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Scattering theory for C^2 long-range potentials

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Abstract. We develop a complete stationary scattering theory for Schrödinger operators on $\mathbb{R}^d$, $d \geq 2$, with C^2 long-range potentials. This extends former results in the literature, in particular Isozaki (1980) and (1982), Ikebe and Isozaki (1982), and Gâtal and Yafaev (1999), which all require a higher degree of smoothness. In this sense, the spirit of our paper is similar to Hörmander [The Analysis of Linear Partial Differential Operators IV (1985), Chapter XXX] and J. Dereziński and C. Gérard [Scattering Theory of Classical and Quantum N-Particle Systems (1997), Section 4.7], which also develop a scattering theory under the C^2 condition, however being very different from ours. While the Agmon–Hörmander theory is based on the Fourier transform and a momentum-space representation, our theory is entirely position-space based and may be seen as more related to our previous approach to scattering theory on manifolds, Ito and Skibsted (2013), (2019), and (2021). The C^2 regularity is natural in the Agmon–Hörmander theory as well as in our theory, in fact probably being "optimal" in the Euclidean setting. We prove equivalence of the stationary scattering theory and a developed position-space based time-dependent scattering theory. Furthermore, we develop a related stationary scattering theory at fixed energy in terms of asymptotics of generalized eigenfunctions of minimal growth. A basic ingredient of our approach is a solution to the eikonal equation constructed from the geometric variational scheme of Cruz-Sampedro and Skibsted (2013). Another key ingredient is strong radiation condition bounds for the limiting resolvents originating in Herbst and Skibsted (1991). They improve formerly known ones by Isozaki (1980) and Saitō (1979) and considerably simplify the stationary approach. We obtain the bounds by a new commutator scheme whose elementary form allows a small degree of smoothness.

Contents

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1. Introduction

1.1. Setting

In the present paper we construct a stationary long-range scattering theory for the Schrödinger operator

$$H = -\frac{1}{2}\Delta + V + q \tag{1.1}$$

on $\mathcal{H} = L^2(\mathbb{R}^d)$ with $d \geq 2$. Here Δ is the ordinary Laplacian on $\mathbb{R}^d$, and we shall often write

$$-\Delta = p \cdot p = p_i p_i, \quad p_i = -\mathrm{i}\partial_i, \quad i = 1, \dots, d,$$

with the Einstein convention being adopted without tensorial superscripts.

We shall address the problem of constructing such theory under a minimal regularity condition on the long-range part V of the potential $V + q$. The second term q is a standard short-range potential. This corresponds to taking $l = 2$ in the following C^l long-range-type condition. For technical reasons we consider below, and throughout the paper, the following more general condition in which $l \geq 2$ is arbitrary (however typically given as $l = 2$). It is a trivial consequence of the condition that H is self-adjoint.

Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, $\mathbb{R}_+ = (0, \infty)$ and $\langle x \rangle = (1 + |x|^2)^{1/2}$ for $x \in \mathbb{R}^d$. For given Banach spaces X and Y, we denote by $\mathcal{L}(X, Y)$ and $\mathcal{C}(X, Y)$ the set of bounded and compact operators $T: X \to Y$, respectively, and for $Y = X$ we abbreviate $\mathcal{L}(X) = \mathcal{L}(X, Y)$ and $\mathcal{C}(X) = \mathcal{C}(X, Y)$.

Condition 1.1. Let $V \in C^l(\mathbb{R}^d; \mathbb{R})$ for some $l \in \{2, 3, \dots\}$, and assume there exist $\sigma \in (0, 1)$, $\rho \in (0, 1]$, and $C > 0$ such that for any $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq l$ and $x \in \mathbb{R}^d$

$$|\partial^\alpha V(x)| \leq C \langle x \rangle^{-m(|\alpha|)}; \quad m(k) = \begin{cases} \sigma + k & \text{for } k = 0, 1, 2, \\ \sigma + 2 + \frac{\rho+1}{2}(k - 2) & \text{for } k = 2, \dots, l. \end{cases} \tag{1.2a}$$

In addition, let $q: \mathbb{R}^d \to \mathbb{R}$ be measurable, and assume there exists $\tau \in (0, 1)$ such that

$$\langle x \rangle^{1+\tau} q(x)(-\Delta + 1)^{-1} \in \mathcal{C}(\mathcal{H}). \tag{1.2b}$$

Finally, assume the operator $H = -(1/2)\Delta + V + q$ does not have positive eigenvalues.

Remarks 1.2. (1) For $l = 2$, the above $V + q$ is called a 2-*admissible potential*, here adapting the terminology of [11, Definition 30.1.3]. Several of our main theorems require only $l = 2$. However, for an intermediate key estimate of independent interest we need $l = 4$ (or with a modification possibly only $l = 3$), see Theorem 1.24

(and Remark 1.25 (2)). This estimate will be used for a certain regularized 4-admissible potential constructed from a given 2-admissible potential, see Remark 1.25 (5). (For the regularized potential the parameter σ is the same and $\rho < \sigma$, arbitrarily.) In this sense, indeed the key estimate serves as an intermediate result for our study of 2-admissible potentials.

(2) We will call V a *classical C^l long-range potential* if there exists $\sigma \in (0, 1)$ and $C > 0$ such that for any $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leq l$ and $x \in \mathbb{R}^d$

$$|\partial^\alpha V(x)| \leq C\langle x\rangle^{-\sigma-|\alpha|}.$$

In addition, V is a *classical C^∞ long-range potential* if it is a classical C^l long-range potential for any $l \geq 2$. Obviously, in these cases, the *order of decay function* $m\colon \mathbb{N}_0 \to \mathbb{R}_+$ is of the simplest form. Nevertheless, its general form is well suited for an induction argument to be used in the proof of Theorem 1.3 (stated below).

(3) The local singularities allowed in (1.2b) is not an important issue/difficulty in this paper. The last assumption on absence of positive eigenvalues is very weak and can be omitted for example if (1.2b) is replaced by assuming boundedness of the function $\langle x\rangle^{1+\tau} q(x)$.

Under Condition 1.1, for $l = 2$ we succeed in fully developing a stationary scattering theory: we characterize the generalized eigenfunctions of minimal growth by their asymptotics and construct the *stationary scattering matrix* as well as the *generalized Fourier transforms*, which unitarily diagonalize the (absolutely) continuous part of H. Such results were formerly obtained by Isozaki [14, 15], Ikebe and Isozaki [12], and Gâtel and Yafaev [8] for classical C^4 or C^3 long-range potentials. In this paper, we extend them to the category of 2-admissible potentials. Note that a similar C^2 condition very naturally appears in the classical long-range scattering theory, see for example [6, Theorem 2.7.1]. In fact, we believe that our condition should be considered as "optimal," although this terminology will not be justified in the paper. Finally, we shall prove that the adjoints of the generalized Fourier transforms coincide with some constructed time-dependent wave operators, verifying that the stationary and the time-dependent approaches are equivalent to each other.

The long-range scattering theory requires a non-trivial comparison dynamics due to non-negligible effects from V at infinity. To virtually eliminate such effects, we solve the *stationary eikonal equation*, or simply the *eikonal equation*,

$$\frac{1}{2}|\nabla_x S(\lambda, x)|^2 + V(x) = \lambda, \quad \lambda > 0, \tag{1.3a}$$

in the stationary theory, and the *time-dependent eikonal equation*, which is more commonly called the *Hamilton–Jacobi equation*,

$$\partial_t K(t, x) + \frac{1}{2}|\nabla_x K(t, x)|^2 + V(x) = 0, \quad t > 0, \tag{1.3b}$$

in the time-dependent theory. In this paper, we solve the former equation (1.3a) by the geometric method of [4] and derive global estimates of the solution. For comparison, we mention that Isozaki [14, 15] in his construction of a solution used a classical PDE-method solving a Cauchy problem, and the cited papers [8, 12] rely on Isozaki's solution. Once a proper solution to (1.3a) is obtained, one can solve (1.3b) by using the Legendre transform, cf. [17].

Another important technical tool is a strong version of the radiation condition bounds for the limiting resolvents, which in fact considerably simplifies the stationary scattering theory. Such "strong radiation condition bounds" were first established by Herbst and Skibsted [9] for classical C^∞ long-range potentials. For a more restrictive class of classical C^∞ long-range potentials (defined by a virial condition), the bounds were derived uniformly in non-negative energies [22], yielding a stationary scattering theory at fixed energy including the threshold zero. In this paper, we present a procedure of proof that works within a low regularity framework (in particular being independent of pseudodifferential operator theory). A similar procedure was invented and applied earlier to the short-range Stark Hamiltonian [2]; however, our setup is different and we need to proceed rather independently. Since the proof still requires fourth (or possibly only third) derivatives of the potential, we shall regularize it up to an error of short-range-type using a regularization scheme of Hörmander [11, Lemma 30.1.1]. This leads to the study of radiation condition bounds of a new classical C^2 long-range potential which conforms with (1.2a) for an $l \geq 3$ but possibly *fails* to be a classical C^3 long-range potential. The short-range error from the Hörmander decomposition (see Lemma 4.1 for the version to be used in our paper) along with the potential q will be treated by the second resolvent identity. Note that the Hörmander decomposition was also employed in [12], however Ikebe and Isozaki considered only classical C^4 long-range potentials.

These two ingredients occupy a considerable part of the paper, and in addition to the entailing stationary and time-dependent scattering theories we consider them as main results of independent interest.

With these preliminaries done, we derive a complete stationary scattering theory. The strong radiation condition bounds yield a very fast construction of generalized Fourier transforms using the "spherical eikonal coordinates." These coordinates were first used in the context of stationary scattering theory in [3] for a different setting and with different proofs. Then we "pull the results back" to assertions in the ordinary spherical coordinates. After a complete stationary theory is obtained, a position-space based time-dependent theory follows naturally, although still being non-trivial. Finally, we mention that our low regularity theory has an application to the 3-body problem. We shall briefly discuss this aspect in Section 1.2.5. Finally, we discuss potential applications to scattering theory on manifolds in Section 1.2.6.

The paper is an improvement and an extension of the unpublished preprint [19].

1.2. Main results

Now, we present a series of main results of the paper.

1.2.1. Stationary eikonal equation. Let us first solve the stationary eikonal equation (1.3a) outside a large ball. Take any $\chi \in C^\infty(\mathbb{R};\mathbb{R})$ such that

$$\chi(t) = \begin{cases} 0 & \text{for } t \le \frac{4}{3}, \\ 1 & \text{for } t \ge \frac{5}{3}, \end{cases} \qquad \chi' \ge 0, \tag{1.4}$$

and set for any $R > 0$ and $x \in \mathbb{R}^d$

$$\chi_R(x) = \chi(|x|/R). \tag{1.5}$$

Theorem 1.3. *Suppose Condition 1.1 for some $l \ge 2$. Fix any closed interval $I \subset \mathbb{R}_+$. Then, it follows that, for all $R \ge R_0$ for some $R_0 > 0$, there exist a real $S \in C^l(I \times (\mathbb{R}^d \setminus \{0\}))$ and $s \in C^l(I \times \mathbb{R}^d)$ such that the following holds.*

(1) *The function S solves*

$$\frac{1}{2}|\nabla_x S|^2 + \chi_R V = \lambda \quad \text{on } I \times (\mathbb{R}^d \setminus \{0\}). \tag{1.6}$$

(2) *For any $\lambda \in I$, $S(\lambda, \cdot)$ coincides with the geodesic distance from the origin with respect to the Riemannian metric $g = 2(\lambda - \chi_R V)\,\mathrm{d}x^2$.*

(3) *The functions S and s are related as*

$$S = \sqrt{2\lambda}|x|(1+s) \quad \text{on } I \times (\mathbb{R}^d \setminus \{0\}),$$

and s vanishes on $I \times \{|x| \le R\}$.

(4) *There exists $C = C(I, R_0) > 0$ (being independent of $R \ge R_0$) such that, for any $k + |\alpha| \le l$ and $(\lambda, x) \in I \times \mathbb{R}^d$,*

$$|\partial_\lambda^k \partial_x^\alpha s(\lambda, x)| \le C\lambda^{-1-k}\langle x\rangle^{-m(k+|\alpha|)+k}. \tag{1.7}$$

Remarks 1.4. (1) For a variation of (1.7), see also Corollary 2.14.

(2) We can extend S and s to be smoothly defined for all $\lambda > 0$, however, allowing $R = R(\lambda)$ to be λ-dependent possibly with $R(\lambda) \to \infty$ as $\lambda \to 0_+$. On the other hand, a bound corresponding to (1.7) can be kept uniform in $\lambda > 0$. This can be seen from the proof, but we shall not elaborate on it.

(3) Our bound (1.7) is stronger than [14, Theorem 4.1], where Isozaki obtained (1.7), except for $(k, \alpha) = (3, 0)$, for a classical C^3 long-range potential. Gâtal and Yafaev asserted (1.7) for a classical C^3 long-range potential in [8, Lemma 3.1]; however, it was not proved there, and in fact it was indicated in a paragraph subsequent to it that the assertion requires a classical C^4 long-range potential.

1.2.2. Stationary scattering theory at fixed energy. Next, we construct a stationary scattering theory at fixed energy through the WKB approximation of the limiting resolvent.

Let us briefly review the *limiting absorption principle* for the resolvent

$$R(z) = (H - z)^{-1}, \quad z \in \mathbb{C} \setminus \sigma(H).$$

It is a basic and well-studied topic, for details see, e.g., [1] and the references there. Recall the *Besov spaces*, or the *Agmon–Hörmander spaces*, defined as

$$\begin{aligned} \mathcal{B} &= \{\psi \in L^2_{\mathrm{loc}} \mid \|\psi\|_{\mathcal{B}} < \infty\}, & \|\psi\|_{\mathcal{B}} &= \sum_{m=0}^{\infty} 2^{m/2} \|1_m \psi\|_{\mathcal{H}}, \\ \mathcal{B}^* &= \{\psi \in L^2_{\mathrm{loc}} \mid \|\psi\|_{\mathcal{B}^*} < \infty\}, & \|\psi\|_{\mathcal{B}^*} &= \sup_{m \geq 0} 2^{-m/2} \|1_m \psi\|_{\mathcal{H}}, \\ \mathcal{B}^*_0 &= \{\psi \in \mathcal{B}^* \mid \lim_{m \to \infty} 2^{-m/2} \|1_m \psi\|_{\mathcal{H}} = 0\}. \end{aligned}$$

Here, we let

$$1_0 = 1(\{|x| < 1\}) \quad \text{and} \quad 1_m = 1(\{2^{m-1} \leq |x| < 2^m\}) \quad \text{for } m \in \mathbb{N}, \tag{1.8}$$

with $1(A)$ being the sharp characteristic function of a subset $A \subseteq \mathbb{R}^d$. It is worthwhile recalling that if we define the standard *weighted L^2 spaces* as

$$L^2_s = \langle x \rangle^{-s} \mathcal{H} \quad \text{for } s \in \mathbb{R},$$

then, for any $s > 1/2$,

$$L^2_s \subset \mathcal{B} \subset L^2_{1/2} \subset \mathcal{H} \subset L^2_{-1/2} \subset \mathcal{B}^*_0 \subset \mathcal{B}^* \subset L^2_{-s}.$$

It is proved in [1] that locally uniformly in $\lambda > 0$ there exist the *limiting resolvents*

$$R(\lambda \pm \mathrm{i}0) = \operatorname*{s\text{–}w^{\star}\text{–}lim}_{z \to \lambda \pm \mathrm{i}0_+} R(z) \quad \text{in } \mathcal{L}(\mathcal{B}, \mathcal{B}^*);$$

here the right-hand side operators act on any $\psi \in \mathcal{B}$ as the (positive) ε-limits of $R(\lambda \pm \mathrm{i}\varepsilon)\psi$ in the weak-star topology of $\mathcal{B}^*$, or, equivalently stated, for any $\psi, \phi \in \mathcal{B}$,

$$\langle \phi, R(\lambda \pm \mathrm{i}0)\psi \rangle = \lim_{\varepsilon \searrow 0} \langle \phi, R(\lambda \pm \mathrm{i}\varepsilon)\psi \rangle,$$

(see Theorem 3.17 for more general assertions). In particular, the singular continuous spectrum of H is empty, $\sigma_{\mathrm{sc}}(H) = \emptyset$.

For these limiting resolvents, we discuss the *WKB approximations* as follows, using here and throughout the paper the notation $\mathcal{G} = L^2(\mathbb{S}^{d-1})$.

Theorem 1.5. *Suppose Condition 1.1 for $l = 2$. Let $I \subset \mathbb{R}_+$ be a closed interval, and let $R > 0$. Assume there exists real $S = \sqrt{2\lambda}|x|(1+s) \in C(I; C^2(\{|x| > R\}))$ satisfying the following.*

(i) *For each $\lambda \in I$, $S(\lambda, \cdot)$ solves (1.3a) on $\{|x| > R\}$.*

(ii) *For any compact subset $I' \subseteq I$, there exist $\varepsilon, C > 0$ such that, for any $|\alpha| \leq 2$, $\lambda \in I'$ and $|x| > R$,*

$$|\partial_x^\alpha s(\lambda, x)| \leq C\langle x\rangle^{-\varepsilon-|\alpha|}.$$

In addition, for any $\xi \in \mathcal{G}$ and $(\lambda, x) \in I \times \mathbb{R}^d$, set

$$\phi_\pm^S[\xi](\lambda, x) = \frac{(2\pi)^{1/2}}{(2\lambda)^{1/4}}\chi_R(x)|x|^{-(d-1)/2}\mathrm{e}^{\pm \mathrm{i}S(\lambda,x)}\xi(\hat{x}), \quad \hat{x} = |x|^{-1}x, \tag{1.9}$$

where $\chi_R \in C^\infty(\mathbb{R}^d)$ is from (1.5). Then, the following assertions hold.

(1) *For any $\lambda \in I$, there exist unique $F^\pm(\lambda) \in \mathcal{L}(\mathcal{B}, \mathcal{G})$ such that, for any $\psi \in \mathcal{B}$,*

$$R(\lambda \pm \mathrm{i}0)\psi - \phi_\pm^S[F^\pm(\lambda)\psi](\lambda, \cdot) \in \mathcal{B}_0^*. \tag{1.10}$$

(2) *The mappings $F^\pm: I \times \mathcal{B} \to \mathcal{G}$ are continuous.*

(3) *For any $\lambda \in I$, one has the identities*

$$(H - \lambda)F^\pm(\lambda)^* = 0 \quad \textit{and} \quad F^\pm(\lambda)^* F^\pm(\lambda) = \delta(H - \lambda),$$

where $\delta(H - \lambda) = \pi^{-1}\,\mathrm{Im}\,R(\lambda + \mathrm{i}0) \in \mathcal{L}(\mathcal{B}, \mathcal{B}^*)$.

(4) *For any $\lambda \in I$, the ranges $F^\pm(\lambda)\mathcal{B} \subseteq \mathcal{G}$ are dense.*

Remarks 1.6. (1) For R large enough, the existence of such S is guaranteed by Theorem 1.3, but here it can be slightly more general (thanks to Theorem 1.3, condition (ii) is fulfilled with $\varepsilon = \sigma$ for $I' = I$). Note also that, according to Remark 1.4 (2), we may let $I = \mathbb{R}_+$ if we allow a λ-dependent R.

(2) Clearly, for any $\xi \in \mathcal{G}$ and $\lambda \in I$, one has $\phi_\pm^S[\xi](\lambda, \cdot) \in \mathcal{B}^*$. We may think of these *quasi-modes* as purely outgoing/incoming distorted spherical waves, respectively.

(3) In Theorem 1.10 below, we will see the "completeness property" $F^\pm(\lambda)\mathcal{B} = \mathcal{G}$ for any $\lambda \in I$.

Now, we have stationary versions of scattering quantities.

Definitions 1.7. In the setting of Theorem 1.5, let $\lambda \in I$.

(1) The operators $F^\pm(\lambda): \mathcal{B} \to \mathcal{G}$ are the *restricted stationary wave operators* at energy λ.

(2) The adjoints $F^{\pm}(\lambda)^*: \mathcal{G} \to \mathcal{B}^*$ are the *stationary wave matrices*.

(3) The *stationary scattering matrix at energy* $\lambda \in I$ is the unitary operator $\mathsf{S}(\lambda)$ on $\mathcal{G}$ obeying

$$F^+(\lambda) = \mathsf{S}(\lambda) F^-(\lambda). \tag{1.11}$$

Indeed, the scattering matrix is well defined, stated as follows.

Corollary 1.8. *In the setting of Theorem 1.5, at any energy $\lambda \in I$ the stationary scattering matrix $\mathsf{S}(\lambda)$ uniquely exist. Moreover, the mapping $I \ni \lambda \mapsto \mathsf{S}(\lambda) \in \mathcal{L}(\mathcal{G})$ is strongly continuous.*

Remarks 1.9. (1) The stationary scattering matrix $\mathsf{S}(\lambda)$ is defined pointwise for *all* $\lambda \in I$, not only for a.e. $\lambda \in I$, unlike in the abstract construction commonly adopted in the time-dependent approach.

