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# STATIONARY SCATTERING THEORY ON MANIFOLDS

**by Kenichi ITO & Erik SKIBSTED (*)**

Abstract. — Based on our previous work we develop a stationary scattering theory for the Schrödinger operator on a manifold possessing an escape function. A particular class of examples are manifolds with Euclidean and/or hyperbolic ends. Scattering by obstacles, possibly non-smooth and/or unbounded in a certain manner, is included in the theory. We develop the theory largely along the classical lines of Jäger, Saitō and Constantin, and derive in particular WKB-asymptotics of minimal generalized eigenfunctions. As an application we prove a conjecture of Hempel, Post and Weder on cross-ends transmissions in its natural and strong form within the framework of our theory.

Résumé. — Sur la base de nos travaux antérieurs, nous développons une théorie stationnaire de la diffusion pour l'opérateur de Schrödinger sur une variété possédant une fonction d'échappement. Une classe particulière d'exemples sont les variétés à extrémités euclidiennes et/ou hyperboliques. La diffusion par des obstacles, éventuellement non lisses et/ou non bornés d'une certaine manière, est incluse dans la théorie. Nous développons la théorie en grande partie selon les idées classiques de Jäger, Saitō et Constantin, et dérivons en particulier les asymptotiques WKB des fonctions propres généralisées minimales. Comme application, nous prouvons une conjecture de Hempel, Post et Weder sur les transmissions transversales sous sa forme naturelle et forte dans le cadre de notre théorie.

## Contents



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## 1. Introduction

Let $(M, g)$ be a connected Riemannian manifold. In this paper we study stationary scattering theory for the geometric Schrödinger operator

$$H = H_0 + V; \quad H_0 = -\tfrac{1}{2}\Delta = \tfrac{1}{2}p_i^* g^{ij} p_j,\ p_i = -\mathrm{i}\partial_i,$$

on the Hilbert space $\mathcal{H} = L^2(M)$. The potential $V$ is real-valued and bounded, and the self-adjointness of $H$ is realized by the Dirichlet boundary condition. We shall develop a long-range stationary scattering theory to a large extent along the lines of Saitō [27] and Constantin [4], in turn based on works by Jäger [21, 22]. Saitō studies scattering theory for the Schrödinger operator on $L^2(\mathbb{R}^d)$ with a long-range potential, and Constantin studies scattering by an unbounded obstacle in $\mathbb{R}^d$ including a short-range potential, while Jäger develops an abstract theory that he applies to obtain an eigenfunction expansion for a Schrödinger operator. For other previous works on scattering by an unbounded obstacle in $\mathbb{R}^d$ including a short-range potential we refer to [13, 14, 15]; see [30] for a review and comparison of [4] and [13, 14, 15]. We develop a time-dependent scattering theory from the stationary theory of this paper elsewhere [19]. For previous time-dependent short-range scattering theories on manifolds we refer to [4, 15, 17, 18] although this list of references is not complete.

The main goal of this paper is to develop a non-perturbative entirely geometric scattering theory. Whence there are no assumptions like "asymptotically Euclidean" or "asymptotically hyperbolic". Rather our assumptions are stated in terms of an intrinsic "escape function" in a spirit somewhat similar to [5], although our assumptions are considerably weaker than those of [5]. One virtue of this approach, besides its cleanness of being manifestly coordinate-invariant and stable under perturbations, is that a given concrete manifold can possess several such functions potentially entailing useful freedom, meaning that one such function might be better or easier to work with than another one. Of course, there are manifolds not possessing "good" escape functions (for example, this is the case for the parabolic obstacle model of Example 1.20), but they certainly exist for a wide class of manifolds, including those with perturbed Euclidean and hyperbolic ends. In this paper we demonstrate several consequences of the bare existence of a sufficiently good escape function on a manifold.

Our main results are Theorem 1.17, the asymptotic completeness or the existence of unitarily diagonalizing distorted Fourier transforms for $H$, and Theorem 1.18, a characterization of an associated class of minimum generalized eigenfunctions in terms of (zeroth order) WKB-asymptotics. As an application we prove a conjecture of [9] on cross-ends transmissions. It is stated in a strong form in Corollary 1.19. The results of the paper are obtained in terms of an intrinsic escape function geometrically controlled by parameters. This means more precisely that a "good" escape function is one having certain parameters of geometric nature located in a certain region. At the border of these parameter constraints we construct a counterexample for which the minimum generalized eigenfunctions do not have WKB-asymptotics, see Example 1.20. Whence our somewhat technical conditions are more natural than a first reading might indicate and in a sense optimal.

## 1.1. Setting and results from the previous work

Our paper is a continuation of [20], and we start by recalling the setting and various results there partly to fix notation and terminologies. This subsection exhibits only a minimal review, and we refer to [20, Subsection 1.1] for more details and to [20, Subsection 1.2] for several examples of manifolds satisfying the abstract conditions appearing below.

### 1.1.1. Basic setting

We assume an *end* structure on $M$ in a somewhat disguised form.

Condition 1.1. — *Let $(M,g)$ be a connected Riemannian manifold of dimension $d \geqslant 1$. There exist a function $r \in C^\infty(M)$ with image $r(M) = [1,\infty)$ and constants $c > 0$ and $r_0 \geqslant 2$ such that:*

(1) *The gradient vector field* $\omega = \operatorname{grad} r \in \mathfrak{X}(M)$ *is forward complete in the sense that the forward integral curve* $(x(t))_{t \geqslant 0}$ *of* $\omega$ *is defined for any initial point* $x = x(0) \in M$.
(2) *The bound* $|\mathrm{d}r| = |\omega| \geqslant c$ *holds on* $\{x \in M \,|\, r(x) > r_0/2\}$.

Under Condition 1.1 each component of the subset $E = \{x \in M \,|\, r(x) > r_0\}$ is called an *end* of $M$, and, along with Condition 1.2 below, the function $r$ may model a distance function there. The forward completeness condition is our version of the "illumination condition" used in [4] and [13, 14, 15] for the Euclidean unbounded obstacle model (imposed with $r(x) = |x|$ at infinity and requiring $C^2$-regularity of the boundary, see Subsection 1.2 for an elaboration). We note that by Condition 1.1 (2) and the implicit function theorem the $r$-spheres

$$S_R = \{x \in M \,|\, r(x) = R\}; \quad R > r_0/2,$$

are submanifolds of $M$. We will construct the *spherical coordinates* on $E$ in Subsection 1.2.

Let us impose more conditions on the geometry of $E$ in terms of the radius function $r$. Choose $\chi \in C^\infty(\mathbb{R})$ such that

$$\chi(t) = \begin{cases} 1 & \text{for } t \leqslant 1, \\ 0 & \text{for } t \geqslant 2, \end{cases} \quad \chi \geqslant 0, \quad \chi' \leqslant 0, \quad \sqrt{1-\chi} \in C^\infty, \tag{1.1}$$

and set

$$\eta = 1 - \chi(2r/r_0), \quad \tilde{\eta} = |\mathrm{d}r|^{-2}\eta = |\mathrm{d}r|^{-2}\big(1 - \chi(2r/r_0)\big). \tag{1.2}$$

We introduce a "radial" differential operator $A$:

$$A = \operatorname{Re} p^r = \tfrac{1}{2}\big(p^r + (p^r)^*\big); \quad p^r = -\mathrm{i}\nabla^r, \ \nabla^r = \nabla_\omega = g^{ij}(\nabla_i r)\nabla_j, \tag{1.3}$$

and also the "spherical" tensor $\ell$ and the associated differential operator $L$:

$$\ell = g - \tilde{\eta}\, \mathrm{d}r \otimes \mathrm{d}r, \quad L = p_i^* \ell^{ij} p_j. \tag{1.4}$$

As we can see easily, in the spherical coordinates introduced in Subsection 1.2 the tensor $\ell$ may be identified with the pull-back of $g$ to the $r$-spheres. We call $L$ the spherical part of $-\Delta$. Note that if $|\mathrm{d}r| = 1$ then $-L$ acts as the Laplace–Beltrami operator on $S_r$ (in general as a kind of perturbation of this operator, see (2.11)). We remark that the tensor $\ell$ clearly satisfies

$$0 \leqslant \ell \leqslant g, \quad \ell^{\bullet i}(\nabla r)_i = (1 - \eta)\mathrm{d}r, \tag{1.5}$$

where the first bounds of (1.5) are understood as quadratic form estimates on the fibers of the tangent bundle of $M$. The quantities of (1.4) will play a major role in this paper.

Let us recall a local expression of the Levi-Civita connection $\nabla$: If we denote the Christoffel symbol by $\Gamma^k_{ij} = \frac{1}{2}g^{kl}(\partial_i g_{lj} + \partial_j g_{li} - \partial_l g_{ij})$, then for any smooth function $f$ on $M$

$$(\nabla f)_i = (\nabla_i f) = (\mathrm{d}f)_i = \partial_i f, \quad (\nabla^2 f)_{ij} = \partial_i\partial_j f - \Gamma^k_{ij}\partial_k f. \tag{1.6}$$

Note that $\nabla^2 f$ is the geometric Hessian of $f$.

Condition 1.2. — *There exist constants $\tau, C > 0$ such that globally on $M$*

$$\begin{aligned} &|\nabla|\mathrm{d}r|^2| \leqslant Cr^{-1-\tau/2}, && \big|\ell^{\bullet i}\nabla_i\nabla^r|\mathrm{d}r|^2\big| \leqslant Cr^{-1-\tau/2},\\ &|\nabla^k r| \leqslant C \text{ for } k \in \{1,2\}, && \big|\ell^{\bullet i}\nabla_i\Delta r\big| \leqslant Cr^{-1-\tau/2}. \end{aligned} \tag{1.7a}$$

*In addition, there exists $\sigma' > 0$ such that for all $R > r_0/2$, and as quadratic forms on fibers of the tangent bundle of $S_R$,*

$$R\,\iota_R^*\nabla^2 r \geqslant \tfrac{1}{2}\sigma'|\mathrm{d}r|^2\iota_R^* g, \tag{1.7b}$$

*where $\iota_R\colon S_R \hookrightarrow M$ is the inclusion map.*

We remark that here Condition 1.2 is formulated slightly differently from [20]. Firstly, the second bound of (1.7a) is added here. It is not necessary for the results of [20], but it is for those of this paper, see the proofs of Corollaries 2.7 and 2.10. Secondly, (1.7b) is written in a more practical manner in [20], but they are in fact equivalent: Condition 1.2 above and the identity

$$(\nabla^2 r)^{ij}(\nabla r)_j = \tfrac{1}{2}(\nabla|\mathrm{d}r|^2)^i \tag{1.8}$$

actually imply that for any $\sigma \in (0, \sigma')$ there exists $C > 0$ such that globally on $M$

$$r\big(\nabla^2 r - \tfrac{1}{2}\tilde{\eta}^2(\nabla^r|\mathrm{d}r|^2)\mathrm{d}r \otimes \mathrm{d}r\big) \geqslant \tfrac{1}{2}\sigma|\mathrm{d}r|^2\ell - Cr^{-\tau}g. \tag{1.9}$$

This coincides with the inequality assumed in [20].

Next we introduce an effective potential:

$$q = V + \tfrac{1}{8}\tilde{\eta}\big[(\Delta r)^2 + 2\nabla^r\Delta r\big]. \tag{1.10}$$

Condition 1.3. — *There exists a splitting by real-valued functions:*

$$q = q_1 + q_2; \quad q_1 \in C^1(M) \cap L^\infty(M),\ q_2 \in L^\infty(M),$$

*such that for some $\rho', C > 0$ the following bounds hold globally on $M$:*

$$\nabla^r q_1 \leqslant Cr^{-1-\rho'}, \quad |q_2| \leqslant Cr^{-1-\rho'}. \tag{1.11}$$

We remark that in this paper only derivatives of $r$ of order at most five are used quantitatively.

Now let us explain the self-adjoint realizations of $H$ and $H_0$. Since $(M,g)$ can be incomplete, the operators $H$ and $H_0$ are not necessarily essentially self-adjoint on $C^\infty_{\mathrm{c}}(M)$. We realize $H_0$ as a self-adjoint operator by imposing the Dirichlet boundary condition, i.e. $H_0$ is the unique self-adjoint operator associated with the closure of the quadratic form

$$\langle H_0\rangle_\psi = \langle \psi, -\tfrac{1}{2}\Delta\psi\rangle, \quad \psi \in C^\infty_{\mathrm{c}}(M).$$

We denote the form closure and the self-adjoint realization by the same symbol $H_0$. Define the associated Sobolev spaces $\mathcal{H}^s$ by

$$\mathcal{H}^s = (H_0+1)^{-s/2}\mathcal{H}, \quad s \in \mathbb{R}. \tag{1.12}$$

Then $H_0$ may be understood as a closed quadratic form on $Q(H_0) = \mathcal{H}^1$. Equivalently, $H_0$ makes sense also as a bounded operator $\mathcal{H}^1 \to \mathcal{H}^{-1}$, whose action coincides with that for distributions. By the definition of the Friedrichs extension the self-adjoint realization of $H_0$ is the restriction of such distributional $H_0\colon \mathcal{H}^1 \to \mathcal{H}^{-1}$ to the domain:

$$\mathcal{D}(H_0) = \{\psi \in \mathcal{H}^1 \,|\, H_0\psi \in \mathcal{H}\} \subseteq \mathcal{H}.$$

Since $V$ is bounded and self-adjoint by Conditions 1.1–1.3, we can realize the self-adjoint operator $H = H_0 + V$ simply as

$$H = H_0 + V, \quad \mathcal{D}(H) = \mathcal{D}(H_0).$$

In contrast to (1.12) we introduce the Hilbert spaces $\mathcal{H}_s$ and $\mathcal{H}_{s\pm}$ with configuration weights:

$$\mathcal{H}_s = r^{-s}\mathcal{H}, \quad \mathcal{H}_{s+} = \bigcup_{s'>s} \mathcal{H}_{s'}, \quad \mathcal{H}_{s-} = \bigcap_{s'<s} \mathcal{H}_{s'}, \quad s \in \mathbb{R}.$$

We consider the $r$-balls $B_R = \{r(x) < R\}$ and the characteristic functions

$$F_\nu = F(B_{R_{\nu+1}} \setminus B_{R_\nu}),\ R_\nu = 2^\nu,\ \nu \geqslant 0, \tag{1.13}$$

where $F(\Omega) = 1_\Omega$ is used for the characteristic function of a subset $\Omega \subseteq M$. Define the associated Besov spaces $B$ and $B^*$ by

$$\begin{aligned} B &= \{\psi \in L^2_{\mathrm{loc}}(M) \,|\, \|\psi\|_B < \infty\}, \quad \|\psi\|_B = \sum_{\nu=0}^\infty R_\nu^{1/2}\|F_\nu\psi\|_{\mathcal{H}}, \\ B^* &= \{\psi \in L^2_{\mathrm{loc}}(M) \,|\, \|\psi\|_{B^*} < \infty\}, \quad \|\psi\|_{B^*} = \sup_{\nu\geqslant 0} R_\nu^{-1/2}\|F_\nu\psi\|_{\mathcal{H}}, \end{aligned} \tag{1.14}$$

respectively. We also define $B_0^*$ to be the closure of $C_c^\infty(M)$ in $B^*$. Recall the nesting:

$$\mathcal{H}_{1/2+} \subsetneq B \subsetneq \mathcal{H}_{1/2} \subsetneq \mathcal{H} \subsetneq \mathcal{H}_{-1/2} \subsetneq B_0^* \subsetneq B^* \subsetneq \mathcal{H}_{-1/2-}.$$

Using the function $\chi \in C^\infty(\mathbb{R})$ of (1.1), define $\chi_n, \bar{\chi}_n, \chi_{m,n} \in C^\infty(M)$ for $n > m \geqslant 0$ by

$$\chi_n = \chi(r/R_n), \quad \bar{\chi}_n = 1 - \chi_n, \quad \chi_{m,n} = \bar{\chi}_m \chi_n. \tag{1.15}$$

Let us introduce an auxiliary space:

$$\mathcal{N} = \{\psi \in L^2_{\mathrm{loc}}(M) \,|\, \chi_n \psi \in \mathcal{H}^1 \text{ for all } n \geqslant 0\}.$$

This is a space of functions that intuitively satisfy the Dirichlet boundary condition, although possibly with infinite $\mathcal{H}^1$-norm on $M$. Note that under Conditions 1.1–1.3 the manifold $M$ may be, e.g. a half-space in the Euclidean space (see [20, Subsection 1.2]), and there could be a "boundary" even for large $r$, which in our framework appears "invisible" from inside $M$ (see the discussion after Condition 1.12). Recall a similar interpretation of the space $\mathcal{H}^1$.

### 1.1.2. Review of the previous results

Now we gather and review the main results of [20]. Note that all the theorems in this subsection are already proved there.

Our first theorem is Rellich's theorem, the absence of $B_0^*$-eigenfunctions with eigenvalues above a certain "critical energy" $\lambda_0 \in \mathbb{R}$ defined by

$$\lambda_0 = \limsup_{r\to\infty} q_1 = \lim_{R\to\infty} \bigl(\sup\{q_1(x) \,\big|\, r(x) \geqslant R\}\bigr). \tag{1.16}$$

For the Euclidean and the hyperbolic spaces and many other examples the critical energy $\lambda_0$ can be computed explicitly, and the essential spectrum is given by $\sigma_{\mathrm{ess}}(H) = [\lambda_0, \infty)$. The latter is usually seen in terms of Weyl sequences, see [23].

Theorem 1.4. — *Suppose Conditions 1.1–1.3, and let $\lambda > \lambda_0$. If a function $\phi \in L^2_{\mathrm{loc}}(M)$ satisfies that*

1. *$(H - \lambda)\phi = 0$ in the distributional sense,*
2. *$\bar{\chi}_m \phi \in \mathcal{N} \cap B_0^*$ for all $m \geqslant 0$ large enough,*

*then $\phi = 0$ in $M$.*

Next we discuss the limiting absorption principle and the radiation condition related to the resolvent $R(z) = (H - z)^{-1}$. We state a locally uniform bound for the resolvent as a map: $B \to B^*$. For that we need a compactness condition.

Condition 1.5. — *In addition to Conditions 1.1–1.3, there exists an open subset* $\mathcal{I} \subseteq (\lambda_0, \infty)$ *such that for any* $n \geqslant 0$ *and compact interval* $I \subseteq \mathcal{I}$ *the mapping*

$$\chi_n P_H(I) \colon \mathcal{H} \to \mathcal{H}$$

*is compact, where* $P_H(I)$ *denotes the spectral projection onto* $I$ *for* $H$.

Due to Rellich's compact embedding theorem [26, Theorem XIII.65], "boundedness" of $r$-balls provides a criterion for Condition 1.5: If each $r$-ball $B_R$, $R \geqslant 1$, is isometric to a bounded subset of a complete manifold, Condition 1.5 is satisfied for $\mathcal{I} = (\lambda_0, \infty)$. Condition 1.5 in fact includes more general situations where $M$ has multiple ends of different critical energies and $r$-balls are unbounded as in [24].

We fix any $\sigma \in (0, \sigma')$ and then large enough $C > 0$ in agreement with (1.9), and introduce the positive quadratic form

$$h := \nabla^2 r - \tfrac{1}{2}\tilde{\eta}^2(\nabla^r |\mathrm{d}r|^2)\mathrm{d}r \otimes \mathrm{d}r + 2Cr^{-1-\tau} g \geqslant \tfrac{1}{2}\sigma r^{-1}|\mathrm{d}r|^2 \ell + Cr^{-1-\tau} g.$$

For any subset $I \subseteq \mathcal{I}$ we denote

$$I_\pm = \{z = \lambda \pm \mathrm{i}\Gamma \in \mathbb{C} \,|\, \lambda \in I,\ \Gamma \in (0,1)\},$$

respectively. We also use the notation $\langle T \rangle_\phi = \langle \phi, T\phi \rangle$.

Theorem 1.6. — *Suppose Condition 1.5 and let* $I \subseteq \mathcal{I}$ *be a compact interval. Then there exists* $C > 0$ *such that for any* $\phi = R(z)\psi$ *with* $z \in I_\pm$ *and* $\psi \in B$

$$\|\phi\|_{B^*} + \|p^r \phi\|_{B^*} + \langle p_i^* h^{ij} p_j \rangle_\phi^{1/2} + \|H_0 \phi\|_{B^*} \leqslant C\|\psi\|_B. \tag{1.17}$$

In our theory the Besov boundedness (1.17) does not immediately imply the limiting absorption principle, and for the latter we need also radiation condition bounds implied by minor additional regularity and decay conditions.

Condition 1.7. — *In addition to Condition 1.5 there exist splittings* $q_1 = q_{11} + q_{12}$ *and* $q_2 = q_{21} + q_{22}$ *by real-valued functions*

$$q_{11} \in C^2(M) \cap L^\infty(M), \quad q_{12}, q_{21} \in C^1(M) \cap L^\infty(M), \quad q_{22} \in L^\infty(M)$$

*and constants* $\rho, C > 0$ *such that for* $k = 0, 1$

$$\begin{gathered}|\nabla^r q_{11}| \leqslant Cr^{-(1+\rho/2)/2}, \quad |\ell^{\bullet i} \nabla_i q_{11}| \leqslant Cr^{-1-\rho/2}, \quad |\mathrm{d}\nabla^r q_{11}| \leqslant Cr^{-1-\rho/2}, \\ |\mathrm{d}q_{12}| \leqslant Cr^{-1-\rho/2}, \qquad |(\nabla^r)^k q_{21}| \leqslant Cr^{-k-\rho}, \qquad q_{21}\nabla^r q_{11} \leqslant Cr^{-1-\rho}, \\ |q_{22}| \leqslant Cr^{-1-\rho/2}.\end{gathered}$$

Our radiation condition bounds are stated in terms of the distributional radial differential operator $A$ defined in (1.3) and an asymptotic complex phase $a$ given below. Pick a smooth decreasing function $r_\lambda \geqslant 2r_0$ of $\lambda > \lambda_0$ such that

$$\lambda + \lambda_0 - 2q_1 \geqslant 0 \text{ for } r \geqslant r_\lambda/2, \tag{1.18}$$

and that $r_\lambda = 2r_0$ for all $\lambda$ large enough. Then we set

$$\eta_\lambda = 1 - \chi(2r/r_\lambda),$$

and for $z = \lambda \pm \mathrm{i}\Gamma \in \mathcal{I} \cup \mathcal{I}_\pm$

$$b = \eta_\lambda |\mathrm{d}r| \sqrt{2(z - q_1)}, \qquad \widetilde{b} = \widetilde{\eta} b, \tag{1.19a}$$

$$a = b \pm \tfrac{1}{4} \eta_\lambda (p^r q_{11}) / (z - q_1), \tag{1.19b}$$

respectively, where the branch of square root is chosen such that $\operatorname{Re} \sqrt{w} > 0$ for $w \in \mathbb{C} \setminus (-\infty, 0]$. Note that for $z \in \mathcal{I}$ there are two values of $a$ which could be denoted $a_\pm$. For convenience we prefer to use the shorter notation in the bulk of this paper. Note also that the phase $a$ of (1.19b) is an approximate solution to the radial Riccati equation

$$\pm p^r a + a^2 - 2|\mathrm{d}r|^2 (z - q_1) = 0 \tag{1.20}$$

in the sense that it makes the quantity on the left-hand side of (1.20) small for large $r \geqslant 1$. The quantity $b$ of (1.19a) alone already gives an approximate solution to the same equation, however with the second term of (1.19b) a better approximation is obtained, cf. Lemma 2.3. Set

$$\beta_c = \tfrac{1}{2} \min\{\sigma, \tau, \rho\}. \tag{1.21}$$

Here and henceforth we consider $\sigma \in (0, \sigma')$ as a fixed parameter.

