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Computing scattering resonances

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Abstract. The question of whether it is possible to compute scattering resonances of Schrödinger operators – independently of the particular potential – is addressed. A positive answer is given, with the potential merely required to be $\mathcal{C}^1$ and have compact support. The proof is constructive, providing a universal algorithm which only needs to access the values of the potential at any requested point. Numerical examples are provided and compared with known results.

Keywords. Scattering resonance, Solvability Complexity Index, computational complexity

1. Introduction and main result

This paper provides an affirmative answer to the following question:

> *Does there exist a universal algorithm for computing the resonances of Schrödinger operators with complex potentials?*

To the authors' best knowledge this is the first time this question is addressed. Furthermore, the proof of existence provides an actual algorithm (that is, the proof is constructive). We test this algorithm on some standard examples, and compare to known results.

The framework required for this analysis is furnished by the *Solvability Complexity Index* (SCI), which is an abstract theory for the classification of the computational complexity and limitations of algorithms. This framework has been developed over the last decade by Hansen and collaborators (cf. [5, 6, 19]).

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1.1. Quantum resonances

Let us first define what a quantum resonance is. Let $q : \mathbb{R}^d \to \mathbb{C}$ be compactly supported, let

$$H_q := -\Delta + q$$

be the associated Schrödinger operator in $L^2(\mathbb{R}^d)$ and let $\chi : \mathbb{R}^d \to \mathbb{R}$ be some compactly supported function with $\chi \equiv 1$ on $\operatorname{supp}(q)$. It follows from the explicit form of the free fundamental solution (cf. (2.1) below) that the map

$$z \mapsto I + q(-\Delta - z^2)^{-1}\chi$$

is an analytic operator-valued function on $\mathbb{C} \setminus \{0\}$, where q and χ are viewed as multiplication operators. We define:

Definition 1.1 (Resonance). A *resonance* of H_q is defined to be a pole of the meromorphic operator-valued function $z \mapsto (I + q(-\Delta - z^2)^{-1}\chi)^{-1}$.

This definition is independent of the specific choice of χ (so long as $\chi \equiv 1$ on $\operatorname{supp}(q)$), and coincides with the poles of the scattering matrix of q ([23, Prop. 8] and [20, III.5]).

Resonances can be regarded as states whose wave function disperses very slowly in time, and can therefore be considered as "almost bound states". In physics, such phenomena arise in the description of unstable particles and radioactive decay. Resonant states, just like eigenfunctions, can only exist at certain energies. The slow-dispersal-in-time approach to resonances motivates one of the earlier definitions of resonances used in the computational physics literature, namely maximization of the so-called time delay function – see, e.g., Le Roy and Liu [22] and Smith [29]. This approach leads to real resonance energies for real-valued potentials and, in the one dimensional case at least, is closely related to the concept of spectral concentration – see, e.g., Eastham [18], which describes one mechanism by which such concentrations may arise. For additional discussion we refer to the review article [32] and the book [17].

It is widely accepted that the reliable computation of resonances is a challenging task. This is not usually due to the intrinsic ill-posedness of analytic continuation, since that step is usually done explicitly, but rather due to the fact that complex scaling changes resonance problems either into non-selfadjoint spectral problems, for which the pseudospectra may be far from the spectrum [31], or into problems with a nonlinear dependence on the spectral parameter, for which sensitivity to perturbations may also be problematic. In this context we refer to [12] (including the references and discussion therein) where interval-arithmetic was used to compute resonances.

We show that resonances can be computed as the limit of a sequence of approximations, each of which can be computed precisely using finitely many arithmetic operations. The proof is constructive: we define an algorithm and prove its convergence. We emphasize that this *single* algorithm is valid for *any* Schrödinger operator H_q as defined above, so long as q is compactly supported. We implement this algorithm in one dimension and compare its performance to that of Bindel and Zworski [10].

1.2. The Solvability Complexity Index hierarchy

The Solvability Complexity Index (SCI) hierarchy addresses questions which are at the nexus of pure and applied mathematics, as well as computer science:

> *How do we compute objects that are "infinite" in nature if we can only handle a finite amount of information and perform finitely many mathematical operations? Indeed, what do we even mean by "computing" such an object?*

These broad topics are addressed in the sequence of papers [5, 6, 19]. Let us summarize the main definitions:

Definition 1.2 (Computational problem). A *computational problem* is a quadruple $(\Omega, \Lambda, \Xi, \mathcal{M})$, where

(i) Ω is a set, called the *primary set*,

(ii) Λ is a set of complex-valued functions on Ω, called the *evaluation set*,

(iii) $\mathcal{M}$ is a metric space,

(iv) $\Xi : \Omega \to \mathcal{M}$ is a map, called the *problem function*.

Definition 1.3 (General algorithm). Let $(\Omega, \Lambda, \Xi, \mathcal{M})$ be a computational problem. A *general algorithm* is a mapping $\Gamma : \Omega \to \mathcal{M}$ such that for each $T \in \Omega$ there exists a finite subset $\Lambda_\Gamma(T) \subset \Lambda$ such that

(i) the action of Γ on T depends only on $\{f(T)\}_{f\in\Lambda_\Gamma(T)}$,

(ii) for every $S \in \Omega$ with $f(T) = f(S)$ for all $f \in \Lambda_\Gamma(T)$ one has $\Lambda_\Gamma(S) = \Lambda_\Gamma(T)$.

Definition 1.4 (Tower of general algorithms). Let $(\Omega, \Lambda, \Xi, \mathcal{M})$ be a computational problem. A *tower of general algorithms* of height k for $(\Omega, \Lambda, \Xi, \mathcal{M})$ is a family $\Gamma_{n_k,n_{k-1},\dots,n_1} : \Omega \to \mathcal{M}$ of general algorithms (where $n_i \in \mathbb{N}$ for $1 \le i \le k$) such that for all $T \in \Omega$,

$$\Xi(T) = \lim_{n_k\to+\infty} \cdots \lim_{n_1\to+\infty} \Gamma_{n_k,\dots,n_1}(T).$$

Definition 1.5 (Recursiveness). Suppose that for all $f \in \Lambda$ and for all $T \in \Omega$ we have $f(T) \in \mathbb{R}$ or $\mathbb{C}$. We say that $\Gamma_{n_k,n_{k-1},\dots,n_1}(\{f(T)\}_{f\in\Lambda})$ is *recursive* if it can be executed by a Blum–Shub–Smale (BSS) machine [11] that takes $(n_1, \dots, n_k)$ as input and that has an oracle that can access $f(T)$ for any $f \in \Lambda$.

Definition 1.6 (Tower of arithmetic algorithms). Given a computational problem $(\Omega, \Lambda, \Xi, \mathcal{M})$, where Λ is countable, a *tower of arithmetic algorithms* for $(\Omega, \Lambda, \Xi, \mathcal{M})$ is a general tower of algorithms where the lowest mappings $\Gamma_{n_k,\dots,n_1} : \Omega \to \mathcal{M}$ satisfy the following: For each $T \in \Omega$ the mapping $\mathbb{N}^k \ni (n_1, \dots, n_k) \mapsto \Gamma_{n_k,\dots,n_1}(T) = \Gamma_{n_k,\dots,n_1}(\{f(T)\}_{f\in\Lambda(T)})$ is recursive, and $\Gamma_{n_k,\dots,n_1}(T)$ is a finite string of complex numbers that can be identified with an element in $\mathcal{M}$.

Remark 1.7 (Types of towers). One can define many types of towers [5]. In this paper we write *type G* as shorthand for a tower of *general* algorithms, and *type A* as shorthand for a tower of *arithmetic* algorithms. If a tower $\{\Gamma_{n_k,n_{k-1},\dots,n_1}\}_{n_i\in\mathbb{N},\,1\le i\le k}$ is of type τ (where $\tau\in\{A,G\}$ in this paper) then we write

$$\{\Gamma_{n_k,n_{k-1},\dots,n_1}\}\in\tau.$$

Remark 1.8 (Computations over the reals). The computations in this paper are assumed to take place over the real numbers, hence the appearance of a BSS machine in Definition 1.5. One could attempt to adapt our results to Turing machines – and this indeed appears to be plausible – but that is not the purpose of the present paper.

Definition 1.9 (SCI). A computational problem $(\Omega,\Lambda,\Xi,\mathcal{M})$ is said to have a *Solvability Complexity Index* (SCI) of k with respect to a tower of algorithms of type τ if k is the smallest integer for which there exists a tower of algorithms of type τ of height k for $(\Omega,\Lambda,\Xi,\mathcal{M})$. We then write

$$\mathrm{SCI}(\Omega,\Lambda,\Xi,\mathcal{M})_\tau=k.$$

If there exists a tower $\{\Gamma_n\}_{n\in\mathbb{N}}\in\tau$ and $N_1\in\mathbb{N}$ such that $\Xi=\Gamma_{N_1}$ then we define $\mathrm{SCI}(\Omega,\Lambda,\Xi,\mathcal{M})_\tau=0$.

Definition 1.10 (The SCI hierarchy). The SCI *hierarchy* is a hierarchy $\{\Delta_k^\tau\}_{k\in\mathbb{N}_0}$ of classes of computational problems $(\Omega,\Lambda,\Xi,\mathcal{M})$, where each Δ_k^τ is defined as the collection of all computational problems satisfying

$$\begin{aligned}(\Omega,\Lambda,\Xi,\mathcal{M})\in\Delta_0^\tau &\iff \mathrm{SCI}(\Omega,\Lambda,\Xi,\mathcal{M})_\tau=0,\\ (\Omega,\Lambda,\Xi,\mathcal{M})\in\Delta_{k+1}^\tau &\iff \mathrm{SCI}(\Omega,\Lambda,\Xi,\mathcal{M})_\tau\le k,\quad k\in\mathbb{N},\end{aligned}$$

with the special class Δ_1^τ defined as the class of all computational problems in Δ_2^τ with known error bounds:

$$(\Omega,\Lambda,\Xi,\mathcal{M})\in\Delta_1^\tau \iff \begin{array}{l}\exists\{\Gamma_n\}_{n\in\mathbb{N}}\in\tau,\ \exists\varepsilon_n\searrow 0\ \forall T\in\Omega:\\ d(\Gamma_n(T),\Xi(T))\le\varepsilon_n.\end{array}$$

Hence we have $\Delta_0^\tau\subset\Delta_1^\tau\subset\Delta_2^\tau\subset\cdots$.

Remark 1.11. The definition of Δ_1^τ above (using an arbitrary null sequence ε_n) is equivalent to [5, Def. 6.10] where the explicit sequence 2^{-n} is used. In fact, given that $d(\Gamma_n(T),\Xi(T))\le\varepsilon_n$ for some $\varepsilon_n\searrow 0$ one can always achieve $d(\Gamma_{n_k}(T),\Xi(T))\le 2^{-k}$ by choosing an appropriate subsequence n_k.

When the metric space $\mathcal{M}$ has certain ordering properties, one can define further classes that take into account convergence from below/above and associated error bounds. In order not to burden the reader with unnecessary definitions, we provide the definition that is relevant to the case where $\mathcal{M}$ is the space of closed (and bounded) subsets of $\mathbb{R}^d$ together with the Attouch–Wets distance [4] (for a more comprehensive and abstract definition we refer to [5]), which is defined as follows:

Definition 1.12 (Attouch–Wets distance). Let A, B be closed, nonempty sets in $\mathbb{R}^d$. The *Attouch–Wets distance* between them is defined as

$$d_{\mathrm{AW}}(A,B) = \sum_{k=1}^{\infty} 2^{-k} \min\Big\{1, \sup_{|x|<k} |\operatorname{dist}(x,A) - \operatorname{dist}(x,B)|\Big\}.$$

Note that if $A, B \subset \mathbb{R}^d$ are bounded, then d_{AW} is equivalent to the Hausdorff distance.

Remark 1.13. It can be shown (cf. [27, Prop. 2.8]) that a sequence of sets $A_n \subset \mathbb{R}^d$ converges to A in the Attouch–Wets metric if the following two conditions are satisfied:

- If $\lambda_n \in A_n$ and $\lambda_n \to \lambda$, then $\lambda \in A$.
- If $\lambda \in A$, then there exist $\lambda_n \in A_n$ with $\lambda_n \to \lambda$.