(2) Alhough the usual well-known short-range scattering theory (defined for $V + q = q$) is a different subject, let us remark that in this case it is more conventional to define the quasi-modes (1.9) in a slightly different way; more precisely, with (1.9) modified by the factor $\mathrm{e}^{\mp \mathrm{i}\pi(d-3)/4}$. In particular, if also the short-range potential q vanishes, it then follows that in fact $\mathsf{S}(\lambda) \equiv I$.

(3) The dependence of the restricted stationary wave operators on the given function $S(\lambda, x)$ is almost canonically given by (1.9) and (1.10). It is given by an explicit multiplication operator of modulus one, see Remark 4.13 and its appearance in Theorem 1.12 (3).

The stationary scattering theory is intimately related to the asymptotics of the *minimal generalized eigenfunctions* $\phi \in \mathcal{E}_\lambda$, where

$$\mathcal{E}_\lambda = \{\phi \in \mathcal{B}^* \mid (H - \lambda)\phi = 0 \text{ in the distributional sense}\}, \quad \lambda > 0,$$

is a non-trivial subspace of $\mathcal{B}^*$ by Theorem 1.5, and it is minimal in the sense that $\mathcal{E}_\lambda \cap \mathcal{B}_0^* = \{0\}$ (see Remark 4.17 (2)).

Theorem 1.10. *In the setting of Theorem 1.5, let $\lambda \in I$.*

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

$$\phi - \phi_+^S[\xi_+](\lambda, \cdot) + \phi_-^S[\xi_-](\lambda, \cdot) \in \mathcal{B}_0^*. \tag{1.12a}$$

(2) *The above correspondences $\xi_\pm \to \phi$ and $\xi_\mp \to \xi_\pm$ are given by the formulas*

$$\phi = 2\pi \mathrm{i} F^{\pm}(\lambda)^* \xi_\pm \quad \textit{and} \quad \xi_+ = \mathsf{S}(\lambda)\xi_-. \tag{1.12b}$$

(3) *The wave matrices* $F^{\pm}(\lambda)^*$ *are topological linear isomorphisms as* $\mathcal{G} \to \mathcal{E}_\lambda \subseteq \mathcal{B}^*$. *In addition, for any* $\phi \in \mathcal{E}_\lambda$ *and* $\xi_\pm \in \mathcal{G}$ *satisfying* (1.12a), *one has*

$$\|\xi_\pm\|_{\mathcal{G}} = \frac{(2\lambda)^{1/4}}{(2\pi)^{1/2}} \lim_{m\to\infty} 2^{-m/2} \|1_m \phi\|_{\mathcal{H}}, \tag{1.12c}$$

where 1_m *is from* (1.8).

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

Remarks 1.11. (1) We can also express $\xi_\pm \in \mathcal{G}$ as simple oscillatory weak limits of $\phi \in \mathcal{E}_\lambda$ at infinity, see Step III of the proof.

(2) The above result extends in the Euclidean setting [8, 18] to 2-admissible potentials. See also [12].

1.2.3. Generalized Fourier transforms. The stationary scattering theory at fixed energy applies to the construction of the *generalized (or distorted) Fourier transforms*, also referred to as the *stationary wave operators*, which unitarily transform the continuous part of the Schrödinger operator H into a simple multiplication operator.

As in Theorem 1.5, the subset $I \subset \mathbb{R}_+$ denotes a closed interval, and we let $P_H(I)$ denote the corresponding spectral projection for H. We introduce the notation

$$H_I = H_{|\mathcal{H}_I}, \quad \mathcal{H}_I = P_H(I)\mathcal{H}, \quad \widetilde{\mathcal{H}}_I = L^2(I, \mathrm{d}\lambda; \mathcal{G}).$$

Thanks to Theorem 1.5, we can also introduce the operators

$$\mathcal{F}_0^{\pm} = \int_I^{\oplus} F^{\pm}(\lambda)\,\mathrm{d}\lambda\colon \mathcal{B} \to C(I;\mathcal{G}) \cap \widetilde{\mathcal{H}}_I.$$

These operators can be extended as to be acting from $P_H(I)\mathcal{B}$, and then in turn to operators acting from $\mathcal{H}_I$. These assertions are part of the following main theorem (see also Step II in the proof).

Theorem 1.12. *In the setting of Theorem* 1.5, *the following assertions hold.*

(1) *The operators* $\mathcal{F}_0^{\pm}$ *induce unitary operators* $\mathcal{F}^{\pm}\colon \mathcal{H}_I \to \widetilde{\mathcal{H}}_I$, *respectively.*

(2) *The induced unitary operators* $\mathcal{F}^{\pm}$ *satisfy*

$$\mathcal{F}^{\pm} H_I (\mathcal{F}^{\pm})^* = M_\lambda,$$

respectively, where M_λ *denotes the operator of multiplication by* λ *on* $\widetilde{\mathcal{H}}_I$.

(3) *Suppose also* S_1 *satisfies the assumptions of Theorem* 1.5, *and let* $\mathcal{F}_1^{\pm}$ *be the associated unitary operators as above. Then, there exists the limit*

$$\Theta(\lambda,\omega) := \lim_{r\to\infty} (S_1(\lambda, r\omega) - S(\lambda, r\omega))$$

taken locally uniformly in $(\lambda,\omega)\in I\times\mathbb{S}^{d-1}$, *and it follows that*

$$\mathcal{F}_1^{\pm}=\mathrm{e}^{\mp\mathrm{i}\Theta}\mathcal{F}^{\pm}.$$

Remarks 1.13. (1) Under the conditions of Theorem 1.3, one can easily extend the assertion to $I=\mathbb{R}_+$, so that the whole absolutely continuous part $H_{\mathrm{ac}}=H_{|\mathcal{H}_{\mathrm{ac}}}$, $\mathcal{H}_{\mathrm{ac}}=P_H(\mathbb{R}_+)\mathcal{H}$, is diagonalized. One has only to cover $\mathbb{R}_+$ with disjoint intervals and take a direct sum of the associated generalized Fourier transforms, or to adopt a function S defined for all $\lambda>0$ in Theorem 1.5, see Remarks 1.4 (2) and 1.6 (1). This is straightforward.

(2) In [8, 12] the diagonalization was carried out successfully for classical C^4 or C^3 long-range potentials. Our result extends these previous results to the C^2 case. For related work, we refer the reader to [18, 21], still the present C^2 case is not covered in these works. On the other hand, [10], the Agmon–Hörmander theory [11, Chapter XXX], and [6, Section 4.7] cover 2-admissible potentials treated by a momentum-space representation (see [6, Proposition 4.7.4] for an interesting comparison within this theory). These works are fundamentally different from ours (since they are momentum-space based). Moreover, the stationary scattering theory of [11, Chapter XXX] is only developed up to the point of showing asymptotic completeness, while [6, Section 4.7] is entirely time-dependent.

1.2.4. Time-dependent scattering theory. We present our results on time-dependent theory, which relate to the time-dependent eikonal equation (1.3b). For that purpose, we introduce the space-time regions

$$\begin{aligned}\Omega_\mu&=\{(t,x)\in\mathbb{R}_+\times\mathbb{R}^d\mid |x|\geq\mu t\},\quad &\mu>0,\\ \Omega_{\mu,T}&=\{(t,x)\in\Omega_\mu\mid t>T>0\},\quad &T>0.\end{aligned}$$

Theorem 1.14. *Suppose Condition 1.1 for some* $l\geq 2$. *Fix any* $\mu>\mu'>0$ *and let* S *be given as in Theorem 1.3 with* $I=I_{\mu'}=[\mu'^2/2,\infty)$ *(assuming here and for other purposes that* $R>0$ *is sufficiently large). Then, for each* $(t,x)\in\Omega_\mu$, *there exists a unique critical point* $\lambda_c=\lambda_c(t,x)\in I$ *of*

$$\widetilde{K}(\lambda,t,x)=S(\lambda,x)-\lambda t \tag{1.14}$$

considered as a function of $\lambda\in I$. *In addition, if one sets* $K=\widetilde{K}(\lambda_{\mathrm{c}},\cdot,\cdot)$, *then the following hold.*

(1) $K\in C^l(\Omega_\mu)$, *and it solves*

$$\partial_t K+\frac{1}{2}|\nabla_x K|^2+\chi_R V=0\quad \text{on } \Omega_\mu. \tag{1.15}$$

(2) *There exists $C > 0$ (being independent of all large R) such that, for any $k + |\alpha| \le 2$ and $(t, x) \in \Omega_\mu$,*

$$\left|\partial_t^k \partial_x^\alpha \left(K(t,x) - \frac{x^2}{2t}\right)\right| \le C t^{1-k} \langle x\rangle^{-\sigma-|\alpha|}. \tag{1.16}$$

Remark 1.15. For $l \ge 3$, it is possible to extend (1.16) to higher order derivatives (given by $3 \le k + |\alpha| \le l$) with appropriate exponents on the right-hand side. Since such estimates are not needed in the present paper, they will not be presented.

Definition 1.16. In the setting of Theorem 1.14, in particular under the fixed condition $\mu > \mu' > 0$, the function $K \in C^l(\Omega_\mu)$ is called the *Legendre transform* of $S \in C^l(I_{\mu'} \times (\mathbb{R}^d \setminus \{0\}))$.

Theorem 1.17. *Suppose Condition 1.1 with $l = 2$. Let $\mu, T > 0$, and assume $K \in C^2(\Omega_{\mu,T}; \mathbb{R})$ satisfies the following.*

(i) *K solves the Hamilton–Jacobi equation (1.3b) on $\Omega_{\mu,T}$.*

(ii) *There exist $\varepsilon, C > 0$ such tha,t for any $|\alpha| \le 2$ and $(t, x) \in \Omega_{\mu,T}$,*

$$\left|\partial_x^\alpha \left(K(t,x) - \frac{x^2}{2t}\right)\right| \le C t \langle x\rangle^{-\varepsilon-|\alpha|}.$$

In addition, let $J = J_\mu = [\mu^2/2, \infty)$ and define isometries $U^\pm(t)\colon \widetilde{\mathcal{H}}_J \to \mathcal{H}$ as follows: for any $(t, h) \in (T, \infty) \times \widetilde{\mathcal{H}}_J$,

$$(U^\pm(t)h)(x) = \mathrm{e}^{\mp 3\pi \mathrm{i}/4} t^{-1} |x|^{1-d/2} \mathrm{e}^{\pm \mathrm{i} K(t,x)} h(x^2/(2t^2), \hat{x}), \quad \hat{x} = |x|^{-1} x.$$

Then, the following two assertions hold.

(1) *There exist the strong limits*

$$W^\pm := \operatorname*{s-lim}_{t\to\infty} \mathrm{e}^{\pm \mathrm{i} t H} U^\pm(t)\colon \widetilde{\mathcal{H}}_J \to \mathcal{H}. \tag{1.17}$$

They are isometries, mapping $\widetilde{\mathcal{H}}_{J'} \subseteq \widetilde{\mathcal{H}}_J$ into $\mathcal{H}_{J'} \subseteq \mathcal{H}$ for any closed subinterval $J' \subseteq J$.

(2) *Let K_1 also satisfy the same assumptions as K, and let $W_1^\pm$ be the associated isometries as above. Then, there exists the limit*

$$\Phi(\lambda, \omega) := \lim_{t\to\infty} (K_1(t, (2\lambda)^{1/2} t\omega) - K(t, (2\lambda)^{1/2} t\omega)) \tag{1.18a}$$

taken locally uniformly in $(\lambda, \omega) \in J \times \mathbb{S}^{d-1}$, and it follows that

$$W_1^\pm = W^\pm \mathrm{e}^{\pm \mathrm{i}\Phi}. \tag{1.18b}$$

Remarks 1.18. (1) Thanks to Theorem 1.14, such K always exists for large T.

(2) Our choice of *free comparison dynamics* $U^{\pm}(t)$ is motivated in Remark 5.4.

(3) Under the conditions of Theorem 1.14, we can extend $U^{\pm}(t)$ and $W^{\pm}$ to act on $\widetilde{\mathcal{H}}_{\mathbb{R}_+}$ by covering $\mathbb{R}_+$ with disjoint intervals (as in Remark 1.13 (1)) and then taking direct sums of the corresponding restricted evolutions and restricted wave operators, respectively. Note that the summands agree with (1.17), although J and K change from interval to interval, and sum up due to the orthogonality induced by the disjointness of the intervals.

Definition 1.19. The limits $W^{\pm}$ from (1.17) are called the *time-dependent wave operators*. They are *asymptotically complete on* J' (for a closed subinterval $J' \subseteq J$) if they are unitary operators mapping $\widetilde{\mathcal{H}}_{J'}$ onto $\mathcal{H}_{J'}$.

The following result shows that stationary and time-dependent wave operators are essentially mutually inverses. First, we state a general result for classes of solutions to the stationary and the time-dependent eikonal equations, then we specialize to the concrete ones constructed geometrically and by the Legendre transform, in which case they are indeed mutually inverses.

Theorem 1.20. *Suppose Condition 1.1 with* $l = 2$.

(1) *Let* $\mathcal{F}^{\pm}$*, along with a closed interval* $I \subset \mathbb{R}_+$*,* $R > 0$*, and a stationary solution* S *of the eikonal equation, be given as in Theorem 1.12. Let* $W^{\pm}$*, along with* $\mu, T > 0$*,* $J = [\mu^2/2, \infty)$*, and a time-dependent solution* K *of the eikonal equation, be given as in Theorem 1.17. Then, there exists* $\Psi \in C((I \cap J) \times \mathbb{S}^{d-1}; \mathbb{R})$ *such that*

$$(W^{\pm})^* = \mathrm{e}^{\mp \mathrm{i}\Psi} \mathcal{F}^{\pm} \colon \mathcal{H}_{I \cap J} \to \widetilde{\mathcal{H}}_{I \cap J}. \tag{1.19}$$

In particular, $W^{\pm}$ *are asymptotically complete on* $I \cap J$.

(2) *Under the conditions of Theorems 1.3 and 1.14, let* $K \in C^2(\Omega_\mu)$ *denote the Legendre transform of* $S \in C^2(I_{\mu'} \times (\mathbb{R}^d \setminus \{0\}))$*;* $I_{\mu'} = [\mu'^2/2, \infty)$*,* $\mu > \mu' > 0$*. Then, (1.19) holds with* $I = I_{\mu'} = [\mu'^2/2, \infty)$*,* $J = [\mu^2/2, \infty)$*, and with* Ψ *taken identically zero, i.e.,*

$$(W^{\pm})^* = \mathcal{F}^{\pm} \colon \mathcal{H}_J \to \widetilde{\mathcal{H}}_J.$$

In particular, $W^{\pm}$ *are asymptotically complete on* J.

Remark 1.21. The above completeness results resemble asymptotic completeness for 2-admissible potentials as stated in [11, Theorem 30.5.10], however there given with a different free dynamics. Our approach is more related to our previous study in a geometric setting [17, 18], though more regularity of V is imposed there. In the geometric short-range setting [16], we employed only time-dependent methods, but the third order derivative was required for the analogous K, see [16, Condition 1.3 and (1.8b)].

1.2.5. Application to the 3-body problem. Our results apply to a recent development in the stationary scattering theory for 3-body long-range Hamiltonians [23]. Let us see how the application comes about in a slightly simplified form. Below, we only present a brief outline, and refer the reader to [23] for precise definitions, terminologies, and procedure. See also Remark 4.13.

Let $\mathbf{X}$ be a finite-dimensional real inner product space, and $\{\mathbf{X}^a\}_{a\in\mathcal{A}}$ a family of subspaces of $\mathbf{X}$ closed under addition. Consider the 3-body problem, i.e., assume that $\#a_{\min} = 3$. Let $V^a \in C^\infty(\mathbf{X}^a)$, $a \in \mathcal{A} \setminus \{a_{\min}, a_{\max}\}$, be pair potentials, and assume there exists $\mu \in (\sqrt{3}-1, 1)$ such that, for any $\alpha \in \mathbb{N}_0^{\dim \mathbf{X}^a}$,

$$\partial^\alpha V^a(x^a) = \mathcal{O}(\langle x^a\rangle^{-\mu-|\alpha|}).$$

Note that $\sqrt{3}-1 \approx 0,732$. We then define cut-off pair potentials $W^a \in C^\infty(\mathbf{X})$ as

$$W^a(x) = \chi(|x^a|/|x|^\mu)V^a(x^a),$$

where $\chi \in C^\infty(\mathbb{R})$ is chosen in agreement with (1.4).

Lemma 1.22. *The cut-off pair potentials W^a, $a \in \mathcal{A} \setminus \{a_{\min}, a_{\max}\}$, satisfy Condition 1.1 with $l = 2$.*

Proof. For any $\alpha \in \mathbb{N}_0^{\dim \mathbf{X}}$, we have $\partial^\alpha W^a(x) = \mathcal{O}(\langle x\rangle^{-\mu(|\alpha|+\mu)})$. The condition $\mu(2+\mu) > 2$ (required for $|\alpha| = 2$) is fulfilled exactly for $\mu > \sqrt{3}-1$. ∎

Remark 1.23. As a consequence of Lemma 1.22, our results apply to the 3-body Hamiltonian using cut-off pair potentials of long-range-type. In particular, one can derive, in a stationary manner, the asymptotic completeness for the 3-body long-range Hamiltonian along with formulas for scattering quantities, cf. [23] and Remark 4.13. Note that the previous methods in the literature do not apply at this point, since the third derivatives of W^a may not be of the form $\mathcal{O}(\langle x\rangle^{-\sigma-3})$ for some $\sigma \in (0, 1]$.

1.2.6. A further perspective: Generalization to manifolds. Our arguments are not really dependent on a specific structure of the Euclidean space, but rather on solutions to the eikonal equations (1.3a) and (1.3b), and the estimates of their derivatives. In fact, we do not even use the (ordinary) Fourier transform, and neither pseudodifferential operators nor advanced functional calculus. In our previous related works [17,18], we studied in the same spirit long-range scattering theory on a manifold with ends, employing approximate solutions to the eikonal equations. We did not develop a C^2 regularity theory using exact solutions as done in the present paper in the Euclidean setting. Moreover, we used weaker radiation condition bounds entailing a more complicated construction of the stationary scattering theory than presented here. For completeness of presentation, let us note that our older work [16] may be seen as a C^3 scattering theory on a manifold in that it involves an exact C^3 solution to the ("free") time-dependent eikonal equation, however this theory is entirely time-dependent and allows only short-range potentials.

If one could construct a "good solution" on a more general manifold, say for a suitable C^2 perturbation (by the variational method of this paper or by any other means), then the elementary techniques of the present paper would conceivably work there. Hence, the methods of this paper potentially could also contribute to stationary scattering theory on manifolds, in particular to developing a more refined low regularity theory.

1.3. Key bounds

In our stationary scattering theory, it is a major challenge to verify the WKB approximation (1.10). The following strong radiation condition bounds constitute a powerful tool for that verification, and are themselves (along with Theorem 1.3) the most important technical novelty of the paper.

Let $S \in C^l(I \times (\mathbb{R}^d \setminus \{0\}))$ be given in agreement with Theorem 1.3, and define the *gamma observables* (or alternatively referred to as *radiation observables*)

$$\begin{aligned} \gamma &= (\gamma_1, \ldots, \gamma_d) = p \mp (\nabla_x \chi_1 S), \\ \gamma_\parallel &= \mathrm{Re}((\nabla_x \chi_1 S) \cdot \gamma) = (\nabla_x \chi_1 S) \cdot \gamma - \frac{\mathrm{i}}{2}(\Delta_x \chi_1 S), \end{aligned} \tag{1.20}$$

where we have included χ_1 from (1.5) just to cut-off the singularity at the origin. We also set

$$\beta_c = \min\{2, 1 + \sigma + \rho\}.$$

Theorem 1.24. *Suppose Condition 1.1 with $l = 4$ and $q \equiv 0$. Let $I \subset \mathbb{R}_+$ be a closed interval and let $S \in C^4(I \times (\mathbb{R}^d \setminus \{0\})$ be the function from Theorem 1.3 given for each $R \geq R_0$ (for some $R_0 > 0$), and define correspondingly γ_j and $\gamma_\parallel$ as above. Then, the following bounds hold for any compact subset $I' \subseteq I \subset \mathbb{R}_+$.*

(1) *For any $\beta \in (0, \beta_c)$ and $R \geq R_0$, there exists $C > 0$, such that, for all $\lambda \in I'$ and $\psi \in L^2_{\beta+1/2}$,*

$$\|\gamma_\parallel R(\lambda \pm \mathrm{i}0)\psi\|_{L^2_{\beta-1/2}} \leq C\|\psi\|_{L^2_{\beta+1/2}}, \tag{1.21a}$$

$$\|\gamma_i\gamma_j R(\lambda \pm \mathrm{i}0)\psi\|_{L^2_{\beta-1/2}} \leq C\|\psi\|_{L^2_{\beta+1/2}}; \quad i, j = 1, \ldots, d. \tag{1.21b}$$

(2) *For any $\beta' \in (0, \beta_c/2)$, $t > 1/2$, and $R \geq R_0$, there exists $C' > 0$, such that, for all $\lambda \in I'$ and $\psi \in L^2_{\beta'+t}$,*

$$\|\gamma_i R(\lambda \pm \mathrm{i}0)\psi\|_{L^2_{\beta'-t}} \leq C'\|\psi\|_{L^2_{\beta'+t}}; \quad i = 1, \ldots, d. \tag{1.21c}$$

Remarks 1.25. (1) These are "strong" in the sense that $\beta_c > 1$, while Isozaki [14] obtained similar bounds for classical C^3 long-range potentials with $\beta_c < 1$. Such strong versions first appeared in [9] for classical C^∞ potentials.