Theorem 1.8. — *Suppose Condition 1.7, and let $I \subseteq \mathcal{I}$ be a compact interval. Then for all $\beta \in [0, \beta_c)$ there exists $C > 0$ such that for any $\phi = R(z)\psi$ with $\psi \in r^{-\beta} B$ and $z \in I_\pm$*

$$\|r^\beta (A \mp a)\phi\|_{B^*} + \langle p_i^* r^{2\beta} h^{ij} p_j \rangle_\phi^{1/2} \leqslant C \|r^\beta \psi\|_B, \tag{1.22}$$

*respectively.*

The limiting absorption principle reads.

Corollary 1.9. — *Suppose Condition 1.7, and let $I \subseteq \mathcal{I}$ be a compact interval. For any $s > 1/2$ and $\epsilon \in (0, \min\{s - 1/2, \beta_c, (2+\rho)/4\})$ there exists $C > 0$ such that for $k = 0, 1$ and any $z, z' \in I_+$ or $z, z' \in I_-$*

$$\|p^k R(z) - p^k R(z')\|_{\mathcal{B}(\mathcal{H}_s, \mathcal{H}_{-s})} \leqslant C|z - z'|^{\min\{\epsilon, 1\}}. \tag{1.23}$$

*In particular, the operators $p^k R(z)$, $k = 0, 1$, attain uniform limits as $I_\pm \ni z \to \lambda \in I$ in the norm topology of $\mathcal{B}(\mathcal{H}_s, \mathcal{H}_{-s})$, say denoted*

$$p^k R(\lambda \pm \mathrm{i}0) := \lim_{I_\pm \ni z \to \lambda} p^k R(z), \quad \lambda \in I, \tag{1.24}$$

*respectively. These limits $p^k R(\lambda \pm \mathrm{i}0) \in \mathcal{B}(B, B^*)$, and $R(\lambda \pm \mathrm{i}0) : B \to \mathcal{N} \cap B^*$.*

Given the limiting resolvents $R(\lambda \pm \mathrm{i}0)$ the radiation condition bounds for real spectral parameters follow directly from Theorem 1.8.

Corollary 1.10. — *Suppose Condition 1.7, and let $I \subseteq \mathcal{I}$ be a compact interval. Then for all $\beta \in [0, \beta_c)$ there exists $C > 0$ such that for any $\phi = R(\lambda \pm \mathrm{i}0)\psi$ with $\psi \in r^{-\beta}B$ and $\lambda \in I$*

$$\|r^\beta (A \mp a_\pm)\phi\|_{B^*} + \langle p_i^* r^{2\beta} h^{ij} p_j \rangle_\phi^{1/2} \leqslant C \|r^\beta \psi\|_B, \tag{1.25}$$

*respectively.*

For the Euclidean and the hyperbolic spaces without potential $V$ we can assume $\beta_c \geqslant 1 - \epsilon$ for any given (small) $\epsilon > 0$. Hence in these cases the bound (1.25) hold for any $\beta \in [0, 1)$. We remark that for the Euclidean space and a sufficiently regular potential the bound (1.25) is well-known for $\beta \in [0, 1)$, cf. [10, 16, 27]. However in this case one can actually allow $\beta \in [1, 2)$, cf. [10]. If $\beta > 1$ is allowed the existence of the distorted Fourier transform follows easily, cf. [10, 11, 28]. This is demonstrated in Subsection 3.1.

As another application of the radiation condition bounds we have characterized the limiting resolvents $R(\lambda \pm \mathrm{i}0)$. For the Euclidean space such a characterization is usually referred to as the Sommerfeld uniqueness result, see for example [16].

Corollary 1.11. — *Suppose Condition 1.7, and let $\lambda \in \mathcal{I}$, $\phi \in L^2_{\mathrm{loc}}(M)$ and $\psi \in r^{-\beta}B$ with $\beta \in [0, \beta_c)$. Then $\phi = R(\lambda \pm \mathrm{i}0)\psi$ holds if and only if both of the following conditions hold:*

(i) *$(H - \lambda)\phi = \psi$ in the distributional sense.*
(ii) *$\phi \in \mathcal{N} \cap r^\beta B^*$ and $(A \mp a_\pm)\phi \in r^{-\beta} B_0^*$.*

## 1.2. Extended framework

Let $r \geqslant r_0$, $\mathrm{d}\mathcal{A}_r$ be the naturally induced measure on $S_r$ and

$$\mathcal{G}_r = L^2(S_r, \mathrm{d}\widetilde{\mathcal{A}}_r); \quad \mathrm{d}\widetilde{\mathcal{A}}_r = |\mathrm{d}r|^{-1} \mathrm{d}\mathcal{A}_r. \tag{1.26}$$

Recall the co-area formula, cf. [7, Theorem C.5], implying that for all integrable functions $\phi$ supported in $E$

$$\int_E \phi(x)\big(\det g(x)\big)^{1/2}\,\mathrm{d}x = \int_{r_0}^{\infty} \mathrm{d}r \int_{S_r} \phi\,\mathrm{d}\widetilde{\mathcal{A}}_r, \tag{1.27}$$

in particular that for square integrable functions

$$\|1_E\phi\|^2 = \int_{r_0}^{\infty} \|\phi_{|S_r}\|^2_{\mathcal{G}_r}\,\mathrm{d}r.$$

We can describe the measure $\mathrm{d}\widetilde{\mathcal{A}}_r$ in some details using the following condition.

Condition 1.12. — *Let $(M,g)$ be the manifold, $r$ be the function and $c$ and $r_0$ be the constants of Condition 1.1. Let $M_0 = \{x \in M \,|\, r(x) > r_0/2\}$. There exists a Riemannian manifold $(M^{\mathrm{ex}}, g^{\mathrm{ex}})$ of dimension $d$ in which the manifold $(M_0, g)$ is isometrically embedded. There exists an extension $r^{\mathrm{ex}} \in C^\infty(M^{\mathrm{ex}})$ of the restriction $r_{|M_0}$ such that the extended vector field $\omega^{\mathrm{ex}} := \operatorname{grad} r^{\mathrm{ex}}$ is complete in $M^{\mathrm{ex}}$ and $|\omega^{\mathrm{ex}}| \geqslant c$ on $\{x \in M^{\mathrm{ex}} \,|\, r^{\mathrm{ex}}(x) > r_0/2\}$. Let $\widetilde{\omega}^{\mathrm{ex}} = \widetilde{\eta}^{\mathrm{ex}}\omega^{\mathrm{ex}}$ be the complete vector field defined with $\widetilde{\eta}^{\mathrm{ex}} = |\omega^{\mathrm{ex}}|^{-2}\big(1-\chi(2r^{\mathrm{ex}}/r_0)\big)$, and let $\widetilde{y}^{\mathrm{ex}}(t,\cdot) = \exp(t\widetilde{\omega}^{\mathrm{ex}})$ denote the corresponding flow. Then*

$$\forall\,\sigma \in S : \{\widetilde{y}^{\mathrm{ex}}(t,\sigma) \,|\, t \geqslant 0\} \cap M \neq \emptyset,$$

*where $S = S^{\mathrm{ex}}_{r_0} = \{x \in M^{\mathrm{ex}} |\, r^{\mathrm{ex}}(x) = r_0\}$.*

For many examples, cf. [20, Subsection 1.2], the vector field $\omega$ of Condition 1.1 is forward as well as backward complete (i.e. complete) and we can take $(M^{\mathrm{ex}}, g^{\mathrm{ex}}, r^{\mathrm{ex}}) = (M, g, r)$. The typical origin for non-backward completeness for a sub-manifold $M \subseteq M'$, $M$ open in $M'$, is "crossing" of integral curves of $\omega$ at the boundary $\partial M \subseteq M'$. The reader might prefer to think about $(M^{\mathrm{ex}}, g^{\mathrm{ex}})$ and $r^{\mathrm{ex}}$ as given from the outset. Then $M_0 \subseteq M^{\mathrm{ex}}$ would be an invariant subset under the forward flow of the vector field $\omega^{\mathrm{ex}}$. However since most of our conditions are needed for $M$ only (in fact (1.33) is the only quantitative exception) we have pursued the given presentation.

The framework of [4] where $M \subseteq \mathbb{R}^d$ fits into ours by taking $r(x) = |x|$ for $|x| > r_0/2$ with $r_0 > 2$ sufficiently big (and defining the function suitably for $|x| \leqslant r_0/2$). We can then use the conic subset $M^{\mathrm{ex}} = \mathbb{R}_+ M$ of $\mathbb{R}^d$ and $r^{\mathrm{ex}}(x) = (1-\chi(4|x|/r_0))|x|$, $x \in M^{\mathrm{ex}}$. We also remark that for the Euclidean unbounded obstacle model the illumination condition of [4] and [13, 14, 15] appears stronger than needed since it corresponds to using this function $r$ only (the reader may consult Examples 1.16 1) and 2) in [19] for examples of Euclidean unbounded obstacle models that fit into our framework but not into the ones of [4] and [13, 14, 15]). On the other hand the short-range conditions P1, P2 and P3 of [4] do not directly compare to our conditions in the short-range case, say defined by taking $q_{11} = q_{12} = 0$ and $\rho > 1$ in Condition 1.7, although the difference appears minimal.

We note

$$\forall\, \sigma \in S \ \forall\, t \geqslant 0 : \quad r^{\mathrm{ex}}(\widetilde{y}^{\mathrm{ex}}(t, \sigma)) = r_0 + t, \tag{1.28}$$

and that any $x \in E^{\mathrm{ex}} := \{x \in M^{\mathrm{ex}} \,|\, r^{\mathrm{ex}}(x) > r_0\}$ has *spherical coordinates* defined as

$$(r, \sigma) = (r^{\mathrm{ex}}(x), \widetilde{y}^{\mathrm{ex}}(r_0 - r^{\mathrm{ex}}(x), x)) \in (r_0, \infty) \times S.$$

In particular any $x \in E$ has spherical coordinates defined in this way.

Mimicking the constructions (1.26) we introduce

$$\mathcal{G} = L^2(S, \mathrm{d}\widetilde{\mathcal{A}}), \quad \mathrm{d}\widetilde{\mathcal{A}} = \mathrm{d}\widetilde{\mathcal{A}}^{\mathrm{ex}} = |\omega^{\mathrm{ex}}|^{-1} \mathrm{d}\mathcal{A}^{\mathrm{ex}}, \tag{1.29}$$

in terms of the naturally induced measure $\mathrm{d}\mathcal{A}^{\mathrm{ex}}$ on $S$. Now, indeed in spherical coordinates

$$\mathrm{d}\widetilde{\mathcal{A}}_r = \exp\biggl(\int_{r_0}^{r} (\operatorname{div} \widetilde{\omega}^{\mathrm{ex}})(s, \sigma)\, \mathrm{d}s\biggr)\, \mathrm{d}\widetilde{\mathcal{A}} \quad \text{for } x = \widetilde{y}^{\mathrm{ex}}(r - r_0, \sigma) \in S_r.$$

This leads to the isometrical embedding $\mathcal{G}_r \subseteq \mathcal{G}$, $r \geqslant r_0$, given by mapping $\mathcal{G}_r \ni \xi_r \to \xi^{\mathrm{ex}} \in \mathcal{G}$ where

$$\xi^{\mathrm{ex}}(\sigma) = \begin{cases} \exp\Bigl(\int_{r_0}^{r} \tfrac{1}{2} (\operatorname{div} \widetilde{\omega}^{\mathrm{ex}})(s, \sigma)\, \mathrm{d}s\Bigr)\, \xi_r(x) & \text{for } x = \widetilde{y}^{\mathrm{ex}}(r - r_0, \sigma) \in S_r, \\ 0 & \text{otherwise.} \end{cases} \tag{1.30}$$

The formula (1.30) can be understood in terms of (a group of) translations on the extended Hilbert space $\mathcal{H}^{\mathrm{ex}} = L^2(M^{\mathrm{ex}}, g^{\mathrm{ex}})$. We introduce the *normalized extended radial translation* $\widetilde{T}^{\mathrm{ex}}(\tau) : \mathcal{H}^{\mathrm{ex}} \to \mathcal{H}^{\mathrm{ex}}$, $\tau \in \mathbb{R}$, in terms of the self-adjoint operator

$$\widetilde{A} = \widetilde{A}^{\mathrm{ex}} = \operatorname{Re}\bigl(-\mathrm{i} \nabla_{\widetilde{\omega}^{\mathrm{ex}}}\bigr)$$

by $\widetilde{T}^{\mathrm{ex}}(\tau) = \mathrm{e}^{\mathrm{i}\tau \tilde{A}}$. Then (1.30) is naturally rewritten as $\xi^{\mathrm{ex}} = \mathrm{e}^{\mathrm{i}(r - r_0)\tilde{A}} \xi_r$ since for $\psi \in \mathcal{H}^{\mathrm{ex}}$ and $x \in M^{\mathrm{ex}}$

$$(\widetilde{T}^{\mathrm{ex}}(\tau)\psi)(x) = \exp\biggl(\int_0^{\tau} \tfrac{1}{2} (\operatorname{div} \widetilde{\omega}^{\mathrm{ex}})(\widetilde{y}^{\mathrm{ex}}(t, x))\, \mathrm{d}t\biggr)\, \psi(\widetilde{y}^{\mathrm{ex}}(\tau, x)), \tag{1.31}$$

cf. a similar formula in [20] (proven there).

We also note that the relation $x = \widetilde{y}^{\mathrm{ex}}(r - r_0, \sigma)$ of (1.30) naturally defines an embedding $S_r \subseteq S$ given as the map $S_r \ni x \to \sigma \in S$. We shall sometimes slightly abuse notation and write $\sigma \in S_r$, leaving it to the reader to decide from the context whether $\sigma$ should be thought of as a point in the subset $S_r$ of $M$ or rather as a point in the image of this map.

## 1.3. Main results

### 1.3.1. Distorted Fourier transform

We need additional assumptions. The following one suffices for constructing the *distorted Fourier transform* (this terminology is motivated by Theorem 1.17 stated below).

CONDITION 1.13. — *Along with Condition 1.12, Condition 1.7 holds with*

$$2\beta_c = \min\{\sigma,\tau,\rho\} > 1. \tag{1.32}$$

*In addition, the function $\widetilde{b} = \widetilde{b}(\lambda, x)$ has a real $C^1$-extension to $\mathcal{I} \times M^{\mathrm{ex}}$, say denoted by $\widetilde{b}^{\mathrm{ex}}$ (or by $\widetilde{b}$ again for short), and the following bound holds uniformly in the spherical coordinates on $E$ and locally uniformly in $\lambda \in \mathcal{I}$:*

$$\sup_{r_0 \leqslant \check{r} \leqslant r} \left| \ell^{\bullet i}\nabla_i \int_{\check{r}}^{r} \widetilde{b}^{\mathrm{ex}}(s,\sigma)\,\mathrm{d}s \right| \leqslant Cr^{-1/2}. \tag{1.33}$$

If $M^{\mathrm{ex}} = M$ the technical bound (1.33) is a consequence of (parts of) the other conditions and Lemma 2.6. The bound is only used in the proof of Lemma 3.5, and we note that it is not needed if we impose the strengthening (1.40) of (1.32) (however we do need it for the alternative Condition 1.16 (2)).

For any $\psi \in \mathcal{H}_{1+}$ and $r \geqslant r_0$ we introduce a function $\xi(r) \in \mathcal{G}$ using the mapping (1.30), omitting here (and often henceforth) the superscript “ex”:

$$\xi(r)(\sigma) = \exp\left(\int_{r_0}^{r} \left(\mp \mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\right)(s,\sigma)\,\mathrm{d}s\right)[\sqrt{b}R(\lambda \pm \mathrm{i}0)\psi](r,\sigma), \tag{1.34}$$

(and $= 0$ for $\sigma \notin S_r$) or, alternatively,

$$\xi(r) = \mathrm{e}^{\mathrm{i}(r-r_0)(\tilde{A}\mp\tilde{b})}\big[\sqrt{b}R(\lambda \pm \mathrm{i}0)\psi\big]_{|S_r}. \tag{1.35}$$

The notation (1.35) is motivated by (1.31) and the formula

$$(\mathrm{e}^{\mathrm{i}\tau(\tilde{A}\mp\tilde{b})}\psi)(x) = \exp\left(\mp\mathrm{i}\int_0^{\tau} \widetilde{b}(\widetilde{y}(t,x))\,\mathrm{d}t\right)(\mathrm{e}^{\mathrm{i}\tau\tilde{A}}\psi)(x).$$

Then we define the “distorted Fourier transform” by

$$F^{\pm}(\lambda)\psi = \mathcal{G}\text{–}\lim_{r\to\infty} \xi(r); \quad \psi \in \mathcal{H}_{1+}. \tag{1.36}$$

Theorem 1.14. — *Suppose Condition 1.13. Then for any* $\psi \in \mathcal{H}_{1+}$ *there exist the limits* (1.36). *The maps* $\mathcal{I} \ni \lambda \mapsto F^{\pm}(\lambda)\psi \in \mathcal{G}$ *are continuous. Moreover, putting* $\delta(H-\lambda) = \pi^{-1}\operatorname{Im} R(\lambda + \mathrm{i}0)$,

$$\|F^{\pm}(\lambda)\psi\|^2 = 2\pi\langle\psi, \delta(H-\lambda)\psi\rangle. \tag{1.37}$$

By definition the function $F^{\pm}(\lambda)\psi \in \mathcal{G} = L^2(S, \mathrm{d}\widetilde{\mathcal{A}})$, and we note that our construction of $F^{\pm}(\lambda)\psi$ is non-canonical primarily due to the freedom in choosing $\mathcal{G}$. In fact for $M^{\mathrm{ex}} = M$ the only non-canonical feature comes from the dependence of $r_0$ (determining $\mathcal{G}$ in that case), while in general there is an additional freedom in choosing extended functions.

Due to (1.37) the operators $F^{\pm}(\lambda)$ extend as continuous operators $B \to \mathcal{G}$, and for any $\psi \in B$ the maps $F^{\pm}(\cdot)\psi \in \mathcal{G}$ are continuous. In Proposition 1.15 stated below we give a formula for these extensions.

Introduce

$$\mathcal{H}_{\mathcal{I}} = P_H(\mathcal{I})\mathcal{H}, \quad \widetilde{\mathcal{H}}_{\mathcal{I}} = L^2(\mathcal{I}, (2\pi)^{-1}\mathrm{d}\lambda; \mathcal{G}),$$

set $H_{\mathcal{I}} = HP_H(\mathcal{I})$ and let $M_\lambda$ be the operator of multiplication by $\lambda$ on $\widetilde{\mathcal{H}}_{\mathcal{I}}$. We define

$$F^{\pm} = \int_{\mathcal{I}} \bigoplus F^{\pm}(\lambda)\,\mathrm{d}\lambda \colon B \to C(\mathcal{I}; \mathcal{G}).$$

These operators can be extended to proper spaces which is stated as the first part of the following result.

Proposition 1.15. — *Suppose Condition 1.13. The operators* $F^{\pm}$ *considered as maps* $B \cap \mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$ *extend uniquely to isometries* $\mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$. *These extensions obey* $F^{\pm}H_{\mathcal{I}} \subseteq M_\lambda F^{\pm}$. *Moreover for any* $\psi \in B$ *the vectors* $F^{\pm}(\lambda)\psi$ *are given as averaged limits. More precisely introducing for any such* $\psi$ *the integral* $⨍_R \xi(r)\,\mathrm{d}r := R^{-1}\int_R^{2R} \xi(r)\,\mathrm{d}r$, *these vectors are given as*

$$\begin{aligned} F^{\pm}(\lambda)\psi &= \mathcal{G}\text{–}\lim_{R\to\infty} ⨍_R \xi(r)\,\mathrm{d}r \\ &= \mathcal{G}\text{–}\lim_{R\to\infty} ⨍_R \exp\Big(\int_{r_0}^{r}\Big(\mp\mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\Big)(s,\cdot)\,\mathrm{d}s\Big)[\sqrt{b}R(\lambda \pm \mathrm{i}0)\psi](r,\cdot)\,\mathrm{d}r, \end{aligned} \tag{1.38}$$

*and the limits* (1.38) *are attained locally uniformly in* $\lambda \in \mathcal{I}$.

The above extended isometries $F^{\pm} \colon \mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$ are actually unitary under an additional condition, and for this reason we call them the Fourier transformations associated with $H_{\mathcal{I}}$. The new condition consists of two alternatives. The first one is a partial strengthening of Condition 1.13. The other one is primarily a set of bounds on higher order derivatives of various quantities defined on $M$.

For simplicity for any smooth function $f$ on $M$ let us set

$$\nabla' f = \nabla f - (\nabla_{\tilde\omega} f)\nabla r, \quad \nabla'^2 f = \nabla^2 f - (\nabla_{\tilde\omega} f)\nabla^2 r. \tag{1.39}$$

Note that in $E$ the quantity $\nabla' f$ involves spherical derivatives only, which may be seen as a consequence of the formula $\nabla' f = \ell^{\bullet i}(\nabla f)_i$. Although we do not verify it in this paper, in $E$ the spherical part of $\nabla'^2 f$, i.e. $\ell^{\bullet i}\ell^{\bullet j}(\nabla'^2 f)_{ij}$, coincides with the second order derivative ($\nabla' f$ is the first order derivative) computed by the Levi-Civita connections on the $r$-spheres $S_r$ associated with the induced Riemannian metrics $g_r := \iota_r^* g$.

Condition 1.16. — *In addition to Condition 1.13 one of the following two properties holds:*

(1)

$$\min\{\sigma, \tau, \rho\} > 2. \tag{1.40}$$

(2) *The extension* $\widetilde{b}^{\mathrm{ex}}$ *of Condition 1.13 is in* $C^2$*. The restriction* $q_{1|E}$ *belongs to* $C^2(E)$*, and there exists* $C > 0$ *such that*

$$\bigl|\ell^{\bullet i}\ell^{\bullet j}\ell^{\bullet k}(\nabla^3 r)_{ijk}\bigr| \leqslant Cr^{-1-\tau/2}, \tag{1.41a}$$

$$|\ell^{\bullet i}\ell^{\bullet j}(\nabla'^2 q_1)_{ij}| \leqslant Cr^{-1-\rho}, \tag{1.41b}$$

*and*

$$\begin{gathered}\bigl|\ell^{\bullet i}\ell^{\bullet j}(\nabla'^2|\mathrm{d}r|^2)_{ij}\bigr| \leqslant Cr^{-1-\tau}, \quad \bigl|\ell^{\bullet i}\ell^{\bullet j}(\nabla'^2\nabla^r|\mathrm{d}r|^2)_{ij}\bigr| \leqslant Cr^{-1-\tau}, \\ \bigl|\ell^{\bullet i}\ell^{\bullet j}(\nabla'^2\Delta r)_{ij}\bigr| \leqslant Cr^{-1-\tau}.\end{gathered} \tag{1.41c}$$

We remark that there does not appear $r$-derivatives in (1.41b) and hence for $q_1$ it suffices to assume additional $C^2$-smoothness only in the spherical directions. The bounds (1.41b) and (1.41c) allow us to estimate

$$\ell^{\bullet i}\ell^{\bullet j}\bigl(\nabla'^2\bigl(\pm \mathrm{i}\widetilde{b} - \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\bigr)\bigr)_{ij} = O(r^{-1-\min\{\tau,\rho\}}), \tag{1.42}$$

to be used in our verification of (2.36).

