and a relatively compact perturbation preserves self-adjointness and the domain (see Ref. 43, pp. 162, 163, and 340; in that reference, the term “ Δ -compact” is used). The self-adjointness of $H_{\mathbf{k}}$ shows that $(\iota+H_{\mathbf{k}})^{-1}:L^2(\mathbb{T})\rightarrow H^2(\mathbb{T})$ is an isomorphism. The compactness of $(\iota+H_{\mathbf{k}})^{-1}:L^2(\mathbb{T})\rightarrow L^2(\mathbb{T})$ then follows from the fact that the inclusion $H^2(\mathbb{T})\rightarrow L^2(\mathbb{T})$ is compact. $\square$

Note that, in particular, the issue of the domain of our self-adjoint extension does not appear, unlike the related case of conical manifolds.⁴⁴

We are ready now to conclude the proof of Theorem I.1.

Proof: (Proof of Theorem I.1) The only difference between the statements of Theorems I.1 and III.2 is that in the latter, we make the apparently stronger assumption that $u\in H^2(\mathbb{T})$. Let us show that this stronger assumption is not really necessary. Indeed, if $u\in L^2(\mathbb{T})$ is such that $H_{\mathbf{k}}u=\lambda u$, then $(\iota+H_{\mathbf{k}})u=(\iota+\lambda)u\in L^2(\mathbb{T})$. Therefore $u=(\iota+\lambda)(\iota+H_{\mathbf{k}})^{-1}u\in H^2(\mathbb{T})$. $\square$

IV. PROOF OF THEOREM I.2

Although in the case of Theorem I.2, that is, where V satisfies only the weaker Assumption 2, the operator $H_{\mathbf{k}}$ is no longer a multiple of a b -differential operator, we can nevertheless use the weaker regularity theorem from the b -calculus, Theorem II.6, to get the following regularity result, which applies to the case that V satisfies only Assumption 2.

Theorem IV.1: Assume $\rho^2V\in W^{\infty,\infty}(\mathbb{T}\setminus\mathcal{S})$. Suppose $u\in\mathcal{K}_{a+1}^0(\mathbb{T}\setminus\mathcal{S})$ is such that $(H_{\mathbf{k}}-\lambda)u\in\mathcal{K}_{a-1}^{m-1}(\mathbb{T}\setminus\mathcal{S})$, then $u\in\mathcal{K}_{a+1}^{m+1}(\mathbb{T}\setminus\mathcal{S})$. Moreover, there exists a constant $C>0$ such that

$$\|u\|_{\mathcal{K}_{a+1}^{m+1}}\leq C(\|(H_{\mathbf{k}}-\lambda)u\|_{\mathcal{K}_{a-1}^{m-1}}+\|u\|_{\mathcal{K}_{a+1}^0}). \quad (28)$$

Proof: Let us take first $V=0$ and $P_{\lambda}:=\rho^2(H_{\mathbf{k}}-\lambda)$, which is a b -differential operator, by Lemma III.1. Our assumption means that $v:=P_{\lambda}u\in\mathcal{K}_{a+1}^{m-1}(\mathbb{T}\setminus\mathcal{S})$. Now apply the small parametrix Q from Theorem II.6 to both sides to get

$$(1-R_1)u=QP_{\lambda}u=Qv\in\mathcal{K}_{a+1}^{m+1}(\mathbb{T}\setminus\mathcal{S}). \quad (29)$$

Rearranging Eq. (29), we get $u=Qv+R_1u$. Since $R_1u\in\mathcal{K}_{a+1}^{\infty}(\mathbb{T}\setminus\mathcal{S})$, we have $u\in\mathcal{K}_{a+1}^{m+1}(\mathbb{T}\setminus\mathcal{S})$. A more careful look at this rearrangement gives

$$\|u\|_{\mathcal{K}_{a+1}^{m+1}}\leq\|Qv\|_{\mathcal{K}_{a+1}^{m+1}}+\|R_1u\|_{\mathcal{K}_{a+1}^{m+1}}\leq C(\|P_{\lambda}u\|_{\mathcal{K}_{a+1}^{m-1}}+\|u\|_{\mathcal{K}_{a+1}^0}), \quad (30)$$

which is the desired inequality (28).

Let us now take V with $\rho^2V\in W^{\infty,\infty}(\mathbb{T}\setminus\mathcal{S})$. Then $\rho^2(H_{\mathbf{k}}-\lambda)=P_{\lambda}+\rho^2V$. The rest of the proof is based on the general fact that if P_{λ} satisfies a regularity property, then $P_{\lambda}+\rho^2V$ will also satisfy that regularity property since ρ^2V is of lower order, as we will explain next.