(2) Our proof is elementary, relying only on the Cauchy–Schwarz inequality and the product rule for differentiation, and it admits considerably weaker assumptions than in [9, 14]. In fact, it applies even to C^3 potentials by redefining appropriately $\gamma_\parallel$ and $\beta_c > 1$, see Remark 3.16.

(3) See Section 3.2 for a motivation from classical mechanics. The third or higher order derivatives of V appear as purely "quantum effects," and there is no classical interpretation of their appearances. Note also that in our setting these derivatives might not have classical decay.

(4) We may let $I = \mathbb{R}_+$ by letting $C, C' > 0$ from (1.21a)–(1.21c) be dependent on $\lambda \in I$, cf. Remark 1.4 (2).

(5) The potential here is more smooth than in the Section 1.2. We will apply Theorem 1.24 to a regularized potential appearing as a technical tool, see Lemma 4.1.

The rest of the paper is organized as follows. In Section 2, we prove Theorem 1.3 following the scheme of [4]. Section 3 is devoted to the proof of Theorem 1.24, for which a commutator-type argument plays a central role. After these preliminaries, we prove Theorems 1.5, 1.10, and 1.12 and Corollary 1.8 in Section 4, where we see that the strong radiation condition bounds provide simple and intuitive proofs. Finally, in Section 5, we prove Theorems 1.14, 1.17 and 1.20.

2. Eikonal equation

In this section we prove Theorem 1.3. We will follow the framework of Cruz-Sampedro and Skibsted [4], and solve (1.6) in a somewhat abstract manner. The equation we investigate here is of the form

$$(\nabla\Phi) \cdot G^{-1}(\nabla\Phi) = 1, \tag{2.1}$$

with G being a given $(d \times d)$-matrix-valued function on $\mathbb{R}^d$, which is assumed to be sufficiently close to the identity matrix I_d. Note that the *potential* eikonal equation (1.6) is always translated into the *geometric* eikonal equation (2.1) through the change of variables

$$\Phi = (2\lambda)^{-1/2} S, \quad G = (1 - \lambda^{-1}\chi_R V) I_d. \tag{2.2}$$

Thus, the arguments of this section on (2.1) will readily apply to an S solving (1.6).

The paper [4] adopts a variational method, and we recall the precise setting in Section 2.1, quoting some results from there. The existence and smoothness of a solution to (2.1) obtained in [4] yield the corresponding assertions (1)–(3) of Theorem 1.3. Then, in Section 2.2 we discuss the remaining problems, i.e., the smoothness and the uniform bounds (1.7), under our more restrictive assumption of our paper. This completes the proof of Theorem 1.3. At the end of the section, we present Corollary 2.14, a modification of (1.7), which will be used in Sections 4 and 5.

2.1. Terminologies and results from [4]

2.1.1. Class of Riemannian metrics. In this section, we discuss the following class $\mathcal{M}_d^l$ of functions with values in square matrices of order d, or of Riemannian metrics on $\mathbb{R}^d$. Denote the set of all the real symmetric matrices of order d by $\mathcal{S}_d(\mathbb{R})$.

Definition 2.1. For any $l \in \mathbb{N}_0$, we set

$$\widetilde{\mathcal{M}}_d^l = \{G = (g_{ij})_{i,j} : \mathbb{R}^d \to \mathcal{S}_d(\mathbb{R}) \mid G \text{ is of class } C^l,\ \|G\|_l < \infty\}$$

along with

$$\|G\|_l = \sup\{\langle x\rangle^{|\alpha|}|\partial^\alpha g_{ij}(x)| \mid x \in \mathbb{R}^d,\ |\alpha| = 0,\dots,l,\ i,j = 1,\dots,d\}.$$

In addition, we set

$$\mathcal{M}_d^l = \{G \in \widetilde{\mathcal{M}}_d^l \mid \text{there exist } a,b > 0 \text{ such that } aI_d \le G(x) \le bI_d \text{ for all } x \in \mathbb{R}^d\}. \tag{2.3}$$

Remark 2.2. Obviously, $\mathcal{M}_d^l \subseteq \widetilde{\mathcal{M}}_d^l$ is open with respect to $\|\cdot\|_l$. Let I be any closed interval in $\mathbb{R}_+$ (as in Theorem 1.3). If we then let $R > 0$ be large enough, G from (2.2) can be arbitrarily close to I_d in the class $\mathcal{M}_d^2$ uniformly in $\lambda \in I$. This is due to the extra order of decay $\sigma \in (0,1)$ in (1.2a). This uniformity will be vital for our proof of Theorem 1.3.

2.1.2. Energy functional and geodesics. Next, we define a *geodesic* for $G \in \mathcal{M}_d^1$ in a variational manner. For any $p \in (1,\infty)$, we introduce the Banach space

$$X^p = (W_0^{1,p}((0,1);\mathbb{R}))^d, \quad \|\kappa\|_p = \left(\sum_{i=1}^d \int_0^1 |\dot\kappa_i(t)|^p \,\mathrm{d}t\right)^{1/p} \quad \text{for } \kappa \in X^p, \tag{2.4}$$

where $W_0^{1,p}((0,1))$ is the standard Sobolev space with the Dirichlet boundary condition, i.e., the completion of $C_c^\infty((0,1))$ with respect to the norm $\|u\|_{W^{1,p}} := \|\dot u\|_{L^p}$. Note that $\|u\|_{W^{1,p}}$ is equivalent to $\|u\|_{L^p} + \|\dot u\|_{L^p}$ due to the Poincaré inequality. For the moment, we shall particularly use the space $X := X^2$, which is a Hilbert space equipped with the inner product

$$\langle \mu, \nu \rangle_X = \langle \mu, \nu \rangle = \langle I_d; \mu, \nu \rangle = \int_0^1 \dot{\mu}(t) \cdot \dot{\nu}(t)\, \mathrm{d}t; \quad \mu, \nu \in X.$$

Here, the $d \times d$ identity matrix I_d is used symbolically to indicate that this inner product on X generates the norm $\| \cdot \|_2$ defined in (2.4). We shall below consider other quadratic forms on X than the inner product.

For any $\kappa \in X$ and $x \in \mathbb{R}^d$, define a path $\kappa_x \in (H^1(0,1))^d$ from 0 to x as

$$\kappa_x(t) = tx + \kappa(t) \quad \text{for } t \in [0,1].$$

Now, given $G \in \mathcal{M}^1_d$, we consider the *energy functional*

$$\mathcal{E}: \mathbb{R}^d \times X \to \mathbb{R}, \quad \mathcal{E}(x, \kappa) = \int_0^1 \dot{\kappa}_x(t) \cdot G(\kappa_x(t)) \dot{\kappa}_x(t)\, \mathrm{d}t. \tag{2.5}$$

Definition 2.3. Let $x \in \mathbb{R}^d$, and denote the space of the paths κ_x by

$$X_x = \{\kappa_x \in (H^1(0,1))^d \mid \kappa \in X\}.$$

We call $\gamma_x \in X_x$ a *geodesic for* $G \in \mathcal{M}^1_d$ *from* 0 *to* x *in unit time* if the associated $\gamma \in X$ satisfies

$$(\partial_\kappa \mathcal{E})(x, \gamma) = 0 \in X', \tag{2.6}$$

where X' is the dual space of X.

Remarks 2.4. (1) The duality pairing of $\partial_\kappa \mathcal{E}(x, \kappa) \in X'$ and $\mu \in X$ is directly computed as

$$\langle \partial_\kappa \mathcal{E}(x, \kappa), \mu \rangle = \int_0^1 \{2\dot{\mu} \cdot G(\kappa_x)\dot{\kappa}_x + \dot{\kappa}_x \cdot (\mu_i \partial_i G)(\kappa_x)\dot{\kappa}_x\}\, \mathrm{d}t. \tag{2.7}$$

(2) Classically, a geodesic for $G = (g_{ij})_{i,j}$ is defined as a smooth curve $y = y(t)$ in $\mathbb{R}^d$ solving

$$\ddot{y}_i + \frac{1}{2} g^{ij} (\partial_k g_{jl} + \partial_l g_{jk} - \partial_j g_{kl}) \dot{y}_k \dot{y}_l = 0 \quad \text{for } i = 1, \ldots, d, \tag{2.8}$$

where $G^{-1} = (g^{ij})_{i,j}$, or equivalently

$$G\ddot{y} = -((\dot{y} \cdot \nabla)G)\dot{y} + \frac{1}{2}\dot{y} \cdot (\nabla_\bullet G)\dot{y}. \tag{2.9}$$

Clearly, (2.6) is a weak form of (2.9) according to the expression (2.7). A geodesic in the sense of Definition 2.3 is equivalent to an H^1 curve solving the H^{-1} equation (2.9). Note that, due to the Sobolev embedding theorem for $y \in (H^1(0,1))^d$, the right-hand side of (2.9) belongs to $(L^1(0,1))^d \subseteq (H^{-1}(0,1))^d$.

(3) We shall use the notation γ, γ_x exclusively when discussing geodesics, and κ, κ_x or μ, μ_x for general paths. There would be no confusion since, as long as G is close to I_d, a geodesic is unique, see Theorem 2.6.

For any $G \in \mathcal{M}_d^2$ and $x \in \mathbb{R}^d$, there always exists at least one geodesic from 0 to x, given as follows.

Lemma 2.5. *Let $G \in \mathcal{M}_d^2$ with $a, b > 0$ as in (2.3), and let $x \in \mathbb{R}^d$. Then, there exists a minimizer $\gamma \in X$ of $\mathcal{E}(x, \cdot)$, i.e.,*

$$\mathcal{E}(x,\gamma) = \inf\{\mathcal{E}(x,\kappa) \mid \kappa \in X\},$$

and hence the associated γ_x is a geodesic for G. Moreover, for any $t \in [0,1]$,

$$\mathcal{E}(x,\gamma) = \dot\gamma_x(t) \cdot G(\gamma_x(t))\dot\gamma_x(t) \tag{2.10a}$$

and

$$\frac{a}{b}|x|^2 \le |\dot\gamma_x(t)|^2 \le \frac{b}{a}|x|^2, \quad \frac{a}{b}|tx|^2 \le |\gamma_x(t)|^2 \le \frac{b}{a}|tx|^2. \tag{2.10b}$$

Proof. It is a part of [4, Lemma 1]. We omit the proof. ■

In general, a geodesic is not necessarily associated with the minimizer of $\mathcal{E}(x,\cdot)$. However, it is the case when G is sufficiently close to I_d.

Theorem 2.6. *There exists a neighborhood $U \subseteq \mathcal{M}_d^2$ of I_d such that the following holds.*

(1) *For any $G \in U$ and $x \in \mathbb{R}^d$, there exists a unique geodesic $\gamma_x \in X_x$.*

(2) *There exists $c > 0$ such that, for any $G \in U$, $x \in \mathbb{R}^d$ and $\kappa \in X$,*

$$\langle (\partial_\kappa^2 \mathcal{E})(x,\gamma); \kappa, \kappa\rangle \ge c\|\kappa\|_2^2.$$

Moreover, for any $G \in U \cap \mathcal{M}_d^l$ with $l \ge 2$, the map $\mathbb{R}^d \ni x \mapsto \gamma \in X$ from (1) is of class C^{l-1}.

Remark 2.7. The second derivative of $\mathcal{E}(x,\cdot)$ reads for any $\kappa, \mu, \nu \in X$ as

$$\begin{aligned}\langle \partial_\kappa^2 \mathcal{E}(x,\kappa); \mu, \nu\rangle = \int_0^1 \big(&2\dot\mu \cdot G(\kappa_x)\dot\nu + 2\dot\mu \cdot (\nu_i \partial_i G)(\kappa_x)\dot\kappa_x \\ &+ 2\dot\nu \cdot (\mu_i \partial_i G)(\kappa_x)\dot\kappa_x + \dot\kappa_x \cdot (\mu_i \nu_j \partial_i \partial_j G)(\kappa_x)\dot\kappa_x\big)\, \mathrm{d}t.\end{aligned} \tag{2.11}$$

Proof. Assertions (1) and (2) follows from [4, Theorem 1 (a)], if we allow $c > 0$ to be dependent on $G \in U$. However, if we let U be small enough, we can choose c uniformly in $G \in U$ due to [4, Lemma 6]. The last assertion follows from [4, Proposition 2 1)]. Hence, we are done. ∎

2.1.3. Solution to the eikonal equation. We are ready to construct and study a specific solution to the eikonal equation (2.1).

Theorem 2.8. *Let $U \subseteq \mathcal{M}_d^2$ be given as in Theorem 2.6, $l \geq 2$, and define, for each $G \in U \cap \mathcal{M}_d^l$,*

$$\Phi\colon \mathbb{R}^d \to [0,\infty), \quad \Phi(x) = \mathcal{E}(x,\gamma)^{1/2} = (\inf\{\mathcal{E}(x,\kappa) \mid \kappa \in X\})^{1/2} \tag{2.12}$$

Then, for any $x \in \mathbb{R}^d$, the identity

$$\nabla(\Phi(x)^2) = 2G(x)\dot{\gamma}_x(1) \tag{2.13}$$

holds. Moreover, Φ is a C^l solution to (2.1) on $\mathbb{R}^d \setminus \{0\}$.

Proof. The assertion is due to [4, (36)] and [4, Proposition 2.2)], and we omit the proof. ∎

Using the above results, we can prove a part of Theorem 1.3. The proofs of the (λ, x)-smoothness and (4) will given in Section 2.2.

Proof of a part of Theorem 1.3. Suppose Condition 1.1 for some $l \geq 2$ and let I be any given closed interval in $\mathbb{R}_+$ (as in the theorem).

(1) Here we let

$$G(\lambda, x) = (1 - \lambda^{-1}\chi_R(x)V(x))I_d$$

as in (2.2). Let $U \subseteq \mathcal{M}_d^2$ be given as in Theorem 2.6, and take large $R > 0$, so that $G(\lambda,\cdot) \in U \cap \mathcal{M}_d^l$ for all $\lambda \in I$. Then, for such $G(\lambda,\cdot)$, we can find a solution $\Phi(\lambda,\cdot) \in C^l(\mathbb{R}^d \setminus \{0\})$ to (2.1) by Theorem 2.8. Thus, if we set

$$S(\lambda,\cdot) = (2\lambda)^{1/2}\Phi(\lambda,\cdot) \in C^l(\mathbb{R}^d \setminus \{0\}) \tag{2.14}$$

as in (2.2), it obviously solves (1.6). We actually have joint smoothness $S \in C^l(I \times (\mathbb{R}^d \setminus \{0\}))$, but we will verify it later.

(2) By the definition (2.12) and (2.10a), it follows that

$$\Phi(\lambda, x) = \int_0^1 \mathcal{E}(x,\gamma)^{1/2}\,\mathrm{d}t = \int_0^1 \sqrt{\dot{\gamma}_x(t) \cdot G(\gamma_x(t))\dot{\gamma}_x(t)}\,\mathrm{d}t.$$

Hence, $\Phi(\lambda, x)$ is the distance with respect to the Riemannian metric $(2\lambda)^{-1}g$ from the origin to x along γ_x. Using again (2.10a) and the fact that Φ solves (2.1), it follows that indeed $\Phi(\lambda, x)$ is the geodesic distance from the origin to x. Obviously, then $S(\lambda, \cdot)$ is the geodesic distance from the origin with respect to g.

(3) Set, for any $x \in \mathbb{R}^d \setminus \{0\}$,

$$s(\lambda, x) = |x|^{-1}\Phi(\lambda, x) - 1 = (2\lambda)^{-1/2}|x|^{-1}S(\lambda, x) - 1.$$

Then $s(\lambda, \cdot) \in C^l(\mathbb{R}^d \setminus \{0\})$, and it satisfies the asserted identity. Furthermore, it extends smoothly to the origin by letting $s(\lambda, 0) = 0$. In fact, we have $G(\lambda, x) = I$ for $|x| \leq R$, and this implies $\Phi(\lambda, x) = |x|$ or $s(\lambda, x) = 0$ there. The joint smoothness of s follows from that of S (in turn to be given in Section 2.2). ∎

2.2. Improved bounds

In this section, we prove the remaining assertions of Theorem 1.3. As for (1.7), note that the similar bounds from [4, Theorem 1 (b)] do not suffice, so we have to argue properly with the more restrictive assumptions of the present paper. The following proposition is a key for our proof. See (2.4) for the definitions of X^p and $\|\cdot\|_p$. The appearing curve $\gamma \in X$ comes from using Theorem 2.8 with the considered G.

Proposition 2.9. *Suppose Condition 1.1 for some $l \geq 2$ and let I be any given closed interval in $\mathbb{R}_+$ (as in Theorem 1.3). Consider the matrix $G = (1 - \lambda^{-1}\chi_R V)I_d$ with $\lambda \in I$ and $R > 0$.*

For any $\delta \in (0, 1)$, there exists $C > 0$ such that, uniformly in all sufficiently large $R > 0$, $k + |\alpha| = 1, \ldots, l-1$, $p \in [1+\delta, 1+\delta^{-1}]$, $\sigma' \in (0, \sigma]$ with $\sigma' p \leq 1 - \delta$ and $(\lambda, x) \in I \times \mathbb{R}^d$, the corresponding $\gamma \in X$ obeys

$$\|\partial_\lambda^k \partial_x^\alpha \gamma\|_p \leq C\lambda^{-1-k}|x|^{2-m'(k+|\alpha|+1)+k}, \tag{2.15}$$

where $m'(k) = m(k) - \sigma + \sigma'$.

Remarks 2.10. (1) Note that $\gamma = 0$ for $|x| \leq R$. Thus, $|x|$ on the right-hand side of (2.15) can be replaced by $\langle x \rangle$.

(2) Obviously, the strongest x-decay is achived choosing $\sigma' = \sigma$ in (2.15). This will be used in the proof of (1.7) simply by using the estimate for any $p \in (1, \infty)$ with $\sigma p < 1$. The (local) uniformity in p and σ' in the assertion is technically necessary for the proof of Proposition 2.9 itself, which relies on induction in l. However, our proof does not extend to the assertion of having uniformity in $p \in (1, \infty)$ rather than the stated condition $p \in [1+\delta, 1+\delta^{-1}]$.

In the proof of Proposition 2.9, we will repeatedly use the following *Hardy* and *generalized Hölder inequalities*.

Lemma 2.11. *For any $p \in (1, \infty)$ and $\kappa \in X^p$, one has*

$$\Big(\sum_{i=1}^{d} \int_0^1 |t^{-1} \kappa_i(t)|^p \, \mathrm{d}t \Big)^{1/p} \leq \frac{p}{p-1} \|\kappa\|_p. \tag{2.16}$$

Proof. The assertion follows from the one for $d = 1$, which is the well-known Hardy inequality. We omit the details. ■

Lemma 2.12. *Let $p_1, \dots, p_n \in [1, \infty]$, $n \in \mathbb{N}$, satisfy $p_1^{-1} + \cdots + p_n^{-1} = 1$. Then, for any $f_i \in L^{p_i}(0, 1)$, $i = 1, \dots, n$, one has*

$$\int_0^1 |f_1(t)| \cdots |f_n(t)| \, \mathrm{d}t \leq \|f_1\|_{L^{p_1}} \cdots \|f_n\|_{L^{p_n}}. \tag{2.17}$$

Proof. The assertion follows easily by repeated application of the familiar Hölder's inequality. We omit the details. ■

The below lemma will be useful in a reduction procedure in the proof of Proposition 2.9, see Steps I, III, and IV there.

Lemma 2.13. *For any $\delta \in (0, 1)$, take a sufficiently small neighborhood $U \subseteq \mathcal{M}_d^2$ of I_d. Then, it follows that, uniformly in $p, q \in [1 + \delta, 1 + \delta^{-1}]$, with $p^{-1} + q^{-1} = 1$, $G \in U$, $x \in \mathbb{R}^d$, $\mu \in X \cap X^p$, and $\nu \in X \cap X^q$, the corresponding $\gamma \in X$ from Theorem 2.6 obeys*

$$|\langle (\partial_\kappa^2 \mathcal{E})(x, \gamma) - 2I_d; \mu, \nu \rangle| \leq \frac{1}{2} \|\mu\|_p \|\nu\|_q.$$

Proof. Take any $\delta \in (0, 1)$. We first let $U \subseteq \mathcal{M}_d^2$ be small enough that not only Theorem 2.6 is available, but also we can find $a, b > 0$ as in (2.3) uniformly in $G \in U$. Then, by (2.11), (2.10b), Hölder's inequality, and Lemma 2.11, we can bound

$$\begin{aligned}
&|\langle (\partial_\kappa^2 \mathcal{E})(x, \gamma) - 2I_d; \mu, \nu \rangle| \\
&\quad \leq \int_0^1 |2\dot{\mu} \cdot (G - I_d)\dot{\nu} + 2\dot{\mu} \cdot (\nu_i \partial_i G)\dot{\gamma}_x \\
&\qquad\qquad + 2\dot{\nu} \cdot (\mu_i \partial_i G)\dot{\gamma}_x + \dot{\gamma}_x \cdot (\mu_i \nu_j \partial_i \partial_j G)\dot{\gamma}_x| \, \mathrm{d}t \\
&\quad \leq C_1 \|G - I_d\|_2 \int_0^1 (|\dot{\mu}||\dot{\nu}| + |\dot{\mu}||\nu|\langle tx \rangle^{-1}|x| \\
&\qquad\qquad + |\dot{\nu}||\mu|\langle tx \rangle^{-1}|x| + |\mu||\nu|\langle tx \rangle^{-2}|x|^2) \, \mathrm{d}t \\
&\quad \leq C_2 \|G - I_d\|_2 \|\mu\|_p \|\nu\|_q,
\end{aligned}$$

where $C_1, C_2 > 0$ only depend on the constants δ, a, b. Thus, possibly by letting U be smaller, the assertion follows. ■

With these preparations, we can now prove Proposition 2.9.