Theorem 1.17. — *Suppose Condition 1.16. Then the operators* $F^{\pm} : \mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$ *are unitarily diagonalizing transforms for* $H_{\mathcal{I}}$*, that is, they are unitary and*

$$F^{\pm} H_{\mathcal{I}} = M_\lambda F^{\pm},$$

*respectively.*

*Remark.* — For the conclusion of Theorem 1.17 it suffices to assume Condition 1.13 and (3.23) of Lemma 3.8. In fact, Condition 1.16 is here and henceforth used only for the verification of (3.23).

### 1.3.2. Scattering matrix and generalized eigenfunctions

Next for any $\xi \in \mathcal{G}$ let us introduce purely outgoing/incoming approximate generalized eigenfunctions $\phi^{\pm}[\xi] \in B^*$ by, using the spherical coordinates,

$$\begin{aligned}(1.43)\quad &\phi^{\pm}[\xi](r,\sigma)\\ &= \eta_\lambda\big[2|\mathrm{d}r|^2(\lambda-q_1)\big]^{-1/4}\exp\bigg(\int_{r_0}^{r}\Big(\pm\mathrm{i}\widetilde{b}-\tfrac12\operatorname{div}\widetilde{\omega}\Big)(s,\sigma)\,\mathrm{d}s\bigg)\xi(\sigma),\end{aligned}$$

cf. Theorem 1.14. Of course these quantities are well-defined independently of all the estimates of Conditions 1.13 and 1.16. We remark that formulas like (1.43) in the context of Schrödinger operators are referred to as (zeroth order) WKB-approximations. We remark that, although only the real part $\operatorname{Re} a$ is employed in (1.43) instead of the full complex phase $a$, the imaginary part $\operatorname{Im} a$ is already somehow taken into account in the front factor $\eta_\lambda[2|\mathrm{d}r|^2(\lambda-q_1)]^{-1/4}$. In fact for $M^{\mathrm{ex}}=M$, letting $\widetilde{a}=|\mathrm{d}r|^{-2}a$, we can see this from

$$\operatorname{Re}\int_{r_0}^{r}\pm\mathrm{i}\widetilde{a}\,\mathrm{d}s=-\tfrac14\int_{r_0}^{r}\Big[\eta_\lambda\partial_s\ln(\lambda-q_1)+\eta_\lambda|\mathrm{d}r|^{-2}(\nabla^r q_{12})/(\lambda-q_1)\Big]\,\mathrm{d}s$$

by an integration by parts. The spherical waves (1.43) will work as free comparison waves in our theory.

If we denote the oscillatory part of the phase by

$$S(x)=\pm\int_{r_0}^{r(x)}\widetilde{b}(s,\sigma(x))\,\mathrm{d}s,$$

then Condition 1.7 and (1.32) of Condition 1.13 imply that for $M^{\mathrm{ex}}=M$

$$\tfrac12|\mathrm{d}S(x)|^2+q_1-\lambda=O(r^{-1-\epsilon})\quad\text{for all }\epsilon<2\beta_c-1,$$

see Lemma 2.6. Whence in this case $S(\cdot)$ is an approximate solution to the eikonal equation with the effective potential $q_1$ and a short-range error. In the general case of Condition 1.13 the bound (1.33) is barely too weak to give a uniform short-range error, however due to Lemma 2.6 we still have pointwise short-range bounds (i.e. short-range bounds that are not uniform in $\sigma\in S$). Although such a property is basic for the WKB-method (in particular for obtaining higher order expansions) it will only be used in a disguised form in this paper. We remark that under Condition 1.13

for any $\xi \in C^\infty_{\mathrm{c}}(S) \subseteq \mathcal{G}$ the vectors $\phi^\pm[\xi] \in \mathcal{N}$ (here possibly needed cutoff further at infinity), and under Condition 1.16 they are approximate generalized eigenfunctions in the sense $R(\mathrm{i})(H-\lambda)\phi^\pm[\xi] \in B \cap \mathcal{H}^1$ which is a consequence of (3.23), cf. the proof of Lemma 3.9 (see also Example 1.20 where this property just barely does not hold).

Under Condition 1.16 and for any $\lambda \in \mathcal{I}$ the *scattering matrix* $S(\lambda)\colon \mathcal{G} \to \mathcal{G}$ is defined by the identity

$$F^+(\lambda)\psi = S(\lambda)F^-(\lambda)\psi; \quad \psi \in B. \tag{1.44}$$

It follows from (3.28b) that $C^\infty_{\mathrm{c}}(S) \subseteq \operatorname{Ran} F^\pm(\lambda)$, and hence (seen in combination with Theorem 1.14, Proposition 1.15 and a density argument) $S(\,\cdot\,)$ is a well-defined strongly continuous unitary operator. We obtain a characterization of the generalized eigenfunctions in $\mathcal{N} \cap B^*$, i.e. the elements of

$$\mathcal{E}_\lambda := \{\phi \in \mathcal{N} \cap B^* \mid (H-\lambda)\phi = 0\}.$$

Due to Theorem 1.4 these eigenfunctions may be called *minimum eigenfunctions.*

Theorem 1.18. — *Suppose Condition 1.16. Then for any $\lambda \in \mathcal{I}$ the following assertions hold.*

(i) *For any one of $\xi_\pm \in \mathcal{G}$ or $\phi \in \mathcal{E}_\lambda$ the two other quantities in $\{\xi_-, \xi_+, \phi\}$ uniquely exist such that*

$$\phi - \phi^+[\xi_+] + \phi^-[\xi_-] \in B_0^*. \tag{1.45a}$$

(ii) *The correspondences in* (1.45a) *are given by the formulas (recall* (1.35)*)*

$$\phi = \mathrm{i}F^\pm(\lambda)^*\xi_\pm, \quad \xi_+ = S(\lambda)\xi_-, \tag{1.45b}$$

$$\xi_\pm = 2^{-1}\, \mathcal{G}\text{–}\lim_{R\to\infty} ⨍_R \mathrm{e}^{\mathrm{i}(r-r_0)(\tilde{A}^{\mathrm{ex}} \mp \tilde{b}^{\mathrm{ex}})} \big[b^{-1/2}(A \pm b)\phi\big]_{|S_r}\, \mathrm{d}r. \tag{1.45c}$$

*In particular the wave matrices $F^\pm(\lambda)^*\colon \mathcal{G} \to \mathcal{E}_\lambda$ are linear isomorphisms.*

(iii) *The wave matrices $F^\pm(\lambda)^*\colon \mathcal{G} \to \mathcal{E}_\lambda\,(\subseteq B^*)$ are bi-continuous. In fact*

$$2\|\xi_\pm\|^2_{\mathcal{G}} = \lim_{R\to\infty} R^{-1} \int_{B_{2R}\setminus B_R} |b^{1/2}\phi|^2\,(\det g)^{1/2}\mathrm{d}x. \tag{1.45d}$$

(iv) *The operators $F^\pm(\lambda)\colon B \to \mathcal{G}$ and $\delta(H-\lambda)\colon B \to \mathcal{E}_\lambda$ are onto.*

We remark that parts of this theorem overlap with [1, 2, 4, 8, 25, 29].

Finally we give an application of our results to channel scattering theory addressed, but treated very differently, in [9]. Suppose $M^{\mathrm{ex}}$ has $N \geqslant 2$

number of ends, i.e. $E^{\mathrm{ex}} = \{x \in M^{\mathrm{ex}} \,|\, r^{\mathrm{ex}}(x) > r_0\}$ has $N \geqslant 2$ components $E_i$, $i = 1, \dots, N$. (Note that this implies that $M \cap E_i$, $i = 1, \dots, N$, are the components of $E = M \cap E^{\mathrm{ex}}$.) Then the Hilbert space $\mathcal{G}$ splits as

$$\mathcal{G} = \mathcal{G}_1 \oplus \cdots \oplus \mathcal{G}_N; \quad \mathcal{G}_i = L^2(S_i),\ S_i = S \cap \overline{E_i},$$

and, accordingly, the scattering matrix $S(\lambda)$ has a matrix representation

$$S(\lambda) = (S_{ij}(\lambda))_{1 \leqslant i,j \leqslant N}, \quad S_{ij}(\lambda) \in \mathcal{B}(\mathcal{G}_j, \mathcal{G}_i).$$

Corollary 1.19. — *Suppose under Condition 1.16 that $E^{\mathrm{ex}}$ has $N$ number of ends. Decomposing as above for any $\lambda \in \mathcal{I}$ the scattering matrix $S(\lambda)$ into components the off-diagonal ones, $S_{ij}(\lambda)$ with $i \neq j$, are one-to-one mappings.*

*Proof.* — If $\xi_- = (\xi_-^1, \dots, \xi_-^N) \in \mathcal{G}$ is given with $\xi_-^j = 0$ for $j \neq 2$ and $\xi_+^1 = 0$ then $\phi = \mathrm{i}F^+(\lambda)^*\xi_-$ obeys that $1_{M\cap E_1}\phi \in B_0^*$. By using a suitable cutoff of the function $r$ (essentially defined by making it vanish in $M \cap E_j$ for $j \geqslant 2$) we then obtain from Theorem 1.4 that $\phi = 0$. For example we could redefine $r$ and $r_0$ of Condition 1.1 as follows (using the notation (1.1)): First replace $r$ by the function $r1_{M\cap E_1}\big(1 - \chi(r/r_0)\big)$ and then replace the parameter $r_0$ by $4r_0$. With these modifications Conditions 1.1–1.3 are fulfilled (with the other parameters there unchanged), and therefore indeed Theorem 1.4 applies. In particular we deduce that $\xi_-^2 = 0$, showing that $\ker S_{12}(\lambda) = \{0\}$. We can argue in the same way for all other off-diagonal components of the scattering matrix. □

We note that Corollary 1.19 may be seen as a stationary solution to conjectures of [9], see [9, Remark 5.7]. We develop the time-dependent version of our results in [19]. In particular this includes a time-dependent version of Corollary 1.19 directly proving conjectures of [9] in a strong form. The proof is based on Corollary 1.19.

For some examples for which our theory applies we refer the reader to [20, Subsection 1.2]. We close this section with a counterexample for which we can not apply our theory. This counterexample means that our theory is in a sense optimal. For a detailed discussion see also Subsection 3.5.

*Example 1.20.* — Consider a subset $M \subseteq \mathbb{R}^2$ equipped with the Euclidean metric and an end consisting of the "interior" of a parabola, say $x^2 < y$, and $r^2 := x^2/2 + y^2 > r_0^2$. We consider only $V = 0$. The orbits of $\omega = \operatorname{grad} r$ are the branches of parabolas $cy^{1/2} = x$ where $-1 < c < 1$, and Condition 1.7 is fulfilled for any $\sigma < 1$, $\tau = 1$ and $\rho = 2$ (and similarly for Condition 1.16 (2)), in particular we can take $\beta_c = 1/2 - \epsilon$ for any small $\epsilon > 0$. However the barely stronger condition (1.32) is not fulfilled and whence the example is not covered by the theory of this paper (in contrast to [20]). Moreover we can in fact show that the generalized eigenfunctions in $\mathcal{N} \cap B^*$ are *not* of WKB-type as in the theorem stated above, see Subsection 3.5. Let us here note, as an indication of this result, that for any $0 \neq \xi \in C_c^\infty(S) \subseteq \mathcal{G}$

$$(H - \lambda)\phi^\pm[\xi] \in \mathcal{H}_{1/2-} \setminus B,$$

which technically prevents us to construct WKB-solutions.

## 2. Separation of variables and free comparison waves

This is a preliminary section for the proofs of our main results. Here we investigate properties of the purely outgoing/incoming spherical waves $\phi^\pm[\xi]$, which was introduced in Subsection 1.3 as free comparison waves. The later parts of the section rely on geometric estimates for the tensor $\ell$. These estimates are rather complicated in the general coordinates, however, they can be much simplified by separation of the radial and the angular variables in the spherical coordinates. Similarly the Hamiltonian $H$ simplifies in the spherical coordinates.

### 2.1. Elementary tensor analysis

Here we fix our convention for the covariant derivatives. We formulate and use them always in local expressions, but for a coordinate-independent representation, see [3, p. 34].

#### 2.1.1. Derivatives of functions and tensors

We shall denote two tensors by the same symbol if they are related to each other through the canonical identification $TM \cong T^*M$, and distinguish them by super- and subscripts. We denote $TM \cong T^*M$ by $T$ for short, and set $T^p = T^{\otimes p}$. The covariant derivative $\nabla$ acts as a linear operator $\Gamma(T^p) \to \Gamma(T^{p+1})$ and is defined for $t \in \Gamma(T^p)$ by

$$(\nabla t)_{ji_1\cdots i_p} = \nabla_j t_{i_1\cdots i_p} = \partial_j t_{i_1\cdots i_p} - \sum_{s=1}^{p} \Gamma^k_{ji_s} t_{i_1\cdots k\cdots i_p}. \tag{2.1}$$

Here $\Gamma^k_{ij} = \frac{1}{2} g^{kl}(\partial_i g_{lj} + \partial_j g_{li} - \partial_l g_{ij})$ is the Christoffel symbol and $t$ is considered as a section of the $p$-fold cotangent bundle, and we adopt the convention that a new subscript is always added to the left as in (2.1). By the identification $TM \cong T^*M$ it suffices to discuss an expression only for the subscripts. In fact, we have the compatibility condition

$$\nabla_i g_{jk} = \partial_i g_{jk} - \Gamma^l_{ij} g_{lk} - \Gamma^l_{ik} g_{jl} = 0, \tag{2.2}$$

and then by (2.1) and (2.2) the covariant derivative can be computed for the tensors of any type. For example, for $t \in \Gamma(T) = \Gamma(T^1)$

$$\begin{aligned} (\nabla t)_j{}^i &= g^{ik}(\nabla t)_{jk} = g^{ik}\big(\partial_j t_k - \Gamma^l_{jk} t_l\big) \\ &= g^{ik}\big(\partial_j g_{kl} t^l - \Gamma^l_{jk} g_{lm} t^m\big) = \partial_j t^i + \Gamma^i_{jk} t^k, \end{aligned} \tag{2.3}$$

and this extends to the general case with ease. The covariant derivative acts as a derivation with respect to tensor product, i.e. for $t \in \Gamma(T^p)$ and $u \in \Gamma(T^q)$

$$(\nabla(t \otimes u))_{ji_1\cdots i_{p+q}} = (\nabla t)_{ji_1\cdots i_p} u_{i_{p+1}\cdots i_{p+q}} + t_{i_1\cdots i_p} (\nabla u)_{ji_{p+1}\cdots i_{p+q}}. \tag{2.4}$$

The formal adjoint $\nabla^* \colon \Gamma(T^{p+1}) \to \Gamma(T^p)$ is defined to satisfy

$$\int \overline{u_{ji_1\cdots i_p}} (\nabla t)^{ji_1\cdots i_p} (\det g)^{1/2}\, \mathrm{d}x = \int \overline{(\nabla^* u)_{i_1\cdots i_p}} t^{i_1\cdots i_p} (\det g)^{1/2}\, \mathrm{d}x$$

for $u \in \Gamma(T^{p+1})$ and $t \in \Gamma(T^p)$ compactly supported in a coordinate neighbourhood. Actually we can write it in a divergence form: For $u \in \Gamma(T^{p+1})$

$$(\nabla^* u)_{i_1\cdots i_p} = -(\operatorname{div} u)_{i_1\cdots i_p} = -(\nabla u)_j{}^j{}_{i_1\cdots i_p} = -g^{jk}(\nabla u)_{jki_1\cdots i_p}.$$

Finally let us give several remarks. It is clear that for any function $f \in \Gamma(T^0) = C^\infty(M)$ the second covariant derivative $\nabla^2 f = \nabla\nabla f$ is symmetric, i.e.

$$(\nabla^2 f)_{ij} = (\nabla^2 f)_{ji} = \partial_i \partial_j f - \Gamma^k_{ij} \partial_k f, \tag{2.5}$$

and we have expressions for the Laplace–Beltrami operator $\Delta$:

$$\Delta f = (\nabla^2 f)_i{}^i = g^{ij}(\nabla^2 f)_{ij} = \operatorname{tr} \nabla^2 f = \operatorname{div} \nabla f.$$

We note that covariant differentiation and contraction are commuting operations. Whence we have, for example, for $t \in \Gamma(T)$ and $u \in \Gamma(T^{p+1})$

$$\begin{aligned} \nabla_k t^j u_{ji_1\cdots i_p} &= (\nabla t)_k{}^j u_{ji_1\cdots i_p} + t^j (\nabla u)_{kji_1\cdots i_p}, \\ \nabla_j (\nabla t)_i{}^i &= (\nabla^2 t)_{ji}{}^i = g^{ik}(\nabla^2 t)_{jik}. \end{aligned} \tag{2.6}$$

#### 2.1.2. Derivatives of mappings

Next let us present a short description of the derivatives of a mapping (not of a function). Let $y\colon M \to N$ be a general mapping from a Riemannian manifold $(M,g)$ to another $(N,h)$. In geometric literatures the $k$-th derivatives $\nabla^k y$, $k=1,2,\dots$, are tensors defined to satisfy the "chain rule". For instance, the derivatives $\nabla y$ and $\nabla^2 y$ are required to satisfy in local coordinates that for any function $f\in C^\infty(N)$

$$\begin{aligned}[\nabla(f(y))]_i &= (\nabla y)^\alpha{}_i(\nabla f)_\alpha(y),\\ [\nabla^2(f(y))]_{ij} &= (\nabla^2 y)^\alpha{}_{ij}(\nabla f)_\alpha(y) + (\nabla y)^\alpha{}_i(\nabla y)^\beta{}_j(\nabla^2 f)_{\alpha\beta}(y).\end{aligned} \tag{2.7}$$

Here we used the Roman and the Greek alphabets to denote the indices of coordinates $x\in M$ and $y=y(x)\in N$, respectively. Although we are not going to verify this, the above definition is indeed well-justified, and we have the following local expressions for such derivatives:

$$(\nabla y)^\alpha{}_i = \partial_i y^\alpha, \quad (\nabla^2 y)^\alpha{}_{ij} = \partial_i\partial_j y^\alpha - \Gamma^k_{ij}\partial_k y^\alpha + \Gamma^\alpha_{\beta\gamma}(\partial_i y^\beta)(\partial_j y^\gamma). \tag{2.8}$$

Note that we adopted the same convention on the Roman and Greek indices as above: In particular, $\Gamma^k_{ij}$ and $\Gamma^\alpha_{\beta\gamma}$ denote the Christoffel symbols for $(M,g)$ and $(N,g)$, respectively. As for (2.8), we refer e.g. to [6, Section 3].

### 2.2. Separation of radial and angular variables

Using spherical coordinates allows us to decompose various quantities into radial and angular parts. It is clear from (1.27) that we naturally have the identification

$$L^2(E) \cong L^2([r_0,\infty)_r;\mathcal{G}_r), \quad \langle\psi,\phi\rangle_{L^2(E)} = \int_{r_0}^\infty \langle\psi,\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r.$$

Such a decomposition holds also for the Riemannian metric, and hence for the Laplace–Beltrami operator.

Lemma 2.1. — *Suppose Condition 1.1. Then in the spherical coordinates $(r,\sigma)=(r,\sigma^2,\dots,\sigma^d)$ in $E$ one has*

$$g^{ij}(\partial_i r)(\partial_j r) = |\mathrm{d}r|^2, \quad g^{ij}(\partial_i r)(\partial_j\sigma^\alpha) = 0, \tag{2.9}$$

*or*

$$g = |\mathrm{d}r|^{-2}\,\mathrm{d}r\otimes\mathrm{d}r + g_{\alpha\beta}\,\mathrm{d}\sigma^\alpha\otimes\mathrm{d}\sigma^\beta,$$

*where the Greek indices run over* $2, \dots, d$*. In particular, by the definition* (1.4)*, the tensor* $\ell$ *coincides with the spherical part of* $g$*:*

$$\ell = g_{\alpha\beta}\, \mathrm{d}\sigma^\alpha \otimes \mathrm{d}\sigma^\beta \quad \text{on } E,$$

*and the operator* $L$ *can be identified with a direct sum:*

$$L \cong \int_{r_0}^{\infty} \bigoplus L_r \,\mathrm{d}r \quad \text{as quadratic forms on } C_{\mathrm{c}}^\infty(E), \tag{2.10}$$

*where* $L_r$ *is the Laplace–Beltrami operator on* $S_r$ *with respect to the induced metric* $g_r := \iota_r^* g$ *and the (non-Riemannian) density* $\mathrm{d}\widetilde{\mathcal{A}}_r$*, i.e.,*

$$L_r = p_\alpha^* g_r^{\alpha\beta} p_\beta; \quad p_\alpha^* = |\mathrm{d}r|(\det g_r)^{-1/2} p_\alpha |\mathrm{d}r|^{-1}(\det g_r)^{1/2}. \tag{2.11}$$

*Proof. —* The first identity of (2.9) is clear by definition, and hence we prove the second. By differentiating the identity $\sigma^\alpha(\widetilde{y}(t,x)) = \sigma^\alpha(x)$ with respect to $t$ we obtain

$$(\partial_t \widetilde{y}^i(t,x))(\partial_i \sigma^\alpha)(\widetilde{y}(t,x)) = 0,$$

which combined with the flow equation $\partial_t \widetilde{y}^i(t,x) = \widetilde{\omega}^i(\widetilde{y}(t,x))$ implies $(\nabla r)^i(\partial_i \sigma^\alpha) = 0$, which is nothing but the second identity of (2.9).

The rest of the assertions are clear. □

Let us comment on the operator $L_r$ given by the expression (2.11). Denote the spherical part of the derivative $p$ by $p'$, or $p' = -\mathrm{i}\nabla'$, cf. (1.39). The operator $p'$ is well-defined on $C^1(S_r)$ as well as on $C^1(M)$, and we do not distinguish them. It is clear from (2.11) that for any $\xi, \zeta \in C_{\mathrm{c}}^\infty(S_r)$

$$\langle \zeta, L_r \xi\rangle_{\mathcal{G}_r} = \int_{S_r} g_r^{ij}\,\overline{(p_i\zeta)}(p_j\xi)\,\mathrm{d}\widetilde{\mathcal{A}}_r = \langle p'\zeta, p'\xi\rangle_{\mathcal{G}_r}.$$

We can at this point use local coordinates of $S$ to define and implement the integration, since in any case clearly the radial derivative $\partial_r$ does not enter. Hence in what follows we may consider $L_r$ as a self-adjoint operator on $\mathcal{G}_r$ defined by the Friedrichs extension of (2.11) from $C_{\mathrm{c}}^\infty(S_r) \subseteq \mathcal{G}_r$. Then by an approximation argument it follows that for any $\phi \in \mathcal{H}^1$ the restriction $\phi_{|S_r} \in \mathcal{D}(L_r^{1/2}) = \mathcal{D}(p')$ for almost every $r \geqslant r_0$. In fact, we have for all $r \geqslant r_0$

$$\int_{r_0}^{r} \|p'\phi_{|S_s}\|_{\mathcal{G}_s}^2 \,\mathrm{d}s = \int_{B_r \setminus B_{r_0}} \ell^{ij}\,\overline{(p_i\phi)}(p_j\phi)(\det g)^{1/2}\,\mathrm{d}x \leqslant \|\phi\|_{\mathcal{H}^1}^2.$$

### 2.3. Decomposition of Hamiltonian

Throughout this subsection we impose Condition 1.7. In Section 3 we will extensively use the notation

$$\kappa = \min\{1+\tau/2, 1+\rho/2, \rho\}$$

and $\widetilde{\eta}$ of (1.2). Let us recall two results, [20, (1.9)] and [20, Lemma 5.1], respectively. (Recall for Lemma 2.3 that $a$ has two values for $z \in I$, say $a = a_\pm$.)