Let us recall this standard argument for the benefit of the reader. We proceed by induction on m . For $m=0$ this claim is automatically satisfied by the second part of the assumption. For $m\geq 1$ we use the induction hypothesis to get that $u\in\mathcal{K}_{a+1}^m(\mathbb{T}\setminus\mathcal{S})$. Then by Lemma III.3, we get $\rho Vu\in\mathcal{K}_{a+1}^m(\mathbb{T}\setminus\mathcal{S})$ and thus $\rho^2Vu\in\mathcal{K}_{a+2}^m(\mathbb{T}\setminus\mathcal{S})$. By assumption, $(H_{\mathbf{k}}-\lambda)u\in\mathcal{K}_{a-1}^{m-1}(\mathbb{T}\setminus\mathcal{S})$. Thus $P_{\lambda}u=\rho^2(H_{\mathbf{k}}-\lambda)u-\rho^2Vu\in\mathcal{K}_{a+1}^{m-1}(\mathbb{T}\setminus\mathcal{S})+\mathcal{K}_{a+2}^m(\mathbb{T}\setminus\mathcal{S})\subset\mathcal{K}_{a+1}^{m-1}(\mathbb{T}\setminus\mathcal{S})$. We can then use the result for P_{λ} from the first part of the proof to conclude that $u\in\mathcal{K}_{a+1}^{m+1}(\mathbb{T}\setminus\mathcal{S})$. The desired inequality follows from Eq. (30) as follows:

$$\begin{aligned} \|u\|_{\mathcal{K}_{a+1}^{m+1}} &\leq C(\|P_\lambda u\|_{\mathcal{K}_{a+1}^{m-1}} + \|u\|_{\mathcal{K}_{a+1}^0}) \leq C(\|(P_\lambda + \rho^2 V)u\|_{\mathcal{K}_{a+1}^{m-1}} + \|u\|_{\mathcal{K}_{a+1}^m}) \leq C(\|(P_\lambda + \rho^2 V)u\|_{\mathcal{K}_{a+1}^{m-1}} \\ &\quad + \|u\|_{\mathcal{K}_{a+1}^0}) = C(\|(H_k - \lambda)u\|_{\mathcal{K}_{a+1}^{m-1}} + \|u\|_{\mathcal{K}_{a+1}^0}), \end{aligned} \quad (31)$$

where the last inequality is from the induction hypothesis and the last equality is by definition. The proof is now complete. $\square$

Throughout the rest of this section, we shall assume that V satisfies Assumption 2, namely, that $\rho V \in W^{\infty, \infty}(\mathbb{T} \setminus S)$. For such a V , the stronger conditions of the previous result are obviously satisfied.

The following lemma gives us our first piece of Theorem I.2.

Lemma IV.2: *Let $u \in L^2(\mathbb{T})$ be such that $H_k u = \lambda u$. Then $u \in H^2(\mathbb{T})$ and $u \in \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus S)$ for all $m \in \mathbb{Z}_+$ and $\epsilon > 0$.*

Proof: We have already seen in the proof of Theorem I.1 (at the conclusion of the previous section) that $u \in H^2(\mathbb{T})$. Corollary III.9 gives then $u \in \mathcal{K}_{3/2-\epsilon}^2(\mathbb{T} \setminus S)$. Since $(H_k - \lambda)u = 0 \in \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus S)$ for any $m \in \mathbb{Z}_+$, we can use the regularity theorem, Theorem IV.1, to conclude that $u \in \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus S)$. $\square$

In view of Lemma IV.2, to complete the proof of Theorem I.2, we need only to show that if $\rho V \in W^{\infty, \infty}(\mathbb{T} \setminus S)$ and u is an eigenfunction of H_k , then $u \in W^{\infty, \infty}(\mathbb{T} \setminus S)$ and $\Delta^{-1}|u|^2 \in W^{\infty, \infty}(\mathbb{T} \setminus S)$.

To even make sense of this last statement, we first have to define Δ^{-1} . We precompose with the projection of u onto the orthogonal complement of (1). The fact that the resulting map is well defined comes from the following lemma, which is similar to Proposition III.8.

Lemma IV.3: *Let $\{1\}^\perp := \{u \in \mathcal{K}_b^m(\mathbb{T} \setminus S), \int_{\mathbb{T}} u dx = 0\}$, where $b > -\frac{3}{2}$. Then $\Delta: \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S) \cap \{1\}^\perp \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S) \cap \{1\}^\perp$, $m \in \mathbb{Z}_+$, is an isomorphism for all $|a| < \frac{1}{2}$.*

Proof: Let us denote by $\Delta_a: \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S) \cap \{1\}^\perp \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S) \cap \{1\}^\perp$ the induced map. Lemma II.5 gives that the identity map defines a compact operator $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S) \cap \{1\}^\perp \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus S) \cap \{1\}^\perp$. Therefore Δ_a and $-D_a = \Delta - 1$ are compact perturbations of each other on the indicated spaces. Therefore they have the same index (when they are Fredholm). Proposition III.8 then shows that Δ_a has index zero for $|a| < \frac{1}{2}$.

Next we proceed as in the proof of Proposition III.8. Let us assume that $0 \leq a < \frac{1}{2}$. Lemma III.7 shows that $(\Delta_a u, u) = -(\nabla u, \nabla u)$ for $0 \leq a < \frac{1}{2}$, and hence Δ_a is injective on $\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus S) \cap \{1\}^\perp$. This shows that Δ_a is an isomorphism for $0 \leq a < \frac{1}{2}$.