Proof of Proposition 2.9. The proof proceeds by induction in l with the interval $I \subset \mathbb{R}_+$ being fixed. Note that the assertion of the proposition amounts to the statement that for each $l \geq 2$ the bounds (2.15) hold uniformly in various parameters. This is a statement amenable to induction.

Fix any $l \geq 2$ and $I \subset \mathbb{R}_+$ as in the proposition. Fix also any $\delta \in (0,1)$. Then, the conclusion of Lemma 2.13 is available for $G = (1 - \lambda^{-1}\chi_R V)I$ uniformly in $\lambda \in I$ and all sufficiently large $R > 0$. In particular, it follows from the classical implicit function theorem (see e.g. [5, Theorem 15.1] or [13, Theorem C.7]) applied to the equation (2.6) with parameter (λ, x), that the mapping

$$I \times \mathbb{R}^d \to X, \quad (\lambda, x) \mapsto \gamma, \tag{2.18}$$

is of class C^{l-1}, cf. Theorem 2.6.

Step I. We first let $l = 2$, and we start with the case $k = 0$ and $|\alpha| = 1$. It suffices to show that we have, uniformly in $i = 1, \dots, d$, $p, q \in [1+\delta, 1+\delta^{-1}]$, with $p^{-1} + q^{-1} = 1$, $\sigma' \in (0, \sigma]$, with $\sigma' p \leq 1 - \delta$, $(\lambda, x) \in I \times \mathbb{R}^d$, and $\mu \in X \cap X^q$,

$$|\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle| \leq C_1 \lambda^{-1} |x|^{-\sigma'} \|\mu\|_q. \tag{2.19}$$

In fact, if (2.19) holds true, we obtain in combination with Lemma 2.13 that

$$\begin{aligned} |\langle \partial_i \gamma, \mu \rangle| &\leq \frac{1}{2} |\langle 2I_d - (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle| + \frac{1}{2} |\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle| \\ &\leq \frac{1}{4} \|\partial_i \gamma\|_p \|\mu\|_q + \frac{C_1}{2} \lambda^{-1} |x|^{-\sigma'} \|\mu\|_q. \end{aligned} \tag{2.20}$$

Note that any $\mu \in X \cap X^q$ takes the form $\mu(t) = \int_0^t (g(s) - \int_0^1 g(\tau) \mathrm{d}\tau) \mathrm{d}s$ with $g \in L^2((0,1);\mathbb{R})^d \cap L^q((0,1);\mathbb{R})^d$, and vice versa. Using arbitrary g in this class, the standard L^p-L^q duality argument and density of $L^2 \cap L^q$ in L^q allow us to compute

$$\|\partial_i \dot{\gamma}\|_{L^p} = \sup_{\|g\|_{L^q} \leq 1} |\langle \partial_i \dot{\gamma}, g \rangle_{L^2}| = \sup_{\|g\|_{L^q} \leq 1} |\langle \partial_i \gamma, \mu_g \rangle|;$$

$$\mu_g(t) = \int_0^t \left(g(s) - \int_0^1 g(\tau) \mathrm{d}\tau \right) \mathrm{d}s, \quad t \in (0,1).$$

Noting that

$$\|\mu_g\|_q = \|\dot{\mu}_g\|_{L^q} \leq 2\|g\|_{L^q},$$

it now follows from (2.20) that

$$\|\partial_i \gamma\|_p \leq \frac{1}{2} \|\partial_i \gamma\|_p + C_1 \lambda^{-1} |x|^{-\sigma'},$$

yielding the assertion (2.15) for $k = 0$ and $|\alpha| = 1$ with $C = C_2 = 2C_1$.

Step II. Here, we prove (2.19). For that, we first claim that, for any $\mu \in X$,

$$\begin{aligned}\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle = \int_0^1 \big(&2\dot{\mu} \cdot (I_d - G(\lambda, \gamma_x))e_i - 2t\dot{\mu} \cdot (\partial_i G)(\lambda, \gamma_x)\dot{\gamma}_x \\ &- 2\dot{\gamma}_x \cdot (\mu_j \partial_j G)(\lambda, \gamma_x)e_i \\ &- t\dot{\gamma}_x \cdot (\mu_j \partial_i \partial_j G)(\lambda, \gamma_x)\dot{\gamma}_x\big)\, \mathrm{d}t.\end{aligned} \tag{2.21}$$

In fact, if we differentiate (2.6) in x_i, it follows that, for any $\mu \in X$,

$$\langle (\partial_i \partial_\kappa \mathcal{E})(\lambda, x, \gamma), \mu \rangle + \langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle = 0.$$

On the other hand, also differentiating (2.7) in x_i, we have for, any $\kappa, \mu \in X$,

$$\begin{aligned}\langle \partial_i \partial_\kappa \mathcal{E}(\lambda, x, \kappa), \mu \rangle = \int_0^1 \big(&2\dot{\mu} \cdot G(\lambda, \kappa_x)e_i + 2t\dot{\mu} \cdot (\partial_i G)(\lambda, \kappa_x)\dot{\kappa}_x \\ &+ 2\dot{\kappa}_x \cdot (\mu_j \partial_j G)(\lambda, \kappa_x)e_i \\ &+ t\dot{\kappa}_x \cdot (\mu_j \partial_i \partial_j G)(\lambda, \kappa_x)\dot{\kappa}_x\big)\, \mathrm{d}t.\end{aligned}$$

We obtain (2.21) by combining the above identities and using that $\mu(0) = \mu(1) = 0$.

Next, we estimate the right-hand side of (2.21). By using (2.10b), Hölder's inequality, and the Hardy inequality (2.16), we have uniformly in the relevant parameters

$$\begin{aligned}|\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_i \gamma, \mu \rangle| &\le C_3 \lambda^{-1} \int_0^1 \big(|\dot{\mu}||tx|^{-\sigma'} + t|\dot{\mu}||tx|^{-1-\sigma'}|x| \\ &\qquad + |\mu||tx|^{-1-\sigma'}|x| + t|\mu||tx|^{-2-\sigma'}|x|^2\big)\, \mathrm{d}t \\ &\le C_4 \lambda^{-1}|x|^{-\sigma'} \int_0^1 (|\dot{\mu}|t^{-\sigma'} + |\mu|t^{-1-\sigma'})\, \mathrm{d}t \\ &\le C_5 \lambda^{-1}|x|^{-\sigma'}\|\mu\|_q.\end{aligned}$$

We have shown (2.19) and hence indeed (2.15) for $k = 0$ and $|\alpha| = 1$.

Step III. Next, we prove the assertion for $k = 1$ and $|\alpha| = 0$ along the lines of Steps I and II. In fact, we can first reduce it to proving

$$|\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_\lambda \gamma, \mu \rangle| \le C_6 \lambda^{-2}|x|^{1-\sigma'}\|\mu\|_q \tag{2.22}$$

uniformly in the relevant parameters. The reasoning is the same as in Step I with Lemma 2.13, and we omit it. Then, in order to prove (2.22), we deduce the following expression valid for any $\mu \in X$:

$$\begin{aligned}\langle (\partial_\kappa^2 \mathcal{E})(\lambda, x, \gamma); \partial_\lambda \gamma, \mu \rangle = \int_0^1 \big(&-2\dot{\mu} \cdot (\partial_\lambda G)(\lambda, \gamma_x)\dot{\gamma}_x \\ &- \dot{\gamma}_x \cdot (\mu_j \partial_j \partial_\lambda G)(\lambda, \gamma_x)\dot{\gamma}_x\big)\, \mathrm{d}t.\end{aligned} \tag{2.23}$$

Again, this formula follows in a manner similar to the first part of Step II (similar, but actually slightly simpler), and we omit the proof. Then, we bound the right-hand side of (2.23) by using (2.10b), Hölder's inequality, and the Hardy inequality (2.16),

$$\begin{aligned}|\langle(\partial_\kappa^2\mathcal{E})(\lambda,x,\gamma);\partial_\lambda\gamma,\mu\rangle| &\le C_7\lambda^{-2}\int_0^1(|\dot\mu||tx|^{-\sigma'}|x|+|\mu||tx|^{-1-\sigma'}|x|^2)\,\mathrm{d}t\\ &\le C_8\lambda^{-2}|x|^{1-\sigma'}\int_0^1(|\dot\mu|t^{-\sigma'}+|\mu|t^{-1-\sigma'})\,\mathrm{d}t\\ &\le C_9\lambda^{-2}|x|^{1-\sigma'}\|\mu\|_q.\end{aligned}$$

This amounts to (2.22), and we have shown (2.15) for $k=1$ and $|\alpha|=0$.

Step IV. From here to the end of the proof, we let $l\ge 3$. It suffices to discuss only the case $k+|\alpha|=l-1$ since the cases $k+|\alpha|=1,\dots,l-2$ follow by the induction hypothesis. In the following, let for short

$$\begin{aligned}&\beta=(k,\alpha)\in\mathbb{N}_0^{d+1},\\ &|\beta|=k+|\alpha|=l-1,\\ &\partial^\beta=\partial^\beta_{\lambda,x}=\partial_\lambda^k\partial_x^\alpha.\end{aligned}$$

Here, we only note that the proof is reduced to verifying

$$|\langle(\partial_\kappa^2\mathcal{E})(\lambda,x,\gamma);\partial^\beta\gamma,\mu\rangle|\le C_1\lambda^{-1-k}|x|^{2-m'(l)+k}\|\mu\|_q \tag{2.24}$$

uniformly in $\mu\in X\cap X^q$ and the relevant parameters. This is indeed a valid reduction, which may be seen by mimicking Step I. Again, we omit the details.

Step V. To show (2.24), we proceed in parallel to Steps II and III, differentiating (2.6). Indeed, repeated differentiation of (2.6) in (λ,x) yields the Faà di Bruno formula

$$\langle(\partial_\kappa^2\mathcal{E})(\lambda,x,\gamma);\partial^\beta\gamma,\mu\rangle=\sum_{n,\beta^0,\dots,\beta^n}C_*\langle(\partial^{\beta^0}\partial_\kappa^{n+1}\mathcal{E})(\lambda,x,\gamma);\partial^{\beta^1}\gamma,\dots,\partial^{\beta^n}\gamma,\mu\rangle, \tag{2.25}$$

where the indices $n\in\mathbb{N}_0$, $\beta^i=(k^i,\alpha^i)\in\mathbb{N}_0\times\mathbb{N}_0^d$, $i=0,\dots,n$, run over

$$n=0,\dots,l-1,\quad \beta^0+\dots+\beta^n=\beta,\quad 1\le|\beta^i|\le l-2\quad\text{for } i=1,\dots,n. \tag{2.26}$$

Here and below, combinatorial constants are denoted simply by $C_*\in\mathbb{N}$ without distinction.

Let us further write down a detailed expression of the summand of (2.25). Directly differentiating the definition (2.5), we can compute $\partial_\kappa^{n+1}\mathcal{E}(\lambda,x,\kappa)$ as

$$\begin{aligned}\langle\partial_\kappa^{n+1}\mathcal{E}(\lambda,x,\kappa);\mu^1,\dots,\mu^{n+1}\rangle &= \sum_{|\eta|=n+1} C_* \int_0^1 (\partial_x^\eta g_{ab})(\dot\kappa_x)_a(\dot\kappa_x)_b\mu^1_{c_1}\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{|\eta|=n} C_* \int_0^1 (\partial_x^\eta g_{ab})(\dot\kappa_x)_b\mu^1_{c_1}\cdots\dot\mu^i_a\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{|\eta|=n-1} C_* \int_0^1 (\partial_x^\eta g_{ab})\mu^1_{c_1}\cdots\dot\mu^i_a\cdots\dot\mu^j_b\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t.\end{aligned}$$

Here and henceforth, $\dot\mu^i_a$ and $\dot\mu^j_b$ replace the corresponding factors, and for short we omit appropriate summations in $a, b, c_1, \dots, c_{n+1}, i, j$ as well as a specification of the combinatorial constants $C_* \in \mathbb{N}$. Also, we abbreviate $(\partial_x^\eta g_{ab})(\kappa_x) = (\partial_x^\eta g_{ab})$. Let below $\{e_1,\dots,e_d\}$ denote the standard basis in $\mathbb{R}^d$. We then proceed, applying $\partial^{\beta^0} = \partial_\lambda^{k^0}\partial_x^{\alpha^0}$ (as defined above), as

$$\begin{aligned}&\langle\partial^{\beta^0}\partial_\kappa^{n+1}\mathcal{E}(\lambda,x,\kappa);\mu^1,\dots,\mu^{n+1}\rangle \\ &= \sum_{\substack{|\eta|=n+1,\\ e_a+e_b\le\alpha^0}} C_* \int_0^1 t^{|\alpha^0|-2}(\partial^{(k^0,\alpha^0-e_a-e_b+\eta)}g_{ab})\mu^1_{c_1}\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{\substack{|\eta|=n+1,\\ e_b\le\alpha^0}} C_* \int_0^1 t^{|\alpha^0|-1}(\partial^{(k^0,\alpha^0-e_b+\eta)}g_{ab})(\dot\kappa_x)_a\mu^1_{c_1}\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{|\eta|=n+1} C_* \int_0^1 t^{|\alpha^0|}(\partial^{(k^0,\alpha^0+\eta)}g_{ab})(\dot\kappa_x)_a(\dot\kappa_x)_b\mu^1_{c_1}\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{\substack{|\eta|=n,\\ e_b\le\alpha^0}} C_* \int_0^1 t^{|\alpha^0|-1}(\partial^{(k^0,\alpha^0-e_b+\eta)}g_{ab})\mu^1_{c_1}\cdots\dot\mu^i_a\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{|\eta|=n} C_* \int_0^1 t^{|\alpha^0|}(\partial^{(k^0,\alpha^0+\eta)}g_{ab})(\dot\kappa_x)_b\mu^1_{c_1}\cdots\dot\mu^i_a\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t \\ &\quad + \sum_{|\eta|=n-1} C_* \int_0^1 t^{|\alpha^0|}(\partial^{(k^0,\alpha^0+\eta)}g_{ab})\mu^1_{c_1}\cdots\dot\mu^i_a\cdots\dot\mu^j_b\cdots\mu^{n+1}_{c_{n+1}}\,\mathrm{d}t.\end{aligned}$$

We substitute $\kappa = \gamma, \mu^1 = \partial^{\beta^1}\gamma, \dots, \mu^n = \partial^{\beta^n}\gamma$ and $\mu^{n+1} = \mu$ in the above formula, and denote the corresponding six types of integrals on the right-hand side simply as $I_1, \dots, I_6$, respectively. Then it suffices to estimate each such integral in agreement with (2.24).

Step IV. Finally, we bound the above $I_1, \dots, I_6$. They are treated similarly by using (1.2a), (2.10b), the generalized Hölder inequality (2.17), the Hardy inequality (2.16), and the induction hypothesis. We may let $|x| \geq R$ below, see Remark 2.10 (1).

We carefully bound I_1, while we record only key steps for $I_2, \dots, I_6$ (they are treated similarly). Use (1.2a), (2.10b), and $|\eta| = n + 1$, to bound it for $|x| \geq R$ as

$$\begin{aligned} |I_1| &\leq C_2\lambda^{-1-k^0}\int_0^1 t^{|\alpha^0|-2}|tx|^{-m'(|\alpha^0|+|\eta|-2)}|\partial^{\beta^1}\gamma_{c_1}|\cdots|\partial^{\beta^n}\gamma_{c_n}||\mu_{c_{n+1}}|\,\mathrm{d}t \\ &\leq C_3\lambda^{-1-k^0}|x|^{-m'(|\alpha^0|+n-1)}\int_0^1 t^{-\sigma'}|t^{-1}\partial^{\beta^1}\gamma_{c_1}|\cdots|t^{-1}\partial^{\beta^n}\gamma_{c_n}||t^{-1}\mu_{c_{n+1}}|\,\mathrm{d}t. \end{aligned} \tag{2.27}$$

We take large $p_0, \dots, p_n \in (1, \infty)$ and small $\sigma_1', \dots, \sigma_n' \in (0, \sigma]$ such that

$$p_0^{-1} + \dots + p_{n+1}^{-1} = 1 - q^{-1} = p^{-1}, \quad \sigma' p_0 < 1, \quad \sigma_1' p_1 < 1, \ \dots, \ \sigma_{n+1}' p_{n+1} < 1,$$

and apply the generalized Hölder inequality (2.17) and the Hardy inequality (2.16) to (2.27). Note that here and henceforth $\delta \in (0, 1)$, $p \in [1 + \delta, 1 + \delta^{-1}]$ and $\sigma' \in (0, \sigma]$ with $\sigma' p \leq 1 - \delta$ are given parameters as in Proposition 2.9. Then, we use the induction hypothesis with a sufficiently smaller $\delta \in (0, 1)$ (to make sure that $p_i \in [1 + \delta, 1 + \delta^{-1}]$ and $\sigma' p_i \leq 1 - \delta$) and with $m_i'(k) = m(k) - \sigma + \sigma_i'$.

Noting also (2.26) and $|\beta^0| - k^0 + n + 1 = |\alpha^0| + n + 1 \geq 2$ by $e_a + e_b \leq \alpha^0$, it follows that, for $|x| \geq R$,

$$\begin{aligned} |I_1| &\leq C_4\lambda^{-1-k^0}|x|^{2-m'(|\alpha^0|+n+1)}\|\partial^{\beta^1}\gamma\|_{p_1}\cdots\|\partial^{\beta^n}\gamma\|_{p_n}\|\mu\|_q \\ &\leq C_5\lambda^{-1-k}|x|^{2-m'(|\beta^0|-k^0+n+1)+(2-m_1'(|\beta^1|+1)+k^1)+\dots+(2-m_n'(|\beta^n|+1)+k^n)}\|\mu\|_q \\ &\leq C_6\lambda^{-1-k}|x|^{2-m'(|\beta|-k^0+1)+k-k^0}\|\mu\|_q \\ &\leq C_7\lambda^{-1-k}|x|^{2-m'(l)+k}\|\mu\|_q. \end{aligned} \tag{2.28}$$

This agrees with (2.24), as wanted.

As for $I_2, \dots, I_6$, we aim at deducing a bound similar to the first line of (2.28), since then the remaining arguments are essentially the same. More precisely, for the cases where $|\beta^0| - k^0 + n + 1 \geq 2$ is valid, this condition and the induction hypothesis suffice for the final conclusion of (2.28). If $|\beta^0| - k^0 + n + 1 = 1$, we can proceed similarly to reach from the first line of (2.28) to the final line of the estimation.