Lemma 2.2. — *As quadratic forms on $\mathcal{H}^1$,*

$$H = \tfrac{1}{2}A\widetilde{\eta}A + \tfrac{1}{2}L + q_1 + q_4; \quad q_4 = q_2 + \tfrac{1}{4}(\nabla^r\widetilde{\eta})(\Delta r).$$

Lemma 2.3. — *Let $I \subseteq \mathcal{I}$ be a compact interval. There exist $C > 0$ such that uniformly in $z \in I \cup I_+$ or $z \in I \cup I_-$*

$$|a| \leqslant C, \quad \big|\pm p^r a + a^2 - 2|\mathrm{d}r|^2(z-q_1)\big| + \big|\ell^{\bullet i}\nabla_i a\big| \leqslant Cr^{-\kappa}.$$

We may consider Lemma 2.2 as a decomposition of $H$ into a sum of radial and angular components (see the discussion at the end of Subsection 2.2). In the next section we shall use similar decompositions:

Lemma 2.4. — *Let $I \subseteq \mathcal{I}$ be a compact interval. Then as a quadratic form on $\bar{\chi}_n\mathcal{H}^1 \subseteq \mathcal{H}^1$ for any large $n$ and uniformly in $z = \lambda \pm \mathrm{i}\Gamma \in I \cup I_\pm$*

$$H - z = \tfrac{1}{2}(A \pm a)\widetilde{\eta}(A \mp a) + \tfrac{1}{2}L + O(r^{-\kappa}), \tag{2.12a}$$

$$H - z = \tfrac{1}{2}b^{1/2}(\widetilde{A} \pm \widetilde{b})b^{-1/2}(A \mp a) + \tfrac{1}{2}L + O(r^{-\kappa})(A \mp a) + O(r^{-\kappa}), \tag{2.12b}$$

$$H - z = \tfrac{1}{2}\tfrac{a}{\sqrt{b}}(\widetilde{A} \pm \widetilde{b})\tfrac{\sqrt{b}}{a}(A \mp a) + \tfrac{1}{2}L + O(r^{-\kappa})(A \mp a) + O(r^{-\kappa}). \tag{2.12c}$$

*Proof.* — Using Lemma 2.2 we can write

$$\begin{aligned} H - z = \tfrac{1}{2}(A \pm a)\widetilde{\eta}(A \mp a) \pm \tfrac{1}{2}(p^r\widetilde{\eta}a) + \tfrac{1}{2}\widetilde{\eta}a^2 \\ + \tfrac{1}{2}L + q_1 + q_2 + \tfrac{1}{4}(\nabla^r\widetilde{\eta})(\Delta r) - z. \end{aligned}$$

Hence the first identity (2.12a) is obtained applying Lemma 2.3 to the remainder written

$$\begin{aligned} \tfrac{1}{2}\widetilde{\eta}\big[\pm(p^r a) + a^2 - 2|\mathrm{d}r|^2(z-q_1)\big] \\ - (1-\eta)(z-q_1) + q_2 + \tfrac{1}{4}(\nabla^r\widetilde{\eta})(\Delta r \mp 2\mathrm{i}a) = O(r^{-\kappa}). \end{aligned}$$

This is valid with or without the factor $\bar{\chi}_n$. However for (2.12b) and (2.12c) we need this factor to avoid dividing by zero. We use (2.12a) and the identities

$$A\widetilde{\eta} = \widetilde{A} - \tfrac{\mathrm{i}}{2}(\nabla^r \widetilde{\eta}), \tag{2.13a}$$

$$(A \pm a)\widetilde{\eta} = b^{1/2}(\widetilde{A} \pm \widetilde{b})b^{-1/2} + O(r^{-\kappa}), \tag{2.13b}$$

$$(A \pm a)\widetilde{\eta} = ab^{-1/2}(\widetilde{A} \pm \widetilde{b})a^{-1}b^{1/2} + O(r^{-\kappa}). \tag{2.13c}$$

□

The identities

$$(A \mp b)b^{1/2} = b^{1/2}(A \mp b - \tfrac{\mathrm{i}}{2}\nabla^r \ln b) = b^{1/2}(A \mp a + O(r^{-\kappa})) \tag{2.14}$$

would provide more symmetric versions (2.12b) and (2.12c), however these are not useful under our conditions.

## 2.4. First order derivatives of spherical waves

We estimate the first order derivatives of the purely outgoing/incoming spherical waves $\phi^\pm[\xi]$, $\xi \in \mathcal{G}$.

The following estimates are almost clear by their definition.

Lemma 2.5. — *Suppose Condition 1.13, and let $I \subseteq \mathcal{I}$ be a compact interval. Then there exists $C \geqslant 0$ such that for any $\lambda \in I$ and $\xi \in \mathcal{G}$ one has that*

$$\|\phi^\pm[\xi]\|_{B^*} \leqslant C\|\xi\|_{\mathcal{G}}, \tag{2.15}$$

*and that for $(r,\sigma) \in E$, $r \geqslant \max_{\lambda\in I} r_\lambda$,*

$$\big|(A \mp a)\phi^\pm[\xi](r,\sigma)\big| \leqslant Cr^{-1-\min\{\tau,\rho\}/2}\big|\phi^\pm[\xi](r,\sigma)\big|. \tag{2.16}$$

*Proof.* — We introduce the restriction to $r$-spheres

$$\phi_r = \phi^\pm[\xi]_{|S_r} \quad \text{for } r \geqslant r_0, \tag{2.17}$$

and estimate recalling the embedding (1.30),

$$\|\xi\|^2_{\mathcal{G}} \geqslant R^{-1}\int_{r_0}^R \|\xi_{|S_r}\|^2_{\mathcal{G}}\,\mathrm{d}r \geqslant (CR)^{-1}\int_{r_0}^R \|\phi_r\|^2_{\mathcal{G}_r}\,\mathrm{d}r.$$

We obtain (2.15) by taking the supremum over all $R \geqslant r_0$.

For $r \geqslant \max_{\lambda\in I} r_\lambda$ we can calculate

$$\begin{aligned}(A \mp a)\phi^\pm[\xi](r,\sigma) &= \Big[-\tfrac{1}{2}(p^r b)/b \pm |\mathrm{d}r|^2\widetilde{b} + (p^r|\mathrm{d}r|^2)/|\mathrm{d}r|^2 \mp a\Big]\phi^\pm[\xi](r,\sigma)\\ &= \tfrac{1}{4}\Big[(p^r q_{12})/(z-q_1) + 3(p^r|\mathrm{d}r|^2)/|\mathrm{d}r|^2\Big]\phi^\pm[\xi](r,\sigma),\end{aligned}$$

and this implies (2.16). □

Next we consider the spherical derivatives. Their estimates depend on a "decay rate" of the spherical part $\ell$ of $g$. To be precise, in general we can not directly compare two tensors on different base points, but we are going to compare the tensor $\ell(\widetilde{y}(t,x))$ and the *push-forward* $\ell_*(t,x)$ of $\ell(x)$ under the map $\widetilde{y}(t,\cdot)$, defined by

$$\ell_*(t,x) = \Bigl(\ell^{ij}(x)[\partial_i\widetilde{y}^\alpha(t,x)][\partial_j\widetilde{y}^\beta(t,x)]\Bigr)_{\alpha,\beta}.$$

Here the Roman and the Greek indices are used for quantities concerning $x$ and $\widetilde{y}=\widetilde{y}(t,x)$, respectively, differently from those in Lemma 2.1. Let us first formulate and verify such a comparison in technical geometric terminology, although in the spherical coordinates it actually reduces to a mere matrix inequality.

Let us introduce a "backwards hitting time" for $x\in E$ by

$$r^{\mathrm{bht}}(x) = \sup\bigl\{s\leqslant r(x)-r_0 \,\big|\, \widetilde{y}(-s,x)\in M\bigr\}.$$

Recall the notation (1.21), $\beta_c = \frac{1}{2}\min\{\sigma,\tau,\rho\}$.

Lemma 2.6. — *Suppose Conditions 1.1 and 1.2 (and $\sigma\in(0,\sigma')$). Then for all $x\in E$ and $t\in(-r^{\mathrm{bht}}(x),0]$*

$$\ell_*(t,x)\leqslant(d-1)\bigl[(r(x)+t)/r(x)\bigr]^{\sigma'}\ell(\widetilde{y}(t,x)) \tag{2.18}$$

*as quadratic forms on the fibers of the cotangent bundle. In spherical coordinates the estimate (2.18) reads: For any $r>s\geqslant r_0$ and $\sigma\in S_s\subseteq S$*

$$\ell(r,\sigma)\leqslant(d-1)(s/r)^{\sigma'}\ell(s,\sigma). \tag{2.19}$$

*Suppose Condition 1.7. Then for any compact interval $I\subseteq\mathcal{I}$ there exists $C>0$ such that for all $\lambda\in I$ and $(r,\sigma)\in E$ in the spherical coordinates*

$$\int_{r-r^{\mathrm{bht}}(r,\sigma)}^{r}\bigl|p'\widetilde{b}(s,\sigma)\bigr|_{g_r}\,\mathrm{d}s\leqslant Cr^{-\beta_c}. \tag{2.20}$$

*Proof.* — To prove the inequality (2.18) let us consider the trace

$$F(t)=g_{\alpha\beta}(\widetilde{y}(t,x))\ell_*^{\alpha\beta}(t,x)=g_{\alpha\beta}(\widetilde{y}(t,x))\ell^{ij}(x)[\partial_i\widetilde{y}^\alpha(t,x)][\partial_j\widetilde{y}^\beta(t,x)],$$

and compute its derivative in $t$. Differentiate the expression

$$(g^*)_{ij}(t,x):=g_{\alpha\beta}(\widetilde{y}(t,x))[\partial_i\widetilde{y}^\alpha(t,x)][\partial_j\widetilde{y}^\beta(t,x)]$$

and use the compatibility condition (2.2) and the flow equation $\partial_t\widetilde{y}^i=\widetilde{\omega}^i$, and then we have

$$\begin{aligned}\tfrac{\partial}{\partial t}(g^*)_{ij} &= [\Gamma^\delta_{\gamma\alpha}g_{\delta\beta}+\Gamma^\delta_{\gamma\beta}g_{\alpha\delta}]\widetilde{\omega}^\gamma(\partial_i\widetilde{y}^\alpha)(\partial_j\widetilde{y}^\beta)\\ &\qquad+g_{\alpha\beta}(\partial_\gamma\widetilde{\omega}^\alpha)(\partial_i\widetilde{y}^\gamma)(\partial_j\widetilde{y}^\beta)+g_{\alpha\beta}(\partial_\gamma\widetilde{\omega}^\beta)(\partial_i\widetilde{y}^\alpha)(\partial_j\widetilde{y}^\gamma)\\ &=2(\nabla\widetilde{\omega})_{\alpha\beta}(\partial_i\widetilde{y}^\alpha)(\partial_j\widetilde{y}^\beta),\end{aligned} \tag{2.21}$$

which yields

$$F'(t) = 2\ell^{ij}(x)\bigl(\nabla\widetilde{\omega}(\widetilde{y}(t,x))\bigr)_{\alpha\beta}[\partial_i\widetilde{y}^\alpha(t,x)][\partial_j\widetilde{y}^\beta(t,x)].$$

Next we decompose $\nabla\widetilde{\omega} = |\mathrm{d}r|^{-2}\nabla^2 r + (\mathrm{d}|\mathrm{d}r|^{-2})\otimes \mathrm{d}r$ and substitute it into the above formula. The second term does not contribute, which is verified easily in the spherical coordinates. Whence using (1.7b) we obtain

$$F'(t) \geqslant \sigma'(r(x)+t)^{-1}F(t).$$

This implies that for $t\in(-r^{\mathrm{bht}}(x),0]$

$$F(0) \geqslant \bigl[r(x)/(r(x)+t)\bigr]^{\sigma'}F(t),$$

or that

$$\ell_*(t,x) \leqslant (d-1)\bigl[(r(x)+t)/r(x)\bigr]^{\sigma'}g(\widetilde{y}(t,x)).$$

If we write the last inequality in the spherical coordinates, then there does not appear radial components on the left-hand side, so that we can remove radial components also from the right-hand side. Thus the inequality (2.18) follows.

Now for (2.20) we use the spherical coordinates and (2.19) estimating

$$\begin{aligned}\int_{r-r^{\mathrm{bht}}(r,\sigma)}^{r} &\bigl|p'\widetilde{b}(s,\sigma)\bigr|_{g_r}\,\mathrm{d}s\\ &\leqslant C_1\int_{r-r^{\mathrm{bht}}(r,\sigma)}^{r}(s/r)^{\sigma'/2}s^{-1-\min\{\tau,\rho\}/2}\,\mathrm{d}s \leqslant C_2 r^{-\beta_c}. \qquad\square\end{aligned}$$

We apply Lemma 2.6 to estimates of the spherical waves $\phi^\pm[\xi]$. Recall the abbreviated notation $\phi_r$ for the restriction of $\phi^\pm[\xi]$ to $r$-spheres (2.17).

Corollary 2.7. — *Suppose Condition 1.13, and let $I\subseteq\mathcal{I}$ be a compact interval. There exists $C\geqslant 0$ such that for any $\lambda\in I$, $r\geqslant s\geqslant \max_{\lambda\in I} r_\lambda$ and $\xi\in\mathcal{G}$ with $\widetilde{y}(s-r_0,\operatorname{supp}\xi)\subseteq S_s$, the functions $\phi_s\in\mathcal{G}_s$, $\phi_r\in\mathcal{G}_r$ and*

$$\|\phi_r\|_{\mathcal{G}_r} \leqslant C\|\phi_s\|_{\mathcal{G}_s}. \tag{2.22a}$$

*If in addition $\xi\in C^1_{\mathrm{c}}(S)$ (so that $\phi_s\in C^1_{\mathrm{c}}(S_s)$) then*

$$\|p'\phi_r\|_{\mathcal{G}_r} \leqslant C\Bigl(r^{-\beta_c}\|\phi_s\|_{\mathcal{G}_s} + (s/r)^{\sigma/2}\|p'\phi_s\|_{\mathcal{G}_s}\Bigr). \tag{2.22b}$$

*Proof.* — Using the expression (1.43) and the supported property of $\xi$, we can write

$$\phi_r(\sigma) = B(s,r,\sigma)\mathrm{e}^{Y(s,r,\sigma)}\phi_s(\sigma) \tag{2.23}$$

with

$$B(s,r,\sigma)=\big[b(s,\sigma)/b(r,\sigma)\big]^{1/2},\quad Y(s,r,\sigma)=\int_s^r\Big(\pm\mathrm{i}\widetilde{b}-\tfrac12\operatorname{div}\widetilde{\omega}\Big)(t,\sigma)\,\mathrm{d}t.$$

Then (2.22a) is a direct consequence of it.

For the latter assertion we can differentiate as

$$p'\phi_r=\big[p'B(s,r,\cdot)\big]\mathrm{e}^{Y(s,r,\cdot)}\phi_s+\big[p'Y(s,r,\cdot)\big]\phi_r+B(s,r,\cdot)\mathrm{e}^{Y(s,r,\cdot)}p'\phi_s.$$

By (2.19) the contributions from the first and the third terms on the right-hand side above satisfy the desired estimate. As for the second term we use again (2.19) proceeding as in the proof of (2.20), whence estimating as

$$\begin{aligned}(2.24)\quad &\ell^{ij}(r,\cdot)\big[p_iY(s,r,\cdot)\big]\big[p_jY(s,r,\cdot)\big]\\ &\quad\leqslant C_1\bigg(\int_s^r(t/r)^{\sigma'/2}\Big|p'\Big(\pm\mathrm{i}\widetilde{b}-\tfrac12\operatorname{div}\widetilde{\omega}\Big)(t,\cdot)\Big|\,\mathrm{d}t\bigg)^2\leqslant C_2r^{-\min\{\sigma,\tau,\rho\}}.\end{aligned}$$

Then by $\operatorname{div}\widetilde{\omega}=|\mathrm{d}r|^{-2}\Delta r+(\nabla^r|\mathrm{d}r|^{-2})$ and (2.22a) we obtain the assertion. □

## 2.5. Second order derivatives of spherical waves

Next, we estimate the second order spherical derivative $L_r\phi_r$ of the restriction of $\phi^\pm[\xi]$ to $r$-spheres. The main result of this subsection is Corollary 2.10.

We are going to make use of the following formula, which reduces the estimate of $L_r\phi_r$ to that of a geometric second derivative of the mapping $\widetilde{y}(t,\cdot)$.

Lemma 2.8. — *For any $f\in C^2(M)$, if one abbreviates $\widetilde{y}=\widetilde{y}(t,\cdot)$, then*

$$(2.25)\qquad L[f(\widetilde{y})]=-\ell^{ij}(\partial_i\widetilde{y}^\alpha)(\partial_j\widetilde{y}^\beta)(\nabla'^2f)_{\alpha\beta}(\widetilde{y})+(L\widetilde{y})^\alpha(\partial_\alpha f)(\widetilde{y}),$$

*where $\nabla'^2f$ is defined in (1.39), and*

$$\begin{aligned}(2.26)\quad L\widetilde{y}^\alpha=&-\ell^{ij}(\nabla^2\widetilde{y})^\alpha{}_{ij}-\widetilde{\eta}\ell^{ij}(\nabla r)^\alpha(\partial_i\widetilde{y}^\beta)(\partial_j\widetilde{y}^\gamma)(\nabla^2r)_{\beta\gamma}\\ &+\Big[(\nabla^r\widetilde{\eta})(\nabla r)^j+\widetilde{\eta}(\Delta r)(\nabla r)^j+\tfrac12\widetilde{\eta}(\nabla|\mathrm{d}r|^2)^j\Big]\partial_j\widetilde{y}^\alpha.\end{aligned}$$

*Here the Roman and the Greek indices are those concerning $x$ and $\widetilde{y}=\widetilde{y}(t,x)$, respectively. In addition, in the spherical coordinates in $E$ the first term on the right-hand side of (2.25) does not contain an $r$-derivative of $f$, and neither does the second term.*

*Proof.* — For any $f \in C^2(M)$ we have, cf. (2.6),

$$L[f(\widetilde{y})] = -\ell^{ij}\big(\nabla^2 f(\widetilde{y})\big)_{ij} - (\nabla\ell)_i{}^{ij}\big(\nabla f(\widetilde{y})\big)_j.$$

Here note that

$$\begin{aligned}(\nabla\ell)_i{}^{ij} &= -\big[\nabla\big(\widetilde{\eta}\,\mathrm{d}r\otimes\mathrm{d}r\big)\big]_i{}^{ij}\\ &= -(\nabla^r\widetilde{\eta})(\nabla r)^j - \widetilde{\eta}(\Delta r)(\nabla r)^j - \tfrac{1}{2}\widetilde{\eta}(\nabla|\mathrm{d}r|^2)^j,\end{aligned}$$

and hence we have

$$\begin{aligned}[Lf(\widetilde{y})] &= -\ell^{ij}\big(\nabla^2 f(\widetilde{y})\big)_{ij}\\ &\quad + \Big[(\nabla^r\widetilde{\eta})(\nabla r)^j + \widetilde{\eta}(\Delta r)(\nabla r)^j + \tfrac{1}{2}\widetilde{\eta}(\nabla|\mathrm{d}r|^2)^j\Big]\big(\nabla f(\widetilde{y})\big)_j.\end{aligned}$$

Now we use the formulas (2.7), (2.8) and (1.39), and then the expression (2.25) follows.

Let us verify the latter assertion. By (1.39) and (1.6) we have in the spherical coordinates on $E$

$$(\nabla'^2 f)_{\alpha\beta} = \partial_\alpha\partial_\beta f - \Gamma^\gamma_{\alpha\beta}\partial_\gamma f - (\partial_r f)(\nabla^2 r)_{\alpha\beta}. \tag{2.27}$$

In the first term on the right-hand side of (2.25) the terms corresponding to $\alpha = r$ or $\beta = r$ vanish, and hence the $r$-derivative of $f$ could appear only from the latter two terms of (2.27). However, they cancel each other out since by (1.6)

$$-\Gamma^r_{\alpha\beta} = (\nabla^2 r)_{\alpha\beta}. \tag{2.28}$$

As for the second term to the right in (2.25) we note that the left-hand side does not contain an $r$-derivative due to (2.11). Whence it does not contain an $r$-derivative neither. Let us give an alternative more direct proof of the fact that $L\widetilde{y}^r = 0$. Recalling (2.8), we can compute

$$\begin{aligned}L\widetilde{y}^r &= -\ell^{ij}\partial_i\partial_j\widetilde{y}^r + \ell^{ij}\Gamma^k_{ij}\partial_k\widetilde{y}^r - \ell^{ij}\Gamma^r_{\beta\gamma}(\partial_i\widetilde{y}^\beta)(\partial_j\widetilde{y}^\gamma)\\ &\quad - \eta\ell^{ij}(\partial_i\widetilde{y}^\beta)(\partial_j\widetilde{y}^\gamma)(\nabla^2 r)_{\beta\gamma}\\ &\quad + \Big[(\nabla^r\widetilde{\eta})(\nabla r)^j + \widetilde{\eta}(\Delta r)(\nabla r)^j + \tfrac{1}{2}\widetilde{\eta}(\nabla|\mathrm{d}r|^2)^j\Big]\partial_j\widetilde{y}^r.\end{aligned}$$

Then the first term above vanishes (since $\widetilde{y}^r(t,r,\sigma) = r+t$). The third and the fourth terms cancel out by (2.28). Similarly, the second and the fifth cancel out due to (2.28). □

Lemma 2.8 motivates us to estimate the tensor $L\widetilde{y}$ defined by (2.26). We remark for any $x \in E$ and $t \in (-r^{\mathrm{bht}}(x), 0]$ the quantity $(L\widetilde{y}^\alpha(t,x))_{\alpha=1,\dots,d}$ defines a tangent vector at $\widetilde{y}(t,x) \in E$, and that it is in fact tangent to the $r$-sphere $S_{\widetilde{y}(t,x)} = S_{r(x)+t}$ since $L\widetilde{y}^r = 0$.