Finally, the relation $D_a^* = D_{-a}$ shows that Δ_a is an isomorphism also for $-\frac{1}{2} < a \leq 0$. This completes the proof. $\square$

We shall need the following improvements on Lemma IV.2. As above, let χ_p be a smooth function equal to 1 in the neighborhood of $p \in S$. We can assume that the supports of χ_p are disjoint. Let V_s be the linear span of the functions χ_p . We fix $\epsilon \in (0, \frac{1}{2})$ arbitrary.

Lemma IV.4: *If $v \in \mathcal{K}_{3/2-\epsilon}^1(\mathbb{T} \setminus S)$ and $\Delta v \in \mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus S)$, $\epsilon \in (0, \frac{1}{2})$, then $v \in V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)$.*

Proof: We shall use the notation and the results of Lemma IV.3 above. Let us notice that $(\Delta v, 1) = 0$. Hence $v = \Delta^{-1}(\Delta v) + c$, where c is a constant. Since $c \in V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)$, it is enough to show that $\Delta^{-1}(\Delta v) \in V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)$. The map $\Delta: \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S) \rightarrow \mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus S)$ is Fredholm, by Lemma III.6. By the results of Ref. 29, for instance, the index of this map is given by the sum over all boundary components of $\mathbb{T} \setminus S$ of minus the order of the pole of the indicial family of Δ at $\frac{3}{2}$. This shows that each point in S contributes -1 to this index. Hence the index of Δ on these spaces is equal to $-\dim V_s = -\#S$ (the number of elements of S). (This also follows from the results of Ref. 29, 35, and 41, or 45.) Our index calculation shows that the map $\Delta: V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S) \rightarrow \mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus S)$ is still Fredholm, this time of index zero. Since $\mathcal{K}_2^2(\mathbb{T} \setminus S) \subset H^2$ the energy estimate is still satisfied to show that Δ [now acting on the space $V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)$] still has kernel consisting of the multiples of the function (1). We then obtain that

$$\Delta: (V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)) \cap \{1\}^\perp \rightarrow \mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus S) \cap \{1\}^\perp$$

is an isomorphism. Hence $\Delta^{-1}(\mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus S)) \subset V_s + \mathcal{K}_{5/2-\epsilon}^{m+1}(\mathbb{T} \setminus S)$. As explained above, this is enough to complete the result (see Ref. 46 for a similar result). $\square$

We have the following embedding result.

Lemma IV.5: We have $V_s + \mathcal{K}_{5/2-\epsilon}^\infty(\mathbb{T} \setminus \mathcal{S}) \subset W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$, $\epsilon \in (0, \frac{1}{2})$.

Proof: For $\epsilon \in (0, \frac{1}{2})$, we get $\mathcal{K}_{5/2-\epsilon}^2 \subset H^2$. So if $u \in \mathcal{K}_{5/2-\epsilon}^\infty$, then for any α , $\rho^{|\alpha|} \partial^\alpha(u) \in \mathcal{K}_{5/2-\epsilon}^2 \subset H^2$ so all b -derivatives of u must be continuous, hence bounded. So $u \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$. It is also clear that $V_s \subset W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$. This completes the proof. $\square$

A more general result is proved in Ref. 34, showing that the right range of ϵ for which the above result holds true is $\epsilon \in (0, 1)$. The proof provided here is more elementary.

Theorem IV.6: Let V be such that $\rho V \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$ (that is, V satisfies Assumption 2). Let $u \in L^2(\mathbb{T})$ be such that $H_k u = \lambda u$. Then $u \in \mathcal{K}_{5/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S}) + V_s$ for all $m \in \mathbb{Z}_+$ and $\epsilon > 0$. In particular, $u \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$.

Proof: By hypothesis, $u \in L^2(\mathbb{T}) = \mathcal{K}_{3/2-\epsilon}^0(\mathbb{T} \setminus \mathcal{S})$, and $(H_k - \lambda)u = 0 \in \mathcal{K}_{3/2-\epsilon}^{m-1}(\mathbb{T} \setminus \mathcal{S})$ for all m by Theorem IV.1, so we have that $u \in \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ for all m . Then Lemma III.4 (ii) gives that $\rho^{-1} B_{k,V,\lambda} u \in \mathcal{K}_{1/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ for all m . We next apply Lemma IV.4 to $\Delta u = \rho^{-1} B_{k,V,\lambda} u \in \mathcal{K}_{1/2-\epsilon}^{m-1}(\mathbb{T} \setminus \mathcal{S})$ to conclude that $u \in \mathcal{K}_{5/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ for all $m \in \mathbb{Z}_+$. $\square$

The following shows that the potentials appearing in the iterations defined in the Hartree–Fock and density-functional method iterations all satisfy Assumption 2. Hence the eigenfunctions of the corresponding Schrödinger operators will all satisfy the regularity result of Theorem I.2.

Corollary IV.7: Let V and u be as in Theorem IV.6. Then $\Delta^{-1}|u|^2 \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$.