We can bound I_2 similarly to

$$\begin{aligned}|I_2| &\leq C_8 \lambda^{-1-k^0} \int_0^1 t^{|\alpha^0|-1} |tx|^{-m'(|\alpha^0|+|\eta|-1)} |x| |\partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^n} \gamma_{c_n}| |\mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_9 \lambda^{-1-k^0} |x|^{1-m'(|\alpha^0|+n)} \int_0^1 t^{-\sigma'} |t^{-1} \partial^{\beta^1} \gamma_{c_1}| \cdots |t^{-1} \partial^{\beta^n} \gamma_{c_n}| |t^{-1} \mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{10} \lambda^{-1-k^0} |x|^{2-m'(|\alpha^0|+n+1)} \|\partial^{\beta^1} \gamma\|_{p_1} \cdots \|\partial^{\beta^n} \gamma\|_{p_n} \|\mu\|_q,\end{aligned}$$

and from there we proceed as in (2.28) (as explained above). As for I_3, we bound it as

$$\begin{aligned}|I_3| &\leq C_{11} \lambda^{-1-k^0} \int_0^1 t^{|\alpha^0|} |tx|^{-m'(|\alpha^0|+|\eta|)} |x|^2 |\partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^n} \gamma_{c_n}| |\mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{12} \lambda^{-1-k^0} |x|^{2-m'(|\alpha^0|+n+1)} \int_0^1 |t|^{-\sigma'} |t^{-1} \partial^{\beta^1} \gamma_{c_1}| \cdots |t^{-1} \partial^{\beta^n} \gamma_{c_n}| |t^{-1} \mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{13} \lambda^{-1-k^0} |x|^{2-m'(|\alpha^0|+n+1)} \|\partial^{\beta^1} \gamma\|_{p_1} \cdots \|\partial^{\beta^n} \gamma\|_{p_n} \|\mu\|_q.\end{aligned}$$

From I_4, there appears a factor which is either directly bounded by $\|\partial^{\beta^*} \gamma\|_{p_*}$ without the Hardy bound, or alternatively a factor bounded by the L^q-norm of $\dot{\mu}$. Hence, typically I_4 and I_5 are bounded as

$$\begin{aligned}|I_4| &\leq C_{14} \lambda^{-1-k^0} \int_0^1 t^{|\alpha^0|-1} |tx|^{-m'(|\alpha^0|+|\eta|-1)} \\ &\qquad \cdot |\partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^i} \dot{\gamma}_a| \cdots |\partial^{\beta^n} \gamma_{c_n}| |\mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{15} \lambda^{-1-k^0} |x|^{-m'(|\alpha^0|+n-1)} \\ &\qquad \cdot \int_0^1 t^{-\sigma'} |t^{-1} \partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^i} \dot{\gamma}_a| \cdots |t^{-1} \partial^{\beta^n} \gamma_{c_n}| |t^{-1} \mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{16} \lambda^{-1-k^0} |x|^{2-m'(|\alpha^0|+n+1)} \|\partial^{\beta^1} \gamma\|_{p_1} \cdots \|\partial^{\beta^n} \gamma\|_{p_n} \|\mu\|_q,\end{aligned}$$

and

$$\begin{aligned}|I_5| &\leq C_{17} \lambda^{-1-k_0} \int_0^1 t^{|\alpha^0|} |tx|^{-m'(|\alpha^0|+|\eta|)} |x| |\partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^i} \dot{\gamma}_a| \cdots |\partial^{\beta^n} \gamma_{c_n}| |\mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{18} \lambda^{-1-k_0} |x|^{1-m'(|\alpha^0|+n)} \int_0^1 t^{-\sigma'} |t^{-1} \partial^{\beta^1} \gamma_{c_1}| \cdots |\partial^{\beta^i} \dot{\gamma}_a| \cdots \\ &\qquad \cdot |t^{-1} \partial^{\beta^n} \gamma_{c_n}| |t^{-1} \mu_{c_{n+1}}| \, \mathrm{d}t \\ &\leq C_{19} \lambda^{-1-k^0} |x|^{2-m'(|\alpha^0|+n+1)} \|\partial^{\beta^1} \gamma\|_{p_1} \cdots \|\partial^{\beta^n} \gamma\|_{p_n} \|\mu\|_q.\end{aligned}$$

Finally, we can typically bound I_6 as

$$
\begin{aligned}
|I_6| &\le C_{20}\lambda^{-1-k_0} \\
&\quad \cdot \int_0^1 t^{|\alpha^0|}|tx|^{-m'(|\alpha^0|+|\eta|)}|\partial^{\beta^1}\gamma_{c_1}|\cdots|\partial^{\beta^i}\dot\gamma_a|\cdots|\partial^{\beta^j}\dot\gamma_b|\cdots|\partial^{\beta^n}\gamma_{c_1}||\mu_{c_{n+1}}|\,\mathrm{d}t \\
&\le C_{21}\lambda^{-1-k_0}|x|^{-m'(|\alpha^0|+n-1)} \\
&\quad \cdot \int_0^1 t^{-\sigma'}|t^{-1}\partial^{\beta^1}\gamma_{c_1}|\cdots|\partial^{\beta^i}\dot\gamma_a|\cdots|\partial^{\beta^j}\dot\gamma_b|\cdots|t^{-1}\partial^{\beta^n}\gamma_{c_n}||t^{-1}\mu_{c_{n+1}}|\,\mathrm{d}t \\
&\le C_{22}\lambda^{-1-k^0}|x|^{2-m'(|\alpha^0|+n+1)}\|\partial^{\beta^1}\gamma\|_{p_1}\cdots\|\partial^{\beta^n}\gamma\|_{p_n}\|\mu\|_q.
\end{aligned}
$$

Therefore, we are done. ∎

We complete the proof of Theorem 1.3 as follows.

Completion of the proof of Theorem 1.3. Fix a closed interval $I \subset \mathbb{R}_+$ and $p \in (1,\infty)$ with $\sigma p < 1$, and let $R > 0$ be large as in Proposition 2.9. For any $k + |\alpha| \le l$, it suffices to argue for $|x| > R$ since s vanishes for $|x| \le R$. All the estimates below are tacitly understood to be uniform in $\lambda \in I$.

Step I. We first show that, for any $k + |\alpha| \le l - 1$ and $|x| > R$,

$$|\partial_\lambda^k \partial_x^\alpha \dot\gamma(1)| \le C_1\lambda^{-1-k}|x|^{2-m(k+|\alpha|+1)+k}. \tag{2.29}$$

We may let $k + |\alpha| \ge 1$ since the case $k + |\alpha| = 0$ follows from (2.29) with $k = 0$ and $|\alpha| = 1$ and integration. Now, let us use a representation

$$(\partial_\lambda^k \partial_x^\alpha \dot\gamma)(1) = 2\int_{1/2}^1 \left((\partial_\lambda^k \partial_x^\alpha \dot\gamma)(t) + \int_t^1 (\partial_\lambda^k \partial_x^\alpha \ddot\gamma)(\tau)\,\mathrm{d}\tau\right)\mathrm{d}t. \tag{2.30}$$

This is due to the fundamental theorem of calculus, but in fact we have to check integrability of the integrands.

By Proposition 2.9 and Hölder's inequality, it follows that

$$\|\partial_\lambda^k \partial_x^\alpha \dot\gamma\|_{L^1(1/2,1)^d} \le C_2\lambda^{-1-k}|x|^{2-m(k+|\alpha|+1)+k}, \tag{2.31}$$

where the norm on the left-hand side denotes the L^1-norm of a function on the interval $(1/2, 1)$ with values in $\mathbb{R}^d$.

On the other hand, as for $\partial_\lambda^k \partial_x^\alpha \ddot\gamma$, we compute it using the expression

$$\ddot\gamma_n = -\frac{1}{2}g^{nl}(\partial_i g_{jl} + \partial_j g_{il} - \partial_l g_{ij})(\dot\gamma_x)_i(\dot\gamma_x)_j =: -\Gamma_{ij}^n(\dot\gamma_x)_i(\dot\gamma_x)_j \tag{2.32}$$

following from (2.8). By (2.32), the product rule and the chain rule of differentiation we can write

$$\partial_\lambda^k \partial_x^\alpha \ddot{\gamma}_n = \sum C_*(\partial_\lambda^{k^0} \partial_x^\eta \Gamma_{ij}^n)\Big(\prod_{a=1}^{d}\prod_{b=1}^{\eta_a}(\partial_\lambda^{k^{ab}} \partial_x^{\alpha^{ab}} \gamma_x)_a\Big)(\partial_\lambda^{k^1} \partial_x^{\alpha^1} \dot{\gamma}_x)_i(\partial_\lambda^{k^2} \partial_x^{\alpha^2} \dot{\gamma}_x)_j, \tag{2.33}$$

where the indices $k^0, k^{ab}, k^1, k^2 \in \mathbb{N}_0$ and $\eta, \alpha^{ab}, \alpha^1, \alpha^2 \in \mathbb{N}_0^d$ run over

$$\begin{aligned} &k^{ab} + |\alpha^{ab}| \geq 1, \quad k^0 + \sum_{a=1}^{d}\sum_{b=1}^{\eta_a} k^{ab} + k^1 + k^2 = k, \\ &|\eta| = 0, \ldots, k + |\alpha|, \quad \sum_{a=1}^{d}\sum_{b=1}^{\eta_a} \alpha^{ab} + \alpha^1 + \alpha^2 = \alpha. \end{aligned} \tag{2.34}$$

Note we read $\prod_{b=1}^{\eta_a}(\partial_\lambda^{k^{ab}} \partial_x^{\alpha^{ab}} \gamma_x)_a = 1$ if $\eta_a = 0$.

We recall that $\gamma_x(\tau) = \tau x + \gamma(\tau)$, and since $\tau \in [1/2, 1]$, we do not have to worry about inverse powers of τ when estimating $\partial_\lambda^{k^0} \partial_x^\eta \Gamma_{ij}^n$ by Lemma 2.5 (as we did in the proof of Proposition 2.9). On the other hand, when taking x-derivatives of γ_x, there are still contributions from differentiating the first term τx, that in addition to the derivatives of γ need consideration. The latter are treated by Proposition 2.9. We prefer the following uniform treatment:

$$\|(\partial_\lambda^{k^{ab}} \partial_x^{\alpha^{ab}} \gamma_x)_a\|_{L^p(1/2,1)} \leq C_p \lambda^{-k^{ab}} |x|^{-\frac{\rho+1}{2}(k^{ab}+|\alpha^{ab}|-1)+k^{ab}}, \tag{2.35a}$$

$$\|(\partial_\lambda^{k^1} \partial_x^{\alpha^1} \dot{\gamma}_x)_i\|_{L^p(1/2,1)} \leq C_p \lambda^{-k^1} |x|^{1-\frac{\rho+1}{2}(k^1+|\alpha^1|)+k^1}, \tag{2.35b}$$

$$\|(\partial_\lambda^{k^2} \partial_x^{\alpha^2} \dot{\gamma}_x)_j\|_{L^p(1/2,1)} \leq C_p \lambda^{-k^2} |x|^{1-\frac{\rho+1}{2}(k^2+|\alpha^2|)+k^2}. \tag{2.35c}$$

For any term with $\eta \neq 0$ in the expansion (2.33), say denoted by T, we can show an estimate agreeing with (2.31). In fact, by using (2.10b), (2.34), (2.35) with $p = |\eta| + 2$, the generalized Hölder inequality (2.17) (with this p applied to each of the p factors), the Hardy inequality (2.16), and Proposition 2.9, we can estimate

$$\begin{aligned} \|T\|_{L^1(1/2,1)} &\leq C_3 \sum \lambda^{-1-k^0} |x|^{-m(|\eta|+1)} \\ &\quad \cdot \Big(\prod_{a=1}^{d}\prod_{b=1}^{\eta_a} \lambda^{-k^{ab}} |x|^{-\frac{\rho+1}{2}(k^{ab}+|\alpha^{ab}|-1)+k^{ab}}\Big) \\ &\quad \cdot \lambda^{-k^1} |x|^{1-\frac{\rho+1}{2}(k^1+|\alpha^1|)+k^1} \lambda^{-k^2} |x|^{1-\frac{\rho+1}{2}(k^2+|\alpha^2|)+k^2} \\ &\leq C_4 \lambda^{-1-k} |x|^{2-m(k+|\alpha|+1)+k}. \end{aligned}$$

For any term with $\eta = 0$ in the expansion (2.33), we use the following estimates. For $k^1 + |\alpha^1| \geq 1$, the second bound of (2.35) can be replaced by a sharper bound (similar to the first bound of (2.35)),

$$\|(\partial_\lambda^{k^1}\partial_x^{\alpha^1}\dot\gamma_x)_i\|_{L^p(1/2,1)} \le C_p'\lambda^{-k^1}|x|^{-\frac{\rho+1}{2}(k^1+|\alpha^1|-1)+k^1}, \quad k^1+|\alpha^1|\ge 1,$$

and similarly for the third bound for $k^2+|\alpha^2|\ge 1$. Thanks to these sharper bounds, we can then argue similarly for the case $\eta=0$, obtaining an estimate for any such term also agreeing with (2.31). This is straightforward, and we omit the details. Hence, we conclude that

$$\|\partial_\lambda^k\partial_x^\alpha\ddot\gamma\|_{L^1(1/2,1)^d} \le C_5\lambda^{-1-k}|x|^{2-m(k+|\alpha|+1)+k}. \tag{2.36}$$

Clearly, (2.30) and the bounds (2.31) and (2.36) yield (2.29).

Step II. Now, to check the smoothness of S and s in (λ,x) up to order l, it suffices for partial derivatives with $\alpha\neq 0$ to prove the continuity of derivatives of $\dot\gamma_x(1)$ (or of $\dot\gamma(1)$) up to order $l-1$. Here, we use (2.14) and (2.13). However, this is already implicitly done in our treatment of (2.30) in Step I, which is based on the C^{l-1}-smoothness of (2.18) from Proposition 2.9. For derivatives with $\alpha=0$, i.e., containing only λ-derivatives, we differentiate (2.12) in λ, leading (thanks to the stationarity condition $(\partial_\kappa\mathcal{E})(\lambda,x,\gamma)=0$) to

$$2|x|\Phi(\partial_\lambda s) = (\partial_\lambda\mathcal{E})(\lambda,x,\gamma) = \lambda^{-2}\int_0^1 \chi_R V|\dot\gamma_x|^2\,\mathrm{d}t,$$

from which we deduce the formula

$$\partial_\lambda s = 2^{-1}|x|^{-2}(1+s)^{-1}\lambda^{-2}\int_0^1 \chi_R V|\dot\gamma_x|^2\,\mathrm{d}t. \tag{2.37a}$$

Inductively, we can differentiate (2.37b) up to $l-1$ times in λ, manifestly yielding continuous expressions for $\partial_\lambda^k s$, $k=1,\dots,l$.

Step III. We are left with (1.7). Integrating the expression (2.13) using (2.2) and (2.29) for $k+|\alpha|=0$, we obtain

$$S(\lambda,x)^2 = (2\lambda)(x^2+\mathcal{O}(\lambda^{-1}|x|^{2-\sigma})),$$

and hence (1.7) for $k+|\alpha|=0$. Next, by (2.13), (2.2) and Theorem 1.3 (3), we can write

$$\nabla_x s = |x|^{-2}(1+s)^{-1}[\dot\gamma(1) - \lambda^{-1}x\chi_R V - \lambda^{-1}\chi_R V\dot\gamma(1) - xs(2+s)]. \tag{2.37b}$$

Using this representation and (2.29), we can inductively obtain (1.7) for $k = 0$ and all $|\alpha| \le l$. The straightforward details are omitted. Along the same line, any general mixed derivative can be computed and estimated from (2.37b). Hence, we conclude (1.7) for all $k + |\alpha| \le l$, assuming $\alpha \neq 0$.

To treat pure λ-derivatives, we use (2.37a), leading to

$$|\partial_\lambda s| \le C_6 \lambda^{-2} |x|^{-2} \int_0^1 |tx|^{-\sigma} \, |x|^2 \, \mathrm{d}t = C_7 \lambda^{-2} |x|^{-\sigma},$$

showing (1.7) for $k = 1$ and $\alpha = 0$. We can inductively show (1.7) for $|\alpha| = 0$ and all $k \le l$ by repeated λ-differentiation of (2.37a) and check of the resulting expressions. This is more complicated than for mixed derivatives, so let us give some details of the proof. We compute $\partial_\lambda^k \int_0^1 \chi_R V |\dot{\gamma}_x|^2 \, \mathrm{d}t$ by differentiating inside the integral using the product rule. Since $(\chi_R V)(\gamma_x(t))$ is a composition, we need the chain rule to compute λ-derivatives of this factor, more or less as we did in Step I. This leads to multiple factors of $\partial_\lambda^k \gamma_x(t)/t$ for which we have good L^p-bounds. So, the main thing is to bound the derivatives $(\partial_x^\eta(\chi_R V))(\gamma_x(t))$ of the external factor, and for that we mimic Step VI of the proof of Proposition 2.9 by estimating

$$|\partial_x^\eta(\chi_R V)| \le C_8 |tx|^{-m(|\eta|)}.$$

In parallel to the estimation of $\partial_\lambda s$, this yields the factor $|x|^{-m(|\eta|)}$ as well as the factor $t^{-m(|\eta|)} = t^{-\sigma} t^{\sigma - m(|\eta|)}$. Choosing a small enough $p > 1$, the familiar generalized Hölder inequality yields a bound in terms for the L^1-norm of $t^{-\sigma p}$ and (after a redistribution of powers of t^{-1} as in Step VI) products of various X^{p_j}-norms for which Proposition 2.9 applies. We omit the book-keeping details.

Hence, we have proven (1.7) for all $k + |\alpha| \le l$. ■

In Sections 4 and 5 we will actually use the following modification of (1.7).

Corollary 2.14. *For any closed interval $I \subset \mathbb{R}_+$ let $s_R \in C^l(I \times \mathbb{R}^d)$ be given as in Theorem 1.3 for $R \ge R_0$, where $R_0 > 0$ is taken sufficiently large. Then, there exists $C > 0$ such that for any $R \ge R_0$, $\sigma' \in (0, \sigma]$, $k + |\alpha| \le l$, and $(\lambda, x) \in I \times \mathbb{R}^d$*

$$|\partial_\lambda^k \partial_x^\alpha s(\lambda, x)| \le C R^{-\sigma + \sigma'} \lambda^{-1-k} \langle x \rangle^{-m'(k + |\alpha|) + k},$$

where $m'(k)$ is given in Proposition 2.9.

Proof. The assertion follows from the arguments of the subsection with all the estimates involving

$$|\partial^\alpha \chi_R V| \le C_1 \langle x \rangle^{-m(|\alpha|)}$$

replaced by

$$|\partial^\alpha \chi_R V| \le C_2 R^{-\sigma+\sigma'} \langle x\rangle^{-m'(|\alpha|)}.$$

It is straightforward, and we omit repeating the arguments. ■

3. Strong radiation condition bounds

In this section, we prove Theorem 1.24. Our main tool is a commutator-type argument. We adopt a second order differential operator as our conjugate operator, whereas the standard Mourre theory employs a first order one. This might appear rather peculiar, since the resulting operator would be of third order, which usually cannot have a sign. However, we repeatedly use a certain *increment or decrement identity* to make it of even order with a definite sign.

We first introduce the needed notation in Section 3.1, and then discuss classical mechanics interpretations in Section 3.2. Motivated by the classical picture, the main propositions of the section will be presented in Section 3.3. After some preliminaries in Section 3.4, these propositions will be proved in Section 3.5. Finally, in Section 3.6 we will complete the proof of Theorem 1.24.

3.1. Notation

Throughout the section, we assume Condition 1.1 with $l = 4$ and $q \equiv 0$. Let $I \subset \mathbb{R}_+$ be a closed interval, and let $S \in C^4(I \times (\mathbb{R}^d \setminus \{0\}))$ be the function from Theorem 1.3 given for $R \ge R_0 > 0$.

According to Theorem 1.3, $S(\lambda,\cdot)$ is a geodesic distance from the origin. It is convenient to normalize this function and consider $\Phi(\lambda,\cdot) = S(\lambda,\cdot)/\sqrt{2\lambda}$, exactly as done in Section 2, but even then the singularity at the origin might cause problems. Consequently, we regularize $\Phi(\lambda,\cdot)$ as follows.

Lemma 3.1. *For all $R \ge R_0$, there exists $f \in C^4(I \times \mathbb{R}^d)$ such that (with the dependence on $\lambda \in I$ and $R \ge R_0$ being suppressed)*

$$f(x) = (2\lambda)^{-1/2} S(\lambda, x) \quad \textit{for any } \lambda \in I \textit{ and } |x| > R. \tag{3.1}$$

Moreover (with all constants below being independent of λ and R),

(1) *there exist $c, C > 0$ such that, for any $(\lambda, x) \in I \times \mathbb{R}^d$,*

$$c\langle x\rangle \le f(x) \le C\langle x\rangle; \tag{3.2a}$$

(2) *there exists $C' > 0$ such that for, any $|\alpha| \le 4$, $(\lambda, x) \in I \times \mathbb{R}^d$,*

$$|\partial^\alpha f(x)| \le C' f(x)^{1-\min\{|\alpha|, m(|\alpha|)\}}; \tag{3.2b}$$

(3) *there exists* $C'' > 0$ *such that, for any* $(\lambda, x) \in I \times \mathbb{R}^d$,

$$(1 - C'' f^{-\sigma}) I_d \leq (\nabla f) \otimes (\nabla f) + f(\nabla^2 f) \leq (1 + C'' f^{-\sigma}) I_d. \quad (3.2c)$$

Proof. Such modification is clearly possible due to Theorem 1.3. We omit the details. ∎

Remark 3.2. In Section 4, we will use the slight modification of (3.2c) given with $C'' f^{-\sigma}$ replaced by $C''' R^{-\sigma'+\sigma} f^{-\sigma'}$, $\sigma' \in (0, \sigma)$.

3.2. Classical mechanics

Here we present a stationary bound holding along a classical scattering orbit in the phase space $T^*\mathbb{R}^d \cong \mathbb{R}^{2d}$. The arguments of this section are not necessary for our purpose, but they serve as important motivation for our proof of Theorem 1.24. Moreover, the proof here will be directly "lifted" to quantum mechanics, apart from the fact that quantum observables of course do not generally commute.