Lemma 2.9. — *Suppose Conditions 1.1 and 1.2 (and $\sigma \in (0,\sigma')$) along with* (1.41a). *Then there exists $C > 0$ such that uniformly in $x \in E$ and $t \in (-r^{\mathrm{bht}}(x), 0]$*

$$|L\widetilde{y}(t,x)| \leqslant C\big[(r(x)+t)^{1/2}/r(x)\big]^{\min\{\sigma,\tau\}}. \tag{2.29}$$

*Proof.* — Fix $x \in E$, and set

$$F(s) = |L\widetilde{y}(s,x)|^2 = g_{\alpha\beta}[L\widetilde{y}^\alpha(s,x)][L\widetilde{y}^\beta(s,x)].$$

To prove (2.29) we shall establish a differential inequality for $F(s)$, cf. the proof of Lemma 2.6. Obviously, we have

$$F'(s) = (\partial_s g_{\alpha\beta})(L\widetilde{y}^\alpha)(L\widetilde{y}^\beta) + 2g_{\alpha\beta}(\partial_s L\widetilde{y}^\alpha)(L\widetilde{y}^\beta). \tag{2.30}$$

In the sequel we use the spherical coordinates. Since $L\widetilde{y}^r = 0$, we may let the indices $\alpha,\beta \neq r$ on the right-hand side above. Then we can compute the first term of (2.30) as

$$\partial_s g_{\alpha\beta} = \widetilde{\omega}^\gamma(\partial_\gamma g_{\alpha\beta}) = \partial_r g_{\alpha\beta} = 2|\mathrm{d}r|^{-2}(\nabla^2 r)_{\alpha\beta}. \tag{2.31}$$

Here we have used

$$\widetilde{\omega}^\gamma = \delta^{\gamma r}, \quad \partial_r g_{\alpha\beta} = -2|\mathrm{d}r|^{-2}\Gamma^r_{\alpha\beta} = 2|\mathrm{d}r|^{-2}(\nabla^2 r)_{\alpha\beta}. \tag{2.32}$$

The latter follows by letting $\gamma = r$ and $\alpha,\beta \neq r$ in

$$g_{\gamma\delta}\Gamma^\delta_{\alpha\beta} = \tfrac{1}{2}(\partial_\alpha g_{\gamma\beta} + \partial_\beta g_{\gamma\alpha} - \partial_\gamma g_{\alpha\beta}). \tag{2.33}$$

On the other hand, as for the second term of (2.30), we use (2.26) and (2.8) amounting to the formula for $\alpha \neq r$

$$L\widetilde{y}^\alpha = \ell^{ij}\Gamma^k_{ij}\partial_k\widetilde{y}^\alpha - \ell^{ij}\Gamma^\alpha_{\beta\gamma}(\partial_i\widetilde{y}^\beta)(\partial_j\widetilde{y}^\gamma) + \tfrac{1}{2}\widetilde{\eta}(\nabla|\mathrm{d}r|^2)^j\partial_j\widetilde{y}^\alpha.$$

Note that the quantities only with Roman indices do not depend on $s$, and so are $\partial_i\widetilde{y}^\alpha$. Whence

$$\partial_s L\widetilde{y}^\alpha = -\ell^{ij}(\partial_r\Gamma^\alpha_{\beta\gamma})(\partial_i\widetilde{y}^\beta)(\partial_j\widetilde{y}^\gamma), \tag{2.34}$$

and it remains to compute $\partial_r\Gamma^\alpha_{\beta\gamma}$. Differentiate (2.33) in $r$ for $\alpha,\beta,\gamma \neq r$, and then use (2.32) to obtain

$$\begin{aligned}
&2|\mathrm{d}r|^{-2}(\nabla^2 r)_{\gamma\delta}\Gamma^\delta_{\alpha\beta} - 2|\mathrm{d}r|^{-2}(\nabla^2 r)_{\gamma r}\Gamma^r_{\alpha\beta} + g_{\gamma\delta}\partial_r\Gamma^\delta_{\alpha\beta}\\
&\qquad = \partial_\alpha|\mathrm{d}r|^{-2}(\nabla^2 r)_{\gamma\beta} + \partial_\beta|\mathrm{d}r|^{-2}(\nabla^2 r)_{\gamma\alpha} - \partial_\gamma|\mathrm{d}r|^{-2}(\nabla^2 r)_{\alpha\beta},
\end{aligned}$$

or

$$\partial_r\Gamma^\delta_{\alpha\beta} = [\nabla|\mathrm{d}r|^{-2}(\nabla^2 r)]_\alpha{}^\delta{}_\beta + [\nabla|\mathrm{d}r|^{-2}(\nabla^2 r)]_\beta{}^\delta{}_\alpha - |\mathrm{d}r|^{-2}(\nabla^3 r)^\delta{}_{\alpha\beta}. \tag{2.35}$$

Now by (2.30), (2.31), (2.34), (2.35), (2.19) and the assumptions we obtain

$$F'(s) \geqslant \sigma'(r(x)+s)^{-1}F(s) - C\big[(r(x)+s)^{-1+\sigma'-\tau/2}/r(x)^{\sigma'}\big]F(s)^{1/2}.$$

Hence, noting that $F(0) = \frac{1}{4}|\mathrm{d}r|^{-4}|\nabla'|\mathrm{d}r|^2|^2$, we obtain (2.29) by Gronwall's inequality. □

Corollary 2.10. — *Suppose Condition 1.13 and Condition 1.16 (2). Let $I \subseteq \mathcal{I}$ be a compact interval, and fix $\delta \in (0, 2\beta_c)$. Then there exists $C > 0$ such that for any $\lambda \in I$, $r \geqslant s \geqslant \max_{\lambda\in I} r_\lambda$ and $\xi \in C^2_{\mathrm{c}}(S) \subseteq \mathcal{G}$ with $\widetilde{y}(s - r_0, \operatorname{supp}\xi) \subseteq S_s$*

$$\begin{aligned}\|L_r\phi_r\|_{\mathcal{G}_r} \leqslant C\Big((1/r)^\delta\|\phi_s\|_{\mathcal{G}_s} + (s^{1/2}/r)^\delta\|\nabla'\phi_s\|_{\mathcal{G}_s} \\ + (s/r)^\delta\|\ell^{\bullet i}(s,\cdot)\ell^{\bullet j}(s,\cdot)(\nabla'^2\phi_s)_{ij}\|_{\mathcal{G}_s}\Big).\end{aligned}\tag{2.36}$$

*Proof.* — Using the expression (2.23) we can write

$$\begin{aligned}L_r\phi_r = {} & \big[L_rB(s,r,\cdot)\big]\mathrm{e}^{Y(s,r,\cdot)}\phi_s + \big[L_rY(s,r,\cdot)\big]\phi_r \\ & + \ell^{ij}(r,\cdot)\big[p_iY(s,r,\cdot)\big]\big[p_jY(s,r,\cdot)\big]\phi_r + B(s,r,\cdot)\mathrm{e}^{Y(s,r,\cdot)}L_r\phi_s \\ & + 2\ell^{ij}(r,\cdot)\big[p_iB(s,r,\cdot)\big]\big[p_iY(s,r,\cdot)\big]\mathrm{e}^{Y(s,r,\cdot)}\phi_s \\ & + 2\ell^{ij}(r,\cdot)B(s,r,\cdot)\big[p_iY(s,r,\cdot)\big]\mathrm{e}^{Y(s,r,\cdot)}p_j\phi_s \\ & + 2\ell^{ij}(r,\cdot)\big[p_iB(s,r,\cdot)\big]\mathrm{e}^{Y(s,r,\cdot)}p_j\phi_s.\end{aligned}\tag{2.37}$$

The third term of (2.37) satisfies the desired estimate due to (2.24) and (2.22a). The sixth term of (2.37) can be treated using the Cauchy–Schwarz inequality, (2.24) and (2.22b). By the proof of Corollary 2.7

$$\ell^{ij}(r,\cdot)\big[p_iB(s,r,\cdot)\big]\big[p_iB(s,r,\cdot)\big] \leqslant C_3/r^\delta.$$

Then, using the Cauchy–Schwarz inequality, the fifth and seventh terms of (2.37) satisfy the desired estimate.

Next, we consider the second term of (2.37). We can compute by (2.10) and Lemma 2.8 that

$$\begin{aligned}L_rY(s,r,\cdot) = {} & -\ell^{\alpha\beta}(r,\cdot)\int_s^r\Big[\nabla'^2\big(\pm\mathrm{i}\widetilde{b} - \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\big)\Big]_{\alpha\beta}(t,\sigma)\,\mathrm{d}t \\ & + \int_s^r(L\widetilde{y})^\alpha(t-r,r,\sigma)\Big[\nabla'\big(\pm\mathrm{i}\widetilde{b} - \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\big)\Big]_\alpha(t,\sigma)\,\mathrm{d}t.\end{aligned}$$

Then by Condition 1.16 (2), (1.42), (2.19) and Lemma 2.9 we obtain

$$\big|L_rY(s,r,\cdot)\big| \leqslant C_4/r^\delta.$$

This and (2.22a) implies that the second term of (2.37) fits with (2.36). The remaining first and fourth terms of (2.37) are treated similarly; we omit the details of proof. □

## 3. Distorted Fourier transform and stationary scattering theory

In this section we impose Condition 1.13. The first problem is to verify the existence of the limit (1.36) which needs preparation. We state various preliminary results. Of course we need to show that $\xi(r) \in \mathcal{G}$ for all large $r$ before taking the limit, and this is in fact doable for all $\psi \in B$. More generally the following four results are valid with $\phi = R(\lambda \pm \mathrm{i}0)\psi$ for any $\lambda \in \mathcal{I}$ and $\psi \in B$.

LEMMA 3.1. — *For all $\psi \in B$ and $r \geqslant r_0$ the quantity $\xi(r) \in \mathcal{G}$.*

*Proof.* — Introduce $\xi \in C_\mathrm{c}^\infty(S_r)$, $0 \leqslant \xi \leqslant 1$ and look at the push-forward given by $\xi_{r'} = \xi(\widetilde{y}(r-r',\cdot)) \in C_\mathrm{c}^\infty(S_{r'})$, $r' \geqslant r \geqslant r_0$.

Note that the $\mathcal{G}_r$-valued function

$$u(r') := \mathrm{e}^{\mathrm{i}(r'-r)\tilde{A}}\{\xi_{r'}[\sqrt{b}\phi]_{|S_{r'}}\};\ r' \in [r,\infty),$$

is a well-defined absolutely continuous function. In particular by the fundamental theorem of calculus

$$u(r) = \int_r^{r+1} u(s)\mathrm{d}s - \int_r^{r+1}\int_r^s \tfrac{\mathrm{d}}{\mathrm{d}r'}u(r')\mathrm{d}r'\mathrm{d}s,$$

yielding upon computing the derivative

$$\tfrac{\mathrm{d}}{\mathrm{d}r'}u(r') = \mathrm{e}^{\mathrm{i}(r'-r)\tilde{A}}\{\xi_{r'}[\mathrm{i}\widetilde{A}\sqrt{b}\phi]_{|S_{r'}}\},$$

taking the norm inside and using the Cauchy–Schwarz inequality the bound

$$\|\xi[\sqrt{b}\phi]_{|S_r}\|_{\mathcal{G}_r} \leqslant \|1_{B_{r+1}}\sqrt{b}\phi\| + 3^{-1/2}\|1_{B_{r+1}}\widetilde{A}\sqrt{b}\phi\|. \tag{3.1}$$

By taking $\xi \nearrow 1$ we obtain a concrete bound of the trace $[\sqrt{b}\phi]_{|S_r} \in \mathcal{G}_r$. $\square$

In the above proof we only used the property that $\check{\phi} := \sqrt{b}\phi \in \mathcal{N}$ which follows from the fact that $\phi \in \mathcal{N}$. The latter property suffices for the next result too. Note that for any such $\check{\phi}$ and $r \geqslant r_0$ we may for any $R_\nu > r+1$ approximate $\chi_\nu\check{\phi} \in \mathcal{H}^1$ by a sequence $(\check{\phi}_n) \subseteq C_\mathrm{c}^\infty(M) \subseteq \mathcal{H}^1$. Then it follows from (3.1) that $[\check{\phi}_n]_{|S_r} \to \check{\phi}_{|S_r}$ in $\mathcal{G}_r$ for $n \to \infty$.

LEMMA 3.2. — *The quantity $\xi(\cdot) \in \mathcal{G}$ (possibly considered for an arbitrary $\phi \in \mathcal{N}$) is an absolutely continuous $\mathcal{G}$-valued function on $[r_0,\infty)$.*

*Proof.* — We fix any $r_1 > r_0$ and write for $r \in [r_0, r_1]$

$$\begin{aligned}\xi(r) &= \mathrm{e}^{\mathrm{i}(r-r_0)(\tilde{A}\mp\tilde{b})}\big[\sqrt{b}R(\lambda \pm \mathrm{i}0)\psi\big]_{|S_r}\\ &= \mathrm{e}^{\mathrm{i}(r_1-r_0)(\tilde{A}\mp\tilde{b})}\mathrm{e}^{\mathrm{i}(r-r_1)(\tilde{A}\mp\tilde{b})}\big[\sqrt{b}\phi\big]_{|S_r}.\end{aligned}$$

It suffices to show that the $\mathcal{G}_{r_1}$-valued function

$$[r_0, r_1] \ni r \to v(r) = \mathrm{e}^{\mathrm{i}(r-r_1)(\tilde{A}\mp\tilde{b})}\big[\sqrt{b}\phi\big]_{|S_r}$$

is absolutely continuous. Formally

$$v'(r) = \mathrm{e}^{\mathrm{i}(r-r_1)(\tilde{A}\mp\tilde{b})}\big[\mathrm{i}(\widetilde{A}\mp\widetilde{b})\sqrt{b}\phi\big]_{|S_r}, \tag{3.2}$$

i.e. $v(r) = v(r_1) - \int_r^{r_1} v'(s)\,\mathrm{d}s$ with $v'(s)$ given by this formula. If we replace $\sqrt{b}\phi =: \check{\phi} \in \mathcal{N}$ by an approximating sequence $(\check{\phi}_n) \subseteq C_\mathrm{c}^\infty(M)$ as in the remark preceding the lemma (used with $r = r_1$) indeed (3.2) holds true for all $n$. Therefore (3.2) also holds in the limit $n \to \infty$. □

The above proof gives the following formula for the derivative (omitting "ex"):

$$\xi'(r) = \tfrac{\mathrm{d}}{\mathrm{d}r}\xi(r) \tag{3.3}$$

$$= \exp\biggl(\int_{r_0}^{r}\Bigl(\mp\mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\Bigr)(s,\cdot)\,\mathrm{d}s\biggr)[\mathrm{i}(\widetilde{A}\mp\widetilde{b})\sqrt{b}\phi](r,\cdot) \in \mathcal{G}. \tag{3.4}$$

Lemma 3.3. — *The following limit exists and is given as*

$$\lim_{R\to\infty} ⨍_R \|[\sqrt{b}\phi]_{|S_r}\|^2_{\mathcal{G}_r}\,\mathrm{d}r = \pm 2\,\mathrm{Im}\langle\psi,\phi\rangle. \tag{3.5}$$

*Proof.* — Consider for convenience only the upper sign.

$$\int_R^{2R} \|[\sqrt{b}\phi]_{|S_r}\|^2_{\mathcal{G}_r}\,\mathrm{d}r = \int_R^{2R}\bigl(\mathrm{Re}\langle\phi,(b-A)\phi\rangle_{\mathcal{G}_r} + \mathrm{Im}\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}\bigr)\,\mathrm{d}r.$$

By Corollaries 1.9 and 1.10

$$⨍_R \mathrm{Re}\langle\phi,(b-A)\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r \to 0.$$

Next we introduce for any $R \geqslant r_0$ a smooth approximation of the characteristic function of the ball $B_R$ of the form (employing (1.1))

$$\chi_{\epsilon,s}(r) = \chi((r-R-s)/\epsilon);\quad \epsilon > 0,\ s \in [0,R].$$

We compute a Green's identity

$$
\begin{aligned}
(3.6)\quad \int_R^{2R} &\operatorname{Im}\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r \\
&= \lim_{\epsilon\to 0}\operatorname{Im}\int_{r_0}^\infty \Big(\chi(r-2R)/\epsilon)-\chi((r-R)/\epsilon\Big)\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r \\
&= -\lim_{\epsilon\to 0}\operatorname{Im}\int_{r_0}^\infty \Big(\int_0^R \chi'_{\epsilon,s}(r)\,\mathrm{d}s\Big)\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r \\
&= -\lim_{\epsilon\to 0}\operatorname{Im}\int_0^R\int_M (\partial_i\chi_{\epsilon,s})\bar{\phi}g^{ij}(\partial_j\phi)(\det g)^{1/2}\,\mathrm{d}x\mathrm{d}s \\
&= -\lim_{\epsilon\to 0}\operatorname{Im}\int_0^R\int_M (\partial_i\chi_{\epsilon,s}\bar{\phi})g^{ij}(\partial_j\phi)(\det g)^{1/2}\,\mathrm{d}x\mathrm{d}s \\
&= -2\lim_{\epsilon\to 0}\int_0^R \operatorname{Im}\langle\chi_{\epsilon,s}\phi,(H-\lambda)\phi\rangle_{\mathcal{H}}\,\mathrm{d}s \\
&= -2\int_0^R \operatorname{Im}\langle 1_{B_{R+s}}\phi,\psi\rangle_{\mathcal{H}}\,\mathrm{d}s.
\end{aligned}
$$

It follows that

$$
⨍_R \operatorname{Im}\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}\,\mathrm{d}r \to 2\operatorname{Im}\langle\psi,\phi\rangle. \qquad \square
$$

We remark that a small modification of the computation (3.6) yields the more familiar Green's identity

$$
\text{(3.7a)}\qquad \operatorname{Im}\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r} = -2\operatorname{Im}\langle 1_{B_r}\phi,\psi\rangle_{\mathcal{H}} \text{ for almost all } r\geqslant r_0,
$$

yielding in particular that $r\to\operatorname{Im}\langle\phi,\nabla_\omega\phi\rangle_{\mathcal{G}_r}$ is absolutely continuous. A similar computation shows that in fact $r\to\langle\check{\phi},\nabla_\omega\phi\rangle_{\mathcal{G}_r}$ is absolutely continuous for any $\check{\phi}\in\mathcal{N}$ as it follows from the resulting Green's identity

$$
\text{(3.7b)}\quad \langle\check{\phi},\nabla_\omega\phi\rangle_{\mathcal{G}_r} = \langle 1_{B_r}p_i\check{\phi},g^{ij}p_j\phi\rangle + 2\big\langle 1_{B_r}\check{\phi},(V-\lambda)\phi-\psi\big\rangle \quad \text{for } r\geqslant r_0.
$$

However, in comparison, we do not know continuity or even local boundedness of the function $r\to\|\nabla_\omega\phi\|_{\mathcal{G}_r}$.

The following technical result will play a major role (see the proofs of Lemmas 3.5–3.7). Recall that the factor $\bar{\chi}_n$ of Lemma 2.4 was introduced to avoid zeros of $a$ and $b$. This is also the role of the factor $\bar{\chi}_n$ below.

Lemma 3.4. — *Let $I\subseteq\mathcal{I}$ be a compact interval. Then we introduce for any large $n$ a function $f_{\check{r}}(r)$, $r\geqslant\check{r}$, depending on any $\check{r}\geqslant r_0$ as well as on any $\lambda\in I$ and $\check{\phi}\in\mathcal{N}$ as follows: Using spherical coordinates we define for*

$r \geqslant \check r$

$$\begin{aligned}
\check e &= \exp\Big(\int_{\check r}^r \pm 2\mathrm{i}\widetilde b(s,\cdot)\,\mathrm{d}s\Big),\\
D\xi(r) &= \exp\Big(\int_{r_0}^r \Big(\mp\mathrm{i}\widetilde b + \tfrac12 \operatorname{div}\widetilde\omega\Big)(s,\cdot)\,\mathrm{d}s\Big)[\sqrt{b}\mathrm{i}(A\mp a)\phi](r,\cdot)\in\mathcal G,\\
\breve\xi(r) &= \exp\Big(\int_{r_0}^r \Big(\mp\mathrm{i}\widetilde b + \tfrac12 \operatorname{div}\widetilde\omega\Big)(s,\cdot)\,\mathrm{d}s\Big)[\sqrt{b}\breve\phi](r,\cdot)\in\mathcal G,\\
f_{\check r}(r) &= \langle \breve\xi(r), (\check e b^{-1}\overline\chi_n)(r,\cdot) D\xi(r)\rangle_{\mathcal G}.
\end{aligned}$$

*Then the function $f_{\check r}(\cdot)$ is absolutely continuous on $[\check r,\infty)$ with derivative*

$$\begin{aligned}
f'_{\check r}(r) &= T_1+\cdots+T_5;\\
T_1 &= \langle (\widetilde A\mp\widetilde b)\sqrt b\breve\phi, \check e b^{-1/2}\overline\chi_n(A\mp a)\phi\rangle_{\mathcal G_r},\\
T_2 &= -2\langle\breve\phi,\check e\overline\chi_n\psi\rangle_{\mathcal G_r},\\
T_3 &= \langle p'\overline{\check e}\breve\phi, \overline\chi_n p'\phi\rangle_{\mathcal G_r},\\
T_4 &= \langle\breve\phi, O(r^{-\kappa})(A\mp a)\phi\rangle_{\mathcal G_r},\\
T_5 &= \langle\breve\phi, O(r^{-\kappa})\phi\rangle_{\mathcal G_r},
\end{aligned}\tag{3.8}$$

*where the bounds of $T_4$ and $T_5$ are uniform in $\lambda\in I$ and $\check r\geqslant r_0$.*

*Proof.* — First we proceed using (2.12b) somewhat unjustified. Compute (formally)

$$\begin{aligned}
f'_{\check r}(r) = \langle (\widetilde A\mp\widetilde b)\sqrt b\breve\phi, \check e b^{-1/2}\overline\chi_n(A\mp a)\phi\rangle_{\mathcal G_r}&\\
-\langle \sqrt b\breve\phi, (\widetilde A\mp\widetilde b)\check e b^{-1/2}\overline\chi_n(A\mp a)\phi\rangle_{\mathcal G_r}&,
\end{aligned}$$

and then substituting for the second term

$$\begin{aligned}
\sqrt b(\widetilde A\mp\widetilde b)\check e b^{-1/2}\overline\chi_n(A\mp a)&\\
&= \check e\sqrt b(\widetilde A\pm\widetilde b)b^{-1/2}\overline\chi_n(A\mp a)\\
&= 2\check e\overline\chi_n\big(H-\lambda-\tfrac12 L\big)+O(r^{-\kappa})(A\mp a)+O(r^{-\kappa}).
\end{aligned}$$

This yields (3.8). Note that $T_3$ is well-defined since in fact $\overline{\check e}\breve\phi\in\mathcal N$ due to (1.33). By the product rule

$$p'\overline{\check e}\breve\phi = \mp\Big(p'\int_{\check r}^r 2\mathrm{i}\widetilde b(s,\cdot)\,\mathrm{d}s\Big)\overline{\check e}\breve\phi + \overline{\check e}p'\breve\phi,\tag{3.9}$$

yielding that $T_3\in L^1_{\mathrm{loc}}$ as a function of $r$. Similarly for the other terms showing explicitly that $f'_{\check r}\in L^1_{\mathrm{loc}}$. The required (pointwise) uniformity property for $T_4$ and $T_5$ is trivial since the $\check r$-dependence is through the oscillatory factor $\check e$ only.