Proof: We have $|u|^2 = \bar{u}u \in W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S}) \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S}) \subset \mathcal{K}_{3/2-\epsilon}^m(\mathbb{T} \setminus \mathcal{S})$ for all m . Hence $\Delta^{-1}|u|^2 \in V_s + \mathcal{K}_{5/2-\epsilon}^\infty(\mathbb{T} \setminus \mathcal{S}) \subset W^{\infty,\infty}(\mathbb{T} \setminus \mathcal{S})$. $\square$

V. PROOFS OF APPROXIMATION RESULTS

We first address the proof of Theorem I.4. The proof of Theorem I.5 is shorter and is included at the end. The first step in proving Theorem I.4 is to construct our sequence of tetrahedralizations. These will be based on the tetrahedralizations constructed in Ref. 47; thus we refer the reader to that paper for the details and here only give an outline and state the critical properties. The second step is to prove a sequence of simple lemmas used in the estimates. The third step is to prove the estimate separately on smaller regions. Our proof uses the scaling properties of the tetrahedralizations and the following important approximation result.^{48–51} To state this result, let us recall the definition of the “degree m Lagrange interpolant.”

A. Lagrange interpolants and approximation

Let $\mathcal{T} = \{T\}$ be a *mesh* on $\mathbb{T}$, that is, a tetrahedralization of $\mathbb{T}$ with tetrahedra T . We can identify this $\mathcal{T}$ with a mesh $\mathcal{T}'$ of the fundamental region of the lattice $\mathcal{L}$ (that is, to the Brillouin zone of $\mathcal{L}$). We fix in what follows an integer $m \in \mathbb{N}$ that will play the role of the order of approximation. We shall denote by $S(\mathcal{T}, m)$ the finite element space associated with the degree m Lagrange tetrahedron. That is, $S(\mathcal{T}, m)$ consists of all continuous functions $\chi: \mathbb{T} \rightarrow \mathbb{R}$ such that χ coincides with a polynomial of degree $\leq m$ on each tetrahedron $T \in \mathcal{T}$. We shall denote by $u_I = u_{I,\mathcal{T},m} \in S(\mathcal{T}, m)$ the Lagrange interpolant of $u \in H^2(\mathbb{T})$. Let us recall the definition of $u_{I,\mathcal{T},m}$. First, given a tetrahedron T , let $[t_0, t_1, t_2, t_3]$ be the barycentric coordinates on T . The nodes of the degree m Lagrange triangle T are the points of T whose barycentric coordinates $[t_0, t_1, t_2, t_3]$ satisfy $mt_j \in \mathbb{Z}$. The degree m Lagrange interpolant $u_{I,\mathcal{T},m}$ of u is the unique function $u_{I,\mathcal{T},m} \in S(\mathcal{T}, m)$ such that $u = u_{I,\mathcal{T},m}$ at the nodes of each tetrahedron $T \in \mathcal{T}$. The shorter notation u_I will be used only when only one mesh is understood in the discussion. The same definitions and concepts apply to any polyhedral domain $P \subset \mathbb{T}$.

The proof of Theorem I.4 follows from the standard result of any of the following basic references.^{48–51}

Theorem V.1: Let $\mathcal{T}$ be a tetrahedralization of a polyhedral domain $P \subset \mathbb{T}$ with the property that all tetrahedra comprising $\mathcal{T}$ have angles $\geq \alpha$ and edges $\leq h$. Then there exists an absolute constant $C(\alpha, m)$ such that, for any $u \in H^{m+1}(P)$,

$$\|u - u_I\|_{H^1(P)} \leq C(\alpha, m) h^m \|u\|_{H^{m+1}(P)}.$$

B. Constructing the tetrahedralizations

We continue to keep the approximation degree m fixed throughout this section. Fix a parameter $a \in (0, 1/2)$ and let $\kappa = 2^{-m/a}$. In our estimates, we will choose a such that $1+a=3/2-\epsilon$. Let l denote the smallest distance between points in $\mathcal{S}$. Choose an edge length $H < \kappa l/4$ and an initial tetrahedralization of T_0 with tetrahedra with sides $\leq H$ such that all singular points of V (i.e., all points of $\mathcal{S}$) are among the nodes of T_0 . Let α be the minimum of all the angles of the tetrahedra of T_0 .

For each point $p \in \mathcal{S}$, we denote by $\mathcal{V}_p$ the union of all tetrahedra of T_0 that have p as a vertex. Now subdivide these tetrahedra as follows. For any integer $1 \leq j \leq n$, let $\mathcal{V}_{pj}$ denote the union of tetrahedra obtained by scaling the tetrahedra defining $\mathcal{V}_p$ by a factor of κ^j with center p .

An important step in our refinement is to set up a level k uniform refinement of an arbitrary tetrahedron T . This refinement procedure will divide each edge of T into 2^k equal segments. Let $[t_0, t_1, t_2, t_3]$ be barycentric coordinates in T . Then our refinement is obtained by considering all planes $t_j = l/2^k$ and $t_i + t_j = l/2^k$, where i and j are arbitrary indices in $\{0, 1, 2, 3\}$ and $0 \leq l \leq 2^k$ is an arbitrary integer. By definition, the level $k+1$ refinement of T is a refinement of the level k refinement of T .