Definition 1.14 (The SCI hierarchy (Attouch–Wets metric)). Consider the setup in Definition 1.10 assuming further that $\mathcal{M} = (\mathrm{cl}(\mathbb{R}^d), d_{\mathrm{AW}})$. Then we define

$$\Sigma_0^\tau = \Pi_0^\tau := \Delta_0^\tau$$

and for $k = 1, 2, \dots$ we can define the following subsets of Δ_{k+1}^τ:

$$\begin{aligned}
\Sigma_k^\tau = \Big\{(\Omega,\Lambda,\Xi,\mathcal{M}) \in \Delta_{k+1}^\tau \;\Big|\; & \exists \varepsilon_k \searrow 0\ \exists\{\Gamma_{n_k,\dots,n_1}\} \in \tau\ \forall T \in \Omega\ \exists\{X_{n_k}(T)\} \subset \mathcal{M} : \\
& \lim_{n_k\to\infty} \cdots \lim_{n_1\to\infty} \Gamma_{n_k,\dots,n_1}(T) = \Xi(T), \\
& \lim_{n_{k-1}\to\infty} \cdots \lim_{n_1\to\infty} \Gamma_{n_k,\dots,n_1}(T) \subset X_{n_k}(T), \\
& d(X_{n_k}(T), \Xi(T)) \le \varepsilon_k\Big\},
\end{aligned}$$

$$\begin{aligned}
\Pi_k^\tau = \Big\{(\Omega,\Lambda,\Xi,\mathcal{M}) \in \Delta_{k+1}^\tau \;\Big|\; & \exists \varepsilon_k \searrow 0\ \exists\{\Gamma_{n_k,\dots,n_1}\} \in \tau\ \forall T \in \Omega\ \exists\{X_{n_k}(T)\} \subset \mathcal{M} : \\
& \lim_{n_k\to\infty} \cdots \lim_{n_1\to\infty} \Gamma_{n_k,\dots,n_1}(T) = \Xi(T), \\
& \Xi(T) \subset X_{n_k}(T), \\
& d\Big(X_{n_k}(T), \lim_{n_{k-1}\to\infty} \cdots \lim_{n_1\to\infty} \Gamma_{n_k,\dots,n_1}(T)\Big) \le \varepsilon_k\Big\}.
\end{aligned}$$

It can be shown that $\Delta_k^\tau = \Sigma_k^\tau \cap \Pi_k^\tau$ for $k \in \{1,2,3\}$ (see Figure 1). We refer to [5] for a detailed treatment.

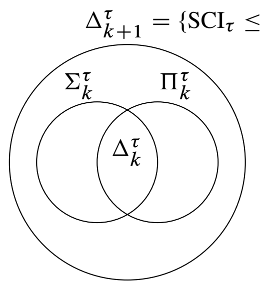

Fig. 1. The SCI hierarchy for $k \in \{1,2,3\}$.

Remark 1.15. For the same reasons mentioned in Remark 1.11, the above definition is equivalent to [5, Def. 6.12].

Informally, these sets can be characterized as follows:

Δ_k^τ: For $k \geq 2$, Δ_k^τ is the class of problems that require at most $k-1$ successive limits to solve with a tower of type τ. We also say that these problem have an SCI value of at most $k-1$. Problems in Δ_1^τ can be solved in one limit with a tower of type τ with known error bounds.

Σ_k^τ: For all $k \in \mathbb{N}$, $\Sigma_k^\tau \subset \Delta_{k+1}^\tau$ is the class of problems in Δ_{k+1}^τ that can be approximated from "below" with known error bounds.

Π_k^τ: For all $k \in \mathbb{N}$, $\Pi_k^\tau \subset \Delta_{k+1}^\tau$ is the class of problems in Δ_{k+1}^τ that can be approximated from "above" with known error bounds.

By an approximation from "above" (resp. "below") we mean that the output of the algorithm is a superset (resp. subset) of the object we are computing (this clearly requires that this object and its approximations belong to a certain topological space) up to the controllable error bound ε_n.

1.3. Main results

We start by defining the computational problems which we shall study.

Primary sets. Let $d \in \mathbb{N}$, fix $M, N > 0$ and let Q_M denote the cube of edge length M centered at the origin. Define the following primary sets:

(1) Ω_{cpt} denotes the class of Schrödinger operators

$$H_q := -\Delta + q \quad \text{on } L^2(\mathbb{R}^d)$$

with $q \in \mathcal{C}_0^1(\mathbb{R}^d; \mathbb{C})$.

(2) $\Omega_{M,N} \subset \Omega_{\mathrm{cpt}}$ denotes the class of Schrödinger operators in Ω_{cpt} with $\operatorname{supp}(q) \subset Q_M$ and $\|q\|_{L^\infty} \leq N$.

Evaluation set. We define the evaluation set Λ to be

$$\Lambda := \{q \mapsto q(x) \mid x \in \mathbb{Q}^d\}. \tag{1.1}$$

Metric space. $\mathcal{M}$ is the space $(\mathrm{cl}(\mathbb{C}), d_{\mathrm{AW}})$ of all closed subsets of $\mathbb{C}$ equipped with the Attouch–Wets metric.

Problem function. $\Xi : \Omega \to \mathcal{M}$ is the map that associates to a particular Schrödinger operator its set of resonances, and we denote it by $\operatorname{Res}(H_q)$.

Then the quadruples $(\Omega, \Lambda, \operatorname{Res}(\cdot), \mathrm{cl}(\mathbb{C}))$, where $\Omega \in \{\Omega_{\mathrm{cpt}}, \Omega_{M,N}\}$, both pose computational problems in the sense of Definition 1.2. Since the evaluation set, metric space and problem function are always the same, we shall omit them in what follows. The main result of the present article is the following.

Theorem 1.16. *The computation of quantum resonances requires*

(1) *one limit for operators belonging to* Ω_{cpt}*:* $\mathrm{SCI}(\Omega_{\mathrm{cpt}})_A = 1$*, i.e.*

$$\Omega_{\mathrm{cpt}} \in \Delta_2^A;$$

(2) *one limit with error bounds from above for operators belonging to* $\Omega_{M,N}$*:*

$$\Omega_{M,N} \in \Pi_1^A.$$

We prove this theorem by explicitly constructing an algorithm which computes the set of resonances in one limit for operators in Ω_{cpt}. This algorithm can be implemented numerically; some numerical experiments are provided in Section 5.

Remark 1.17. Our computations will involve not only the values $q(x)$, but also the values of Hankel functions $H_\nu^{(1)}(z)$, $z \in \mathbb{C}$, $\nu \in \frac{1}{2}\mathbb{N}$, as well as the exponential e^z, $z \in \mathbb{C}$, and taking square roots. These do not have to be included as part of the evaluation set because they can be approximated to arbitrary precision with explicit error bounds. In order to keep the presentation clear and concise, we will assume the values $H_\nu^{(1)}(z)$, e^z are known and not track these explicit errors in our estimates.

The proof of Theorem 1.16 is divided into several steps. First, we obtain quantitative resolvent norm estimates for the operator $K(z) := q(-\Delta - z^2)^{-1}\chi$ from Definition 1.1. These are then used to bound the error between $K(z)$ itself and a discretized version $K_n(z)$, obtained by replacing the potential q by a piecewise constant approximation. Finally, the poles of $(I + K(z))^{-1}$ are identified through a thresholding of the discretized operator function $(I + K_n(z))^{-1}$.

1.4. Comparison to previous results

This paper applies the ideas on complexity of infinite-dimensional problems developed in [5, 6, 19] to the problem of computing quantum resonances. In a separate paper [7] we studied obstacle scattering resonances. Recent years have seen a flurry of activity in this direction. We point out [8, 15, 16] where some of the theory of spectral computations has been further developed; [27] where this has been applied to certain classes of unbounded operators; [3] where solutions of PDEs were considered; and [14] where the authors give further examples of how to perform certain spectral computations with error bounds.

The approach developed in [12] for resonances in 1D uses interval arithmetic and automatic differentiation to solve initial value problems with guaranteed error bounds. An interval arithmetic implementation of the argument principle allows the number of resonances to be counted in any user-specified rectangle in the complex plane. Compared to the PDE methods, the most significant difference is that the input required is not just a black box providing point values of the potential, but source code in a form which is amenable to automatic differentiation pre-processing. This includes all cases with symbolically defined potentials.

Organization of the paper. Section 2 contains a short discussion of Definition 1.1 and meromorphic continuation. In Section 3 we prove some estimates for convergence of finite-dimensional approximations of linear operators, which are then used in Section 4 to construct an explicit algorithm which computes resonances in one limit, thereby proving Theorem 1.16. Section 5 is dedicated to numerical experiments. In Appendix A we review some properties of the fundamental solution to the free Helmholtz operator $-\Delta - z^2$ which plays an important role throughout this paper.

2. Analytic continuation

We use this section for a more detailed discussion of Definition 1.1 and to fix some notations and conventions. First, for $x \in \mathbb{R}^d$ and $z \in \mathbb{C}$ let

$$G(x,z) := \begin{cases} \frac{\mathrm{i}}{4}\left(\frac{z}{2\pi|x|}\right)^{(d-2)/2} H^{(1)}_{(d-2)/2}(z|x|), & d \geq 2, \\ \frac{\mathrm{i}}{2z} e^{\mathrm{i}z|x|}, & d = 1, \end{cases} \tag{2.1}$$

where $H^{(1)}_\nu$ denotes the Hankel function of the first kind. For $\mathrm{Im}(z) > 0$ the Green function $G(x,z)$ is the fundamental solution to the free Helmholtz operator $-\Delta - z^2$ (cf. [28, Ch. 22]) satisfying

$$(-\Delta_x - z^2)G = \delta_{x=0}.$$

For the sake of self-containedness, we prove the existence of $z \mapsto (I + q(-\Delta - z^2)^{-1}\chi)^{-1}$ as a meromorphic operator-valued function on the domain

$$\mathbb{C}^{\mathrm{ext}} := \begin{cases} \mathbb{C} & \text{if } d \text{ is odd}, \\ \text{logarithmic cover of } \mathbb{C} & \text{if } d \text{ is even}. \end{cases}$$

This result follows from the classical analytic Fredholm theorem (cf. e.g. [25, Sec. VI.5]):

Theorem 2.1 (Analytic Fredholm theorem). *Let $D \subset \mathbb{C}$ be open and connected and let $F : D \to L(\mathcal{H})$ be an analytic operator-valued function such that $F(z)$ is compact for all $z \in D$. Then, either*

(i) $(I + F(z))^{-1}$ *exists for no $z \in D$, or*

(ii) $(I + F(z))^{-1}$ *exists for all $z \in D \setminus S$, where S is a discrete subset of D. In this case, $z \mapsto (I + F(z))^{-1}$ is meromorphic in D, analytic in $D \setminus S$, the residues at the poles are finite rank operators, and if $z \in S$ then* $\ker(I + F(z)) \neq \{0\}$.

Next, recall that Q_M denotes the cube of edge length M in $\mathbb{R}^d$ centered at the origin. Let $\chi := \chi_{Q_M}$ be the indicator function of Q_M. Note that the operator-valued function $z \mapsto q(-\Delta - z^2)^{-1}\chi$ is an analytic function on $\mathbb{C}^{\mathrm{ext}} \setminus \{0\}$. This follows from the explicit representation of the free fundamental solution (2.1) (cf. Remark A.2).

Lemma 2.2. *The function $\mathbb{C}^+ \ni z \mapsto (I + q(-\Delta - z^2)^{-1}\chi)^{-1}$ has a meromorphic continuation to $\mathbb{C}^{\mathrm{ext}}$. Moreover, the residues at the poles are finite rank operators.*

Proof. The operator $q(-\Delta - z^2)^{-1}\chi$ is compact by the Fréchet–Kolmogorov theorem and the inverse $(I + q(-\Delta - z^2)^{-1}\chi)^{-1}$ exists for $\mathrm{Im}(z) > 0$ large enough, by the Neumann series. Hence, the claim follows from the analytic Fredholm theorem, together with Remark A.2 in the appendix. ■

The above observations lead us to study the spectrum of the compact operator

$$K(z) := q(-\Delta - z^2)^{-1}\chi, \quad z \in \mathbb{C}^{\mathrm{ext}}. \tag{2.2}$$

Since the integral kernel for the free resolvent is given explicitly by (2.1) as an analytic function of $z \in \mathbb{C}^{\mathrm{ext}} \setminus \{0\}$, we have an explicit representation of (2.2) as an integral operator on $L^2(\mathbb{R}^d)$:

$$(q(-\Delta - z^2)^{-1}\chi f)(x) = q(x) \int_{\mathbb{R}^d} G(x-y, z)\chi(y) f(y)\, dy, \quad z \in \mathbb{C}^{\mathrm{ext}} \setminus \{0\}. \tag{2.3}$$

3. Abstract error estimates

We recall that the resonances of $H_q = -\Delta + q$ are defined to be the poles of $\mathbb{C}^{\mathrm{ext}} \ni z \mapsto (I + K(z))^{-1}$ where $K(z) = q(-\Delta - z^2)^{-1}\chi$ is a compact operator. In this section we prove general abstract estimates for approximations of families of linear operators. These are largely independent of the rest of this paper and will be applied in the proof of Theorem 1.16. Abusing notation, our generic abstract analytic operator family is denoted $K(z)$.