3.2.1. Free Hamiltonian. Let us start with the trivial case with $V \equiv 0$, for simplicity. Hence, we consider the free classical Hamiltonian

$$H_0^{\mathrm{cl}}(x, \xi) = \frac{1}{2}\xi^2 \quad \text{for } (x, \xi) \in \mathbb{R}^{2d},$$

and the associated Hamilton equations

$$\dot{x} = \xi, \quad \dot{\xi} = 0.$$

Then, for any initial data $(y, \eta) \in \mathbb{R}^{2d}$, we have an explicit classical orbit

$$x(t) = \eta t + y, \quad \xi(t) = \eta.$$

Assuming the orbit has a positive energy

$$\lambda = H_0^{\mathrm{cl}}(x(t), \xi(t)) = \frac{1}{2}\eta^2 > 0,$$

which is fixed, we discuss the asymptotic relation between observables along the orbit. Obviously, it follows that (forward in time)

$$\xi = \sqrt{2\lambda}|x|^{-1}x + \mathcal{O}(t^{-1}) \quad \text{as } t \to \infty, \quad (3.3)$$

and hence the momentum ξ is comparable to $\sqrt{2\lambda}|x|^{-1}x$. However, we would like to express it in a stationary manner without time parameter. For that purpose, note

$$|x| = \sqrt{2\lambda}t + \mathcal{O}(1) \quad \text{as } t \to \infty.$$

This implies that the quantity $|x|$ is an “effective time” up to a constant factor, allowing us to replace the time parameter. Now, let us introduce the “classical gamma observables” as

$$\gamma^{\mathrm{cl}} = \xi - (\nabla S_0), \quad \gamma^{\mathrm{cl}}_{\parallel} = (\nabla S_0)\cdot\gamma^{\mathrm{cl}}; \quad S_0 = \sqrt{2\lambda}|x|, \tag{3.4}$$

cf. (1.20). Then we obtain a stationary expression of (3.3) as

$$\gamma^{\mathrm{cl}} = \mathcal{O}(|x|^{-1}). \tag{3.5}$$

Furthermore, it follows that

$$\gamma^{\mathrm{cl}}_{\parallel} = H^{\mathrm{cl}}_0 - \lambda - \frac{1}{2}(\gamma^{\mathrm{cl}})^2 = -\frac{1}{2}(\gamma^{\mathrm{cl}})^2 = \mathcal{O}(|x|^{-2}).$$

Note that the bound $\gamma^{\mathrm{cl}}_{\parallel} = \mathcal{O}(|x|^{-2})$ is sharper than the bound resulting from substituting (3.5) into the middle expression of (3.4) . This is our starting point.

3.2.2. Perturbed Hamiltonian. Next, we turn to the general case of a classical C^2 long-range potential V. We discuss the perturbed classical Hamiltonian

$$H^{\mathrm{cl}}(x,\xi) = \frac{1}{2}\xi^2 + \chi_R(x)V(x) \quad \text{for } (x,\xi)\in\mathbb{R}^{2d}, \tag{3.6}$$

cf. (1.6). The associated Hamilton equations are given as

$$\dot{x} = \xi, \quad \dot{\xi} = -\nabla(\chi_R V). \tag{3.7}$$

We are interested in the asymptotic stationary estimates along a forward scattering orbit $(x(t),\xi(t))$ (meaning beyond (3.7) that $|x(t)|\to\infty$ for $t\to\infty$) with a fixed positive energy

$$\lambda = H^{\mathrm{cl}}(x(t),\xi(t)) > 0.$$

Parallel to the free, case we can study details of propagation along this orbit in terms of the classical gamma observables given as

$$\gamma = \gamma^{\mathrm{cl}} = \xi - (\nabla S) \quad \text{and} \quad \gamma_{\parallel} = \gamma^{\mathrm{cl}}_{\parallel} = (\nabla S)\cdot\gamma^{\mathrm{cl}}, \tag{3.8}$$

where as in (1.20) the function S comes from Theorem 1.3. Until the end of Section 3.2, we drop the superscript $^{\mathrm{cl}}$ for short.

Proposition 3.3. *Fix any $\lambda > 0$, and define γ and $\gamma_{\parallel}$ as above. Let $(x(t),\xi(t))$, $t\in\mathbb{R}$, be a classical orbit for the Hamiltonian (3.6) with energy λ such that*

$$|x(t)|\to\infty \quad \text{as } t\to+\infty.$$

Then, for any $\beta\in(0,2)$, there exists $C>0$ such that for $t\geq 0$ and along the orbit $(x(t),\xi(t))$,

$$\gamma^2 \leq Cf^{-\beta} \quad \text{and} \quad |\gamma_{\parallel}| \leq Cf^{-\beta}.$$

Remarks 3.4. (1) This is the classical counterpart of Theorem 1.24 intuitively explaining why the operator $\gamma_\parallel$ accepts a doubled weight compared to the operators γ_i. See also [9].

(2) Proposition 3.3 holds true for V satisfying Condition 1.1 with $l = 2$, but we need to let $l = 4$ in Theorem 1.24 since higher order derivatives of S are involved in the quantum mechanical case. Note that, due to this, the range of β gets narrower in Theorem 1.24 than in Proposition 3.3.

Proof. All the below classical quantities are considered along the forward scattering orbit $(x(t), \xi(t))$, and the dependence on $t \geq 0$ is suppressed. It suffices to argue only for large $t \geq 0$, so that we may consider x to stay away from the origin, in fact quantitatively as $|x(t)| > 2R$. Hence, by (1.6), we have the identity for large t

$$0 = H^{\mathrm{cl}} - \lambda = \frac{1}{2}\gamma^2 + \gamma_\parallel. \tag{3.9}$$

This identity is important (it will be used repeatedly) and deserves to be named the *classical increment or decrement identity*. By (3.9), it suffices to show the bound

$$P^{\mathrm{cl}} := (f^\beta \gamma_\parallel)^2 \leq C_1, \tag{3.10}$$

and for that we compute the time-derivative of P^{cl}. However, the time-derivative coincides with the Poisson bracket, hence $D := \mathrm{d}/\mathrm{d}t = \{H^{\mathrm{cl}}, \cdot\}$. In any case, we easily compute

$$DP^{\mathrm{cl}} = 2\beta f^{2\beta-1}\gamma_\parallel^2(Df) + 2f^{2\beta}\gamma_\parallel(D\gamma_\parallel), \tag{3.11}$$

motivating us to show that the right-hand side eventually is negative along the orbit.

We compute and bound the first term on the right-hand side by using (3.8), (3.9), and (1.6) as

$$\begin{aligned}
&2\beta f^{2\beta-1}\gamma_\parallel^2(Df)\\
&\quad = 2\beta f^{2\beta-1}\gamma_\parallel^2(\nabla f)\cdot\xi\\
&\quad = 2\beta(2\lambda)^{-1/2} f^{2\beta-1}\gamma_\parallel^2(\gamma_\parallel + |\nabla S|^2)\\
&\quad = 2\beta(2\lambda)^{-1/2} f^{2\beta-1}\gamma_\parallel^2\Big(-\frac{1}{2}\gamma^2 + 2\lambda - 2\chi_R V\Big)\\
&\quad \leq -\beta(2\lambda)^{-1/2} f^{2\beta-1}\gamma_\parallel^2\gamma^2 + 2\beta(2\lambda)^{1/2} f^{2\beta-1}\gamma_\parallel^2 + C_2 f^{2\beta-1-\sigma}\gamma_\parallel^2.
\end{aligned}$$

To compute the second term of (3.11), we note the identity obtained by differentiating the equation (1.6)

$$(\nabla^2 S)\nabla S = \frac{1}{2}\nabla|\nabla S|^2 = -\nabla(\chi_R V). \tag{3.12}$$

Then, by (3.8), (3.12), and (3.9), this second term is computed as

$$\begin{aligned}2f^{2\beta}\gamma_\parallel(D\gamma_\parallel) &= 2f^{2\beta}\gamma_\parallel(\xi\cdot(\nabla^2 S)\gamma + (\nabla S)\cdot(-(\nabla\chi_R V) - (\nabla^2 S)\xi))\\ &= 2f^{2\beta}\gamma_\parallel(\gamma\cdot(\nabla^2 S)\gamma - (\nabla S)\cdot(\nabla^2 S)(\nabla S) - (\nabla S)\cdot(\nabla\chi_R V))\\ &= -(2\lambda)^{1/2} f^{2\beta}\gamma^2\gamma\cdot(\nabla^2 f)\gamma.\end{aligned}$$

Combining the above computations and using (3.2c) and (3.9), we bound (3.11) as

$$\begin{aligned}DP^{\mathrm{cl}} \le\ & -(2\lambda)^{1/2} f^{2\beta-1}\gamma^2\gamma\cdot(\beta(\nabla f)\otimes(\nabla f) + (f\nabla^2 f))\gamma\\ & + 2\beta(2\lambda)^{1/2} f^{2\beta-1}\gamma_\parallel^2 + C_2 f^{2\beta-1-\sigma}\gamma_\parallel^2\\ \le\ & -(\min\{1,\beta\})(2\lambda)^{1/2} f^{2\beta-1}\gamma^4(1 - C_3 f^{-\sigma})\\ & + 2\beta(2\lambda)^{1/2} f^{2\beta-1}\gamma_\parallel^2 + C_2 f^{2\beta-1-\sigma}\gamma_\parallel^2\\ \le\ & -(\min\{4-2\beta, 2\beta\})(2\lambda)^{1/2} f^{2\beta-1}\gamma_\parallel^2 + C_4 f^{2\beta-1-\sigma}\gamma_\parallel^2,\end{aligned}$$

so that, for any sufficiently large t,

$$DP^{\mathrm{cl}} \le -c_1 f^{-1} P^{\mathrm{cl}} \le 0. \tag{3.13}$$

Hence, indeed P^{cl} is bounded as $t \to \infty$, verifying (3.10), and we are done. ∎

Remark 3.5. We have presented a stationary proof without explicit time parameter, so that the scheme extends to the quantum setup, see Proposition 3.6 and its proof. We could have given a simpler proof computing $D(f^\beta\gamma_\parallel)$, however we are not aware of any analogous procedure in quantum mechanics. Note that, in the literature on scattering theory of Schrödinger operators, conjugate operators are usually of first order, and consequently our scheme of proof (not being of this sort) is rather non-conventional.

3.3. Main propositions of the section

Clearly, we can assume that the arbitrary compact subset $I' \subseteq I$ in Theorem 1.24 is taken as $I' = I$, and hence that also I is compact. We make these assumption in the remaining part of the section.

To prove Theorem 1.24, we are going to compute and bound a quantum observable corresponding to the expression $D((f^\beta\gamma_\parallel^{\mathrm{cl}})^2)$ appearing in the proof of Proposition 3.3. As a quantum observable corresponding to (3.10), we consider

$$P = \gamma_\parallel\theta^{2\beta}\gamma_\parallel, \quad \beta\in(0,2). \tag{3.14}$$

where $\gamma_\parallel$ is the radiation observable from (1.20). Here the weight function

$$\theta = \theta(f) = \theta(f(x))$$

is defined as

$$\theta = \theta_{\delta,\nu}(f) = \int_0^f \Bigl(1 + \frac{t}{\nu}\Bigr)^{-1-\delta} \mathrm{d}t; \quad \nu \geq 1,\ \delta > 0.$$

It is a refinement of the so-called *Yosida approximation* of f. Note that θ is bounded for each $\nu \geq 1$, but that

$$\theta' \uparrow 1 \ \text{ and } \ \theta \uparrow f \quad \text{pointwise as } \nu \to \infty,$$

where θ' denotes the derivative of θ as a function of f.

The main propositions of the section present upper and lower bounds of a "distorted commutator"

$$2\,\mathrm{Im}(P(H-z))$$

with

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

Note that it is comparable with $DP^{\mathrm{cl}} = \{H^{\mathrm{cl}}, P^{\mathrm{cl}}\}$ considered before in classical mechanics. In fact, if $z = \lambda \in I$, it is nothing but the commutator $\mathrm{i}[H, P]$.

Proposition 3.6. *Define P and θ as above with $\beta \in (0,2)$ and $\delta > 0$ arbitrarily fixed. Then, there exist $c > 0$ and $\nu_0 \geq 1$ such that, for all $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$, $R \geq R_0$, and $\nu \geq \nu_0$ (with the constant $C > 0$ being independent of $\lambda \in I$ but possibly depending on $R \geq R_0$),*

$$\begin{aligned}\pm 2\,\mathrm{Im}(P(H-z)) \leq & -c\gamma_\| \theta' \theta^{2\beta-1}\gamma_\| + C\Gamma f^{-2}\theta^{2\beta} \\ & + Cf^{-1-2\beta_c+3\delta}\theta^{2\beta} + C(H-z)^* f^{1+\delta}\theta^{2\beta-\delta}(H-z)\end{aligned}$$

as quadratic forms on $\mathcal{D}(H)$.

Proposition 3.7. *Suppose the same setting of Proposition 3.6, and let $\varepsilon \in (0,1]$. Then, there exists $\nu_0 \geq 1$ such that, for all $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$, $R \geq R_0$ and $\nu \geq \nu_0$ (with the constant $C > 0$ being independent of $\lambda \in I$ but possibly depending on $R \geq R_0$),*

$$\begin{aligned}\pm 2\,\mathrm{Im}(P(H-z)) \geq & -\varepsilon\gamma_\| \theta' \theta^{2\beta-1}\gamma_\| - C\Gamma f^{-2}\theta^{2\beta} \\ & - Cf^{-1-2\beta_c+3\delta}\theta^{2\beta} - C(H-z)^* f^{1+\delta}\theta^{2\beta-\delta}(H-z)\end{aligned}$$

as quadratic forms on $\mathcal{D}(H)$.

Remark 3.8. Proposition 3.6 is obviously a quantum analogue of (3.13) with some negligible errors coming from commutation of observables, while Proposition 3.7 only says that the left-hand side of Proposition 3.6 is negligible too. In the proof of Theorem 1.24, we shall take expectation of these bounds in the state $\phi = R(z)\psi$, and take the limits $\Gamma \to 0_+$ and $\nu \to \infty$. Then, the second, third, and fourth terms on the right-hand sides of Propositions 3.6 and 3.7 are in fact negligible for $\beta < \beta_c$ and δ taken small. This is due to the factor Γ, the limiting absorption principle bounds and cancellation of $H - z$ and $R(z)$, respectively. We will give the details in Section 3.6.

The propositions will be proved in Section 3.5, after some preliminaries in Section 3.4.

3.4. Preliminaries

Here, we gather some identities and estimates that will be frequently cited in the remaining of Section 3. Throughout Section 3.4, we adapt the setting of Proposition 3.6. In particular, $\beta \in (0,2)$ and $\delta > 0$ are fixed along with I, R, S, and f from Section 3.1.

We first record several bounds for the weight θ. We denote the derivatives of θ in f by primes or similar superscripts such as $\theta', \theta'', \dots, \theta^{(k)}$.

Lemma 3.9. *There exist $c_0, C_0 > 0$ such that, uniformly in $\lambda \in I$ and $\nu \geq 1$,*

$$c_0 \min\{\nu, f\} \leq \theta \leq \min\{C_0 \nu, f\}, \quad \theta' \leq f^{-1}\theta.$$

Furthermore, for any $k \in \mathbb{N}$ there exist $c_k, C_k > 0$ such that, uniformly in $\lambda \in I$ and $\nu \geq 1$,

$$c_k \nu^{1-k} f^{-k-\delta} \theta^{k+\delta} \leq (-1)^{k-1}\theta^{(k)} \leq C_k \nu^{1-k} f^{-k-\delta}\theta^{k+\delta}.$$

Remark 3.10. In the rest of the section, we will mostly use the simplified bounds

$$c_1 f^{-1-\delta}\theta^{1+\delta} \leq \theta' \leq f^{-1}\theta, \quad |\theta^{(k)}| \leq C_k' f^{-k}\theta.$$

Proof. According to whether $f \leq \nu$ or $f \geq \nu$, we have

$$\theta \geq \int_0^f 2^{-1-\delta}\,\mathrm{d}s = 2^{-1-\delta} f \quad \text{or} \quad \theta \geq \int_0^\nu 2^{-1-\delta}\,\mathrm{d}s = 2^{-1-\delta}\nu,$$

respectively. On the other hand,

$$\theta = \delta^{-1}\nu\Big(1 - \Big(\frac{1+f}{\nu}\Big)^{-\delta}\Big) \leq \delta^{-1}\nu \quad \text{and} \quad \theta \leq \int_0^f \mathrm{d}s = f.$$

Hence, we obtain the asserted bounds for θ.

We also have

$$\theta' = (1 + f/\nu)^{-1-\delta} = f^{-1}\int_0^f \Big(\frac{1+f}{\nu}\Big)^{-1-\delta}\,\mathrm{d}s \leq f^{-1}\theta.$$

In addition, for any $k \in \mathbb{N}$, we can find a constant $C_k > 0$ such that

$$\begin{aligned}\theta^{(k)} &= (-1)^{k-1} C_k \nu^{1-k} (1 + f/\nu)^{-k-\delta} \\ &= (-1)^{k-1} C_k \nu^{1-k} f^{-k-\delta} (f^{-1} + \nu^{-1})^{-k-\delta}.\end{aligned}$$

Here, the last factor satisfies

$$\frac{1}{2} \min\{\nu, f\} \le (f^{-1} + \nu^{-1})^{-1} \le \min\{\nu, f\}.$$

Hence, we are done. ■

We next present a simple key identity corresponding to (3.9). It involves gamma observables of different orders, and hence it can be used either to increment or decrement the order of a differential operator (it will be used both ways many times).

Lemma 3.11. *For any $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$ on the subset $\{|x| > 2R\}$, the identities*

$$H - z = \frac{1}{2}\gamma^2 \pm \gamma_\parallel \mp \mathrm{i}\Gamma \tag{3.15}$$

hold.

Proof. The assertion is straightforward by (1.6) and (1.20). (Recall that throughout the section, $q \equiv 0$ in (1.1).) ■

The following commutator relations of the gamma observables are also important.

Lemma 3.12. *For any $\lambda \in I$ and $i, j = 1, \dots, d$, one has on $\{|x| \ge 2\}$*

$$[\gamma_i, \gamma_j] = 0, \tag{3.16a}$$

$$[\gamma_\parallel, \gamma_i] = \mathrm{i}\,\mathrm{Re}((\nabla \partial_i S) \cdot \gamma), \tag{3.16b}$$

$$[\gamma_\parallel, \gamma^2] = 2\mathrm{i}\gamma \cdot (\nabla^2 S)\gamma - \frac{\mathrm{i}}{2}(\Delta^2 S). \tag{3.16c}$$

Proof. By conjugation by $\mathrm{e}^{\mp \mathrm{i} S}$, relation (3.16a) reduces to that for p, which is trivial. We can verify (3.16b) immediately by (1.20) and (3.16a). As for (3.16c), we use (3.16b) to compute

$$\begin{aligned}[\gamma_\parallel, \gamma^2] &= \Big(\mathrm{i}\gamma \cdot (\nabla \partial_i S) - \frac{1}{2}(\partial_i \Delta S)\Big)\gamma_i + \gamma_i \Big(\mathrm{i}(\nabla \partial_i S) \cdot \gamma + \frac{1}{2}(\partial_i \Delta S)\Big) \\ &= 2\mathrm{i}\gamma \cdot (\nabla^2 S)\gamma - \frac{\mathrm{i}}{2}(\Delta^2 S).\end{aligned}$$

Thus, we obtain the assertion. ■

Lastly, we present several handy "ellipticity estimates." We will often use the following identities holding, for any $a \in C^\infty(\mathbb{R}^d;\mathbb{R})$,

$$p \cdot ap = \mathrm{Re}(ap^2) + \frac{1}{2}(\Delta a), \tag{3.17a}$$

$$p \cdot (p \cdot ap)p = p^2 ap^2 - p \cdot (\nabla^2 a)p + p \cdot (\Delta a)p. \tag{3.17b}$$

The lemma below implies that any compactly supported differential operator of order at most four is bounded by the last two terms of Propositions 3.6 and 3.7. For short, we shall denote their sum as

$$Q = f^{-1-2\beta_c+3\delta}\theta^{2\beta} + (H-z)^* f^{1+\delta}\theta^{2\beta-\delta}(H-z). \tag{3.18}$$

Lemma 3.13. *For any $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R})$, there exists $C > 0$ such that, uniformly in $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$, $R \geq R_0$, and $\nu \geq 1$,*

$$\eta \leq CQ, \quad \gamma \cdot \eta\gamma \leq CQ, \quad \gamma \cdot (\gamma \cdot \eta\gamma)\gamma \leq CQ. \tag{3.19}$$

Proof. The first bound from (3.19) is trivial. For the second and third bounds, it suffices to show the bounds with γ replaced by p. As for the second, we use (3.17a) and the Cauchy–Schwarz inequality to bound it for any $N \geq 0$ as

$$\begin{aligned} p \cdot \eta p &= 2\,\mathrm{Re}(\eta(H-z)) - 2\eta(V-z) + \frac{1}{2}(\Delta\eta) \\ &\leq C_1 f^{-N} + C_1(H-z)^* f(H-z). \end{aligned}$$

The second bound follows by choosing $N = 5$, which suffices since $5 \geq 1 + 2\beta_c$. Lastly, we rewrite the left-hand side of the third bound of (3.19) by using (3.17b) as

$$\begin{aligned} p \cdot (p \cdot \eta p)p = {}& 4(H-z)^*\eta(H-z) - 8\,\mathrm{Re}(\eta(V-z^*)(H-z)) \\ &+ 4\eta|V-z|^2 - p \cdot (\nabla^2\eta)p + p \cdot (\Delta\eta)p. \end{aligned}$$

The third bound then follows by the Cauchy–Schwarz inequality and the first and second bounds. ∎

The next lemma implies various forms of negligible terms can be absorbed into the leading term $\gamma_\parallel \theta'\theta^{2\beta-1}\gamma_\parallel$, or $\gamma \cdot (\gamma \cdot \theta'\theta^{2\beta-1}\gamma)\gamma$, cf. Lemma 3.15.