Next we give a rigorous derivation of (3.8) using (2.12b) differently (this argument will not be repeated for the derivation of similar formulas in the proof of Lemmas 3.6 and 3.7). We already argued that all of the above terms make sense and agree with the conclusion of the lemma. We claim that indeed $f_{\check r}$ is absolutely continuous. Note that due to (3.7b) and the fact that $\bar{\check e}\check\phi \in \mathcal{N}$ we have the representation

$$f_{\check r}(r) = \langle 1_{B_r} p_i \bar\chi_n \bar{\check e}\check\phi, g^{ij} p_j \phi\rangle + 2\big\langle 1_{B_r} \bar\chi_n \bar{\check e}\check\phi, (V-\lambda)\phi - \psi\big\rangle + \big\langle \bar\chi_n \bar{\check e}\check\phi, (\tfrac12 \Delta r \mp \mathrm{i}a)\phi\big\rangle_{\mathcal{G}_r}. \tag{3.10}$$

Clearly the first and second terms are absolutely continuous, and by Lemma 3.2 the last one is too.

It is of course doable to compute $f'_{\check r}$ using (3.10). However the result is not immediately consistent with the representation from our informal computation. Instead we shall proceed as follows: It remains to show that for $r_1 > \check r$

$$f_{\check r}(r_1) = \int^{r_1} (T_1 + T_2 + T_3 + T_4 + T_5)\,\mathrm{d}r. \tag{3.11}$$

Let for $r_1 > \check r$

$$\chi_\epsilon(r) = \chi((r - r_1)/\epsilon); \quad \epsilon > 0.$$

We compute on one hand

$$\begin{aligned} &\langle (\widetilde A \pm \widetilde b) b^{1/2} \chi_\epsilon \bar\chi_n \bar{\check e}\check\phi, b^{-1/2}(A \mp a)\phi\rangle \\ &\quad = \langle \chi'_\epsilon \bar\chi_n \bar{\check e}\check\phi, \mathrm{i}(A\mp a)\phi\rangle + \langle \chi_\epsilon (\widetilde A \pm \widetilde b) b^{1/2} \bar\chi_n \bar{\check e}\check\phi, b^{-1/2}(A\mp a)\phi\rangle \\ &\quad = \int \chi'_\epsilon(r) f_{\check r}(r)\,\mathrm{d}r + \langle \chi_\epsilon (\widetilde A \pm \widetilde b) b^{1/2} \bar\chi_n \bar{\check e}\check\phi, b^{-1/2}(A\mp a)\phi\rangle, \end{aligned}$$

and on the other hand using (2.12b) (considering $L$ as a form)

$$\begin{aligned} &\langle (\widetilde A \pm \widetilde b) b^{1/2} \chi_\epsilon \bar\chi_n \bar{\check e}\check\phi, b^{-1/2}(A \mp a)\phi\rangle \\ &\quad = \langle \chi_\epsilon \bar\chi_n \bar{\check e}\check\phi, 2\psi - 2\big(\tfrac12 L + O(r^{-\kappa})(A\mp a) + O(r^{-\kappa})\big)\phi\rangle. \end{aligned}$$

Since $f_{\check r}$ is continuous at $r_1$ we obtain using that the right-hand sides are equal and by letting $\epsilon \to 0$ that

$$\begin{aligned}
&- f_{\check r}(r_1) + \langle 1_{B_{r_1}}(\widetilde{A} \pm \widetilde{b})b^{1/2}\bar\chi_n\bar{\check e}\check\phi, b^{-1/2}(A \mp a)\phi\rangle \\
&\qquad = \langle 1_{B_{r_1}}\bar\chi_n\bar{\check e}\check\phi, 2\psi - 2\big(\tfrac12 L + O(r^{-\kappa})(A \mp a) + O(r^{-\kappa})\big)\phi\rangle \\
&\qquad = 2\langle 1_{B_{r_1}}\check\phi, \check e\bar\chi_n\psi\rangle - \langle 1_{B_{r_1}}p'\bar{\check e}\check\phi, \bar\chi_n p'\phi\rangle \\
&\qquad\qquad - \langle 1_{B_{r_1}}\check\phi, O(r^{-\kappa})(A \mp a)\phi\rangle - \langle 1_{B_{r_1}}\check\phi, O(r^{-\kappa})\phi\rangle.
\end{aligned}$$

Moreover

$$\begin{aligned}
&\langle 1_{B_{r_1}}(\widetilde{A} \pm \widetilde{b})b^{1/2}\bar\chi_n\bar{\check e}\check\phi, b^{-1/2}(A \mp a)\phi\rangle \\
&\quad = \langle 1_{B_{r_1}}(\widetilde{A} \mp \widetilde{b})b^{1/2}\bar\chi_n\check\phi, \check e b^{-1/2}(A \mp a)\phi\rangle \\
&\quad = \langle 1_{B_{r_1}}(\widetilde{A} \mp \widetilde{b})b^{1/2}\check\phi, \check e\bar\chi_n b^{-1/2}(A \mp a)\phi\rangle + \langle 1_{B_{r_1}}\check\phi, O(r^{-\kappa})(A \mp a)\phi\rangle.
\end{aligned}$$

We conclude (3.11). $\square$

### 3.1. Proof of Theorem 1.14 in the easy case

Suppose in addition to Condition 1.13 that Condition 1.16 (1) holds and consider only $\psi \in \mathcal{H}_{3/2+}$. We show that (1.36) exists. For convenience we consider only the upper sign. Note that the estimate of Corollary 1.10 holds for some $\beta > 1$.

We compute, cf. (2.14) and (2.13a),

$$\begin{aligned}
(\widetilde{A} - \widetilde{b})b^{1/2} &= b^{1/2}(\widetilde{A} - \widetilde{b} - \tfrac{\mathrm{i}}{2}\widetilde{\omega}^i\nabla_i \ln b) \\
&= b^{1/2}(\widetilde{A} - \widetilde{a} + O(r^{-2})) \\
&= b^{1/2}\widetilde{\eta}(A - a + O(r^{-2})).
\end{aligned}$$

Using then in turn (3.3) and the Cauchy–Schwarz inequality we obtain for $\beta$ slightly bigger than 1

$$\begin{aligned}
&\int_{r_0}^{\infty} \|\tfrac{\mathrm{d}}{\mathrm{d}r}\xi(r)\|_{\mathcal{G}}\,\mathrm{d}r \\
&\qquad \leqslant C_\beta\bigg(\int_{r_0}^{\infty} r^{2\beta-1}\big\|[\sqrt{b}|\mathrm{d}r|^{-2}\big(A - a + O(r^{-2})\big)\phi]_{|S_r}\big\|^2_{\mathcal{G}_r}\,\mathrm{d}r\bigg)^{1/2} \\
&\qquad \leqslant C_1\|\big(A - a\big)\phi\|_{\beta-1/2} + C_2 \\
&\qquad \leqslant C_3 < \infty.
\end{aligned}$$

Whence the existence of (1.36) follows by integration.

The constant $C_3$ can be chosen locally uniform in $\lambda > \lambda_0$ and arbitrary small if we replace $\int_{r_0}^\infty$ by $\int_R^\infty$, $R > r_0$ big. Whence the limit (1.36) is attained locally uniformly in $(\lambda_0, \infty)$. In addition, since for finite $r$ the map $\lambda \to \xi(r)$ is continuous (cf. (3.1)), we obtain continuity of the map $(\lambda_0, \infty) \ni \lambda \to F^+(\lambda)\psi \in \mathcal{G}$.

Let us also note that due to Lemma 3.3

$$\|F^+(\lambda)\psi\| = 2\,\mathrm{Im}\langle\psi, \phi\rangle$$

follows from the computation

$$\|F^+(\lambda)\psi\|_{\mathcal{G}}^2 = \lim_{R\to\infty} R^{-1}\int_R^{2R} \|\xi(r)\|_{\mathcal{G}}^2\,\mathrm{d}r = \lim_{R\to\infty} \fint_R \|[\sqrt{b}\phi]_{|S_r}\|_{\mathcal{G}_r}^2\,\mathrm{d}r.$$

### 3.2. Proof of Theorem 1.14 in the general case

In this subsection we prove the existence of the limit (1.36) for $\psi \in \mathcal{H}_{1+}$ under Condition 1.13 and then the remaining assertions of Theorem 1.14. We shall consider only the upper sign, since the lower sign can be dealt with in parallel. Throughout the subsection we fix any compact interval $I \subseteq \mathcal{I}$.

For the remaining part of this section let $\psi \in \mathcal{H}_{1+}$ and $\phi = R(\lambda + \mathrm{i}0)\psi$, $\lambda \in I \subseteq \mathcal{I}$.

Lemma 3.5. — *The following limit exists and is given as*

$$\lim_{r\to\infty} \|\xi(r)\|_{\mathcal{G}}^2 = 2\,\mathrm{Im}\langle\psi, \phi\rangle_{\mathcal{H}}. \tag{3.12}$$

*Proof.* — We use Lemma 3.4 taking there $\check{\phi} = \phi$. By evaluating at $r = \check{r}$ and integrating the derivative on the interval $[\check{r}, \infty)$ we then obtain that

$$\lim_{r\to\infty} f_r(r) = 0.$$

At this point note that all of the terms $T_1, \ldots, T_5$ are integrable due to the Cauchy–Schwarz inequality, Corollaries 1.9 and 1.10, (1.33) and (3.9) (note that if $M^{\mathrm{ex}} = M$ the bound (1.33) follows from (2.20)). Next by taking the imaginary part and using (3.7a) we obtain

$$0 = \lim_{r\to\infty} \mathrm{Im}\langle\phi, \nabla_\omega\phi - \mathrm{i}b\phi\rangle_{\mathcal{G}_r} = 2\,\mathrm{Im}\langle\psi, \phi\rangle_{\mathcal{H}} - \lim_{r\to\infty} \|\sqrt{b}\phi(r)\|_{\mathcal{G}_r}^2.$$

Whence indeed

$$\lim_{r\to\infty} \|\xi(r)\|_{\mathcal{G}}^2 = \lim_{r\to\infty} \|\sqrt{b}\phi(r)\|_{\mathcal{G}_r}^2 = 2\,\mathrm{Im}\langle\psi, \phi\rangle_{\mathcal{H}}. \qquad \square$$

*Remark.* — It follows from the above proof that the limit (3.12) is attained uniformly in $\lambda \in I$. This property will be used in the proof of Proposition 1.15.

Next decompose

$$\xi = \xi(r) = \exp\Big(\int_{r_0}^{r} \Big(-\mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\Big)(s,\cdot\,)\,\mathrm{d}s\Big)[\sqrt{b}\phi](r,\cdot\,)$$

as

$$(3.13)\qquad \begin{aligned} \xi &= a^{-1}\xi_+ + a^{-1}\xi_-;\\ \xi_\pm &= 2^{-1}\exp\Big(\int_{r_0}^{r} \Big(-\mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\Big)(s,\cdot\,)\,\mathrm{d}s\Big)[\sqrt{b}(a \pm A)\phi](r,\cdot\,). \end{aligned}$$

At this point the reader is *WARNED* about our use of notation: The quantities $a$ and $\phi$ are considered with the *upper sign only* in this subsection, so for the cases $\pm$ in (3.13) these quantities are the *same* (not to be mixed up with the convention of Lemmas 2.4 and 3.4).

LEMMA 3.6. — *There exists the weak limit*

$$F := \operatorname*{w-\mathcal{G}-lim}_{r\to\infty} \xi(r).$$

*Proof.* — Let $g \in C_{\mathrm{c}}^\infty(S) \subseteq \mathcal{G}$ be given. Due to Lemma 3.5 it suffices to show the existence of

$$C_\pm := \lim_{r\to\infty} \langle g, a^{-1}(r)\xi_\pm(r)\rangle_{\mathcal{G}}.$$

*Step I ($C_- = 0$).* — Writing

$$g = \exp\Big(\int_{r_0}^{r} \tfrac{1}{2}\operatorname{div}\widetilde{\omega}(s,\cdot\,)\,\mathrm{d}s\Big)u(r)$$

we note that $u(r') \in C_{\mathrm{c}}^\infty(S_{r'})$ for $r' \geqslant R_n$ with $n$ large enough. We can write $u(r) = \mathrm{e}^{\mathrm{i}(r'-r)\tilde{A}}u(r') \in C_{\mathrm{c}}^\infty(S_r)$ for $r \geqslant r'$. Let $\overline{\chi}_n = 1 - \chi(r/R_n)$ so that $\overline{\chi}_n u \in \mathcal{N}$ (and such that all zeros of $a$ and $b$ are in $B_{R_n}$). Introduce then for $r \geqslant r_0$

$$\begin{aligned} \check{\phi} &= \exp\Big(\int_{r_0}^{r} \mathrm{i}\widetilde{b}(s,\cdot\,)\,\mathrm{d}s\Big)b^{-1/2}\overline{\chi}_n u(r),\\ \check{\xi} &= \exp\Big(\int_{r_0}^{r} \Big(-\mathrm{i}\widetilde{b} + \tfrac{1}{2}\operatorname{div}\widetilde{\omega}\Big)(s,\cdot\,)\,\mathrm{d}s\Big)[\sqrt{b}\check{\phi}](r,\cdot\,) \in \mathcal{G}. \end{aligned}$$

Note that we can consider $\check{\phi}$ as an element of $\mathcal{N}$ and that $\check{\xi}(r) = g$. Also note that $\xi_- = \mathrm{i}2^{-1}D\xi$ in terms of notation of Lemma 3.4. We introduce as in Lemma 3.4

$$\check{e} = \exp\Big(\int_{\check{r}}^{r} 2\mathrm{i}\widetilde{b}(s,\cdot)\,\mathrm{d}s\Big);\; r \geqslant \check{r} \geqslant r_0.$$

By the proof of Lemma 3.4 with this choice of $\check{\phi}$ (and by using (2.12c) rather than (2.12b)) it follows by evaluating at $r = \check{r} \geqslant 2R_n$ and integrating the derivative

$$\begin{aligned}\tfrac{2}{\mathrm{i}}\tfrac{\mathrm{d}}{\mathrm{d}r}\langle\check{\xi}(r), \check{e}a^{-1}\xi_-(r)\rangle_{\mathcal{G}} &= \langle(\widetilde{A}-\widetilde{b})\sqrt{b}\check{\phi}, \check{e}a^{-1}\sqrt{b}(A-a)\phi\rangle_{\mathcal{G}_r}\\ &\quad - \langle\sqrt{b}\check{\phi}, (\widetilde{A}-\widetilde{b})\check{e}a^{-1}\sqrt{b}(A-a)\phi\rangle_{\mathcal{G}_r}\\ &= -\langle\sqrt{b}\check{\phi}, \check{e}(\widetilde{A}+\widetilde{b})a^{-1}\sqrt{b}(A-a)\phi\rangle_{\mathcal{G}_r}\end{aligned}$$

on the interval $[\check{r},\infty)$ that $C_- = \lim_{r\to\infty}\langle g, a^{-1}\xi_-(r)\rangle_{\mathcal{G}}$ exists and in fact is given by $C_- = 0$. Note that the analogue of the expression $T_1$ of Lemma 3.4 of the derivative vanishes, and that the corresponding terms $T_2,\dots,T_5$ are integrable (uniformly in $\check{r}$). For example it follows from Lemma 2.6 and Corollary 2.7 that

$$\|p'\bar{\check{e}}\tfrac{b}{\bar{a}}\check{\phi}\|_{\mathcal{G}_r} \leqslant C\big((r')^{1/2}\|p'u(r')\|_{\mathcal{G}_{r'}} + \|u(r')\|_{\mathcal{G}_{r'}}\big)r^{-1/2};\; r \geqslant r'. \tag{3.14}$$

(Here $C$ may depend on the support of $g$.) This estimate can be applied with $r' = 2R_n$ (for example) to treat the analogue of the expression $T_3$ of Lemma 3.4.

*Step II ($C_+$ exists).* — Similarly we have

$$2\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}r}\langle\check{\xi}(r), a^{-1}\xi_+(r)\rangle_{\mathcal{G}} = -\langle\sqrt{b}\check{\phi}, (\widetilde{A}-\widetilde{b})a^{-1}\sqrt{b}(A+a)\phi\rangle_{\mathcal{G}_r}$$

To show that $C_+$ exists it suffices to argue that the derivative is integrable (since now there is no factor $\check{e}$ and whence no $\check{r}$-dependence to control). As in Step I there are four terms to consider, say $T_2,\dots,T_5$. More precisely these terms are the contributions from four terms arising by the following computation. We compute using (2.13a), (2.13c) and in the last step (2.12a)

$$\begin{aligned}&\tfrac{a}{\sqrt{b}}(\widetilde{A}-\widetilde{b})\tfrac{\sqrt{b}}{a}(A+a)\\ &= (A-\bar{a})\widetilde{\eta}(A+a) + O(r^{-\kappa})(A-a) + O(r^{-\kappa})\\ &= (A-a)\widetilde{\eta}(A+a) + \widetilde{\eta}4\mathrm{i}(\operatorname{Im} a)a + \big(\widetilde{\eta}2\mathrm{i}(\operatorname{Im} a) + O(r^{-\kappa})\big)(A-a) + O(r^{-\kappa})\\ &= (A+a)\widetilde{\eta}(A-a) + \widetilde{\eta}\big(2(p^r a) + 4\mathrm{i}(\operatorname{Im} a)a\big) + O(r^{-\kappa/2})(A-a) + O(r^{-\kappa})\\ &= (A+a)\widetilde{\eta}(A-a) + O(r^{-\kappa/2})(A-a) + O(r^{-\kappa})\\ &= 2(H-\lambda) - L + O(r^{-\kappa/2})(A-a) + O(r^{-\kappa}).\end{aligned}$$

We can now proceed as in Step I. In particular we can use (3.14) with $\check{e} = 1$ to treat the term $T_3$ which is the analogue of $T_3$ of Lemma 3.4. □

Lemma 3.7. — *The quantity $F$ is the strong limit*

$$F = \mathcal{G}\text{–}\lim_{r\to\infty} \xi(r).$$

*Proof.* — Due to Corollary 1.10 there exists $C_1 > 0$ and a sequence $r_n \to \infty$ such that

$$\|(A-a)\phi\|^2_{\mathcal{G}_{r_n}} + \|p'\phi\|^2_{\mathcal{G}_{r_n}} \leqslant C_1/r_n. \tag{3.15}$$

To show the existence of the strong limit it suffices to show that

$$\lim_{n\to\infty} \langle \xi(r_n), F - \xi(r_n)\rangle_{\mathcal{G}} = 0. \tag{3.16}$$

In fact, (3.16) along with Lemma 3.5 shows that

$$\lim_{r\to\infty} \|\xi(r)\|_{\mathcal{G}} = \|F\|_{\mathcal{G}},$$

which, combined with Lemma 3.6, in turn implies the assertion by [31, Theorem 8, p. 124]. Due to (3.15) it suffices in turn to show that

$$\lim_{n\to\infty}\lim_{m\to\infty} \langle \xi(r_n), (a^{-1}\xi_+)(r_m) - (a^{-1}\xi_+)(r_n)\rangle_{\mathcal{G}} = 0. \tag{3.17}$$

Now we claim that proceeding as in Step II of the proof of Lemma 3.6 (replacing $g \to \xi(r_n)$ and now integrating from $r_n$) indeed (3.17) follows. Note for the analogue term $T_3$ that Lemma 2.6, Corollary 2.7 and a density argument yield

$$\|p'\tfrac{b}{\bar a}\check{\phi}_n\|_{\mathcal{G}_r} \leqslant C_2\big(r_n^{1/2}\|p'\phi\|_{\mathcal{G}_{r_n}} + \|\phi\|_{\mathcal{G}_{r_n}}\big)r^{-1/2};$$
$$r \geqslant r_n, \quad \check{\phi}_n = \mathrm{e}^{\mathrm{i}(r_n - r)(\tilde A - \tilde b)}[\phi]_{S_{r_n}}.$$

In combination with (3.15) we then obtain

$$\|p'\tfrac{b}{\bar a}\check{\phi}_n\|_{\mathcal{G}_r} \leqslant C_3 r^{-1/2},$$

which suffices for integrability and smallness $o(n^0)$ of the integral (due to the Cauchy–Schwarz inequality and Corollary 1.10) essentially showing (3.17). □

*Proof of Theorem 1.14.* — The definition (1.36) is justified by Lemma 3.7. Clearly (1.37) follows from Lemma 3.5.

It remains to show the continuity statement. We shall basically follow the scheme of [4]. Due to (1.37), Corollary 1.9 and the density of $C^\infty_{\mathrm{c}}(S) \subseteq \mathcal{G}$ the continuity of the map $I \ni \lambda \to F^+(\lambda)\psi \in \mathcal{G}$ follows if we can show the continuity of $\langle F^+(\cdot)\psi, g\rangle_{\mathcal{G}}$ for any $\psi \in \mathcal{H}_{1+}$ and $g \in C^\infty_{\mathrm{c}}(S)$. Let us for any such $g$ introduce approximate generalized eigenfunctions $\phi^\pm[g] \in \mathcal{N} \cap B^*$ by specifying in the spherical coordinates

$$\begin{aligned}(3.18)\quad &\phi^\pm[g](r,\sigma)\\ &\quad = \bar\chi_n(r) b(r,\sigma)^{-1/2} \exp\biggl(\int_{r_0}^{r} \Bigl(\pm\mathrm{i}\widetilde{b} - \tfrac12 \operatorname{div}\widetilde{\omega}\Bigr)(s,\sigma)\,\mathrm{d}s\biggr) g(\sigma).\end{aligned}$$

The factor $\bar\chi_n$ is chosen as a cut-off function, possibly depending on $I$ and the support of $g$, to assure the property $\phi^\pm[g] \in \mathcal{N}$ (as in the proof of Lemma 3.6). Note that these vectors are essentially the same as those introduced at (1.43) (this is why we are using the same notation). We shall use the previous notation $\xi$, $\xi_+$ and $\phi$. First calculate (for $m$ sufficiently large)

$$\begin{aligned}2\langle\psi, \chi_m\phi^+[g]\rangle &= -\mathrm{i}\langle (A+\bar a)\phi, \chi_m'\phi^+[g]\rangle + \langle (A+\bar a)\phi, \chi_m \widetilde{\eta}(A-a)\phi^+[g]\rangle\\ &\quad + \int_{r_0}^\infty \chi_m(r)\bigl(\langle p'\phi, p'\phi^+[g]\rangle_{\mathcal{G}_r} + \langle \phi, O(r^{-\kappa})\phi^+[g]\rangle_{\mathcal{G}_r}\bigr)\,\mathrm{d}r,\end{aligned}$$

cf. (2.12a). Note for the first term to the right that

$$\langle (A+\bar a)\phi, \chi_m'\phi^+[g]\rangle = \int_{r_0}^\infty \chi_m'(r)\langle (A+\bar a)\phi, \phi^+[g]\rangle_{\mathcal{G}_r}\,\mathrm{d}r,$$

and

$$\begin{aligned}\langle (A+\bar a)\phi, \phi^+[g]\rangle_{\mathcal{G}_r} &= \langle (\bar a - a)\phi, \phi^+[g]\rangle_{\mathcal{G}_r} + 2\langle (b^{-1}\xi_+)(r), g\rangle_{\mathcal{G}}\\ &= 2\langle (a^{-1}\xi_+)(r), g\rangle_{\mathcal{G}} + 2\langle ((b^{-1}-a^{-1})\xi_+)(r), g\rangle_{\mathcal{G}}\\ &\qquad + 2\mathrm{i}\langle (\operatorname{Im} a)\phi, \phi^+[g]\rangle_{\mathcal{G}_r}.\end{aligned}$$

Note for the second term to the right that

$$\begin{aligned}(3.19)\quad \bigl(A - a + O(r^{-\kappa})\bigr)\phi^+[g] &= \bigl(b^{-1/2}(A-b)b^{1/2} + \tfrac{\mathrm{i}}{2}\nabla_\omega \ln|\mathrm{d}r|^2\bigr)\phi^+[g]\\ &= O(r^{-\infty}),\end{aligned}$$

in fact here the last term vanishes for $r$ large. These considerations allow us to take $m \to \infty$ and we obtain (using that $\langle (a^{-1}\xi_+)(r), g\rangle_{\mathcal{G}} \to \langle F^+(\lambda)\psi, g\rangle_{\mathcal{G}}$ for $r \to \infty$) that

$$\begin{aligned}2\mathrm{i}\langle F^+(\lambda)\psi, g\rangle_{\mathcal{G}} &= 2\langle \psi, \phi^+[g]\rangle - \langle (A+\bar a)\phi, \widetilde{\eta}(A-a)\phi^+[g]\rangle\\ &\quad - \int_{r_0}^\infty \bigl(\langle p'\phi, p'\phi^+[g]\rangle_{\mathcal{G}_r} + \langle \phi, O(r^{-\kappa})\phi^+[g]\rangle_{\mathcal{G}_r}\bigr)\,\mathrm{d}r.\end{aligned}$$

By tracing the $\lambda$-dependence we conclude from this representation that indeed $\langle F^+(\cdot)\psi, g\rangle_{\mathcal{G}}$ is continuous. □

The last formula reads more compactly (although less precisely)

$$\mathrm{i}\langle F^+(\lambda)\psi, g\rangle_{\mathcal{G}} - \langle\psi, \phi^+[g]\rangle = -\langle\phi, (H-\lambda)\phi^+[g]\rangle, \tag{3.20}$$

where the right-hand side is given an interpretation very similar to (2.12a).