Let $\mathcal{H}$ be a separable Hilbert space and denote by $L(\mathcal{H})$ the space of bounded operators on $\mathcal{H}$. Let $\mathcal{H}_n \subset \mathcal{H}$ be a finite-dimensional subspace, $P_n : \mathcal{H} \to \mathcal{H}_n$ the orthogonal projection and $K : \mathbb{C}^{\mathrm{ext}} \to L(\mathcal{H})$ continuous in operator norm. Moreover, let $K_n : \mathbb{C}^{\mathrm{ext}} \to L(\mathcal{H}_n)$ be analytic for every $n \in \mathbb{N}$. Assume that for any compact subset $B \subset \mathbb{C}^{\mathrm{ext}}$ there exist a sequence $a_n \downarrow 0$ and a constant $C > 0$ such that for all $z \in B$,

$$\|K(z) - K_n(z)P_n\|_{L(\mathcal{H})} \le C a_n, \tag{3.1}$$

$$\|P_n K(z)|_{\mathcal{H}_n} - K_n(z)\|_{L(\mathcal{H}_n)} \le C a_n, \tag{3.2}$$

$$\|K(z) - P_n K(z) P_n\|_{L(\mathcal{H})} \le C a_n. \tag{3.3}$$

3.1. Error estimates

With the above setup, and assuming (3.1)–(3.3) to hold true, we now prove a sequence of abstract lemmas which then allow us to define an abstract algorithm for computing poles, and prove its convergence (cf. Lemma 3.5).

Lemma 3.1. *If $z \in \mathbb{C}^{\mathrm{ext}}$ is such that $-1 \notin \sigma(K(z))$, then*

$$(1 - C a_n \|(I + K(z))^{-1}\|_{L(\mathcal{H})}) \|(I + K_n(z))^{-1}\|_{L(\mathcal{H}_n)} \le \|(I + K(z))^{-1}\|_{L(\mathcal{H})},$$

where we use the convention that $\|(I + K_n(z))^{-1}\|_{L(\mathcal{H})} = +\infty$ if $-1 \in \sigma(K_n(z))$.

Proof. Whenever the left hand side is non-positive the assertion is trivially true, so we may assume that $1 - Ca_n \|(I + K(z))^{-1}\|_{L(\mathcal{H})} > 0$. In this case, the assertion follows by a Neumann series argument, as follows. We have

$$\begin{aligned} I + K_n(z)P_n &= I + K(z) + (K_n(z)P_n - K(z)) \\ &= (I + K(z))[I + (I + K(z))^{-1}(K_n(z)P_n - K(z))]. \end{aligned} \tag{3.4}$$

Because $Ca_n < \frac{1}{\|(I+K(z))^{-1}\|}$, the second factor in (3.4) is invertible by the Neumann series and

$$[I + (I + K(z))^{-1}(K_n(z)P_n - K(z))]^{-1} = \sum_{j=0}^{\infty}\big((I + K(z))^{-1}(K_n(z)P_n - K(z))\big)^j.$$

Hence,

$$\begin{aligned} &\|(I + K_n(z)P_n)^{-1}\|_{L(\mathcal{H})} \\ &\quad \leq \Big\|\sum_{j=0}^{\infty}\big((I + K(z))^{-1}(K_n(z) - K(z))\big)^j\Big\|_{L(\mathcal{H})}\|(I + K(z))^{-1}\|_{L(\mathcal{H})} \\ &\quad \leq \sum_{j=0}^{\infty}\|(I + K(z))^{-1}\|_{L(\mathcal{H})}^{j+1}\|K_n(z)P_n - K(z)\|_{L(\mathcal{H})}^{j} \\ &\quad \leq \sum_{j=0}^{\infty}\|(I + K(z))^{-1}\|_{L(\mathcal{H})}^{j+1}(Ca_n)^j \\ &\quad = \|(I + K(z))^{-1}\|_{L(\mathcal{H})}\sum_{j=0}^{\infty}\|(I + K(z))^{-1}\|_{L(\mathcal{H})}^{j}(Ca_n)^j \\ &\quad = \frac{\|(I + K(z))^{-1}\|_{L(\mathcal{H})}}{1 - \|(I + K(z))^{-1}\|_{L(\mathcal{H})}Ca_n} \end{aligned}$$

for any $n \in \mathbb{N}$. It remains to replace the $L(\mathcal{H})$ norm on the left hand side by the $L(\mathcal{H}_n)$ norm. This follows from Claim 3.2, completing the proof. ∎

Claim 3.2. *We have $\|(I + K_n(z))^{-1}\|_{L(\mathcal{H}_n)} \leq \|(I + K_n(z)P_n)^{-1}\|_{L(\mathcal{H})}$ for all z for which both operators are boundedly invertible.*

Proof. For $x \in \mathcal{H}_n$ we have $(I + K_nP_n)^{-1}x = (I + K_n)^{-1}x$, because if $u \in \mathcal{H}_n$ solves $(I + K_n)u = x$, then $(I + K_nP_n)u = x$ and by invertibility $u = (I + K_nP_n)^{-1}x$. We conclude that

$$\sup_{x\in\mathcal{H}_n,\,\|x\|=1}\|(I + K_nP_n)^{-1}x\|_{\mathcal{H}} = \sup_{x\in\mathcal{H}_n,\,\|x\|=1}\|(I + K_n)^{-1}x\|_{\mathcal{H}_n}$$

and therefore

$$\sup_{x\in\mathcal{H},\,\|x\|=1}\|(I + K_nP_n)^{-1}x\|_{\mathcal{H}} \geq \sup_{x\in\mathcal{H}_n,\,\|x\|=1}\|(I + K_n)^{-1}x\|_{\mathcal{H}_n}.$$ ∎

Lemma 3.3. *If $z \in \mathbb{C}^{\mathrm{ext}}$ is such that either $-1 \in \sigma(K(z))$ or $\|(I+K(z))^{-1}\|_{L(\mathcal{H})} \geq \frac{1}{Ca_n}$, then either $-1 \in \sigma(P_n K(z) P_n)$ or*

$$\|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})} \geq \frac{1}{2Ca_n}.$$

Proof. If $-1 \in \sigma(K(z))$, then unless $-1 \in \sigma(P_n K(z) P_n)$, we have

$$\begin{aligned} I + K(z) &= I + P_n K(z) P_n + (K(z) - P_n K(z) P_n) \\ &= (I + P_n K(z) P_n)[I + (I + P_n K(z) P_n)^{-1}(K(z) - P_n K(z) P_n)]. \end{aligned}$$

We now argue by contradiction. If we had $\|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})} < \frac{1}{2Ca_n}$, then we would have $\|(I + P_n K(z) P_n)^{-1}(K(z) - P_n K(z) P_n)\|_{L(\mathcal{H})} < 1$ and $I + K(z)$ would be invertible by the Neumann series, contradicting our assumption that $-1 \in \sigma(K(z))$. Thus we must have $\|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})} \geq \frac{1}{2Ca_n}$.

Now let us turn to the case where $-1 \notin \sigma(K(z))$ and $\|(I + K(z))^{-1}\|_{L(\mathcal{H})} \geq \frac{1}{Ca_n}$. The same calculation as in the proof of Lemma 3.1 shows that

$$\big(1 - Ca_n \|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})}\big)\|(I + K(z))^{-1}\|_{L(\mathcal{H})} \leq \|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})}$$

from which it follows easily that $\frac{1}{2Ca_n} \leq \|(I + P_n K(z) P_n)^{-1}\|_{L(\mathcal{H})}$. ∎

Lemma 3.4. *Let $B \subset \mathbb{C}^{\mathrm{ext}}$ be compact and assume that $\|K(z) - K(w)\| \leq C|z - w|$ for some $C > 0$ for all $z, w \in B$. If $-1 \in \sigma(K(z))$, then $\|(I + K(w))^{-1}\| \geq \frac{1}{C|z-w|}$.*

Proof. Assume that $I + K(w)$ is invertible. Then

$$I + K(z) = (I + K(w))[I + (I + K(w))^{-1}(K(z) - K(w))]. \tag{3.5}$$

If we had $\|(I + K(w))^{-1}\| \, \|(K(z) - K(w))\| < 1$, then the right hand side of (3.5) would be invertible by the Neumann series – a contradiction. Hence one must have

$$\|(I + K(w))^{-1}\| \geq \|(K(z) - K(w))\|^{-1} \geq \frac{1}{C|z - w|}.$$ ∎

3.2. An abstract algorithm for computing poles

We now demonstrate how the assumptions (3.1)–(3.3) allow us to construct an abstract algorithm that computes the poles of $(I + K(z))^{-1}$. By an *abstract algorithm* we mean a sequence of subsets of $\mathbb{C}^{\mathrm{ext}}$, which is constructed from K_n and which converges in Attouch–Wets metric to $\{z \in \mathbb{C}^{\mathrm{ext}} \mid -1 \in \sigma(K(z))\}$. Note that this is not yet an *arithmetic algorithm* in the sense of Definition 1.3, since the sets are not computed from a finite amount of information in finitely many steps.

Let $B \subset \mathbb{C}^{\mathrm{ext}}$ be compact and define the lattice $\mathcal{L}_n := a_n^{-1}(\mathbb{Z} + \mathrm{i}\mathbb{Z}) \cap B$. Since we assume that a_n is explicitly known and $K_n(z)$ can be computed in finitely many steps, we can define the set

$$\Theta_n^B(K) = \left\{ z \in \mathcal{L}_n \;\middle|\; \|(I + K_n(z))^{-1}\|_{L(\mathcal{H}_n)} \geq \frac{1}{2\sqrt{a_n}} \right\}. \tag{3.6}$$

Moreover, by [5, Prop. 10.1], determining whether $\|(I+K_n(z))^{-1}\|_{L(\mathcal{H}_n)} \geq \frac{1}{2\sqrt{a_n}}$ can be done with finitely many arithmetic operations on the matrix elements of $K_n(z)$ for each $z \in \mathcal{L}_n$.

Lemma 3.5. *The assumptions* (3.1)–(3.3) *imply the convergence*

$$\Theta_n^B(K) \to \{z \in B \mid -1 \in \sigma(K(z))\}$$

in the Attouch–Wets metric.

Proof. I. Excluding spectral pollution. Assume that $z_n \in \Theta_n^B(K)$ with $z_n \to z_0$ for some $z_0 \in B$. Then for each n we have $\|(I + K_n(z_n))^{-1}\|_{L(\mathcal{H}_n)} \geq \frac{1}{2\sqrt{a_n}}$ and hence by Lemma 3.1,

$$\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} \geq \left(1 - Ca_n\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})}\right)\frac{1}{2}a_n^{-1/2}$$

(with the convention that $\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} = +\infty$ if $-1 \in \sigma(K(z_n))$). Whenever $\sqrt{a_n} \leq 2/C$ this leads to

$$\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} \geq \frac{1}{2}\frac{a_n^{-1/2}}{1 + C\sqrt{a_n}/2} \geq \frac{1}{4}a_n^{-1/2}.$$

It follows that $\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} \to +\infty$ as $n \to +\infty$ and hence $I + K(z_0)$ is not invertible (this follows by yet another Neumann series argument, together with norm continuity of K). Hence z_0 is a pole.

II. Spectral inclusion. Assume now that z is a pole, i.e. $-1 \in \sigma(K(z))$. Our reasoning will have the structure

$$\begin{gathered}
-1 \in \sigma(K(z)) \\
\Downarrow \\
\exists z_n \in \mathcal{L}_n : \|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} \text{ large} \\
\Downarrow \\
\|(I + P_nK(z_n)P_n)^{-1}\|_{L(\mathcal{H})} \text{ large} \\
\Downarrow \\
\|(I + P_nK(z_n)|_{\mathcal{H}_n})^{-1}\|_{L(\mathcal{H}_n)} \text{ large} \\
\Downarrow \\
\|(I + K_n(z_n))^{-1}\|_{L(\mathcal{H}_n)} \text{ large,}
\end{gathered}$$

with a quantitative estimate in each step. To this end, note first that if $-1 \in \sigma(K(z))$ for some $z \in B$, then there exist $\nu, c, \varepsilon > 0$ (independent of n) such that for all ζ in an ε-neighborhood of z,

$$\|(I + K(\zeta))^{-1}\|_{L(\mathcal{H})} \geq c|z - \zeta|^{-\nu}. \tag{3.7}$$

Indeed, since all singularities of $(I + K(z))^{-1}$ are of finite order by the analytic Fredholm theorem, this follows from the Laurent expansion of meromorphic operator-valued functions.