Lemma 3.14. *For any $\varepsilon > 0$ and $R \geq R_0$, there exist $C = C(\delta) > 0$ and $\nu_0 = \nu_0(\delta) \geq 1$, such that, for all $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$ and $\nu \geq \nu_0$,*

$$\gamma_\parallel f^{-1-\delta}\theta^{2\beta}\gamma_\parallel \leq \varepsilon\gamma_\parallel\theta'\theta^{2\beta-1}\gamma_\parallel + CQ, \tag{3.20a}$$

$$\gamma \cdot f^{-1-\beta_c+\delta}\theta^{2\beta}\gamma \leq \varepsilon\gamma_\parallel\theta'\theta^{2\beta-1}\gamma_\parallel + CQ. \tag{3.20b}$$

$$\gamma \cdot (\gamma \cdot f^{-1-\delta}\theta^{2\beta}\gamma)\gamma \leq \varepsilon\gamma \cdot (\gamma \cdot \theta'\theta^{2\beta-1}\gamma)\gamma + CQ, \tag{3.20c}$$

Proof. Let $\varepsilon > 0$. By Lemma 3.9, we can find $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R})$, such that, uniformly in $\nu \geq \nu_0$ for some $\nu_0 \geq 1$ chosen sufficiently large,

$$f^{-1-\delta}\theta^{2\beta} \leq \varepsilon\theta'\theta^{2\beta-1} + \eta.$$

Then, we conclude (3.20a) and (3.20c) by Lemma 3.13. To prove (3.20b), note that, by conjugation by $\mathrm{e}^{\pm \mathrm{i}\chi_1 S}$, we can rewrite (3.17a) as

$$\gamma \cdot a\gamma = \mathrm{Re}(a\gamma^2) + \frac{1}{2}(\Delta a). \tag{3.21}$$

In addition, set

$$t = 1 + \beta_c - \delta.$$

Then, by (3.21), (1.5), Lemmas 3.11 and 3.9, the Cauchy–Schwarz inequality, and Lemma 3.13, we can estimate (using the cut-off function χ_{2R} from (1.5))

$$\begin{aligned}\gamma \cdot f^{-t}\theta^{2\beta}\gamma &\leq \mp 2\,\mathrm{Re}(\chi_{2R} f^{-t}\theta^{2\beta}\gamma_\|) + 2\,\mathrm{Re}(\chi_{2R} f^{-t}\theta^{2\beta}(H-z)) \\ &\quad + C_1 f^{-t-2}\theta^{2\beta} + \mathrm{Re}((1-\chi_{2R}) f^{-t}\theta^{2\beta}\gamma^2) \\ &\leq \gamma_\| f^{-1-\delta}\theta^{2\beta}\gamma_\| + C_1 f^{-t-2}\theta^{2\beta} + C_2 f^{-2t+1+\delta}\theta^{2\beta} \\ &\quad + C_2(H-z)^* f^{-1-\delta}\theta^{2\beta}(H-z) + C_2 Q.\end{aligned}$$

Applying in turn (3.20a), this yields (3.20b). ∎

The final lemma says $4\gamma_\|\theta'\theta^{2\beta-1}\gamma_\|$ and $\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma$ are interchangeable up to small errors.

Lemma 3.15. *For any $\varepsilon > 0$ and $R \geq R_0$, there exist $C > 0$ and $\nu_0 \geq 1$ such that, for all $z = \lambda + \mathrm{i}\Gamma \in I_+$ and $\nu \geq \nu_0$,*

$$\pm\{4\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| - \gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma\} \leq \varepsilon\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| + C\Gamma f^{-2}\theta^{2\beta} + CQ.$$

The same bounds also hold uniformly in $z = \lambda - \mathrm{i}\Gamma \in I_-$ and $\nu \geq \nu_0$.

Proof. We discuss only $z = \lambda + \mathrm{i}\Gamma \in I_+$ since the other is proved in the same manner. Similarly to (3.21), by conjugation by $\mathrm{e}^{-\mathrm{i}\chi_1 S}$, we have (3.17b) rewritten as

$$\gamma\cdot(\gamma\cdot a\gamma)\gamma = \gamma^2 a\gamma^2 - \gamma\cdot(\nabla^2 a)\gamma + \gamma\cdot(\Delta a)\gamma.$$

Then, it follows by Lemma 3.9 that

$$\pm\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma \leq \pm\gamma^2\theta'\theta^{2\beta-1}\gamma^2 + C_1\gamma\cdot f^{-3}\theta^{2\beta}\gamma. \tag{3.22}$$

The second term on the right-hand side of (3.22) can be bounded by (3.20b), and hence it suffices to discuss the first term of (3.22). With the localization factor χ_{2R}

inserted in this term, we are allowed to isolate γ^2 in (3.15) and substitute into the two appearing factors of γ^2. After expansion, we then use the Cauchy–Schwarz inequality to absorb cross terms into the diagonal ones. Hence, it follows that

$$\begin{aligned}\pm\gamma^2\theta'\theta^{2\beta-1}\gamma^2 &= \pm 4(-\gamma_\| + \mathrm{i}\Gamma + (H-z))^*\chi_{2R}\theta'\theta^{2\beta-1}(-\gamma_\| + \mathrm{i}\Gamma + (H-z))\\ &\quad \pm \gamma^2(1-\chi_{2R})\theta'\theta^{2\beta-1}\gamma^2\\ &\le (\pm 4+\varepsilon)\gamma_\|\chi_{2R}\theta'\theta^{2\beta-1}\gamma_\| + C_2\Gamma^2 f^{-1}\theta^{2\beta} + C_2 Q.\end{aligned}$$

We can remove χ_{2R} from the first term on the right-hand side above by retaking $C_2 > 0$ larger, and hence it suffices to discuss the second term. By the expression (1.20), the Cauchy–Schwarz inequality, and Lemma 3.9, we can proceed as

$$\begin{aligned}\Gamma^2 f^{-1}\theta^{2\beta} &= \frac{1}{2}\Gamma\,\mathrm{Re}((\nabla f^{-1}\theta^{2\beta})\cdot\gamma) + \frac{1}{2}\Gamma(\nabla f^{-1}\theta^{2\beta})\cdot(\nabla S)\\ &\quad - \Gamma\,\mathrm{Im}(f^{-1}\theta^{2\beta}(H-z))\\ &le\ C_3\gamma_\| f^{-2}\theta^{2\beta}\gamma_\| + C_3\Gamma f^{-2}\theta^{2\beta} + C_3 Q.\end{aligned} \tag{3.23}$$

The first term on the right-hand side of (3.23) can be bounded as asserted by using (3.20a). Hence, we obtain the assertion. ■

3.5. Upper and lower bounds for the distorted commutator

Here, we prove Propositions 3.6 and 3.7. We start with Proposition 3.6.

Proof of Proposition 3.6. We proceed in four steps.

Step I. Let us prove the assertion only for the upper sign, since the lower one follows in the same manner. With reference to the constants $0 < c \le C$ of (3.2a) and the function χ of (1.4), we introduce the smooth cut-off function $\tilde\chi = \chi(f/4CR)$. Then,

$$\mathrm{supp}\,\tilde\chi \subseteq \{|x| > 2R\}, \quad \tilde\chi = 1, \quad \text{on } \{|x| \ge 8RC/c\}.$$

In particular, (3.15) applies on the support of $\tilde\chi$. Hence, by (3.14) and Lemma 3.11 we can split the distorted commutator on the left-hand side of the assertion as

$$\begin{aligned}2\,\mathrm{Im}(P(H-z)) &= \mathrm{Im}(\gamma_\|\tilde\chi\theta^{2\beta}\gamma_\|\gamma^2) + 2\,\mathrm{Im}(\gamma_\|\tilde\chi\theta^{2\beta}\gamma_\|^2)\\ &\quad + 2\,\mathrm{Im}(\gamma_\|(1-\tilde\chi)\theta^{2\beta}\gamma_\|(H-\lambda)) - 2\Gamma\gamma_\|\theta^{2\beta}\gamma_\|.\end{aligned} \tag{3.24}$$

In the following steps, we will further compute and bound each term of (3.24).

First, we comment on our notation. Throughout the proof, we fix $\varepsilon > 0$ such that, for some $c_1 > 0$, it follows that, uniformly in $\lambda \in I$,

$$(2\lambda)^{1/2}\min\{4-2\beta, 2\beta\} - 19\varepsilon > c_1 > 0. \tag{3.25}$$

We shall consider only $\nu \geq \nu_0$ with appropriate $\nu_0 \geq 1$ tacitly retaken each time we apply Lemmas 3.14 or 3.15. In addition, we shall adopt the notation Q from (3.18). We particularly note that, when computing (3.24), once a derivative hits $\tilde{\chi}$, the corresponding term is immediately bounded by $C_1 Q$ for some $C_1 > 0$ due to Lemma 3.13. We shall also tacitly implement such estimates.

Step II. Now, we start with the first term on the right-hand side of (3.24). By (1.20) and (3.16c), we can compute it as

$$\begin{aligned}\operatorname{Im}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}\gamma_\parallel \gamma^2) &= \operatorname{Im}(\gamma_\parallel [\tilde{\chi}\theta^{2\beta}, \gamma]\cdot \gamma\gamma_\parallel) + \operatorname{Im}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}[\gamma_\parallel, \gamma^2]) \\ &= (2\lambda)^{-1/2}\operatorname{Re}(\gamma_\parallel (\tilde{\chi}\theta^{2\beta})'\gamma_\parallel^2) + 2\operatorname{Re}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}\gamma\cdot(\nabla^2 S)\gamma) \\ &\quad - \frac{1}{2}\operatorname{Re}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}(\Delta^2 S)).\end{aligned}$$

By the Cauchy–Schwarz inequality, (3.12), (3.2b), and Lemmas 3.13 and 3.14, we can bound it as

$$\begin{aligned}\operatorname{Im}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}\gamma_\parallel \gamma^2) &\leq 2\beta(2\lambda)^{-1/2}\operatorname{Re}(\gamma_\parallel^2 \tilde{\chi}\theta'\theta^{2\beta-1}\gamma_\parallel) \\ &\quad + 2\operatorname{Re}(\gamma_\parallel \gamma\cdot \tilde{\chi}\theta^{2\beta}(\nabla^2 S)\gamma) + \varepsilon\gamma_\parallel \theta'\theta^{2\beta-1}\gamma_\parallel + C_2 Q.\end{aligned} \tag{3.26a}$$

The second term of (3.24) can be computed by (1.20), (1.6), and Lemma 3.14 as

$$\begin{aligned}2\operatorname{Im}(\gamma_\parallel \tilde{\chi}\theta^{2\beta}\gamma_\parallel^2) &= \gamma_\parallel (\nabla S)\cdot(\nabla\tilde{\chi}\theta^{2\beta})\gamma_\parallel \\ &\leq (2\beta(2\lambda)^{1/2} + \varepsilon)\gamma_\parallel \theta'\theta^{2\beta-1}\gamma_\parallel + C_3 Q.\end{aligned} \tag{3.26b}$$

The third and fourth terms of (3.24) is bounded trivially as

$$2\operatorname{Im}(\gamma_\parallel (1-\tilde{\chi})\theta^{2\beta}\gamma_\parallel (H-\lambda)) - 2\Gamma\gamma_\parallel \tilde{\chi}\theta^{2\beta}\gamma_\parallel \leq C_4 Q. \tag{3.26c}$$

Hence, by (3.24) and (3.26a)–(3.26c), we obtain

$$\begin{aligned}2\operatorname{Im}(P(H-z)) &\leq 2\beta(2\lambda)^{-1/2}\operatorname{Re}(\gamma_\parallel^2 \tilde{\chi}\theta'\theta^{2\beta-1}\gamma_\parallel) + 2\operatorname{Re}(\gamma_\parallel \gamma\cdot\tilde{\chi}\theta^{2\beta}(\nabla^2 S)\gamma) \\ &\quad + (2\beta(2\lambda)^{1/2} + 2\varepsilon)\gamma_\parallel \theta'\theta^{2\beta-1}\gamma_\parallel + C_5 Q.\end{aligned} \tag{3.27}$$

Step III. We continue to compute (3.27). We next increment the order of the first and second terms of (3.27) by substituting the following version of (3.15):

$$\gamma_\parallel = -\frac{1}{2}\gamma^2 - \mathrm{i}\Gamma + (H-z)^*, \tag{3.28}$$

In fact, using (3.28), we can rewrite the first and second terms of (3.27) as

$$\begin{aligned}&2\beta(2\lambda)^{-1/2}\operatorname{Re}(\gamma_\parallel^2 \tilde{\chi}\theta'\theta^{2\beta-1}\gamma_\parallel) + 2\operatorname{Re}(\gamma_\parallel \gamma\cdot\tilde{\chi}\theta^{2\beta}(\nabla^2 S)\gamma) \\ &\quad = -\beta(2\lambda)^{-1/2}\operatorname{Re}(\gamma^2\gamma_\parallel \tilde{\chi}\theta'\theta^{2\beta-1}\gamma_\parallel) - \operatorname{Re}(\gamma^2\gamma\cdot\tilde{\chi}\theta^{2\beta}(\nabla^2 S)\gamma) \\ &\qquad + 2\beta(2\lambda)^{-1/2}\operatorname{Re}((H-z)^*\gamma_\parallel \tilde{\chi}\theta'\theta^{2\beta-1}\gamma_\parallel) \\ &\qquad + 2\operatorname{Re}((H-z)^*\gamma\cdot\tilde{\chi}\theta^{2\beta}(\nabla^2 S)\gamma).\end{aligned} \tag{3.29}$$

Let us discuss each term on the right-hand side. The first term of (3.29) can be bounded, by using (3.16b), the Cauchy–Schwarz inequality, and Lemma 3.14, as

$$\begin{aligned} &-\beta(2\lambda)^{-1/2}\operatorname{Re}(\gamma^2\gamma_\| \tilde\chi\theta'\theta^{2\beta-1}\gamma_\|) \\ &\quad= -\beta(2\lambda)^{-1/2}\{\gamma\cdot\gamma_\|\tilde\chi\theta'\theta^{2\beta-1}\gamma_\|\gamma + \operatorname{Re}(\gamma\cdot[\gamma,\gamma_\|]\tilde\chi\theta'\theta^{2\beta-1}\gamma_\|) \\ &\qquad + \operatorname{Re}(\gamma\cdot\gamma_\|[\gamma,\tilde\chi\theta'\theta^{2\beta-1}]\gamma_\|) + \operatorname{Re}(\gamma\cdot\gamma_\|\tilde\chi\theta'\theta^{2\beta-1}[\gamma,\gamma_\|])\} \\ &\quad\le -\beta(2\lambda)^{-1/2}\gamma\cdot\gamma_\|\tilde\chi\theta'\theta^{2\beta-1}\gamma_\|\gamma + \varepsilon\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| \\ &\qquad + \varepsilon\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma + C_6 Q. \end{aligned} \tag{3.30a}$$

The second term of (3.29) can be bounded, by using (3.2b) and Lemma 3.14, as

$$\begin{aligned} -\operatorname{Re}(\gamma^2\gamma\cdot\tilde\chi\theta^{2\beta}(\nabla^2 S)\gamma) &= -\gamma\cdot(\gamma\cdot\tilde\chi\theta^{2\beta}(\nabla^2 S)\gamma)\gamma + \frac{1}{2}\gamma\cdot(\Delta\tilde\chi\theta^{2\beta}(\nabla^2 S))\gamma \\ &\le -\gamma\cdot(\gamma\cdot\tilde\chi\theta^{2\beta}(\nabla^2 S)\gamma)\gamma + \varepsilon\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| + C_7 Q. \end{aligned} \tag{3.30b}$$

As for the third and fourth terms of (3.29), by the Cauchy–Schwarz inequality, (3.2b), and Lemma 3.14, we have

$$\begin{aligned} &2\beta(2\lambda)^{-1/2}\operatorname{Re}((H-z)^*\gamma_\|\tilde\chi\theta'\theta^{2\beta-1}\gamma_\|) + 2\operatorname{Re}((H-z)^*\gamma\cdot\tilde\chi\theta^{2\beta}(\nabla^2 S)\gamma) \\ &\quad\le C_8(\gamma_\|\theta'\theta^{2\beta-1}\gamma_\|)f^{1-\delta}\theta^{-2\beta}(\gamma_\|\theta'\theta^{2\beta-1}\gamma_\|) \\ &\qquad + C_8(\gamma\cdot\theta^{2\beta}(\nabla^2 S)\gamma)f^{1-\delta}\theta^{-2\beta}(\gamma\cdot\theta^{2\beta}(\nabla^2 S)\gamma) + C_8 Q \\ &\quad\le \varepsilon\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| + \varepsilon\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma + C_9 Q. \end{aligned} \tag{3.30c}$$

Hence, by (3.27), (3.29), and (3.30a)–(3.30c), we conclude that

$$\begin{aligned} 2\operatorname{Im}(P(H-z)) \le{}& -\beta(2\lambda)^{-1/2}\gamma\cdot\gamma_\|\tilde\chi\theta'\theta^{2\beta-1}\gamma_\|\gamma - \gamma\cdot(\gamma\cdot\tilde\chi\theta^{2\beta}(\nabla^2 S)\gamma)\gamma \\ &+ 2\varepsilon\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma + (2\beta(2\lambda)^{1/2} + 5\varepsilon)\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| \\ &+ C_{10} Q. \end{aligned} \tag{3.31}$$

Step IV. Now, we use (3.2c) to the right-hand side of (3.31). Also using Lemmas 3.9 and 3.14, we obtain

$$\begin{aligned} 2\operatorname{Im}(P(H-z)) \le{}& -((2\lambda)^{1/2}\min\{1,\beta\} - 3\varepsilon)\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma \\ &+ (2\beta(2\lambda)^{1/2} + 6\varepsilon)\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| + C_{11} Q. \end{aligned} \tag{3.32}$$

Next, we rewrite the first term of (3.32) by using Lemma 3.15, so that

$$\begin{aligned} 2\operatorname{Im}(P(H-z)) \le{}& -((2\lambda)^{1/2}\min\{4-2\beta,2\beta\} - 19\varepsilon)\gamma_\|\theta'\theta^{2\beta-1}\gamma_\| \\ &+ C_{12}\Gamma f^{-2}\theta^{2\beta} + C_{12} Q. \end{aligned}$$

Hence, by (3.25) we obtain the assertion. ∎

Next we prove Proposition 3.7. Compared to Proposition 3.6, it is much simpler.

Proof of Proposition 3.7. Let us discuss only the upper sign. Similarly to the proof of Proposition 3.6, we adopt Q from (3.18). By the definition (3.14), the Cauchy–Schwarz inequality, Lemma 3.9, (1.20), and Lemma 3.14, we can bound, for any $\varepsilon \in (0, 1]$,

$$\begin{aligned}\operatorname{Im}(P(H-z)) &\geq -\varepsilon\gamma_\parallel \theta^{2\beta}\gamma_\parallel \theta'\theta^{-2\beta-1}\gamma_\parallel \theta^{2\beta}\gamma_\parallel - C_1\varepsilon^{-1}Q \\ &\geq -C_2\varepsilon\gamma\cdot(\gamma\cdot\theta'\theta^{2\beta-1}\gamma)\gamma - C_2\varepsilon\gamma_\parallel\theta'\theta^{2\beta-1}\gamma_\parallel - C_2\varepsilon^{-1}Q,\end{aligned}$$

where $C_* > 0$ are independent of $\varepsilon \in (0, 1]$. Then, by Lemma 3.15,

$$\operatorname{Im}(P(H-z)) \geq -C_3\varepsilon\gamma_\parallel\cdot\theta'\theta^{2\beta-1}\gamma_\parallel - C_3\Gamma f^{-2}\theta^{2\beta} - C_3\varepsilon^{-1}Q,$$

and we are done. ∎

Remark 3.16. We can modify the arguments of Section 3.5 to be applicable to the case $l = 3$, avoiding fourth derivatives of S. For that, we should employ

$$\tilde{\gamma}_\parallel = (\nabla S)\cdot\gamma - \frac{\mathrm{i}(d-1)}{2}(2\lambda)^{1/2}f^{-1}, \quad \tilde{\beta}_c = 1+\sigma$$

instead of $\gamma_\parallel$, β_c, respectively. Note that, although $\tilde{\gamma}_\parallel$ is not symmetric, it well approximates $\gamma_\parallel$, thanks to Theorem 1.3, and we can avoid $\Delta^2 S$ coming from (3.16c). The fourth order derivatives of S appear also from other parts of the above arguments, but we can manage them by the Cauchy–Schwarz inequality. We omit the details. Note also that, although $\tilde{\beta}_c$ is worse than β_c, it is still greater than 1, and the associated radiation condition bounds are stronger than the ordinary ones.

3.6. Proof of strong radiation condition bounds

Finally, in this section we prove Theorem 1.24. We will use the standard limiting absorption principle bounds on the following form.