### 3.3. Properties of distorted Fourier transform

We first prove Proposition 1.15. Throughout this subsection we continue to consider only the upper sign.

*Proof of Proposition 1.15.* — We first prove (1.38) for $\psi \in B$. It is a direct consequence of Theorem 1.14 that (1.38) holds for $\psi \in \mathcal{H}_{1+}$, and we have already seen that the left-hand side extends continuously in $\psi \in B$. Hence it suffices to show the existence and continuity of the right-hand side in $B$. By Theorem 1.6 these matters reduce to the following estimate, a version of which appears in a similar context in [28]: For any $\psi \in B$

$$\sup_{R>r_0} \left\| \fint_R \xi(r)\,\mathrm{d}r \right\|_{\mathcal{G}} \leqslant C\|\phi\|_{B^*}. \tag{3.21}$$

To show (3.21) we write $\xi(r) = \mathrm{e}^{\mathrm{i}(r-r_0)(\tilde{A}^{\mathrm{ex}}-\tilde{b}^{\mathrm{ex}})}u(r)$ and note that

$$\left\| \fint_R \xi(r)\,\mathrm{d}r \right\|_{\mathcal{G}} \leqslant \fint_R \|u(r)\|_{\mathcal{G}_r}\,\mathrm{d}r.$$

Next for any $R > r_0$ we choose $n \geqslant 0$ such that $R_n \leqslant 2R < R_{n+1}$ and use the Cauchy–Schwarz inequality to obtain

$$\begin{aligned} \left\| \fint_R \xi(r)\,\mathrm{d}r \right\|_{\mathcal{G}}^2 &\leqslant \fint_R \|u(r)\|_{\mathcal{G}_r}^2\,\mathrm{d}r \\ &\leqslant 2\sum_{\nu=0}^{n} (R_\nu/R_n) R_\nu^{-1} \|F_\nu \sqrt{b}\phi\|^2 \\ &\leqslant 4\|\sqrt{b}\phi\|_{B*}^2. \end{aligned}$$

Hence we have shown (3.21) and therefore that (1.38) holds for any $\psi \in B$.

To show that $\fint_R \xi(r)\,\mathrm{d}r \to F^{\pm}(\lambda)\psi$ locally uniformly in $\lambda$ we can assume that $\psi \in \mathcal{H}_{1+}$. Next note that

$$\left\| F^+(\lambda)\psi - \fint_{R_1} \xi(r_1)\,\mathrm{d}r_1 \right\|_{\mathcal{G}}^2 \leqslant \lim_{R_2\to\infty} \fint_{R_1}\fint_{R_2} \|\xi(r_2)-\xi(r_1)\|_{\mathcal{G}}^2\,\mathrm{d}r_2\mathrm{d}r_1.$$

We look at $R_2 > 2R_1$ and write

$$\begin{aligned}\|\xi(r_2)-\xi(r_1)\|_{\mathcal{G}}^2 &= \|\xi(r_2)\|_{\mathcal{G}}^2 - \|\xi(r_1)\|_{\mathcal{G}}^2 - 2\operatorname{Re}\langle\xi(r_1),\xi(r_2)-\xi(r_1)\rangle_{\mathcal{G}}\\ &= \|\xi(r_2)\|_{\mathcal{G}}^2 - \|\xi(r_1)\|_{\mathcal{G}}^2 - 2\operatorname{Re}\langle\xi(r_1),(a^{-1}\xi_-)(r_2)\rangle_{\mathcal{G}}\\ &\quad + 2\operatorname{Re}\langle\xi(r_1),(a^{-1}\xi_-)(r_1)\rangle_{\mathcal{G}}\\ &\quad - 2\operatorname{Re}\langle\xi(r_1),(a^{-1}\xi_+)(r_2)-(a^{-1}\xi_+)(r_1)\rangle_{\mathcal{G}}.\end{aligned}$$

The first term contributes to the $R_2$-limit by $2\operatorname{Im}\langle\psi,\phi\rangle$ due to Lemma 3.3, the second term by $-\fint_{R_1}\|\xi(r_1)\|_{\mathcal{G}}^2\,\mathrm{d}r_1$, the third term by 0 (cf. Corollary 1.10), the fourth term by $\fint_{R_1} 2\operatorname{Re}\langle\xi(r_1),(a^{-1}\xi_-)(r_1)\rangle_{\mathcal{G}}\,\mathrm{d}r_1$ and the last term by $o(R_1^0)$ (by the proof of Lemma 3.7). We readily check that $\fint_{R_1} 2\operatorname{Re}\langle\xi(r_1),(a^{-1}\xi_-)(r_1)\rangle_{\mathcal{G}}\,\mathrm{d}r_1 \to 0$ locally uniformly in $\lambda$, and similarly that $\fint_{R_1}\|\xi(r_1)\|_{\mathcal{G}}^2\,\mathrm{d}r_1 \to 2\operatorname{Im}\langle\psi,\phi\rangle$ and the quantity $o(R_1^0)\to 0$ locally uniformly in $\lambda$. This is by Corollary 1.10 and the proofs of Lemmas 3.3 and 3.7, respectively.

Next, we note that $B\cap\mathcal{H}_{\mathcal{I}}$ is dense in $\mathcal{H}_{\mathcal{I}}$. In fact for any $\psi\in B$ and any $f\in C_{\mathrm{c}}^\infty(\mathcal{I})$ the vector $f(H)\psi\in B$, cf. [12, Theorem 14.1.4]. Due to Stone's formula and (1.37) we have

$$\|F^+\psi\|_{\widetilde{\mathcal{H}}_{\mathcal{I}}} = \|\psi\|_{\mathcal{H}_{\mathcal{I}}};\quad \psi\in B\cap\mathcal{H}_{\mathcal{I}},$$

so the operator $F^+$ extends as an isometry from $B\cap\mathcal{H}_{\mathcal{I}}\subseteq\mathcal{H}_{\mathcal{I}}$ to an isometry $\mathcal{H}_{\mathcal{I}}\to\widetilde{\mathcal{H}}_{\mathcal{I}}$ (denoted also by $F^+$). It remains to show that $F^+H_{\mathcal{I}}\subseteq M_\lambda F^+$ or equivalently that $F^+(H_{\mathcal{I}}-\mathrm{i})^{-1} = (M_\lambda-\mathrm{i})^{-1}F^+$. Whence it suffices to show that

$$F^+(H-\mathrm{i})^{-1}\psi = (M_\lambda-\mathrm{i})^{-1}F^+\psi \quad \text{for any } \psi\in B\cap\mathcal{H}_{\mathcal{I}}.$$

Using the resolvent equations

$$R(\lambda\pm\mathrm{i}0)R(\mathrm{i}) = (\lambda-\mathrm{i})^{-1}R(\lambda\pm\mathrm{i}0) - (\lambda-\mathrm{i})^{-1}R(\mathrm{i}), \tag{3.22}$$

we obtain

$$F^+(\lambda)R(\mathrm{i})\psi = \lim_{R\to\infty}\fint_R(\lambda-\mathrm{i})^{-1}\xi(r)\,\mathrm{d}r = (\lambda-\mathrm{i})^{-1}F^+(\lambda)\psi.$$

Note that due to the Cauchy–Schwarz inequality the second term of (3.22) does not contribute to the limit. ☐

Now we embark on the proof of Theorem 1.17. Theorem 1.17 is clearly a direct consequence of Lemmas 3.8 and 3.9 below.

Note that under the conditions of the lemma below a priori we can write

$$R(\mathrm{i})L\phi^+[g] = \mathrm{w}^\star\text{-}B^*\text{-}\lim_{m\to\infty}R(\mathrm{i})\chi_m L\phi^+[g]\in B^*,$$

meaning that for any $\check{\psi} \in B$

$$\begin{aligned}\langle R(\mathrm{i})L\phi^+[g], \check{\psi}\rangle &= \langle p'\phi^+[g], p'R(-\mathrm{i})\check{\psi}\rangle \\ &= \lim_{m\to\infty}\int \chi_m(r)\langle p'\phi^+[g], p'R(-\mathrm{i})\check{\psi}\rangle_{\mathcal{G}_r}\,\mathrm{d}r.\end{aligned}$$

Lemma 3.8. — *Suppose Condition 1.16. For any $g \in C_\mathrm{c}^\infty(S)$ let $\phi^+[g] \in \mathcal{N}\cap B^*$ be given by* (3.18) *(where $n$ is large, but locally independent of $\lambda > \lambda_0$). Then*

$$R(\mathrm{i})L\phi^+[g] = \mathrm{w}\text{–}B\text{–}\lim_{m\to\infty} R(\mathrm{i})\chi_m L\phi^+[g] \in B,$$

*meaning that the vector $\psi = R(\mathrm{i})L\phi^+[g]$, a priori in $B^*$, actually is in $B$ and that for all $\check{\phi} \in B^*$*

$$\begin{aligned}\langle \psi, \check{\phi}\rangle &= \langle p'\phi^+[g], p'R(-\mathrm{i})\check{\phi}\rangle \\ &= \lim_{m\to\infty}\int \chi_m(r)\langle p'\phi^+[g], p'R(-\mathrm{i})\check{\phi}\rangle_{\mathcal{G}_r}\,\mathrm{d}r.\end{aligned}$$

*In fact*

$$R(\mathrm{i})L\phi^+[g] \in B\cap\mathcal{H}^1. \tag{3.23}$$

*Proof.* — Write with $\check{r} = R_n$ (recall that possibly $n$ depends on the support of $g$)

$$\phi^+ = \bar{\chi}_n(r)b^{-1/2}\mathrm{e}^{\mathrm{i}(\check{r}-r)(\tilde{A}-\tilde{b})}u; \quad u = \mathrm{e}^{\mathrm{i}(r_0-\check{r})(\tilde{A}-\tilde{b})}g \in C_\mathrm{c}^1(S_{\check{r}}).$$

First let us assume Condition 1.16 (1). We decompose

$$R(\mathrm{i})L\phi^+ = (R(\mathrm{i})r^{-s}p')(p'r^s\phi^+); \quad s > 1/2. \tag{3.24}$$

Since the first factor is bounded as $\mathcal{H} \to \mathcal{H}_s\cap\mathcal{H}^1 \subseteq B\cap\mathcal{H}^1$, it suffices to show that the second factor belongs to $\mathcal{H}$ for some $s > 1/2$. We combine Condition 1.16 (1) with Lemma 2.6 and Corollary 2.7 and conclude that indeed $p'r^s\phi^+ \in \mathcal{H}$ for some $s > 1/2$. Of course the conclusion $R(\mathrm{i})L\phi^+ = \mathrm{w}\text{–}B\text{–}\lim_{m\to\infty}(R(\mathrm{i})r^{-s}p')\chi_m(p'r^s\phi^+)$ follows from this argument.

Next, assuming Condition 1.16 (2), we note that $u \in C_\mathrm{c}^2(S_{\check{r}})$ and decompose

$$R(\mathrm{i})L\phi^+ = \big(R(\mathrm{i})r^{-s}\big)\bigg(\int\bigoplus r^sL_r\phi^+\,\mathrm{d}r\bigg); \quad s > 1/2,$$

and proceed by using Corollary 2.10 to bound $L_r\phi^+$. Next we introduce a factor $\chi_m$ as above and conclude similarly. □

Lemma 3.9. — *If for all $g \in C_\mathrm{c}^\infty(S)$ the vector $\phi^+[g]$ of* (3.18) *(depending on $\lambda > \lambda_0$) satisfies* (3.23)*, then $F^+\colon \mathcal{H}_\mathcal{I} \to \widetilde{\mathcal{H}}_\mathcal{I}$ is a unitary diagonalizing transform.*

*Proof.* — We consider for $\lambda \in \mathcal{I}$ the operator $F^+(\lambda)\colon B \to \mathcal{G}$ of Proposition 1.15. From the same result we know that $F^+$ is an isometry.

*Step I.* — First we show that $F^+(\lambda)$ has dense range. This is equivalent to showing that $F^+(\lambda)^* : \mathcal{G} \to B^*$ is injective, and for that we will use the representation (3.20) of $F^+(\lambda)^* g$ for $g \in C_{\mathrm{c}}^\infty(S)$. For the term on the right-hand side for such $g$ we claim the bound

$$(A + a)R(\lambda - \mathrm{i}0)(H - \lambda)\phi^+[g] \in B_0^*. \tag{3.25}$$

To obtain (3.25) we use (3.22), reducing the problem to show that

$$(A + a)\psi_+,\ (A + a)R(\lambda - \mathrm{i}0)\psi_+ \in B_0^*; \quad \psi_+ = R(\mathrm{i})(H - \lambda)\phi^+[g].$$

The interpretation of $\psi_+$ is given as in the proof of Theorem 1.14 which amounts to expanding $(H - \lambda)\phi^+[g]$ into a sum of three terms, cf. (2.12a). Each term is in $B \cap \mathcal{H}^1$, so consequently $\psi_+ \in B \cap \mathcal{H}^1$. Note that at this point we use (3.19) and (3.23). Using that $\psi_+ \in B \cap \mathcal{H}^1$ we deduce (3.25) by Corollary 1.10.

Now using (3.19), (3.20) and (3.25) we obtain

$$g = \mathcal{G}\text{–}\lim_{R\to\infty} \fint_R \mathrm{e}^{\mathrm{i}(r - r_0)(\tilde{A}^{\mathrm{ex}} - \tilde{b}^{\mathrm{ex}})} \left[\tfrac{b^{1/2}\mathrm{i}}{2a}(a + A)F^+(\lambda)^* g\right]_{|S_r} \mathrm{d}r, \tag{3.26}$$

and since

$$(a + A)F^+(\lambda)^* = (\lambda - \mathrm{i})\big\{(a + A)R(\mathrm{i})\big\}F^+(\lambda)^* \in \mathcal{B}(\mathcal{G}, B^*),$$

we conclude (3.26) for all $g \in \mathcal{G}$ by a continuity argument essentially identical with the one given in the first part of the proof of Proposition 1.15. In particular indeed $F^+(\lambda)^* : \mathcal{G} \to B^*$ is injective.

*Step II.* — We prove the unitarity of $F^+\colon \mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$. Since we know $F^+ H_{\mathcal{I}} \subseteq M_\lambda F^+$ from Proposition 1.15 it then follows that $F^+ H_{\mathcal{I}} = M_\lambda F^+$, and the proof is done.

By using Proposition 1.15 (possibly in combination with (3.31)) we obtain that

$$F^+(\lambda)f(H)\psi = f(\lambda)F^+(\lambda)\psi \text{ for all } f \in C_{\mathrm{c}}^\infty(\mathcal{I}) \text{ and } \psi \in B. \tag{3.27}$$

Assuming $g(\,\cdot\,) \in \ker(F^+)^* \subseteq \widetilde{\mathcal{H}}_{\mathcal{I}}$ it suffices to show that $g(\lambda) = 0$ for a.e. $\lambda \in \mathcal{I}$. We shall mimic the proof of [1, Theorem 1.1]. For any $f \in C_{\mathrm{c}}^\infty(\mathcal{I})$ and $\psi \in B$

$$\int_{\mathcal{I}} f(\lambda)\big\langle g(\lambda), F^+(\lambda)\psi\big\rangle_{\mathcal{G}} \,\mathrm{d}\lambda = \big\langle (F^+)^* g(\cdot), f(H)\psi\big\rangle_{\mathcal{H}_{\mathcal{I}}} = 0.$$

Apply this to the elements of a countable and dense subset, say $\{\psi_k\}_{k=1}^\infty \subseteq B$, and we conclude that there exists a set $N \subseteq \mathcal{I}$ of measure 0 such that

$$\left\langle g(\lambda), F^+(\lambda)\psi_k \right\rangle_{\mathcal{G}} = 0 \text{ for all } k \in \mathbb{N} \text{ and } \lambda \in \mathcal{I} \setminus N.$$

Since $\{F^+(\lambda)\psi_k\}_{k=1}^\infty \subseteq \mathcal{G}$ is dense (by Step I) we conclude that $g(\cdot) = 0$. Hence $F^+ \colon \mathcal{H}_{\mathcal{I}} \to \widetilde{\mathcal{H}}_{\mathcal{I}}$ is surjective and therefore unitary. □

*Remarks 3.10.* — We used above the representation in terms of the vectors $\phi^\pm[g] \in \mathcal{N}$ of (3.18) (here stated for both signs)

$$\begin{aligned} &\pm \mathrm{i} F^\pm(\lambda)^* g = \phi^\pm[g] - \psi_\pm - (\lambda - \mathrm{i}) R(\lambda \mp \mathrm{i}0)\psi_\pm; \\ &\qquad\qquad g \in C_{\mathrm{c}}^\infty(S), \quad \psi_\pm = R(\mathrm{i})(H-\lambda)\phi^\pm[g] \in B \cap \mathcal{H}^1. \end{aligned} \tag{3.28a}$$

For comparison we obtain using Corollary 1.11

$$0 = \phi^\pm[g] - \psi_\pm - (\lambda - \mathrm{i}) R(\lambda \pm \mathrm{i}0)\psi_\pm.$$

In particular

$$\phi^\pm[g] - (\lambda - \mathrm{i}) R(\lambda \pm \mathrm{i}0)\psi_\pm \in B_0^*,$$

which leads to

$$g = (\lambda - \mathrm{i}) F^\pm(\lambda)\psi_\pm; \quad g \in C_{\mathrm{c}}^\infty(S), \quad \psi_\pm = R(\mathrm{i})(H-\lambda)\phi^\pm[g]. \tag{3.28b}$$

The formulas (3.28a) and (3.28b) will be used in Section 3.4, however we stress that the vectors of (3.18) are given with a cutoff to make them elements of $\mathcal{N}$. The vectors $\phi^\pm[g]$ given by (1.43) do not necessarily enjoy this property, and in fact the above formulas might not be valid in general when $\phi^\pm[g]$ (with $g \in C_{\mathrm{c}}^\infty(S)$) are given by (1.43).

*Proof of Theorem 1.17.* — The statement is obvious from Proposition 1.15 and Lemmas 3.8 and 3.9. □

### 3.4. Scattering matrix and characterization of generalized eigenfunctions

In this subsection we prove Theorem 1.18. Throughout the subsection we assume Condition 1.16, and we fix $\lambda \in \mathcal{I}$.

We begin with a partial uniqueness result.

Lemma 3.11. — *Suppose $\phi \in \mathcal{E}_\lambda$ and $\xi_\pm \in \mathcal{G}$ satisfy*

$$\phi - \phi^+[\xi_+] + \phi^-[\xi_-] \in B_0^*. \tag{3.29}$$

*Then $\xi_\pm$ are uniquely determined by $\phi$. Moreover*

$$\|\xi_+\|^2_{\mathcal{G}} + \|\xi_-\|^2_{\mathcal{G}} = \lim_{R\to\infty} R^{-1}\int_{B_{2R}\setminus B_R} b|\phi|^2\,(\det g)^{1/2}\mathrm{d}x, \tag{3.30a}$$

$$\|\xi_+\|_{\mathcal{G}} = \|\xi_-\|_{\mathcal{G}}. \tag{3.30b}$$

*Proof.* — The uniqueness statement follows from (3.30a), which in turn is proved as follows:

$$\begin{aligned}
&\lim_{R\to\infty} R^{-1}\int_{B_{2R}\setminus B_R} b|\phi|^2\,(\det g)^{1/2}\mathrm{d}x\\
&= \lim_{R\to\infty} R^{-1}\int_{B_{2R}\setminus B_R} b|\phi^+[\xi_+]-\phi^-[\xi_-]|^2\,(\det g)^{1/2}\mathrm{d}x\\
&= \|\xi_+\|^2_{\mathcal{G}} + \|\xi_-\|^2_{\mathcal{G}} - 2\,\mathrm{Re}\lim_{R\to\infty} \fint_R \left\langle \xi_+, \exp\left(-2\mathrm{i}\int_{r_0}^r \widetilde{b}(s,\cdot)\,\mathrm{d}s\right)\xi_-\right\rangle_{\mathcal{G}} \mathrm{d}r
\end{aligned}$$

The last term vanishes as may be seen by first writing

$$\exp\left(-2\mathrm{i}\int_{r_0}^r \widetilde{b}(s,\cdot)\,\mathrm{d}s\right) = (-2\mathrm{i}\widetilde{b})^{-1}\tfrac{\mathrm{d}}{\mathrm{d}r}\exp\left(-2\mathrm{i}\int_{r_0}^r \widetilde{b}(s,\cdot)\,\mathrm{d}s\right)$$

and then integrate by parts picking up a sum of decaying factors. Note that indeed $\frac{\mathrm{d}}{\mathrm{d}r}\widetilde{b}(r,\cdot) = o(R^0)$ uniformly in the angle variable (so that the Cauchy–Schwarz inequality applies).