Let us apply now the level 1 of refinement to all tetrahedra comprising $\mathcal{V}_p$. Then we deform the new nodes on the sides containing p to divide their edge in the ratio κ . Then we deform all the other edges and planes accordingly. This will give a new tetrahedralization of $\mathcal{V}_p$ such that all tetrahedra defining $\mathcal{V}_{p1}$ are contained in this new tetrahedralization. In particular, we have obtained a tetrahedralization of $\mathcal{R}_{p1} := \mathcal{V}_p \setminus \mathcal{V}_{p1}$. Then we dilate this refinement to a similar refinement of $\mathcal{R}_{pj} := \mathcal{V}_{p(j-1)} \setminus \mathcal{V}_{pj}$.

We can now define the tetrahedralization (or mesh) $\mathcal{T}_n$ of T . Define

$$P := T \setminus \bigcup_{p \in \mathcal{S}} \mathcal{V}_p. \quad (32)$$

We first decompose T as the union

$$T = P \cup_{p \in \mathcal{S}} (\bigcup_{j=1}^n \mathcal{R}_{pj} \cup \mathcal{V}_{pn}). \quad (33)$$

Then we apply to each tetrahedron $T \in P$ contained in P the level n refinement. Then we apply to each tetrahedron $T \subset \mathcal{R}_{pj}$ the level $n-j$ refinement. The tetrahedra defining $\mathcal{V}_{pn}$ are not refined. The resulting tetrahedra (including the ones defining $\mathcal{V}_{pn}$) define the tetrahedralization $\mathcal{T}_n$. The fact that $\mathcal{T}_n$ is a tetrahedralization follows from the way our refinement was performed. This and more details of these constructions are given in Ref. 47.

Let us denote by $u_{I,n} = u_{I,\mathcal{T}_n,m}$ the degree m Lagrange interpolant of u associated with the mesh $\mathcal{T}_n$. By construction, the restriction of $\mathcal{T}_n$ to $\mathcal{R}_{pj}$ scales to the restriction of $\mathcal{T}_{n-j+1}$ to $\mathcal{R}_{p1}$. This gives the following.

Lemma V.2: We have $u_{I,n}(x) = u_{I,n-j+1}(\kappa^{-(j-1)}(x))$, for all $x \in \mathcal{R}_{pj}$, where $\kappa^{-(j-1)}(x) := p + (x - p)/\kappa^{(j-1)}$ is the dilation with ratio $\kappa^{-(j-1)}$ and center p .

The size of each simplex of $\mathcal{T}_n$ contained in P is $\geq h2^{-n}$. Similarly, the size of each simplex of $\mathcal{T}_n$ contained in $\mathcal{R}_{pj}$ is $\geq C\kappa^j 2^{-(n-j)}$. All angles of the tetrahedra used in our meshes are bounded uniformly from below by an angle $\alpha > 0$ (independent of the order of refinement n). This shows that the volumes of the tetrahedra are $\geq Ch2^{-3n}$ for the tetrahedra in P . Similarly, the volumes of the tetrahedra in $\mathcal{R}_{pj}$ are $\geq C\kappa^{3j} 2^{-3(n-j)}$. The constant $C > 0$ is independent of n or j . Since the volume of $\mathcal{R}_{pj}$ is $\leq C\kappa^{3j}$, we obtain that the total number of simplices of $\mathcal{T}_n$ is $\leq C2^{3n}$. Hence

$$\dim S(\mathcal{T}_n, m) \leq C2^{3n}. \quad (34)$$

C. Preliminary lemmas

None of the lemmas of this subsection is very difficult and analogous results have been proven in various papers, but it is useful to have them collected here.

Lemma V.3: Let D be a small neighborhood of a point $p \in \mathcal{S}$ such that on D , ρ is given by

distance to p . Let $0 < \gamma < 1$ and denote by γD the region obtained by radially shrinking around p by a factor of γ . Then

$$\|u\|_{\mathcal{K}_a^m(D)} = (\gamma)^{a-3/2} \|u\|_{\mathcal{K}_a^m(\gamma D)}.$$

Proof: Let x denote the coordinates on γD . For simplicity of notation, we will denote here by ∂_x a derivative with respect to any of these coordinates.

$$\|u\|_{\mathcal{K}_a^m(\gamma D)}^2 = \sum_{|\alpha| \leq m} \|\rho^{|\alpha|-a} \partial_x^\alpha u\|_{L^2(\gamma D)}^2 = \sum_{|\alpha| \leq m} \int_{\gamma D} \rho^{2|\alpha|-2a} (x) |\partial_x^\alpha u|^2 dx.$$