It follows from (3.7) that for any z_n such that $|z - z_n| \leq a_n$ one will have, for all n with $a_n < 1$,

$$\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} \geq c|z - z_n|^{-\nu} \geq c a_n^{-\nu} \geq c a_n^{-1}.$$

We conclude that for any pole z there exists a sequence $z_n \in \mathcal{L}_n$ such that $z_n \to z$ as $n \to +\infty$ and $\|(I + K(z_n))^{-1}\|_{L(\mathcal{H})} > c/a_n$ for all but finitely many $n \in \mathbb{N}$.

Next, Lemma 3.3 shows that $\|(I + P_n K(z_n) P_n)^{-1}\|_{L(\mathcal{H})} > \frac{c}{2a_n}$. Studying this norm further, we have

$$(I_{\mathcal{H}} + P_n K(z_n) P_n)^{-1} = (I_{\mathcal{H}_n} + P_n K(z_n)|_{\mathcal{H}_n})^{-1} \oplus I_{\mathcal{H}_n^{\perp}}$$

and thus

$$\|(I_{\mathcal{H}} + P_n K(z_n) P_n)^{-1}\|_{L(\mathcal{H})} = \max\{\|(I_{\mathcal{H}_n} + P_n K(z_n)|_{\mathcal{H}_n})^{-1}\|_{L(\mathcal{H}_n)}, 1\}.$$

Hence, as long as $a_n < c/2$, we have

$$\|(I + P_n K(z_n) P_n)^{-1}\|_{L(\mathcal{H})} = \|(I + P_n K(z_n)|_{\mathcal{H}_n})^{-1}\|_{L(\mathcal{H}_n)}.$$

We conclude that if z is a pole, then there exists $z_n \in \mathcal{L}_n$ such that

$$\|(I + P_n K(z_n)|_{\mathcal{H}_n})^{-1}\|_{L(\mathcal{H}_n)} > \frac{c}{2a_n} \tag{3.8}$$

(n large enough). A similar reasoning to that in Lemma 3.1 (using (3.2)) shows that now

$$\begin{aligned}(1 - C a_n \|(I + K_n(z_n))^{-1}\|_{L(\mathcal{H}_n)}) &\|(I + P_n K(z_n)|_{\mathcal{H}_n})^{-1}\|_{L(\mathcal{H}_n)} \\ &\leq \|(I + K_n(z_n))^{-1}\|_{L(\mathcal{H}_n)},\end{aligned}$$

and rearranging terms, together with (3.8), gives

$$\|(I + K_n(z_n))^{-1}\|_{L(\mathcal{H}_n)} \geq \frac{c}{2(1 + Cc)a_n}$$

and therefore $z_n \in \Theta_n^B(K)$ for large enough n. The assertion about Attouch–Wets convergence now follows from Remark 1.13. ■

4. Definition of the algorithm

In this section we apply the abstract results of Section 3 to our resonance problem and prove Theorem 1.16. The proof (contained in Sections 4.3 and 4.4) relies on the following weaker result which is proved in Section 4.2:

Theorem 4.1. *Let Q_M denote the cube of edge length M centered at the origin. Let $\Omega_M \subset \Omega_{\mathrm{cpt}}$ denote the class of Schrödinger operators H_q in Ω_{cpt} with* $\operatorname{supp}(q) \subset Q_M$. *Then $\Omega_M \in \Delta_2^A$.*

We first define

$$K(z) := q(-\Delta - z^2)^{-1}\chi$$

to be the operator appearing in Definition 1.1. We recall that it is given by the expression

$$(q(-\Delta - z^2)^{-1}\chi f)(x) = q(x)\int_{\mathbb{R}^d} G(x-y,z)\chi(y)f(y)\,dy, \quad z \in \mathbb{C}^{\text{ext}} \setminus \{0\}.$$

With a slight abuse of notation and where there is no risk of confusion, we retain the symbol K for the integral kernel of $K(z)$, that is,

$$K(x,y) := q(x)G(x-y,z)\chi(y)$$

for any fixed z. Since the supports of both q and χ are contained within the cube Q_M, we have $\operatorname{supp}(K) \subset Q_M \times Q_M$. We will construct an operator approximation K_n of K, which satisfies (3.1)–(3.3) and in addition

(H1) the matrix elements of K_n can be computed in finitely many steps from a finite subset $\Lambda_n \subset \Lambda$ (cf. (1.1) and Def. 1.3);

(H2) the convergence rate a_n is explicitly known (i.e. the sequence a_n can be used to define the algorithm).

To this end, let us define $\mathcal{H}_n$ and P_n as follows:

$$\mathbb{R}^d = \bigcup_{i\in\frac{1}{n}\mathbb{Z}^d} S_{n,i} := \bigcup_{i\in\frac{1}{n}\mathbb{Z}^d} \left([0,1/n)^d + i\right), \tag{4.1}$$

$$\mathcal{H}_n = \left\{ f \in L^2(Q_M) \;\middle|\; f|_{S_{n,i}} \text{ constant } \forall i \in \tfrac{1}{n}\mathbb{Z}^d \cap Q_M \right\},$$

$$P_n f(x) = \sum_{i\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} \left(n^d \int_{S_{n,i}} f(t)\,dt \right) \chi_{S_{n,i}}(x). \tag{4.2}$$

Furthermore, we have to make a concrete choice for the approximation K_n. An obvious choice is the integral kernel

$$K_n(x,y) := \sum_{i,j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} K(i,j)\chi_{S_{n,i}}(x)\chi_{S_{n,j}}(y),$$

i.e. a piecewise constant approximation of $K(\cdot,\cdot)$ which can be computed from the values of K on the lattice $n^{-1}\mathbb{Z}^d$ (in dimensions greater than 1, the fundamental solution G has a singularity at $x = y$; hence, we put $K_n := 0$ for $i = j$ in this case). As in (3.6), our algorithm is

$$\Theta_n^B(q) = \left\{ z \in \mathcal{L}_n \;\middle|\; \|(I + K_n(\cdot,\cdot))^{-1}\|_{L(\mathcal{H}_n)} \geq \frac{1}{2\sqrt{a_n}} \right\}$$

where we abuse notation and write $\Theta_n^B(q)$ rather than $\Theta_n^B(K)$ to emphasize that the sole input of this problem is the particular potential q.

4.1. Error estimates

We will now show that the operators K, K_n satisfy (3.1)–(3.3). To streamline the presentation, we will restrict ourselves to $d \geq 3$ in our computations, the cases $d \leq 2$ being entirely analogous with minor changes in the formulas. Constants independent of n will be denoted C and their value may change from line to line.

Proof of (3.3). Using the definitions (4.1)–(4.2), we have

$$Kf(x) - P_n K P_n f(x) = \int_{\mathbb{R}^d} K(x,y) f(y)\, dy - \int_{\mathbb{R}^d} P_n^x K(x,y) P_n f(y)\, dy,$$

where $P_n^x K(x,y)$ means $(P_n K(\cdot, y))(x)$. Using L^2-selfadjointness of P_n, we conclude that

$$\begin{aligned} Kf(x) - P_n K P_n f(x) &= \int_{\mathbb{R}^d} K(x,y) f(y)\, dy - \int_{\mathbb{R}^d} P_n^y P_n^x K(x,y) f(y)\, dy \\ &= \int_{\mathbb{R}^d} (K(x,y) - P_n^y P_n^x K(x,y)) f(y)\, dy. \end{aligned}$$

Note that $P_n^y P_n^x K(x,y)$ simply yields a step function approximation of $K(x,y)$ like (4.2), but in dimension $2d$. By applying Young's inequality [30, Th. 0.3.1] we conclude that

$$\|Kf - P_n K P_n f\|_{L^2(\mathbb{R}^d)} \leq \eta_n \|f\|_{L^2(\mathbb{R}^d)},$$

where

$$\begin{aligned} \eta_n = \max \Big\{ &\sup_{x \in \mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy, \\ &\sup_{y \in \mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dx \Big\}. \end{aligned} \tag{4.3}$$

Thus, all we have to do is estimate the L^∞-L^1 difference between K and its projection onto step functions. To this end, fix $x \in Q_M$, let $\varepsilon > 2/n$ and decompose the integrals as follows:

$$\begin{aligned} &\int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy = \int_{Q_M} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy \\ &= \int_{Q_M \setminus B_\varepsilon(x)} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy + \int_{B_\varepsilon(x)} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy. \end{aligned} \tag{4.4}$$

The integral over $B_\varepsilon(x)$ can be estimated by $\int_{B_\varepsilon(x)} 2|K(x,y)|\, dy$, while for the remaining integral we can use the fact that the derivative of K is bounded, as follows. Let $j \in \frac{1}{n}\mathbb{Z}^d$ be such that $x \in S_{n,j}$ (see Figure 2). Let $i \in \frac{1}{n}\mathbb{Z}^d$ be such that $|i - j| > \varepsilon/2$. Then

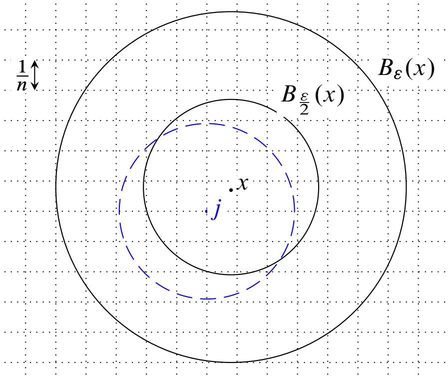

Fig. 2. Sketch of the geometry in the calculation leading to (4.5). The sum over i includes all cells whose nodes are outside the dashed ball centered at j.

$$\begin{aligned}\int_{S_{n,i}} |K(x,y) - P_n^y P_n^x K(x,y)|\,dy &= \int_{S_{n,i}} \left| K(x,y) - \fint_{S_{n,i}\times S_{n,j}} K(s,t)\,ds\,dt \right| dy \\ &\le \int_{S_{n,i}} \fint_{S_{n,i}\times S_{n,j}} |K(x,y) - K(s,t)|\,ds\,dt\,dy \\ &= \int_{S_{n,i}} \fint_{S_{n,i}\times S_{n,j}} \left| \int_0^1 \nabla K(\tau\left(\begin{smallmatrix} x\\ y\end{smallmatrix}\right) + (1-\tau)\left(\begin{smallmatrix} s\\ t\end{smallmatrix}\right)) \cdot (\left(\begin{smallmatrix} x\\ y\end{smallmatrix}\right) - \left(\begin{smallmatrix} s\\ t\end{smallmatrix}\right))\,d\tau \right| ds\,dt\,dy \\ &\le \int_{S_{n,i}} \fint_{S_{n,i}\times S_{n,j}} \int_0^1 |\nabla K(\tau\left(\begin{smallmatrix} x\\ y\end{smallmatrix}\right) + (1-\tau)\left(\begin{smallmatrix} s\\ t\end{smallmatrix}\right))|\,|\left(\begin{smallmatrix} x\\ y\end{smallmatrix}\right) - \left(\begin{smallmatrix} s\\ t\end{smallmatrix}\right)|\,d\tau\,ds\,dt\,dy \\ &\le \int_{S_{n,i}} \fint_{S_{n,i}\times S_{n,j}} \int_0^1 \|\nabla K\|_{L^\infty(S_{n,i}\times S_{n,j})} \frac{2\sqrt{d}}{n}\,d\tau\,ds\,dt\,dy.\end{aligned}$$

Summing over i, we finally obtain (cf. Figure 2)

$$\begin{aligned}\int_{\mathbb{R}^d\setminus B_\varepsilon(x)} |K(x,y) - P_n^y P_n^x K(x,y)|\,dy &\le \sum_{i:|i-j|>\varepsilon/2} \int_{S_{n,i}} |K(x,y) - P_n^y P_n^x K(x,y)|\,dy \\ &\le \sum_{i:|i-j|>\varepsilon/2} \int_{S_{n,i}} \fint_{S_{n,i}\times S_{n,j}} \int_0^1 \|\nabla K\|_{L^\infty(S_{n,i}\times S_{n,j})} \frac{2\sqrt{d}}{n}\,d\tau\,ds\,dt\,dy \\ &\le \frac{2\sqrt{d}}{n} \|\nabla K\|_{L^\infty(Q_M\setminus B_{\varepsilon/2}(x))} \int_{Q_M\setminus B_{\varepsilon/4}(x)} dy \\ &= |Q_M| \frac{2\sqrt{d}}{n} \|\nabla K\|_{L^\infty(Q_M\setminus B_{\varepsilon/2}(x))} \\ &\le |Q_M| \frac{2\sqrt{d}}{n} \|q\|_{\mathcal{C}^1} C \left(\frac{\varepsilon}{2}\right)^{1-d} \\ &\le C \frac{|Q_M|}{n} \varepsilon^{1-d}, \end{aligned} \tag{4.5}$$

where the fifth line follows from (A.2) in the appendix, and the bound $\|q\|_{\mathcal{C}^1} < +\infty$. Using (4.5) in (4.4), we conclude that

$$\int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy \le C \frac{|Q_M|}{n} \varepsilon^{1-d} + \int_{B_\varepsilon(x)} 2|K(x,y)|\, dy,$$

so

$$\sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dy \le C \frac{|Q_M|}{n} \varepsilon^{1-d} + C'\varepsilon^2,$$

where in the last line we have used (A.1) and the boundedness of q again.