As for (3.30b) first note that $A\phi \in B^*$, which comes from the representation $A\phi = (\lambda-\mathrm{i})AR(\mathrm{i})\phi$ and the fact that $AR(\mathrm{i}) \in \mathcal{B}(B^*)$. Then we compute

$$\begin{aligned}
0 &= \lim_{n\to\infty}\langle \mathrm{i}[H,\chi_n]\rangle_\phi\\
&= \lim_{n\to\infty}\langle A\chi_n'\rangle_\phi\\
&= \lim_{n\to\infty}\langle A\phi, \chi_n'(\phi^+[\xi_+]-\phi^-[\xi_-])\rangle\\
&= \lim_{n\to\infty}\langle \phi, \chi_n'(A\phi^+[\xi_+]-A\phi^-[\xi_-])\rangle\\
&= \lim_{n\to\infty}\langle \phi, \chi_n'(b\phi^+[\xi_+]+b\phi^-[\xi_-])\rangle\\
&= \lim_{n\to\infty}\langle \phi^+[\xi_+]-\phi^-[\xi_-], \chi_n' b(\phi^+[\xi_+]+\phi^-[\xi_-])\rangle\\
&= \|\xi_+\|^2_{\mathcal{G}} - \|\xi_-\|^2_{\mathcal{G}},
\end{aligned}$$

where in the last step we integrated by parts as in the proof of (3.30a). □

Next, we construct $\xi_\pm \in \mathcal{G}$ from $\phi \in \mathcal{E}_\lambda$. Note for comparison that $F^\pm(\lambda)^*\xi \in \mathcal{E}_\lambda$ for any $\xi \in \mathcal{G}$ (readily proven by using $F^\pm(\lambda)^* = (\lambda-\mathrm{i})R(\mathrm{i})F^\pm(\lambda)^*$, cf. the proof of Lemma 3.9).

Lemma 3.12. — *For any $\phi \in \mathcal{E}_\lambda$ there exist $\xi_\pm \in \mathcal{G}$ such that* (1.45b) *hold.*

*Proof.* — We use the scheme of proof of [28, Proposition 6.2]. By the definition of $S(\lambda)$ it suffices to show that for any $\phi \in \mathcal{E}_\lambda$ the representation $\phi = \mathrm{i}F^+(\lambda)^*\xi$ for some $\xi \in \mathcal{G}$ holds.

Pick $f \in C_\mathrm{c}^\infty(\mathbb{R})$ with $f(t) = t$ in neighbourhood of $t = \lambda$. Whence $f(H)\phi = \lambda\phi$. We introduce (for a fixed large $m$)

$$\phi_\pm = \tfrac{1}{2b}\bar{\chi}_m(A \pm b)\phi \in B^*, \quad \xi_n = F^+(\lambda)\chi_n\big(f(H) - \lambda\big)\phi_+;\ n \in \mathbb{N}.$$

The sequence $(\xi_n) \subseteq \mathcal{G}$ is bounded. Indeed since $F^+(\lambda)\big(f(H) - \lambda\big) = 0$ (cf. (3.27)) we compute using (3.31) (stated below) and estimate uniformly in $n \in \mathbb{N}$ and in $g \in C_\mathrm{c}^\infty(S)$, $\|g\|_\mathcal{G} = 1$,

$$\begin{aligned} \langle g, \xi_n\rangle_\mathcal{G} &= \mathrm{i}\langle F^+(\lambda)^*g, \big(A\chi_n' + \mathrm{i}|\mathrm{d}r|^2\chi_n''/2\big)f'(H)\phi_+\rangle_{B^*\times B},\\ |\langle g, \xi_n\rangle_\mathcal{G}| &\leqslant C_1|\big(\|AF^+(\lambda)^*g\|_{B^*} + \|F^+(\lambda)^*g\|_{B^*}\big) \leqslant C_2. \end{aligned}$$

Next we choose a weakly convergent subsequence of $(\xi_n)$, cf. [31, Theorem 1, p. 126]. Whence, possibly upon changing notation, $\mathrm{w}\text{–}\lim_{n\to\infty}\xi_n =: \xi \in \mathcal{G}$. For this $\xi$ and with $\breve{f}(t) := (f(t) - \lambda)(t - \lambda)^{-1}$ we compute

$$\begin{aligned} \mathrm{i}F^+(\lambda)^*\xi &= \mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–}\lim}\,\mathrm{i}F^+(\lambda)^*F^+(\lambda)\chi_n\big(f(H) - \lambda\big)\phi_+\\ &= \mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–}\lim}\big(R(\lambda + \mathrm{i}0) - R(\lambda - \mathrm{i}0)\big)\chi_n\big(f(H) - \lambda\big)\phi_+\\ &= \mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–}\lim}\Big(R(\lambda + \mathrm{i}0)\chi_n\big(f(H) - \lambda\big)\phi_+\\ &\qquad\qquad + R(\lambda - \mathrm{i}0)\chi_n\big(f(H) - \lambda\big)(\phi - \phi_+)\Big)\\ &= \mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–}\lim}\Big(\breve{f}(H)\chi_n\phi + R(\lambda + \mathrm{i}0)[\chi_n, f(H)]\phi_+\\ &\qquad\qquad + R(\lambda - \mathrm{i}0)[\chi_n, f(H)](\phi - \phi_+)\Big)\\ &= \breve{f}(H)\phi + \mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–}\lim}\Big(R(\lambda + \mathrm{i}0)[\chi_n, f(H)]\phi_+\\ &\qquad\qquad + R(\lambda - \mathrm{i}0)[\chi_n, f(H)](\phi - \phi_+)\Big). \end{aligned}$$

The first term simplifies as $\breve{f}(H)\phi = \phi$. To compute the last term we represents in a standard fashion (in terms of an almost analytic extension $\widetilde{f}$)

$$f(H) = \int_\mathbb{C} R(z)\mathrm{d}\mu(z);\ \mathrm{d}\mu(z) = -(2\pi\mathrm{i})^{-1}\bar{\partial}\widetilde{f}(z)\mathrm{d}z\mathrm{d}\bar{z}, \tag{3.31}$$

allowing us to compute

$$[\chi_n, f(H)] = -\mathrm{i}\int_\mathbb{C} R(z)\big(A\chi_n' + \mathrm{i}|\mathrm{d}r|^2\chi_n''/2\big)R(z)\mathrm{d}\mu(z).$$

Whence due to Corollary 1.11 (note also that the second term with the factor $\chi_n''$ does not contribute to the limit)

$$\begin{aligned}
&\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, R(\lambda+\mathrm{i}0)[\chi_n, f(H)]\phi_+ \\
&\qquad = -\mathrm{i}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}} \int_{\mathbb{C}} R(z)R(\lambda+\mathrm{i}0)A\chi_n' R(z)\mathrm{d}\mu(z)\phi_+ \\
&\qquad = \mathrm{i}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}} \int_{\mathbb{C}} R(z)R(\lambda+\mathrm{i}0)b\chi_n' R(z)\mathrm{d}\mu(z)\phi_+ \\
&\qquad = \mathrm{i}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}} \int_{\mathbb{C}} R(z)R(\lambda+\mathrm{i}0)R(z)\mathrm{d}\mu(z)b\chi_n'\phi_+ \\
&\qquad = -\tfrac{\mathrm{i}}{2}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, f'(H)R(\lambda+\mathrm{i}0)\chi_n'\bar{\chi}_m(A+b)\phi \\
&\qquad = -\tfrac{\mathrm{i}}{2}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, f'(H)R(\lambda+\mathrm{i}0)(A+b)\chi_n'\phi \\
&\qquad = 0.
\end{aligned}$$

Similarly, using that $\phi-\phi_+=\chi_m\phi-\phi_-$,

$$\begin{aligned}
&\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, R(\lambda-\mathrm{i}0)[\chi_n, f(H)](\phi-\phi_+) \\
&\qquad = -\tfrac{\mathrm{i}}{2}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, f'(H)R(\lambda-\mathrm{i}0)\chi_n'\bar{\chi}_m\big((A-b)\phi\big) \\
&\qquad = -\tfrac{\mathrm{i}}{2}\,\mathrm{w}^\star\text{–}\underset{n\to\infty}{B^*\text{–lim}}\, f'(H)R(\lambda-\mathrm{i}0)(A-b)\chi_n'\phi \\
&\qquad = 0.
\end{aligned}$$

Whence we have shown that $\phi=\mathrm{i}F^+(\lambda)^*\xi$ for the constructed $\xi$. □

Lemma 3.13. — *For all $\psi\in B$ and all $\lambda\in\mathcal{I}$*

$$\sqrt{b}R(\lambda\pm\mathrm{i}0)\psi-1_M\mathrm{e}^{\mathrm{i}(r_0-r)(\tilde{A}^{\mathrm{ex}}\mp\tilde{b}^{\mathrm{ex}})}F^{\pm}(\lambda)\psi\in B_0^*. \tag{3.32}$$

*Proof.* — This is obvious from Lemma 3.7 for $\psi\in\mathcal{H}_{1+}$. The general case is treated by an approximation argument (as in the proof of [28, Corollary 5.5]). □

A construction of $\phi\in\mathcal{E}_\lambda$ from $\xi_\pm\in\mathcal{G}$ may intuitively seem most feasible when $\xi_\pm$ satisfies the Dirichlet boundary condition. We first give such construction for $\xi_\pm\in C_\mathrm{c}^\infty(S)$ and shortly extend it allowing any $\xi_\pm\in\mathcal{G}$.

Lemma 3.14. — *For any $\xi_-\in C_\mathrm{c}^\infty(S)$ introduce $\phi^-[\xi_-]\in\mathcal{N}\cap B^*$ by* (3.18) *(rather than by* (1.43)*) and define then $\phi\in\mathcal{E}_\lambda$ and $\xi_+\in\mathcal{G}$ by*

$$\begin{aligned}
&\phi=\psi_-+(\lambda-\mathrm{i})R(\lambda+\mathrm{i}0)\psi_--\phi^-[\xi_-],\\
&\xi_+=(\lambda-\mathrm{i})F^+(\lambda)\psi_-;\quad \psi_-=R(\mathrm{i})(H-\lambda)\phi^-[\xi_-].
\end{aligned} \tag{3.33}$$

*Then* (1.45a) *and* (1.45b) *hold for $\{\xi_-,\xi_+,\phi\}$.*

*Proof.* — Note that $\psi_- \in B$, cf. the proof of Lemma 3.9, and that (1.45a) holds with the approximate eigenfunctions of (1.43) if the estimate is valid for those defined by (3.18) (obviously the difference is in $B_0^*$). We combine (3.28a) and (3.28b) (with the lower sign only) and Lemma 3.13 (with the upper sign). □

Similarly we can first specify $\xi_+ \in C_c^\infty(S)$ (the proof is similar).

Lemma 3.15. — *For any $\xi_+ \in C_c^\infty(S)$ introduce $\phi^+[\xi_+] \in \mathcal{N} \cap B^*$ by* (3.18) *and define $\phi \in \mathcal{E}_\lambda$ and $\xi_- \in \mathcal{G}$ by*

$$\begin{aligned} \phi &= \phi^+[\xi_+] - \psi_+ - (\lambda - \mathrm{i})R(\lambda - \mathrm{i}0)\psi_+, \\ \xi_- &= (\lambda - \mathrm{i})F^-(\lambda)\psi_+; \quad \psi_+ = R(\mathrm{i})(H-\lambda)\phi^+[\xi_+]. \end{aligned} \tag{3.34}$$

*Then* (1.45a) *and* (1.45b) *hold for* $\{\xi_-, \xi_+, \phi\}$.

*Proof of Theorem 1.18.* — Let any $\xi_- \in \mathcal{G}$ be given, and choose a sequence $\xi_{-,n} \in C_c^\infty(S)$ such that $\xi_{-,n} \to \xi_-$ in $\mathcal{G}$ as $n \to \infty$. By Lemma 3.14 we have

$$\mathrm{i}F^-(\lambda)^*\xi_{-,n} - \phi^+[S(\lambda)\xi_{-,n}] + \phi^-[\xi_{-,n}] \in B_0^*$$

(with the approximate eigenfunctions of (1.43)). Then by the continuity of $F^-(\lambda)^*$, $S(\lambda)$ and $\phi^\pm[\cdot]$ we obtain, letting $n \to \infty$,

$$\mathrm{i}F^-(\lambda)^*\xi_- - \phi^+[S(\lambda)\xi_-] + \phi^-[\xi_-] \in B_0^*. \tag{3.35}$$

Whence (1.45a) and (1.45b) hold for $\{\xi_-, S(\lambda)\xi_-, \mathrm{i}F^-(\lambda)^*\xi_-\}$, and the existence part of (i) follows when $\xi_- \in \mathcal{G}$ is given first. We can proceed similarly using Lemma 3.15 when $\xi_+ \in \mathcal{G}$ is given first, and whence, with Lemma 3.12, the existence part of (i) is completed. In addition, the correspondences for either $\xi_- \in \mathcal{G}$ or $\xi_+ \in \mathcal{G}$ given first are given by (1.45b).

To complete (i) it remains to prove the uniqueness part. Note that we already have a partial result in Lemma 3.11 (for $\phi$ given first). Let $\xi_- \in \mathcal{G}$ be given and suppose that $\phi - \phi^+[\xi_+] + \phi^-[\xi_-] \in B_0^*$ for some $\phi \in \mathcal{E}_\lambda$ and $\xi_+ \in \mathcal{G}$. By linearity we may assume that $\xi_- = 0$, and it suffices to show that $\xi_+ = 0$ and $\phi = 0$. Clearly by Lemma 3.11 the vector $\xi_+ = 0$ and whence $\phi \in B_0^*$. By Theorem 1.4 it then follows that $\phi = 0$. We can argue similarly if $\xi_+ \in \mathcal{G}$ is given. We have shown (i) and the formulas (1.45b). The assertion (1.45c) for the upper sign follows from (3.26). We can argue similarly for the lower sign. Whence (ii) is shown.

The formulas (1.45d) are immediate consequences of (3.30a) and (3.30b), and in combination with (i) and (ii) we conclude that indeed $F^\pm(\lambda)^*\colon \mathcal{G} \to \mathcal{E}_\lambda\ (\subseteq B^*)$ are bi-continuous. We have shown (iii).

Finally, since $F^{\pm}(\lambda)^*$ are injective and have closed range in $B^*$ (by (iii)), Banach's closed range theorem [31, Theorem p. 205] implies that the range of $F^{\pm}(\lambda)$ for both signs coincides with $\mathcal{G}$. We conclude that the range of $\delta(H-\lambda) = (2\pi)^{-1}F^{\pm}(\lambda)^*F^{\pm}(\lambda)$ coincides with $\mathcal{E}_\lambda$. Hence (iv) is shown. □

### 3.5. Counterexamples, open problems

We consider modifications of the model of Example 1.20 and show that the asymptotics of the generalized eigenfunctions in $B^*$ for these models are *not* given by (1.45a). Fix $\kappa \in (0,1)$, let $\theta := xy^{-\kappa}$ for $y > 0$ and let $r^2 := \kappa x^2 + y^2$. Consider $M \subseteq \mathbb{R}^2$ with an end described as

$$E = \{(x,y) \in \mathbb{R} \times \mathbb{R}_+ \,|\, r > r_0,\ -1 < \theta < 1\},$$

which is a cylinder in the variables $r$ and $\theta$. The (inverse) metric in these coordinates are

$$g^{rr} = N_r := |\mathrm{d}r|^2, \quad g^{\theta\theta} = N_\theta := |\mathrm{d}\theta|^2, \quad g^{r\theta} = 0.$$

Using the short-hand notation $|g| = \det g = N_r^{-1}N_\theta^{-1}$ we compute

$$\begin{aligned}
|g|^{1/4}\Delta|g|^{-1/4} &= \partial_r N_r \partial_r + \partial_\theta N_\theta \partial_\theta + W_r + W_\theta;\\
&\qquad W_r = -N_r(\partial_r \ln|g|)^2/16 - (\partial_r N_r \partial_r \ln|g|)/4,\\
&\qquad W_\theta = -N_\theta(\partial_\theta \ln|g|)^2/16 - (\partial_\theta N_\theta \partial_\theta \ln|g|)/4.
\end{aligned}$$

We also compute

$$\begin{aligned}
&\partial_r x = \tfrac{\kappa x}{rN_r}, \quad \partial_\theta x = \tfrac{1}{y^\kappa N_\theta}, \quad \partial_r y = \tfrac{y}{rN_r}, \quad \partial_\theta y = -\tfrac{\kappa\theta}{yN_\theta},\\
&N_r = 1 - (\kappa-\kappa^2)\theta^2 y^{2\kappa} r^{-2}, \quad N_\theta = y^{-2\kappa} + \tfrac{\kappa^2\theta^2}{y^2},\\
&\partial_r N_r = 2(1-\kappa N_r^{-1})(\kappa-\kappa^2)\theta^2 y^{2\kappa} r^{-3} = O(r^{2\kappa-3}),\\
&\partial_\theta N_r = -2(1-\kappa^2 N_\theta^{-1}\theta^2 y^{-2})(\kappa-\kappa^2)\theta y^{2\kappa} r^{-2} = O(r^{2\kappa-2}),\\
&\partial_r^2 N_r = O(r^{2\kappa-4}), \quad \partial_\theta^2 N_r = O(r^{2\kappa-2}),\\
&\partial_r N_\theta = -\tfrac{2\kappa}{rN_r}\big(y^{-2\kappa} + \kappa\theta^2 y^{-2}\big) = O(r^{-1-2\kappa}),\\
&\partial_\theta N_\theta = \tfrac{2\kappa^2\theta}{y^2 N_\theta}\big(y^{-2\kappa} + \kappa\theta^2 y^{-2}\big) + \tfrac{2\kappa^2\theta}{y^2} = \tfrac{4\kappa^2\theta}{r^2}\big(1 + O\big(r^{2\kappa-2}\big)\big),\\
&\partial_r^2 N_\theta = O(r^{-2-2\kappa}), \quad \partial_\theta^2 N_\theta = \tfrac{4\kappa^2}{r^2}\big(1 + O\big(r^{2\kappa-2}\big)\big).
\end{aligned}$$

Using these formulas and $\partial_* \ln|g| = -(\partial_* N_r)/N_r - (\partial_* N_\theta)/N_\theta$ we get

$$W_r = O(r^{-2}), \quad W_\theta = O(r^{-2}).$$

We consider for $\kappa \in (0,1/2]$ the approximate outgoing eigenfunction (corresponding to any $\lambda > 0$ and here with $r_0 = r_0(\lambda)$ chosen big enough)

$$\begin{aligned}\phi^+ &:= \bar\chi_n |g|^{-1/4} b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} u(\theta)\\ &\approx C(\lambda) r^{-\kappa/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} u(\theta).\end{aligned}\tag{3.36}$$

Here

$$b = \sqrt{2(\lambda - \tfrac{\mu(\lambda)}{r^{2\kappa}})} \approx \sqrt{2\lambda} - \tfrac{\mu(\lambda)}{\sqrt{2\lambda}} r^{-2\kappa},$$

$u = u(\theta)$ is any Dirichlet eigenstate of the operator on $L^2((-1,1),\mathrm{d}\theta)$ given by

$$H_D := \begin{cases} -\frac12 \partial_\theta^2 & \text{for } \kappa < 1/2,\\ -\frac12 \partial_\theta^2 - \frac{\lambda\theta^2}{4} & \text{for } \kappa = 1/2,\end{cases}$$

and $\mu(\lambda)$ is the corresponding eigenvalue. To see why this is an approximate eigenfunction we first note that $\phi^+ \in \mathcal{N} \cap B^*$. We claim that in fact

$$(H-\lambda)\phi^+ \in \begin{cases} r^{2\kappa-2} B^* \subseteq B & \text{for } \kappa < 1/2,\\ r^{-2} B^* \subseteq B & \text{for } \kappa = 1/2.\end{cases}$$

We compute for $\kappa = 1/2$ (skipping the details for $\kappa < 1/2$)

$$\begin{aligned}\partial_r N_r \partial_r \big(b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} u\big) &= \big(-b^2 + \tfrac{\lambda\theta^2}{2r} + O(r^{-2})\big) b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} u,\\ \partial_\theta N_\theta \partial_\theta \big(b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} u\big) &= b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} \big(\tfrac1r \partial_\theta^2 u + O(r^{-2})\big).\end{aligned}$$

In the first identity we substitute $b^2 = 2(\lambda - \frac{\mu(\lambda)}{r})$. Then we collect our computations and indeed obtain

$$(H-\lambda)\phi^+ = (H-\lambda)\phi^+ - |g|^{-1/4} b^{-1/2} \mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} r^{-1}\big(H_D - \mu(\lambda)\big) u \in r^{-2} B^*.$$

Next we define

$$\phi_u = \phi^+ - R(\lambda - \mathrm{i}0)(H-\lambda)\phi^+.$$

This $\phi_u$ is in $\mathcal{E}_\lambda$ with non-trivial prescribed outgoing asymptotics. If we look at all eigenstates of $H_D$, say numbered by $k \in \mathbb{N}$, we obtain several generalized eigenfunctions this way. Note that for $\kappa = 1/2$

$$\mathrm{e}^{\mathrm{i}\int_{r_0}^r b\,\mathrm{d}r} \approx \mathrm{e}^{\mathrm{i}\sqrt{2\lambda} r} \exp\big(-\mathrm{i}\tfrac{\mu(\lambda)}{\sqrt{2\lambda}} \ln r\big).$$

Due to the non-trivial factor

$$\exp\big(-\mathrm{i}\tfrac{\mu(\lambda,k)}{\sqrt{2\lambda}} \ln r\big)$$

the asymptotics (1.45a) is readily seen to be *incorrect* (seen by using just two of the constructed generalized eigenfunctions). By a similar reasoning this conclusion is also valid for $\kappa < 1/2$.

The methods of this paper (in combination with other ingredients) should yield a modification of Theorem 1.18 where the asymptotics of *any* $\phi \in \mathcal{E}_\lambda$ should be provided by functions of the form (3.36) and their incoming counterparts, say in combination denoted by $\{\phi_k^\pm | k \in \mathbb{N}\}$. This would intuitively yield the identification of the limiting space as $\mathcal{G} = l^2(\mathbb{N})$, but we shall not elaborate at this point.

For $\kappa \in (1/2, 1)$ we do not know how to construct approximate outgoing eigenfunctions in $\mathcal{N} \cap B^*$. If for example we take $b = \sqrt{2\lambda}$ and $u$ any nonzero function in the domain of the Dirichlet Laplacian on $(-1, 1)$ in (3.36) we obtain

$$(H - \lambda N_r)\phi^+ \in r^{-2\kappa} B^* \subseteq B,$$

which shows that

$$(H - \lambda)\phi^+ \notin B,$$

since $1 - N_r \approx (\kappa - \kappa^2)\theta^2 r^{2\kappa - 2}$ is long-range for $\kappa \in (1/2, 1)$. The reader might think that a better approximation to the eikonal equation than $\sqrt{2\lambda} r$ could be given to construct concrete approximate outgoing eigenfunctions in $\mathcal{N} \cap B^*$ to cure this deficiency, however a closer examination indicates that this is not feasible (note that the forward flow property is a severe restriction). The ansatz (1.43) has a similar deficiency. Whence the asymptotics of the generalized eigenfunctions in $\mathcal{E}_\lambda$ is not known to us for $\kappa \in (1/2, 1)$.

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