Do the change of variables $w = \gamma^{-1}x$. Then $\partial_x = \gamma^{-1} \partial_w$, γD becomes D , and dx becomes $\gamma^3 dw$. Further, since $\rho(x) = \text{distance to } p$, $\rho(x) = \gamma \rho(w)$. Thus we get

$$\begin{aligned} \|u\|_{\mathcal{K}_a^m(\gamma D)}^2 &= \sum_{|\alpha| \leq m} \int_D (\gamma \rho(w))^{2|\alpha|-2a} |\gamma^{-|\alpha|} \partial_w^\alpha u|^2 \gamma^3 dw = \gamma^{3-2a} \sum_{|\alpha| \leq m} \int_D \rho(w)^{2|\alpha|-2a} |\partial_w^\alpha u|^2 dw \\ &= (\gamma^{3/2-a} \|u\|_{\mathcal{K}_a^m(D)})^2, \end{aligned} \quad (35)$$

as required. $\square$

Lemma V.4: If $m \geq m'$, $a \geq a'$, and $0 < \rho < \delta$ on D , then

$$\|v\|_{\mathcal{K}_{a'}^{m'}(D)} \leq c(m) \delta^{a-a'} \|v\|_{\mathcal{K}_a^m(D)}.$$

Proof: We have

$$\begin{aligned} \|v\|_{\mathcal{K}_{a'}^{m'}(D)}^2 &= \sum_{|\alpha| \leq m'} \|\rho^{|\alpha|-a'} \partial^\alpha v\|_{L^2(D)}^2 \leq \sum_{|\alpha| \leq m} \int_D |\rho^{a-a'} \rho^{|\alpha|-a} \partial^\alpha v|^2 dx \leq \sum_{|\alpha| \leq m} \int_D \delta^{2(a-a')} |\rho^{|\alpha|-a} \partial^\alpha v|^2 dx \\ &= \delta^{2(a-a')} \|v\|_{\mathcal{K}_a^m(D)}^2, \end{aligned} \quad (36)$$

as stated. $\square$

Lemma V.5: For any m , if $\rho \leq b$, then

$$\|v\|_{\mathcal{K}_0^m(D)} \leq b^a \|v\|_{H^m(D)}.$$

Proof: We compute

$$\|v\|_{\mathcal{K}_0^m(D)}^2 = \sum_{|\alpha| \leq m} \int_D |\rho^{|\alpha|} \partial^\alpha v|^2 dx \leq \sum_{|\alpha| \leq m} \int_D b^{2|\alpha|} |\partial^\alpha v|^2 dx = b^{2a} \|v\|_{H^m(D)}^2, \quad (37)$$

which gives the result. $\square$

Lemma V.6: If $1 \geq \rho > \beta > 0$ on D , and $m \geq a$, then

$$\|v\|_{H^m(D)} \leq \delta^{a-m} \|v\|_{\mathcal{K}_a^m(D)}.$$

Proof: We have

$$\|v\|_{\mathcal{K}_a^m(D)}^2 = \sum_{|\alpha| \leq m} \int_D |\rho^{|\alpha|-a} \partial^\alpha v|^2 dx.$$

Since $\rho \leq 1$ and $|\alpha| \leq m$, we get $\rho^{|\alpha|-a} \geq \rho^{m-a}$. Thus this is

$$\geq \sum_{|\alpha| \leq m} \int_D \rho^{2(m-a)} |\partial^\alpha v|^2 dx \geq \sum_{|\alpha| \leq m} \int_D \delta^{2(m-a)} |\partial^\alpha v|^2 dx = \delta^{m-a} \|v\|_{H^m(D)}.$$

□

Lemma V.7: If $0 \leq \rho \leq \delta \leq 1$ on D and $a \geq m$, then

$$\|v\|_{H^m(D)} \leq \delta^{a-m} \|v\|_{\mathcal{K}_a^m(D)}.$$

Proof:

$$\|v\|_{\mathcal{K}_a^m(D)} = \sum_{|\alpha| \leq m} \int_D |\rho^{|\alpha|-a} \partial^\alpha v|^2 dx.$$

Since $a > m \geq |\alpha|$ and $\rho \leq \delta \leq 1$, we know $\rho^{2|\alpha|-2a} \geq \delta^{2|\alpha|-2a} \geq \delta^{2m-2a}$; thus this is

$$\geq \sum_{|\alpha| \leq m} \int_D \delta^{2(m-a)} |\partial^\alpha v|^2 dx = \delta^{2(m-a)} \|v\|_{H^m(D)}^2.$$

The proof is complete. □

D. Breaking the estimates into regions and proof of Theorem I.4

Now we can prove Theorem I.4 stated in Sec. I. Recall that $\mathcal{V}_p$ consists of the tetrahedra of the initial mesh $\mathcal{T}_0$ that have p as a vertex and that all the regions $\mathcal{V}_p$ are away from each other (they are closed and disjoint). We used this to define $\mathbb{P} := \mathbb{T} \setminus \bigcup_p \mathcal{V}_p$. The region $\mathcal{V}_{pj}$ is obtained by dilating $\mathcal{V}_p$ with the ratio $\kappa^j < 1$ and center p . Finally, recall that $\mathcal{R}_{pj} = \mathcal{V}_{p(j-1)} \setminus \mathcal{V}_{pj}$. Let R be any of the regions $\mathbb{P}$, $\mathcal{R}_{pj}$, or $\mathcal{V}_{pn}$. Since the union of these regions is $\mathbb{T}$, it is enough to prove that

$$\|u - u_{I, \mathcal{T}_n, m}\|_{\mathcal{K}_1^1(R \setminus S)} \leq C \dim(S_n)^{-m/3} (\|u\|_{\mathcal{K}_{3/2-\epsilon}^{m+1}(R \setminus S)} + \max_{p \in S \cap R} |u(p)|). \quad (38)$$

The result will follow by squaring all these inequalities and adding them up.