With an analogous calculation for $\sup_{y\in\mathbb{R}^d} \int_{\mathbb{R}^d} |K(x,y) - P_n^y P_n^x K(x,y)|\, dx$ (which we omit here), and recalling that η_n was defined by (4.3), we conclude that for all $\varepsilon > 0$,

$$\eta_n \le \frac{1}{n} C\varepsilon^{1-d} + C'\varepsilon^2.$$

Choosing $\varepsilon := n^{-1/(d+1)}$, we conclude that

$$\|Kf - P_n K P_n f\|_{L^2(\mathbb{R}^d)} \le \frac{C + C'}{n^{2/(d+1)}} \|f\|_{L^2(\mathbb{R}^d)} \tag{4.6}$$

and hence $\|K - P_n K P_n\|_{L(L^2(\mathbb{R}^d))} \to 0$ as $n \to +\infty$ with rate (at least) $a_n = n^{-2/(d+1)} \le n^{-1/d}$.

Remark 4.2. Note that the constants C, C' all depend on the spectral parameter z, but are bounded for z in compact subsets of $\mathbb{C}^{\mathrm{ext}}$, because K depends continuously on z.

Proof of (3.2) *and* (H1). An orthonormal basis of $\mathcal{H}_n$ is given by the functions

$$e_i := n^{d/2} \chi_{S_{n,i}}, \quad i \in \tfrac{1}{n}\mathbb{Z}^d \cap Q_M,$$

so that

$$P_n f = \sum_{j\in\frac{1}{n}\mathbb{Z}\cap Q_M} \langle f, e_j\rangle_{L^2} e_j$$

in this basis. It is then easily seen that in this basis K_n has the matrix elements

$$(K_n)_{ij} = n^{-d} K(i,j).$$

Note that this proves (H1): The matrix elements of K_n can be calculated in finitely many arithmetic operations from the finite set $\Lambda_n := \{K(i,j) \,|\, i,j \in \frac{1}{n}\mathbb{Z} \cap Q_M\} \subset \Lambda$. Similarly, it can be seen that the matrix elements of $P_n K|_{\mathcal{H}_n}$ in this basis are given by

$$(P_n K)_{ij} = n^d \int_{S_{n,i}} \int_{S_{n,j}} K(x,y)\, dx\, dy =: n^{-d} \langle K\rangle_{ij},$$

where we have introduced the notation $\langle\cdot\rangle_{ij}$ for the mean value on $S_{n,i} \times S_{n,j}$. Let $f = \sum_j f_j e_j \in \mathcal{H}_n$. From the above, and Young's inequality, we conclude that

$$\|(P_n K - K_n) f\|_{L^2}^2 = \sum_{i\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} \left| \sum_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d} (K(i,j) - \langle K\rangle_{ij}) f_j \right|^2 \le \tilde{\eta}_n^2 \|f\|_{L^2}^2,$$

where

$$\tilde{\eta}_n := \max\Big\{ \sup_{i\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} \sum_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d}|K(i,j)-\langle K\rangle_{ij}|,$$
$$\sup_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} \sum_{i\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d}|K(i,j)-\langle K\rangle_{ij}|\Big\}.$$

Hence, we have reduced the problem to estimating these ℓ^∞-ℓ^1 differences. This can be done similarly to (4.4), by separating $(Q_M \times Q_M) \cap (\frac{1}{n}\mathbb{Z} \times \frac{1}{n}\mathbb{Z})$ into an ε-region around $i = j$ and the rest:

$$\begin{aligned}
&\sum_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d}|K(i,j)-\langle K\rangle_{ij}| \\
&\quad= \sum_{|j-i|>\varepsilon} n^{-d}|K(i,j)-\langle K\rangle_{ij}| + \sum_{|j-i|\le\varepsilon} n^{-d}|K(i,j)-\langle K\rangle_{ij}| \\
&\quad\le Cn^{-1}\sum_{|j-i|>\varepsilon} n^{-d}\|\nabla K\|_{L^\infty(\{|x-y|>\varepsilon\})} + \sum_{|j-i|\le\varepsilon} n^{-d}|K(i,j)-\langle K\rangle_{ij}| \\
&\quad\le Cn^{-1}\varepsilon^{-d+1} + \sum_{|j-i|\le\varepsilon} n^{-d}|K(i,j)-\langle K\rangle_{ij}|,
\end{aligned} \tag{4.7}$$

where we have used (A.2) and the $\mathcal{C}^1$-boundedness of q in the last line. To estimate the last term on the right hand side, note that $|K(i,j)-\langle K\rangle_{ij}| \le C|j-i|^{-(d-2)}$ near $i = j$ (cf. (A.1)). Next, note that the sum $n^{-d}\sum_{j:|j-i|\le\varepsilon}\frac{1}{|j-i|^{d-2}}$ can be interpreted as an integral over a piecewise constant function, which approximates $(x,y)\mapsto |x-y|^{2-d}$. But this function is dominated by $(x,y)\mapsto |x-y|^{1-d}$ when $|x-y|$ is small, and therefore we have

$$\begin{aligned}
n^{-d}\sum_{j:|j-i|\le\varepsilon}\frac{1}{|j-i|^{d-2}} &\le C\int_{B_{2\varepsilon}(x)}|x-y|^{1-d}\,dy = C\int_0^{2\varepsilon} r^{1-d}\,\omega_d r^{d-1}\,dr \\
&= 2C\omega_d\varepsilon,
\end{aligned} \tag{4.8}$$

where ω_d denotes the volume of the unit sphere in $\mathbb{R}^d$. Note that the above calculation is uniform in i, because q is bounded. Plugging (4.8) into (4.7), we arrive at

$$\sum_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d}|K(i,j)-\langle K\rangle_{ij}| \le Cn^{-1}\varepsilon^{-d+1} + 2C\omega_d\,\varepsilon.$$

Choosing $\varepsilon = n^{-1/d}$ yields

$$\sum_{j\in\frac{1}{n}\mathbb{Z}^d\cap Q_M} n^{-d}|K(i,j)-\langle K\rangle_{ij}| \le C' n^{-1/d}. \tag{4.9}$$

Finally, swapping i and j will give an analogous estimate and we can conclude that $\tilde{\eta}_n \to 0$ with rate $a_n = n^{-1/d}$.

Remark 4.3. Note again that the constants C, C' depend on z, but are bounded for z in compact subsets of $\mathbb{C}^{\mathrm{ext}}$, since K depends continuously on z.

Proof of (3.1) *and* (H2). Estimate (3.1) in fact follows from (3.3) and (3.2). Indeed, writing K_n and K as block operator matrices with respect to the decomposition $\mathcal{H} = \mathcal{H}_n \oplus \mathcal{H}_n^\perp$, we have

$$K = \begin{pmatrix} P_n K|_{\mathcal{H}_n} & D_1 \\ D_2 & D_3 \end{pmatrix}$$

with some operators D_1, D_2, D_3. Estimate (3.3) shows that

$$\left\| \begin{pmatrix} 0 & D_1 \\ D_2 & D_3 \end{pmatrix} \right\|_{L(\mathcal{H})} < C a_n, \tag{4.10}$$

whereas estimate (3.2) shows that

$$\|P_n K|_{\mathcal{H}_n} - K_n\|_{L(\mathcal{H}_n)} = \left\| \begin{pmatrix} P_n K|_{\mathcal{H}_n} - K_n & 0 \\ 0 & 0 \end{pmatrix} \right\|_{L(\mathcal{H})} < C a_n. \tag{4.11}$$

Together, (4.10) and (4.11) imply that

$$\|K(z) - K_n(z) P_n\|_{L(\mathcal{H})} = \left\| \begin{pmatrix} P_n K|_{\mathcal{H}_n} - K_n & D_1 \\ D_2 & D_3 \end{pmatrix} \right\|_{L(\mathcal{H})} < 2C a_n.$$

The explicit rates obtained in (4.6) and (4.9) prove that our approximation scheme satisfies (H2).

4.2. *Proof of Theorem* 4.1

The results of Section 4.1 imply that for any compact $B \subset \mathbb{C}^{\mathrm{ext}}$, $\Theta_n^B(q) \to \mathrm{Res}(H_q) \cap B$ in the Attouch–Wets metric. It remains to extend the algorithm Θ_n^B from a single compact set $B \subset \mathbb{C}^{\mathrm{ext}}$ to the entire complex plane. This is done via a diagonal-type argument.

4.2.1. Odd dimensions. We choose a tiling of $\mathbb{C}$, where we start with a square $B_1 = \{z \in \mathbb{C} \mid |\mathrm{Re}(z)| \le 1/2, -1 \le |\mathrm{Im}(z)| \le 0\}$ and then add squares in a counterclockwise spiral manner as shown in Figure 3. Next, we define our algorithm as follows. We let

$$\begin{aligned}
\Gamma_1(q) &:= \Theta_1^{B_1}(q), \\
\Gamma_2(q) &:= \Theta_2^{B_1}(q) \cup \Theta_2^{B_2}(q), \\
\Gamma_3(q) &:= \Theta_3^{B_1}(q) \cup \Theta_3^{B_2}(q) \cup \Theta_3^{B_3}(q), \\
&\ \vdots \\
\Gamma_n(q) &:= \bigcup_{j=1}^{n} \Theta_n^{B_j}(q).
\end{aligned}$$

Lemma 3.5 ensures that each $\Theta_n^{B_k}$ converges to $\mathrm{Res}(H_q) \cap B_k$ for fixed k and since the $\{B_k\}$ form a tiling of $\mathbb{C}$, it follows that $\Gamma_n(q) \to \mathrm{Res}(H_q)$ in the Attouch–Wets metric.

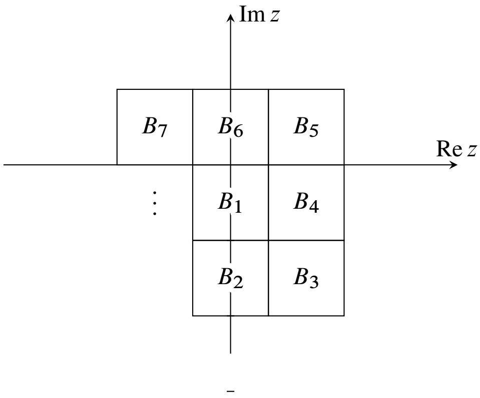

Fig. 3. Tiling of the complex plane.

4.2.2. Even dimensions. In even dimensions we have to cover not only the complex plane $\mathbb{C}$, but its logarithmic covering space, which is equivalent to covering infinitely many copies of the complex plane. A similar strategy to the odd-dimensional case, together with a diagonal-type argument, does the job in this case. Indeed, we can construct a cover by boxes B_n as follows (cf. Figure 4):

(1) Start with box B_1 (defined as in the odd-dimensional case) on the first Riemann sheet.
(2) Add a box B_2 below B_1 on sheet number 1 and add a box B_1 on sheet number 2.
(3) Add a box B_3 on sheet number 1, add a box B_2 on sheet number 2 and a box B_1 on sheet number 3.
(4) …

Next, define again

$$\begin{aligned}
\Gamma_1(q) &:= \Theta_1^{B_1^{(1)}}(q),\\
\Gamma_2(q) &:= \Theta_2^{B_1^{(1)}}(q) \cup \Theta_2^{B_2^{(1)}}(q) \cup \Theta_2^{B_1^{(2)}}(q),\\
\Gamma_3(q) &:= \Theta_3^{B_1^{(1)}}(q) \cup \Theta_3^{B_2^{(1)}}(q) \cup \Theta_3^{B_3^{(1)}}(q) \cup \Theta_3^{B_1^{(2)}}(q) \cup \Theta_3^{B_2^{(2)}}(q) \cup \Theta_3^{B_3^{(1)}}(q),\\
&\ \ \vdots\\
\Gamma_n(q) &:= \bigcup_{k=1}^{n} \bigcup_{j=1}^{n-k+1} \Theta_n^{B_j^{(k)}}(q).
\end{aligned}$$

Lemma 3.5 ensures that each $\Theta_n^{B_j^{(k)}}$ converges to $\operatorname{Res}(H_q) \cap B_j^{(k)}$ for fixed k and since the $\{B_j^{(k)}\}$ form a tiling of $\mathbb{C}^{\mathrm{ext}}$, it follows that $\Gamma_n(q) \to \operatorname{Res}(H_q)$ in the Attouch–Wets metric.

Having proved convergence for all dimensions $d \in \mathbb{N}$, it follows that $\Omega_M \in \Delta_2^A$ and therefore the proof of Theorem 4.1 is complete.

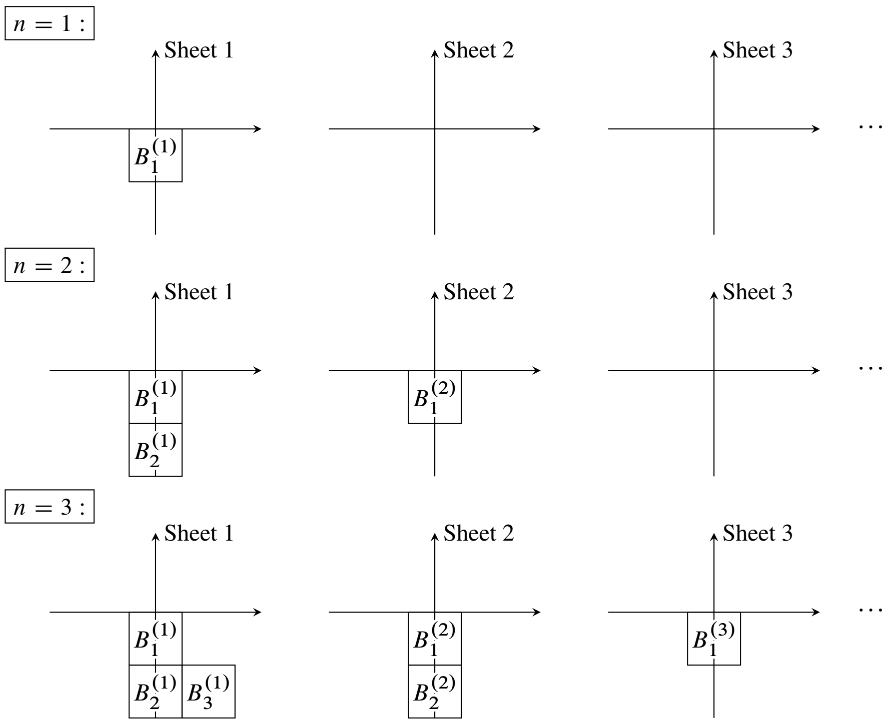

Fig. 4. Tiling of the logarithmic Riemann surface.

4.3. *Proof of Theorem* 1.16 (1)

Given $M > 0$, recall that $Q_M = [-M/2, M/2]^d \subset \mathbb{R}^d$. We denote the d-dimensional grid introduced in (4.1) by $\mathcal{G}_{M,n} := \frac{1}{n}\mathbb{Z}^d \cap Q_M$. For $n \in \mathbb{N}$ let $\Gamma_{M,n}$ be the algorithm defined in Section 4.2 (i.e. the discretization in $\Gamma_{M,n}$ is based on $\mathcal{G}_{M,n}$). For any element $H_q \in \Omega_{\mathrm{cpt}}$, consider the algorithm defined by the following pseudocode.

Algorithm 1: Compute resonances on Ω_{cpt}

Initialize $M, n := 1$ and $m := M + 1$;
while *True* **do**
  if $q(j) = 0$ *for all* $j \in \mathcal{G}_{m,n} \setminus \mathcal{G}_{M,n}$, **then**
    define $\Gamma_n(q) := \Gamma_{M,n}(q)$;
    increment m by 1 and proceed to $n + 1$;
  else
    increment m by 1, set $M := m - 1$ and repeat the current step;
  end
end

Algorithm 1 defines sequences $\{M_n\}_{n\in\mathbb{N}}$ and $\{m_n\}_{n\in\mathbb{N}}$ and an algorithm $\Gamma_n : \Omega_{\mathrm{cpt}} \to \mathrm{cl}(\mathbb{C})$. Note that $m_n \nearrow +\infty$, because it gets incremented by at least 1 in every step.

By Lemma 4.4 below, the sequence $\{M_n\}_{n\in\mathbb{N}}$ is eventually constant, i.e. there exists $N \in \mathbb{N}$ such that $M_n = M_N$ for all $n \geq N$ and one has $H_q \in \Omega_{M_N}$. Hence $\Gamma_n(q) = \Gamma_{M_N,n}(q)$ for all $n \geq N$ and

$$\lim_{n\to+\infty} \Gamma_n(q) = \lim_{n\to+\infty} \Gamma_{M_N,n}(q) = \mathrm{Res}(H_q),$$

where the last equality follows from the convergence of the algorithm $\Gamma_{M_N,n}(q)$ and the fact that $H_q \in \Omega_{M_N}$. This completes the proof of Theorem 1.16 (1): $\Omega_{\mathrm{cpt}} \in \Delta_2^A$.

Lemma 4.4. *The sequence $\{M_n\}_{n\in\mathbb{N}}$ is eventually constant and if $N > 0$ is such that $M_n = M_N$ for all $n > N$, then $H_q \in \Omega_{M_N}$.*

Proof. The fact that $\{M_n\}_{n\in\mathbb{N}}$ is eventually constant follows immediately from the boundedness of $\mathrm{supp}(q)$ and Algorithm 1. Now let $N \in \mathbb{N}$ be as in the assertion. To prove that $H_q \in \Omega_{M_N}$, assume for contradiction that $q(x) \neq 0$ for some $x \notin Q_{M_N}$. Then by continuity $q \neq 0$ on a ball $B_\varepsilon(x)$. Hence, as long as $n^{-1} < \varepsilon$ one would have $q(j_n) \neq 0$ for some lattice point $j_n \in \frac{1}{n}\mathbb{Z} \cap B_\varepsilon(x)$. In particular, q would be nonzero on $\mathcal{G}_{m,n} \setminus \mathcal{G}_{M,n}$. But then, as long as $m_n > |x| + \varepsilon$, Algorithm 1 would force M_n to increase by 1, contradicting the fact that M_n is constant for $n \geq N$. ∎

4.4. Proof of Theorem 1.16 (2)

To prove that $\Omega_{M,N} \in \Pi_1^A$, we need to construct sets $X_n(q) \subset \mathbb{C}$ such that $\mathrm{Res}(H_q) \subset X_n(q)$ and $d_{\mathrm{AW}}(X_n(q), \Gamma_n(q)) \leq \varepsilon_n$ for some explicit error ε_n for all $q \in \Omega_{M,N}$ (cf. Definition 1.14). These involve estimates of the Green function which was defined in (2.1). We begin with two lemmas.

Lemma 4.5. *One has $\|K(z) - K(w)\|_{L^2\to L^2} \leq \|q\|_\infty \|G(\cdot,z) - G(\cdot,w)\|_{L^1(Q_{3M}(0))}$ for all $z, w \in \mathbb{C}$.*

Proof. For $f \in L^2(\mathbb{R}^d)$ and $z, w \in \mathbb{C}$ a direct calculation with Young's inequality gives

$$\begin{aligned}\|(K(z) - K(w))f\|_{L^2(\mathbb{R}^d)} &= \|q \cdot [(G(\cdot,z) - G(\cdot,w)) * (\chi f)]\|_{L^2(Q_M)} \\ &\leq \|q\|_\infty \|(G(\cdot,z) - G(\cdot,w)) * (\chi f)\|_{L^2(Q_M)} \\ &\leq \|q\|_\infty \|G(\cdot,z) - G(\cdot,w)\|_{L^1(B_R)} \|f\|_{L^2(\mathbb{R}^d)},\end{aligned}$$

where the second line follows from Hölder's inequality, and the third follows from Young's inequality. The radius R must be large enough such that $Q_M + x \subset B_R$ for all $x \in Q_M$ (which is satisfied by $R = 3M$). ∎

Lemma 4.6. *For any compact set $B \subset \mathbb{C}$ and for any $R > 0$ there exists an explicit constant $C_{B,R} > 0$ such that $\|G(\cdot,z) - G(\cdot,w)\|_{L^1(B_R(0))} \leq C_{B,R}|z - w|$ for any $z, w \in B$.*

The proof of Lemma 4.6 is postponed to Appendix A.2. Now to construct $X_n(q)$, suppose that $B \subset \mathbb{C}$ is compact and $z \in B$ is a resonance of q, i.e. $-1 \in \sigma(K(z))$. Then combining Lemmas 3.4, 4.5, 4.6 we conclude that for any $z_n \in \mathcal{L}_n$ with $|z - z_n| < a_n = n^{-1/d}$ one has

$$\|(I + K(z_n))^{-1}\| \geq (C_{B,3M}\|q\|_\infty a_n)^{-1}$$

(with explicit $C_{B,R}$, $R = 3M$ as in Lemma 4.6). This explicit bound replaces (3.7) in the proof of Lemma 3.5. Proceeding as in the proof of Lemma 3.5, we obtain the following. If $-1 \in \sigma(K(z))$, then $\|(I + K_n(z_n))^{-1}\| \geq \frac{1}{2C_{B,3M}\|q\|_\infty + 2C} a_n^{-1}$, hence $z_n \in \Gamma_n(q)$ as long as $(2C_{B,3M}\|q\|_\infty + 2C)a_n \leq 2\sqrt{a_n}$ (inserting $a_n = n^{-1/d}$ and using $\|q\|_\infty \leq N$ yields an explicit value $n = n(B)$ for which this inequality is satisfied). Because $|z - z_n| < a_n$ (by choice) and $z_n \in \Gamma_n(q)$, we conclude that

$$\operatorname{Res}(H_q) \cap B \subset B_{a_n}(\Theta_n^B(q)) \tag{4.12}$$

for compact subsets $B \subset \mathbb{C}$ as long as $n > n(B)$.

Next, fix $\rho > 0$. According to our choice of numbering $\{B_j\}_{j\in\mathbb{N}}$ (cf. Section 4.2.1) we have $|z| \leq \rho$ for all $z \in B_j$, $j \leq 4\rho^2$ and thus

$$B_\rho(0) \subset \bigcup_{j \leq 4\rho^2} B_j \tag{4.13}$$

(with similar formulas for $B_j^{(k)}$ if d is even). Combining (4.12) and (4.13) we have

$$\operatorname{Res}(H_q) \cap B_\rho(0) \subset B_{a_n}(\Gamma_n(q)) \tag{4.14}$$

as long as $n \geq \max\{4\rho^2, n(B_\rho(0))\}$.

Lemma 4.7. *There exists an explicitly computable sequence $\{\rho_n\}_{n\in\mathbb{N}}$ of nonnegative numbers with $\rho_n \nearrow +\infty$ such that $n \geq \max\{4\rho_n^2, n(B_{\rho_n}(0))\}$ for all $n \in \mathbb{N}$.*

Proof. Let $\rho_1 := 0$. Then trivially $\operatorname{Res}(H_q) \cap B_{\rho_1}(0) \subset B_{a_n}(\Gamma_n(q))$ for all n, so $n(B_{\rho_1}(0)) = 1$. Consequently, $1 \geq \max\{4\rho_1^2, n(B_{\rho_1}(0))\}$. The remaining ρ_k are constructed inductively as follows. Assume ρ_{k-1} has been constructed. Compute $m := \max\{4(\rho_{k-1} + 1)^2, n(B_{\rho_{k-1}+1}(0))\}$. If $m \leq k$ let $\rho_k := \rho_{k-1} + 1$, otherwise let $\rho_k := \rho_{k-1}$.