Since $2^{-nm} \leq C \dim(S_n)^{-m/3}$, by Eq. (34), it is enough to prove

$$\|u - u_{I, \mathcal{T}_n, m}\|_{\mathcal{K}_1^1(R \setminus S)} \leq C 2^{-nm} (\|u\|_{\mathcal{K}_{3/2-\epsilon}^{m+1}(R \setminus S)} + \max_{p \in S \cap R} |u(p)|). \quad (39)$$

If $R = \mathbb{P}$, the estimate of Eq. (39) follows right away from Theorem V.1. For the other estimates, we need to choose $0 < \kappa \leq 2^{-m/a}$, where $1 + a = 3/2 - \epsilon$, with $a \in (0, \frac{1}{2})$.

We next establish the desired interpolation estimate on the region $R = \mathcal{R}_{pj}$, for any fixed $p \in S$ and $j = 1, 2, \dots, n$. Let $w(x) = u(\kappa^{j-1}x)$. From Lemmas V.3 and V.2, we have

$$\|u - u_{I, n}\|_{\mathcal{K}_1^1(\mathcal{R}_{pj})} = (\kappa^{j-1})^{1/2} \|w - w_{I, n-j+1}\|_{\mathcal{K}_1^1(\mathcal{R}_{p1})}.$$

Now we can apply Theorem V.1 with $h = 2^{-(n-j+1)}H$ to get that this is

$$\leq C(\kappa^{j-1})^{1/2} 2^{-m(n-j+1)} \|w\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{R}_{p1})}.$$

Now applying Lemma V.3 to scale back again and using also $\kappa = 2^{-m/a}$, we get that this last quantity is equal to

$$= C(\kappa^{j-1})^a 2^{-m(n-j+1)} \|u\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{R}_{pj})} \leq C 2^{-nm} \|u\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{R}_{pj})}.$$

This proves the estimate of Eq. (39) for $R = \mathcal{R}_{pj}$.

It remains to prove this estimate for $R = \mathcal{V}_{pn}$. Then on $\mathcal{V}_{pn}$, we have $u = v + u(p)$, where $v(p) = 0$. For any function w on $\mathcal{V}_{pn}$, we let $w_n(x) = w(\kappa^n x)$, a function on $\mathcal{V}_p$. For simplicity, below, we shall denote all interpolants in the same way [so $u_I = u_{I, n}$ and $u_{n, I} = (u_n)_{I, 0}$]. So

$$\|u - u_I\|_{\mathcal{K}_1^1(\mathcal{V}_{pn})} = (\kappa^n)^{1/2} \|(u - u_I)_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)}$$

by scaling Lemma V.3 and

$$(\kappa^n)^{1/2} \|(u - u_I)_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)} = (\kappa^n)^{1/2} \|u_n - u_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}$$

by Lemma V.2 (which follows from the definition of the tetrahedralizations $\mathcal{T}_k$ and from the fact that interpolation commutes with changes of variables). Then the decomposition $u = v + u(p)$ gives

$$\begin{aligned} (\kappa^n)^{1/2} \|u_n - u_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} &= (\kappa^n)^{1/2} \|(v + u(p))_n - (v + u(p))_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} = (\kappa^n)^{1/2} \|v_n + u(p) - v_{n,I} \\ &\quad - u(p)\|_{\mathcal{K}_1^1(\mathcal{V}_p)} = (\kappa^n)^{1/2} \|v_n - v_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} \end{aligned} \quad (40)$$

by properties of interpolation. Now let χ be a smooth cutoff function on $\mathcal{V}_p$ which =0 in a neighborhood of p and =1 at every other interpolation point of $\mathcal{V}_p$. Then

$$(\kappa^n)^{1/2} \|v_n - v_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} \leq (\kappa^n)^{1/2} (\|v_n - \chi v_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi v_n - v_{n,I}\|_{\mathcal{K}_1^1(\mathcal{V}_p)})$$

by the triangle inequality and

$$= (\kappa^n)^{1/2} (\|v_n - \chi v_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi v_n - (\chi v_n)_I\|_{\mathcal{K}_1^1(\mathcal{V}_p)})$$

by properties of interpolation, since $\chi v_n = v_n$ at each interpolation point. This is

$$\leq C(\kappa^n)^{1/2} (\|v_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi v_n - (\chi v_n)_I\|_{\mathcal{K}_1^1(\mathcal{V}_p)})$$

by bounds on χ and its first derivatives. Now, since χv_n is in $H^{m+1}(\mathcal{V}_p)$, we can apply the standard result of Theorem V.1 and the fact that χv_n is supported away from the singularity to get

$$\begin{aligned} &\leq C(\kappa^n)^{1/2} (\|v_n\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi v_n\|_{H^{m+1}(\mathcal{V}_p)}) \leq C(\kappa^n)^{1/2} \|v_n\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{V}_p)} = C(\kappa^n)^a \|v\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{V}_p)} \\ &\leq C 2^{-mn} \|v\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{V}_p)}. \end{aligned} \quad (41)$$