To show that $\rho_k \nearrow +\infty$, note that by definition for any k the only two possibilities are $\rho_{k+1} = \rho_k$ or $\rho_{k+1} = \rho_k + 1$. This proves monotonicity. Moreover, the divergence $\rho_k \nearrow +\infty$ could only fail if for all k larger than some $k_0 \in \mathbb{N}$ one had $\rho_{k+1} \equiv \rho_k$. This is not possible, however, because for $k \geq m$ the definition of ρ_k enforces $\rho_{k+1} = \rho_k + 1$. ∎

This motivates the following definition. Choose a sequence ρ_n as in Lemma 4.7. Then define

$$X_n(q) := B_{a_n}(\Gamma_n(q)) \cup (\mathbb{C} \setminus B_{\rho_n}(0)).$$

Then by the definition of the Attouch–Wets distance d_{AW} one has

$$\begin{aligned} d_{\mathrm{AW}}(\Gamma_n(q), X_n(q)) &= \sum_{j=1}^{\infty} 2^{-j} \min\Big\{1, \sup_{\substack{p\in\mathbb{C}\\ |p|<j}} \Big| \inf_{a\in\Gamma_n(q)} |a-p| - \inf_{b\in X_n(q)} |b-p| \Big| \Big\} \\ &\le \sum_{j=1}^{\rho_n} 2^{-j} \min\Big\{1, \sup_{\substack{p\in\mathbb{C}\\ |p|<j}} \Big| \inf_{a\in\Gamma_n(q)} |a-p| - \inf_{b\in X_n(q)} |b-p| \Big| \Big\} + \sum_{j=\rho_n+1}^{\infty} 2^{-j} \\ &\le a_n \sum_{j=1}^{\rho_n} 2^{-j} + 2^{-\rho_n} \le a_n + 2^{-\rho_n} \end{aligned} \tag{4.15}$$

where the second inequality follows from the definition of $X_n(q)$. Moreover, by (4.14) we have

$$\mathrm{Res}(H_q) \subset X_n(q). \tag{4.16}$$

Together, (4.15) and (4.16) imply $\Omega_{M,N} \in \Pi_1^A$ with explicit error $\varepsilon_n = a_n + 2^{-\rho_n}$.

5. Numerical results

Software to compute resonances has been in existence for decades [1,13,26]. The authors of [9] recently proposed a collection of MATLAB codes to compute resonance poles and scattering of plane waves efficiently ("MatScat" [10]). In this section we compare the results of our algorithm to that of MatScat.

In order to study the actual numerical performance of our algorithm, we coded a MATLAB routine for the one-dimensional case with $\mathrm{supp}(q) \subset [a,b]$ (for some known $a < b$), which computes the set

$$\Big\{z \in \mathcal{L}_n \cap B \;\Big|\; \Big\| \big(\mathbb{1}_{n\times n} + (K(i,j))_{i,j\in\frac{b-a}{n}\mathbb{Z}\cap[a,b]}\big)^{-1} \Big\| > C\Big\},$$

where the region B in the complex plane, the lattice distance of $\mathcal{L}_n$ and the cutoff threshold C were treated as independent parameters.

Comparison of results. Figures 5 and 6 show the output of MatScat (black dots) versus the output of our algorithm (blue regions) for a Gaussian well and trapping potential, respectively. As the plots show, there is agreement between the two.

Limitations. As mentioned before, MatScat has been developed with the goal to create an efficient algorithm to compute resonances fast. Indeed, the computation of the black dots in Figure 5 takes less than a second, while computing the regions with our algorithm takes several hours on a personal computer. We stress that our MATLAB code was written mainly for illustration purposes and that there is considerable room for improvement in numerical efficiency. Moreover, considering rounding errors and storage limitations of actual computers, our algorithm can only yield reliable results in a certain region, as the following heuristic calculations make clear.

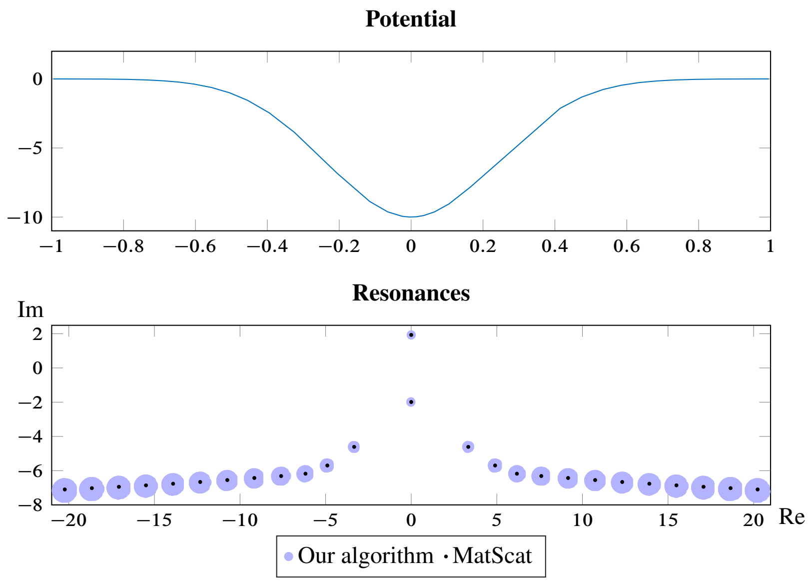

Fig. 5. Comparison of the result of [10] (black) and our algorithm (blue) for a Gaussian well supported between −1 and 1. The chosen parameter values: $n = 100$; threshold for resolvent norm: $C = 200$; number of lattice points in the shown region of the complex plane: $M \times 4M = 1000 \times 4000$.

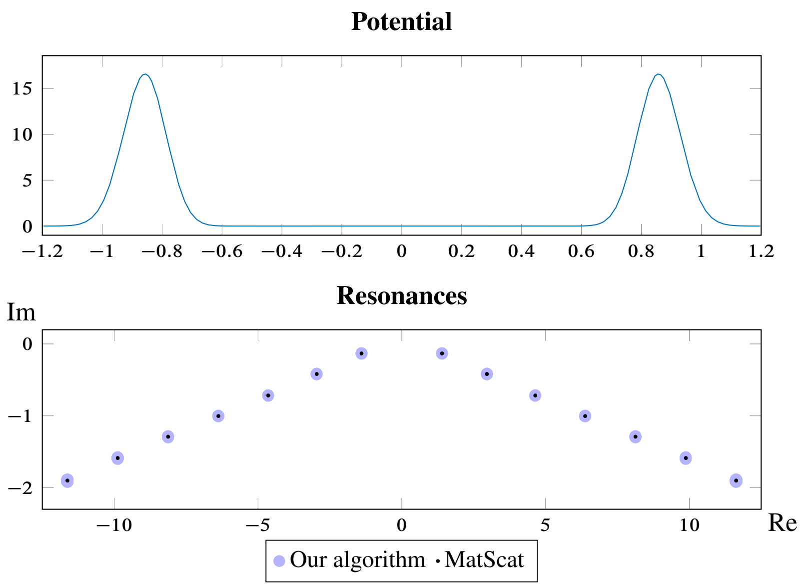

Fig. 6. Comparison of the result of [10] (black) and our algorithm (blue) for a smooth trapping potential supported between −1.2 and 1.2. The chosen parameter values: $n = 100$; threshold for resolvent norm: $C = 200$; number of lattice points in the shown region of the complex plane: $M \times 10M = 1000 \times 10000$.

- *Imaginary part of z:* Since the fundamental solution $G(x,z) = \frac{1}{2iz}e^{iz|x|}$ grows exponentially with $-\operatorname{Im}(z)$ and $x \in [-a,a]$, a limit is reached when $|\operatorname{Im}(z)| \sim \frac{\log(2M)}{2a}$, where M is the largest number the machine can store with adequate precision[1] (for the interval $[-a,a] = [-1,1]$ and $M = 10^{16}$ this bound yields $\operatorname{Im}(z) \gtrsim -18.8$).
- *Real part of z:* Similarly, a natural bound on $\operatorname{Re}(z)$ is reached when the period of $e^{iz|x|}$ is less than twice the lattice spacing $2/n$, i.e. when $|\operatorname{Re}(z)| \lesssim \pi n$ (for $n = 30$ this bound yields $|\operatorname{Re}(z)| \lesssim 94$).

Numerical experiments have confirmed the above bounds (see Figure 7). Note that the bound on $\operatorname{Im}(z)$ is fixed by the machine precision, while the bound on $|\operatorname{Re}(z)|$ can be raised by increasing n.

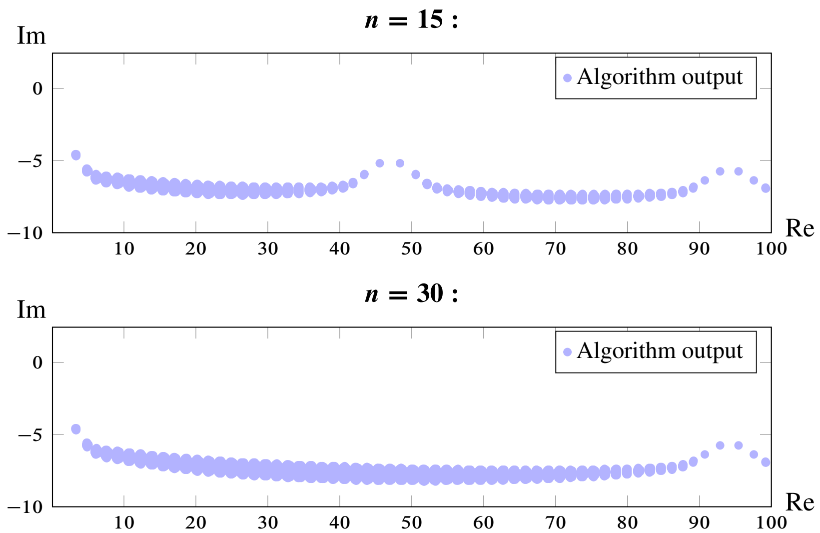

Fig. 7. Numerical artefacts for large real part of z. Top: Output of our algorithm for Gaussian well potential on the interval $[-1,1]$ with $n = 15$. Bottom: Output for the same problem with $n = 30$. The locations of the spurious peaks agree with the bound $|\operatorname{Re}(z)| \sim \pi n$ in each case.

Remark 5.1. We note that our algorithm is not restricted to one dimension or real-valued potentials. Indeed, the algorithm Γ_n only uses the bound $\operatorname{supp}(q) \subset Q_M$, and higher-dimensional implementations of Γ_n can be coded similarly to the one-dimensional one.

Appendix A. Fundamental solution

In this appendix we gather some well-known results about the fundamental solution for the Helmholtz equation. These facts are used to show that the abstract framework of Section 3 holds in the context of our algorithm as defined in Section 4, namely that (3.1)–(3.3)

[1]This means that M is the largest number such that $M + 1 > M$ in machine arithmetic.

hold. We remind the reader of the definition of the fundamental solution:

$$G(x,z) = \begin{cases} \frac{\mathrm{i}}{4}\left(\frac{z}{2\pi|x|}\right)^{(d-2)/2} H^{(1)}_{(d-2)/2}(z|x|), & d \geq 2, \\ \frac{\mathrm{i}}{2z} e^{\mathrm{i}z|x|}, & d = 1. \end{cases}$$

A.1. Asymptotics near 0

We start by obtaining some asymptotic expressions for $G(x,z)$. We adopt the notation of [2] and write $f(\zeta) \sim \zeta^{\nu}$ if f and ζ^{ν} are *asymptotically equal*, i.e. $|f(\zeta) - \zeta^{\nu}| = O(|\zeta|^{\nu+1})$ as $|\zeta| \to 0$.

Remark A.1. By the asymptotic expansion of the Hankel functions

$$H^{(1)}_{\nu}(\zeta) \sim \begin{cases} -\frac{\Gamma(\nu)}{\pi}\left(\frac{\zeta}{2}\right)^{-\nu}, & \nu > 0, \\ \frac{2\mathrm{i}}{\pi}\log(\zeta), & \nu = 0, \end{cases}$$

where Γ denotes the Gamma function and log denotes the principal branch of the logarithm (cf. [2, Ch. 9.1.9]), we find that the fundamental solution satisfies the small $|x|$ asymptotics

$$\begin{aligned} G(x,z) &\sim -\frac{\mathrm{i}\Gamma\left(\frac{d-2}{2}\right)}{\pi}\left(\frac{z|x|}{2}\right)^{-(d-2)/2} \frac{\mathrm{i}}{4}\left(\frac{z}{2\pi|x|}\right)^{(d-2)/2} \\ &= \frac{\Gamma\left(\frac{d-2}{2}\right)}{4\pi^{d/2}} \frac{1}{|x|^{d-2}} \quad \text{as } |x| \to 0, \end{aligned}$$

for $d \geq 3$, and

$$G(x,z) \sim -\frac{1}{2\pi}\log(z|x|) \quad \text{as } |x| \to 0,$$

for $d = 2$. Hence

$$|G(x,z)| \leq C_z \cdot \begin{cases} \frac{1}{|x|^{d-2}}, & d \geq 3, \\ \log(|x|), & d = 2, \end{cases} \tag{A.1}$$

for all x in a neighborhood of 0, where $C_z > 0$ is uniformly bounded for z in a compact subset of $\mathbb{C}$. Similar formulas hold for the derivatives of G. Indeed, identities for Hankel functions (cf. [2, Ch. 9.1.30]) show that

$$|\nabla G(x,z)| \leq \frac{C_z}{|x|^{d-1}} \quad \text{for } d \geq 2. \tag{A.2}$$

Remark A.2. From the representation of $G(x,z)$ in terms of Hankel functions it follows that G can be continued analytically in z through the branch cut $\mathbb{R}_+$. In fact, it can be shown that G can be continued to

- the Riemann surface of the complex square root if d is odd,
- the Riemann surface of the complex logarithm if d is even

(cf. [17, Ch. 3.1.4]). The estimates (A.1) and (A.2) remain valid in either case.

A.2. Lipschitz bounds

In this section we give the proof of Lemma 4.6. For the reader's convenience, some long calculations are omitted.

Proof of Lemma 4.6. We recall that the lemma states that for any compact set $B \subset \mathbb{C}$ and for any $R > 0$ there exists an explicit constant $C_{B,R} > 0$ such that $\|G(\cdot, z) - G(\cdot, w)\|_{L^1(B_R(0))} \le C_{B,R}|z - w|$ for any $z, w \in B$. We focus on the case $d \ge 3$, the other cases being similar. Introducing $\zeta := z|x|$, we write

$$G(x, z) = \frac{\mathrm{i}}{4}\left(\frac{1}{2\pi}\right)^{(d-2)/2} |x|^{-(d-2)}\zeta^{(d-2)/2} H^{(1)}_{(d-2)/2}(\zeta).$$

From the recurrence relations for Bessel functions it follows that

$$\frac{d}{d\zeta}(\zeta^\nu H^{(1)}_\nu(\zeta)) = \zeta^\nu H^{(1)}_{\nu-1}(\zeta). \tag{A.3}$$

Now consider some compact set $B \subset \mathbb{C}$ and let $z, w \in B$. For any fixed $x \in \mathbb{R}^d \setminus \{0\}$ we have, by (A.3),

$$\begin{aligned}
|G(x, z) - G(x, w)| &\le |z - w| \left\| \frac{dG(x, \cdot)}{dz} \right\|_{L^\infty(B)} \\
&= |z - w| \frac{1}{4}\left(\frac{1}{2\pi}\right)^{(d-2)/2} |x|^{-(d-2)} \left\| \frac{d}{dz}\zeta^{(d-2)/2} H^{(1)}_{(d-2)/2}(\zeta) \right\|_{L^\infty(B)} \\
&= |z - w| \frac{1}{4}\left(\frac{1}{2\pi}\right)^{(d-2)/2} |x|^{-(d-3)} \left\| \frac{d}{d\zeta}\zeta^{(d-2)/2} H^{(1)}_{(d-2)/2}(\zeta) \right\|_{L^\infty(B)} \\
&= |z - w| \frac{1}{4}\left(\frac{1}{2\pi}\right)^{(d-2)/2} |x|^{-(d-3)} \|\zeta^{(d-2)/2} H^{(1)}_{(d-4)/2}(\zeta)\|_{L^\infty(B)}.
\end{aligned}$$

Integrating both sides in x over $B_R(0)$ we obtain

$$\begin{aligned}
&\|G(\cdot, z) - G(\cdot, w)\|_{L^1(B_R(0))} \\
&\qquad \le |z - w| \left(\frac{1}{2\pi}\right)^{(d-2)/2} \frac{S_{d-1}R^3}{12} \|\zeta^{(d-2)/2} H^{(1)}_{(d-4)/2}(\zeta)\|_{L^\infty(B)},
\end{aligned}$$

where S_{d-1} denotes the $(d-1)$-dimensional measure of the unit sphere. Hence it is enough to find an explicit bound for $\|\zeta^{(d-2)/2} H^{(1)}_{(d-4)/2}(\zeta)\|_{L^\infty(B)}$. This will be sketched in the following. We will write $\nu := (d-2)/2$ to simplify notation.

Even dimension ($\nu \in \mathbb{N}$)*:* By definition, $H^{(1)}_\nu = J_\nu + \mathrm{i}Y_\nu$ (where Y_ν denote the Bessel functions of the second kind), hence $|H^{(1)}_\nu| \le |J_\nu| + |Y_\nu|$. For $\nu > -1/2$ one has the bound

$$|J_\nu(\zeta)| \le \frac{(\zeta/2)^\nu e^{|\mathrm{Im}(\zeta)|}}{\Gamma(\nu + 1)} \tag{A.4}$$

(cf. [24, (10.14.4)]). To bound $|Y_\nu|$, consider the following series expansion, which holds for $\nu = n \in \mathbb{N}$ [21, (5.5.1)]:

$$\begin{aligned} Y_n(\zeta) = &-\frac{1}{\pi}\sum_{k=0}^{n-1}\frac{(n-k-1)!}{k!}\Big(\frac{\zeta}{2}\Big)^{2k-n} \\ &+\frac{1}{\pi}\sum_{j=0}^{\infty}(-1)^j\frac{(\zeta/2)^{n+2j}}{j!(n+j)!}\Big[2\log\Big(\frac{\zeta}{2}\Big)-\psi(j+1)-\psi(n+j+1)\Big], \end{aligned} \tag{A.5}$$

where $\psi(m) = -\gamma + \sum_{j=1}^{m}\frac{1}{j}$ and γ is the Euler–Mascheroni constant. The expansion (A.5) shows that the highest order term in $Y_n(\zeta)$ is ζ^{-n}. Thus, $|\zeta^n Y_{n-1}(\zeta)|$ is bounded for ζ in compact subsets of $\mathbb{C}$. A tedious calculation using (A.5) yields an explicit bound $|\zeta^n Y_{n-1}(\zeta)| \le C$.

Odd dimension ($\nu \in \mathbb{N}+1/2$)*:* For $\nu \in \mathbb{N}+1/2$ one has $H_\nu^{(1)} = (-1)^{\nu+1}\mathrm{i}(J_{-\nu} - e^{\mathrm{i}\nu\pi}J_\nu)$ (cf. [21, (5.6.4)]). For positive ν, $|J_\nu(\zeta)|$ can be bounded by (A.4). The summand $J_{-\nu}$ can be expressed in terms of J_μ with $\mu > 0$ by successive application of the relation

$$J_{\nu-1}(\zeta) = \frac{2\nu}{\zeta}J_\nu(\zeta) - J_{\nu+1}(\zeta). \tag{A.6}$$

The highest power of ζ^{-1} that appears after $\lceil\nu\rceil$ applications of (A.6) is $\zeta^{-\lceil\nu\rceil}$; hence $|\zeta^\nu J_{-(\nu-1)}(\zeta)|$ is bounded on compact sets by an explicit constant. ∎

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References

[1] Abramov, A. A., Aslanyan, A., Davies, E. B.: Bounds on complex eigenvalues and resonances. J. Phys. A **34**, 57–72 (2001) Zbl 1123.81415 MR 1819914

[2] Abramowitz, M., Stegun, I. A.: Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. National Bureau of Standards Applied Mathematics Series 55, U.S. Government Printing Office, Washington, DC (1964) Zbl 0171.38503 MR 0167642

[3] Becker, S., Hansen, A. C.: Computing solutions of Schrödinger equations on unbounded domains – on the brink of numerical algorithms. arXiv:2010.16347 (2020)

[4] Beer, G.: Topologies on Closed and Closed Convex Sets. Math. Appl. 268, Kluwer, Dordrecht (1993) Zbl 0792.54008 MR 1269778

[5] Ben-Artzi, J., Colbrook, M. J., Hansen, A. C., Nevanlinna, O., Seidel, M.: Computing spectra – on the solvability complexity index hierarchy and towers of algorithms. arXiv:1508.03280 (2015)

[6] Ben-Artzi, J., Hansen, A. C., Nevanlinna, O., Seidel, M.: New barriers in complexity theory: on the solvability complexity index and the towers of algorithms. C. R. Math. Acad. Sci. Paris **353**, 931–936 (2015) Zbl 1343.68078 MR 3411224

[7] Ben-Artzi, J., Marletta, M., Rösler, F.: Computing the sound of the sea in a seashell. Found. Comput. Math. **22**, 697–731 (2022) Zbl 07536701 MR 4433111

[8] Ben-Artzi, J., Marletta, M., Rösler, F.: Universal algorithms for computing spectra of periodic operators. Numer. Math. **150**, 719–767 (2022) Zbl 1486.35157 MR 4394000

[9] Bindel, D., Zworski, M.: Symmetry of bound and antibound states in the semiclassical limit. Lett. Math. Phys. **81**, 107–117 (2007) Zbl 1161.81430 MR 2336226

[10] Bindel, D., Zworski, M.: Theory and computation of resonances in 1d scattering. http://www.cs.cornell.edu/~bindel/cims/matscat/ (2006)

[11] Blum, L., Cucker, F., Shub, M., Smale, S.: Complexity and Real Computation. Springer, New York (1998) Zbl 0872.68036 MR 1479636

[12] Bögli, S., Brown, B. M., Marletta, M., Tretter, C., Wagenhofer, M.: Guaranteed resonance enclosures and exclosures for atoms and molecules. Proc. Roy. Soc. London Ser. A Math. Phys. Engrg. Sci. **470**, art. 20140488, 17 pp. (2014) Zbl 1371.81347 MR 3272932

[13] Brown, B. M., Eastham, M. S. P., McCormack, D. K. R.: Resonances and analytic continuation for exponentially decaying Sturm–Liouville potentials. J. Comput. Appl. Math. **116**, 181–193 (2000) Zbl 0979.34018 MR 1741794

[14] Colbrook, M. J., Roman, B., Hansen, A. C.: How to compute spectra with error control. Phys. Rev. Lett. **122**, art. 250201, 6 pp. (2019) MR 3980052

[15] Colbrook, M. J.: On the computation of geometric features of spectra of linear operators on Hilbert spaces. arXiv:1908.09598 (2019)

[16] Colbrook, M. J., Hansen, A. C.: The foundations of spectral computations via the solvability complexity index hierarchy. J. Eur. Math. Soc., to appear

[17] Dyatlov, S., Zworski, M.: Mathematical Theory of Scattering Resonances. Grad. Stud. Math. 200, Amer. Math. Soc., Providence, RI (2019) Zbl 1454.58001 MR 3969938

[18] Eastham, M. S. P.: On the location of spectral concentration for perturbed discrete spectra. Mathematika **46**, 145–154 (1999) Zbl 0959.34068 MR 1750651

[19] Hansen, A. C.: On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators. J. Amer. Math. Soc. **24**, 81–124 (2011) Zbl 1210.47013 MR 2726600

[20] Lax, P. D., Phillips, R. S.: Scattering Theory. 2nd ed., Pure Appl. Math. 26, Academic Press, Boston, MA (1989) Zbl 0697.35004 MR 1037774

[21] Lebedev, N. N.: Special Functions and their Applications. Prentice-Hall, Englewood Cliffs, NJ (1965) Zbl 0131.07002 MR 0174795

[22] LeRoy, R., Liu, W.: Energies and widths of quasibound levels (orbiting resonances) for spherical potentials. J. Chem. Phys. **69**, 3622–3631 (1978)

[23] Melrose, R.: Polynomial bound on the number of scattering poles. J. Funct. Anal. **53**, 287–303 (1983) Zbl 0535.35067 MR 724031

[24] NIST Digital Library of Mathematical Functions. http://dlmf.nist.gov/

[25] Reed, M., Simon, B.: Methods of Modern Mathematical Physics. I. 2nd ed., Academic Press, New York (1980) Zbl 0459.46001 MR 751959

[26] Rittby, M., Elander, N., Brändas, E.: Weyl's theory and the complex-rotation method applied to phenomena associated with a continuous spectrum. Phys. Rev. A (3) **24**, 1636–1639 (1981) MR 627126

[27] Rösler, F.: On the solvability complexity index for unbounded selfadjoint and Schrödinger operators. Integral Equations Operator Theory **91**, art. 54, 23 pp. (2019) Zbl 1435.35269 MR 4040617

[28] Serov, V.: Fourier Series, Fourier Transform and Their Applications to Mathematical Physics. Appl. Math. Sci. 197, Springer, Cham (2017) Zbl 1422.42001 MR 3729317

[29] Smith, F. T.: Lifetime matrix in collision theory. Phys. Rev. (2) **118**, 349–356 (1960) Zbl 0092.19001 MR 116934

[30] Sogge, C. D.: Fourier Integrals in Classical Analysis. 2nd ed., Cambridge Tracts in Math. 210, Cambridge Univ. Press, Cambridge (2017) Zbl 1361.35005 MR 3645429

[31] Trefethen, L. N., Embree, M.: Spectra and Pseudospectra. Princeton Univ. Press, Princeton, NJ (2005) Zbl 1085.15009 MR 2155029

[32] Zworski, M.: Resonances in physics and geometry. Notices Amer. Math. Soc. **46**, 319–328 (1999) Zbl 1177.58021 MR 1668841