Since constants are in $\mathcal{K}_{1+a}^{m+1}(R)$, we have that $\|v\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{V}_p)} \leq \|u\|_{\mathcal{K}_{1+a}^{m+1}(\mathcal{V}_p \setminus \mathcal{S})} + |u(p)|$. This proves the estimate of Eq. (39) for $R = V_{pn}$ and completes the proof of Theorem I.4.

E. Proof of approximation Theorem I.5

We now address Theorem I.5. A much more detailed discussion of the following issues will be included in the sequel to this paper, where also numerical tests will be included.

Proof: (Proof of Theorem I.5) Let $v \in H^s(\mathbb{T})$. Then the standard estimate of the growth of the Fourier coefficients of v [see Eq. (3)] gives that

$$\|v - P_N v\|_{H^1(\mathbb{T})} \leq C N^{-(s-1)} \|v\|_{H^s(\mathbb{T})}, \quad (42)$$

and no better estimate will hold for any v in $H^s(\mathbb{T})$. Now consider u as in the hypotheses of the theorem. By Theorem I.1, $u \in H^{5/2-\epsilon}(\mathbb{T})$. So putting the estimate above with the fact that $\dim(\mathcal{S}_N) \sim N^3$ proves the first relation.

For the second relation, let us assume for simplicity that $l=1$. We remove the order ρ term from the expansion for u in Theorem I.1 by choosing $h_p \in C^\infty(S^2)$ such that

$$v := u - \sum_p \rho h_p \chi_p \in \mathcal{K}_{7/2-\epsilon}^\infty(\mathbb{T} \setminus \mathcal{S}) \subset H^{7/2-\epsilon}(\mathbb{T}).$$

Note that we did not have to subtract the first singular function $\phi_0=1$ since it is already smooth and that we may fix ρ and χ_p depending only on $\mathcal{S}$ (if we choose differently we obtain an equivalent norm p below).

We then approximate v with elements in S_N . By the same standard arguments as for the first part of the theorem, this approximation is of order $N^{5/2-\epsilon}$. Now we can approximate the h_p with linear combinations h_{pN} of spherical harmonics such that $\sum_p \rho h_{pN} \chi_p \in W_s$. This approximation is of order k for any k since v is smooth in polar coordinates around any singular point. To be precise, since each $h_p \in C^\infty(S^2)$, for s sufficiently large we have

$$\|h_p - h_{pN}\|_{H^1(S^2)} \leq CN^{-a(s-1)/2} \|h_p\|_{H^s(S^2)},$$

where a is the constant used to define the spaces $S'_{N,a,l}$. Thus integrating, we get in a neighborhood U_p of each $p \in \mathcal{S}$,

$$\|\rho \chi_p (h_p - h_{pN})\|_{H^1(U_p)} \leq C \|h_p - h_{pN}\|_{H^1(S^2)} \leq CN^{-a(s-1)/2} \|h_p\|_{H^s(S^2)}.$$

Since for sufficiently large N the dimension of the enlarged space S'_N is $\dim(S_{N,3,1}) \leq CN^3$ (from Weyl's theorem on the asymptotics of eigenvalues as in Sec. I), all together we obtain

$$\begin{aligned} \|u - P'_N u\|_{H^1(\mathbb{T})} &\leq \|v - P_N v\|_{H^1(\mathbb{T})} + \sum_p \|\rho \chi_p (h_p - h_{pN})\|_{H^1(\mathbb{T})} \leq CN^{-(5/2-\epsilon)} \|v\|_{H^{7/2-\epsilon}(\mathbb{T})} \\ &\quad + CN^{-a(s-1)} \sum_p \|h_p\|_{H^s(S^2)} \leq C(\dim(S'_{N,3,1}))^{-(5-\epsilon)/6} p(u), \end{aligned} \quad (43)$$

by choosing $s > 5/2 - \epsilon$ and setting $p(u) = \|v\|_{H^{7/2-\epsilon}(\mathbb{T})} + \sum_p \|h_p\|_{H^s(S^2)}$ for the decomposition given as above. $\square$

The general case $l \geq 1$ is completely similar. In addition, we note that for potentials satisfying Assumption 1, better (i.e., smaller) approximation space than $S'_{N,a,l}$ could be used to approximate the eigenfunctions u of H_k . This could be done by looking in more detail at the expansion of Theorem I.1. Using the eigenfunction equation, supplemental information may be derived about the functions $\phi_k(x')$ in this expansion. Using this information would allow us to restrict to a smaller space of supplementary orbital functions. This is similar to the technique used in the case of the usual Schrödinger operator for the hydrogen atom.²⁴ Again, this will be discussed in more detail in a later paper.

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