Theorem 3.17. *There exists $C > 0$ such that, uniformly in $z \in I_\pm$ and $\psi \in \mathcal{B}$,*

$$\|R(z)\psi\|_{\mathcal{B}^*} \leq C\|\psi\|_{\mathcal{B}}, \quad \|\Delta R(z)\psi\|_{\mathcal{B}^*} \leq C\|\psi\|_{\mathcal{B}}.$$

Moreover, for any $t > 1/2$, there exist uniform limits in $\lambda \in I$,

$$R(\lambda \pm \mathrm{i}0) = \lim_{I_\pm \ni z \to \lambda} R(z), \quad \Delta R(\lambda \pm \mathrm{i}0) = \lim_{I_\pm \ni z \to \lambda} \Delta R(z),$$

in the norm topology of $\mathcal{L}(L^2_t, L^2_{-t})$.

Remark 3.18. We do not need to assume $q \equiv 0$ for this result.

Proof. This is the standard result in the theory of the Schrödinger operators, and we omit a proof. We refer the reader to [1]. ∎

Proof of Theorem 1.24. We note that, by the density argument, it suffices to prove the asserted bounds (1.21a)–(1.21c) for $\psi \in C_c^\infty(\mathbb{R}^d)$.

(1) Let $\beta \in (0, \beta_c)$, and choose $\delta > 0$ such that

$$2\beta + 3\delta < 2\beta_c, \quad \delta \leq 2\beta. \tag{3.33}$$

By Propositions 3.6 and 3.7, we can find $C_1 > 0$ and $\nu_0 \geq 1$ such that, uniformly in $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$ and $\nu \geq \nu_0$,

$$\begin{aligned} \gamma_\| \theta' \theta^{2\beta-1} \gamma_\| \leq C_1 \Gamma f^{-2} \theta^{2\beta} + C_1 f^{-1-2\beta_c+3\delta} \theta^{2\beta} \\ + C_1 (H - z)^* f^{1+\delta} \theta^{2\beta-\delta} (H - z). \end{aligned} \tag{3.34}$$

Take the expectation of the above inequality in the state $\phi = R(z)\psi$ for any $z = \lambda \pm \mathrm{i}\Gamma \in I_\pm$ and $\psi \in C_c^\infty(\mathbb{R}^d)$, and we obtain, by (3.33) and, Theorem 3.17

$$\begin{aligned} \|\theta'^{1/2}\theta^{\beta-1/2}\gamma_\| \phi\|_{\mathcal{H}}^2 &\leq C_1 \Gamma \|f^{-1}\theta^\beta \phi\|_{\mathcal{H}}^2 + C_1 \|f^{-1/2-\beta_c+3\delta/2}\theta^\beta \phi\|_{\mathcal{H}}^2 \\ &\quad + C_1 \|f^{(1+\delta)/2}\theta^{\beta-\delta/2}\psi\|_{\mathcal{H}}^2 \\ &\leq C_1 \Gamma \|f^{-1}\theta^\beta \phi\|_{\mathcal{H}}^2 + C_2 \|f^\beta \psi\|_{L^2_{1/2}}^2. \end{aligned}$$

Next, we take the limit $\Gamma \to 0_+$, and obtain, by Theorem 3.17,

$$\|\theta'^{1/2}\theta^{\beta-1/2}\gamma_\| R(\lambda \pm \mathrm{i}0)\psi\|_{\mathcal{H}} \leq C_2 \|f^\beta \psi\|_{L^2_{1/2}}.$$

Finally, we let $\nu \to \infty$, and then, by the monotone convergence theorem, the bound (1.21a) follows.

Combining Lemma 3.15 and (3.34), we also have

$$\begin{aligned} \gamma \cdot (\gamma \cdot \theta' \theta^{2\beta-1} \gamma)\gamma \leq C_3 \Gamma f^{-2} \theta^{2\beta} + C_3 f^{-1-2\beta_c+3\delta} \theta^{2\beta} \\ + C_3 (H - z)^* f^{1+\delta} \theta^{2\beta-\delta} (H - z). \end{aligned}$$

Hence, we can verify (1.21b) similarly to (1.21a).

(2) Let $\psi, \psi' \in C_c^\infty(\mathbb{R}^d)$, and consider a quantity

$$F(\zeta) = \langle \psi', (\gamma \cdot f^{2\beta'} \gamma)^\zeta f^{-t} R(\lambda \pm \mathrm{i}0) f^{-t} f^{-2\beta'\zeta} \psi \rangle.$$

It is obviously analytic in $0 < \operatorname{Re}\zeta < 1$. For $\operatorname{Re}\zeta = 0$, we have, by Theorem 3.17,

$$|F(\zeta)| \leq C_4 \|\psi'\|_{\mathcal{H}} \|\psi\|_{\mathcal{H}},$$

and, for $\operatorname{Re}\zeta = 1$, by (1.21b), (1.21a), and Theorem 3.17,

$$|F(\zeta)| \le C_5 \|\psi'\|_{\mathcal{H}} \|\psi\|_{\mathcal{H}}.$$

Hence, we obtain by the Hadamard three-lines theorem

$$|\langle \psi', (\gamma \cdot f^{2\beta'}\gamma)^{1/2} f^{-t} R(\lambda \pm \mathrm{i}0) f^{-t} f^{-\beta'} \psi\rangle| = \left| F\left(\frac{1}{2}\right)\right| \le C_6 \|\psi'\|_{\mathcal{H}} \|\psi\|_{\mathcal{H}},$$

or, for any $\psi'' \in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$,

$$\|(\gamma \cdot f^{2\beta'}\gamma)^{1/2} f^{-t} R(\lambda \pm \mathrm{i}0)\psi''\|_{\mathcal{H}} \le C_6 \|f^{\beta'}\psi''\|_{L^2_t}.$$

However, we can rewrite the square of the left-hand side by using the inner product and Theorem 3.17 as

$$\begin{aligned} \|(\gamma \cdot f^{2\beta'}\gamma)^{1/2} f^{-t} R(\lambda \pm \mathrm{i}0)\psi''\|^2_{\mathcal{H}} &= \sum_{i=1}^d \|f^{\beta'}\gamma_i f^{-t} R(\lambda \pm \mathrm{i}0)\psi''\|^2_{\mathcal{H}} \\ &\ge \sum_{i=1}^d \|f^{\beta'}\gamma_i R(\lambda \pm \mathrm{i}0)\psi''\|^2_{L^2_{-t}} - C_7 \|\psi''\|^2_{\mathcal{B}}. \end{aligned}$$

Therefore, we obtain (1.21c). ∎

4. Stationary scattering theory

In this section, we discuss the stationary scattering theory for H, proving Theorems 1.5, 1.10, and 1.12 and Corollary 1.8. In order to use the strong radiation condition bounds of Theorem 1.24, we need more regularity for the potential than required in these assertions. Section 4.1 reviews a decomposition $V = V_{\mathrm{S}} + V_{\mathrm{L}}$ due to Hörmander [11, Lemma 30.1.1], so that the strong radiation condition bounds are available for $H_{\mathrm{L}} = -(1/2)\Delta + V_{\mathrm{L}}$. Then, in Section 4.2 we introduce the spherical eikonal coordinates associated with V_{L}, and study its geometry. In these coordinates, we can quickly construct the stationary wave operators for H_{L}, mimicking the procedure of [22]. They are then fused to those for H by a change of coordinates and the second resolvent identity. This is implemented in Section 4.3, and the proofs of Theorem 1.5 and Corollary 1.8 are done. The proofs of Theorems 1.10 and 1.12 are rather routine, and they are presented in Sections 4.4 and 4.5, respectively. Then, our stationary scattering theory is completed.

4.1. Hörmander's regularization

The asserted Theorem 1.24 requires four derivatives on the potential V, which clearly is not at disposal for a 2-admissible potential. Consequently, to implement the radiation condition bounds of the theorem we need first to regularize V. This is done by using the scheme of Hörmander [11, Lemma 30.1.1].

Lemma 4.1. *Suppose Condition 1.1 with $l = 2$.*

(1) *For any $\rho \in (0, \sigma)$, there exists a splitting*

$$V = V_{\mathrm{S}} + V_{\mathrm{L}}; \quad V_{\mathrm{S}} \in C^2(\mathbb{R}^d; \mathbb{R}), \ \ V_{\mathrm{L}} \in C^\infty(\mathbb{R}^d; \mathbb{R}),$$

satisfying the following: there exists $C > 0$ such that, for any $|\alpha| \le 2$ and $x \in \mathbb{R}^d$,

$$|\partial^\alpha V_{\mathrm{S}}(x)| \le C \langle x\rangle^{-1-\sigma+\rho-|\alpha|(\rho+1)/2}, \tag{4.1a}$$

and, for any $\alpha \in \mathbb{N}_0^d$, there exists $C_\alpha > 0$ such that, for any $x \in \mathbb{R}^d$,

$$|\partial^\alpha V_{\mathrm{L}}(x)| \le C_\alpha \langle x\rangle^{-m(|\alpha|)}, \tag{4.1b}$$

where m is defined by (1.2a) with the parameters σ and ρ (and for any $l \ge 2$).

(2) *For any $\rho \in (0, \sigma)$ and $\varepsilon, \delta > 0$, there exists a splitting*

$$V = V'_{\mathrm{S}} + V'_{\mathrm{L}}; \quad V'_{\mathrm{S}} \in C^2(\mathbb{R}^d; \mathbb{R}), \ \ V'_{\mathrm{L}} \in C^\infty(\mathbb{R}^d; \mathbb{R}),$$

satisfying the following: for any $|\alpha| \le 2$ and $x \in \mathbb{R}^d$,

$$|\partial^\alpha V'_{\mathrm{S}}(x)| \le \varepsilon \langle x\rangle^{-1-\sigma+\rho+\delta-|\alpha|(\rho+1)/2},$$

and, for any $\alpha \in \mathbb{N}_0^d$, there exists $C_\alpha > 0$ such that, for any $x \in \mathbb{R}^d$,

$$|\partial^\alpha V'_{\mathrm{L}}(x)| \le C_\alpha \langle x\rangle^{-m(|\alpha|)},$$

where m is given as in (4.1b). The constants C_α can, for $|\alpha| \le 2$, be chosen independently of $\varepsilon, \delta > 0$.

Remarks 4.2. (1) Ikebe and Isozaki [12] adopted a decomposition similar to (1) for classical C^4 long-range potentials. Note that our $\partial^\alpha V_{\mathrm{L}}$ has worse decay rate than theirs for $|\alpha| \ge 3$.

(2) Assertion (2) will only be employed in Section 5.2.2, the last part of the paper, for the proof of Theorem 1.20 (2).

Proof. (1) Although the bounds for V_{S} are slightly better than in [11, Lemma 30.1.1], the same proof works well. Let us review it since we will use its modification below for assertion (2). Fix any real $\eta \in C^\infty(\{|x| < 2\})$ with $\eta = 1$ for $|x| \le 1$, and set

$$V_0(x) = \eta(x)V(x), \quad V_n(x) = (\eta(2^{-n}x) - \eta(2^{1-n}x))V(x) \quad \text{for } n \in \mathbb{N}.$$

We also take a real $\chi \in C_c^\infty(\mathbb{R}^d)$ such that

$$\int_{\mathbb{R}^d} \chi \, dx = 1, \quad \int_{\mathbb{R}^d} x_j \chi(x) \, dx = 0 \quad \text{for } j = 1, \dots, d,$$

and set

$$\chi_n(x) = 2^{-dn(1+\rho)/2} \chi(2^{-n(1+\rho)/2} x).$$

Then, we define

$$V_L = \sum_{n \in \mathbb{N}_0} \chi_n * V_n, \quad V_S = V - V_L,$$

and they satisfy the asserted bounds. We omit further details.

(2) For $N_1, N_2 \in \mathbb{N}$, we consider

$$V_L' = \sum_{n \geq N_1} \chi_n * V_n + \sum_{n < N_1} \chi_{N_2} * V_n, \quad V_S' = V - V_L'.$$

With a proper adjustment of the parameters (fix first N_1 large and then suitably large N_2), indeed V_S' and V_L' satisfy the asserted bounds. We are done. ∎

The main part of the section is devoted to the analysis of V_L from Lemma 4.1 (1), while the effects from $V_S + q$ are taken into account only in the last steps. Note that the bound (4.1b) clearly agrees with Condition 1.1 for any $l \geq 2$, and thus the results from the previous sections are available for V_L. We denote

$$H_L = -\frac{1}{2}\Delta + V_L, \quad R_L(z) = (H_L - z)^{-1} \quad \text{for } z \in \mathbb{C} \setminus \sigma(H_L),$$

and

$$R_L(\lambda \pm i0) = \operatorname*{s\text{–}w^\star\text{–}lim}_{z \to \lambda \pm i0_+} R_L(z) \quad \text{in } \mathcal{L}(\mathcal{B}, \mathcal{B}^*) \quad \text{for } \lambda > 0.$$

Throughout the section, we fix any closed interval $I \subset \mathbb{R}_+$, and let $S_L \in C^{l'}(I \times (\mathbb{R}^d \setminus \{0\}))$ and $s_L \in C^{l'}(I \times \mathbb{R}^d)$ be given as in Theorem 1.3 for V_L and any fixed $l' > 1 + 2/\rho$. We will actually possibly need to take $R > 0$ larger than needed for Theorem 1.3 in Sections 4.2.3 and 5.1, implementing Corollary 2.14, but the R-dependence is suppressed.

Remark 4.3. This specific requirement $l' > 1 + 2/\rho$ will be needed only in the proof of Lemma 5.3. Otherwise, it suffices to take $l' = 4$, so that Theorem 1.24 is available. Although Theorem 1.3 does not provide bounds for $k + |\alpha| > l'$, nevertheless $s_L \in C^\infty(I \times \mathbb{R}^d)$, and similarly for S_L. This is a consequence of the fact that $V_L \in C^\infty(\mathbb{R}^d)$ and the implicit function theorem, see the proof of Theorem 1.3 (1).

4.2. Spherical eikonal coordinates

4.2.1. Eikonal flow at fixed energy. In order to define so-called spherical eikonal coordinates, in which the function $S_{\mathrm{L}}(\lambda,\cdot)$, $\lambda\in I$, introduced in Section 4.1, plays the role of *eikonal distance* from the origin, consider the *eikonal flow* y satisfying, for any given $(\lambda,\theta)\in I\times\mathbb{S}^{d-1}$,

$$\frac{\partial}{\partial t}y(\lambda,t,\theta)=(|\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}})(\lambda,y(\lambda,t,\theta)) \tag{4.3a}$$

with

$$\lim_{t\to 0_+}y(\lambda,t,\theta)=0\quad\text{and}\quad\lim_{t\to 0_+}\frac{\partial}{\partial t}y(\lambda,t,\theta)=(2\lambda)^{-1/2}\theta. \tag{4.3b}$$

Lemma 4.4. *The solution y to (4.3a) with (4.3b) is smooth in $(\lambda,t,\theta)\in I\times\mathbb{R}_+\times\mathbb{S}^{d-1}$, and for any $\lambda\in I$ it induces a (smooth) diffeomorphism*

$$y(\lambda,\cdot,\cdot)\colon\mathbb{R}_+\times\mathbb{S}^{d-1}\to\mathbb{R}^d\setminus\{0\}. \tag{4.4}$$

In addition, for any $(\lambda,t,\theta)\in I\times\mathbb{R}_+\times\mathbb{S}^{d-1}$ one has

$$S_{\mathrm{L}}(\lambda,y(\lambda,t,\theta))=t. \tag{4.5}$$

Remarks 4.5. (1) From a geometric point of view, the flow $y(\lambda,\cdot,\cdot)$ is nothing but the exponential map from the unit-sphere in the tangent space at the origin in the space $\mathbb{R}^d$ equipped with the metric $g_L=2(\lambda-\chi_R V_L)\,\mathrm{d}x^2$.

(2) The flow $y(\lambda,\cdot,\cdot)$ constitutes a family of reparametrized classical orbits of energy λ for the classical Hamiltonian

$$H_{\mathrm{L}}^{\mathrm{cl}}(x,\xi)=\frac{1}{2}\xi^2+\chi_R(x)V_{\mathrm{L}}(x).$$

In fact, if we set

$$z(\tau)=y(\lambda,t,\theta),\quad \tau=\int_0^t|\nabla S_{\mathrm{L}}(\lambda,y(\lambda,s,\theta))|^{-2}\,\mathrm{d}s,$$

then, by using (1.6),

$$\frac{\mathrm{d}}{\mathrm{d}\tau}z=\nabla S_{\mathrm{L}},\quad\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}z=(\nabla^2S_{\mathrm{L}})(\nabla S_{\mathrm{L}})=-\nabla(\chi_R V_{\mathrm{L}}),$$

cf. (3.7). The reparametrizing factor $|\nabla S_{\mathrm{L}}|^{-2}$ in (4.3a) is the proper normalization guaranteeing (4.5). This point of view was taken in the proof of an analogous statement [3, Proposition 2.2].

Proof of Lemma 4.4. By Theorem 1.3 (2), we conclude that y is defined at least on $I \times (0, (2\lambda)^{1/2}R] \times \mathbb{S}^{d-1}$, and

$$y(\lambda, t, \theta) = (2\lambda)^{-1/2} t\theta \quad \text{for } (\lambda, t, \theta) \in I \times (0, (2\lambda)^{1/2}R] \times \mathbb{S}^{d-1}. \tag{4.6}$$

On the other hand, by (4.3a), (4.3b), and (4.6)

$$\frac{\partial}{\partial t} S_{\mathrm{L}}(\lambda, y(\lambda, t, \theta)) = 1 \quad \text{and} \quad \lim_{t \to 0_+} S_{\mathrm{L}}(\lambda, y(\lambda, t, \theta)) = 0.$$

This implies $y(\lambda, t, \theta)$ never hits the origin for $t > (2\lambda)^{1/2}R$, and neither it can reach infinity in finite time. Hence, the vector field $|\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}}$ is forward complete, and y is globally defined on $I \times \mathbb{R}_+ \times \mathbb{S}^{d-1}$, satisfying (4.5).

Next, we note that $y(\lambda, \cdot, \cdot)$ is bijective. In fact, by the uniqueness for the initial-value problem of ODEs, the injectivity follows. To see the surjectivity, starting at any given point in $x \in \mathbb{R}^d \setminus \{0\}$, we solve the ODE (4.3a) in the backward time-direction. Then, we obtain a "crossing" initial angle θ from where indeed the forward flow for a proper time t satisfies $y(\lambda, t, \theta) = x$. (Alternatively, $y(\lambda, \cdot, \cdot)$ is bijective, since any $x \in \mathbb{R}^d \setminus \{0\}$ can be connected to the origin by a unique geodesic, cf. Theorems 1.3 (2) and 2.6 (1).)

Finally, we show that $y(\lambda, \cdot, \cdot)$ is a diffeomorphism. Note that the maps $y(\lambda, \cdot, \cdot)$ and $y(\cdot, \cdot, \cdot)$ are smooth, viewed as a solution to an initial-value problem with data specified on the sphere $(2\lambda)^{-1/2}\mathbb{S}^{d-1} \simeq \mathbb{S}^{d-1}$ at time $t = 1$. Thus, it suffices to check the non-degeneracy of the map. Take any local coordinates $\theta' = (\theta'_2, \dots, \theta'_d)$ of $\mathbb{S}^{d-1}$, and let J' be the Jacobian of (4.4) in these local coordinates. Now, we claim that, for any (λ, t, θ'),

$$\partial_t J'(\lambda, t, \theta') = (\nabla \cdot |\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}})(\lambda, y(\lambda, t, \theta'))J'(\lambda, t, \theta'). \tag{4.7}$$

In fact, differentiating the defining expression of the Jacobian, we can write

$$\partial_t J' = \sum_{i=1}^{d} \det \mathcal{J}^{(i)},$$

where $\mathcal{J}^{(i)}$ are matrix-valued functions whose components are given by

$$\mathcal{J}^{(i)}_{jk} = \begin{cases} \partial_k y_j & \text{for } j \neq i, \\ \partial_t \partial_k y_i & \text{for } j = i, \end{cases} \qquad j = 1, \dots, d, \ \ k = t, \theta'_2, \dots, \theta'_d.$$

However, thanks to the flow equation (4.3a), we can compute

$$\partial_t \partial_k y_i = \partial_k (|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_i) = (\partial_l |\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_i)\partial_k y_l.$$

Thus, we obtain the claimed identity (4.7), noting that the determinant is alternating and multilinear. By (4.6), J' is non-vanishing for $t \in (0, (2\lambda)^{1/2}R]$, and hence with (4.7) we can conclude that so it is for all $t > 0$. We are done. ■

Now, the spherical eikonal coordinates are defined as follows.

Definition 4.6. The *spherical eikonal coordinates* on $\mathbb{R}^d \setminus \{0\}$ at energy $\lambda \in I$ are the entries of the inverse of (4.4). We denote them by (t, θ), or by (λ, t, θ) to clarify the λ-dependence. They are also denoted by (t, θ') or (λ, t, θ') if local coordinates $\theta' = (\theta'_2, \ldots, \theta'_d)$ of $\mathbb{S}^{d-1}$ are specified. We call $t = S_{\mathrm{L}}(\lambda, y(\lambda, t, \theta))$ and θ (or θ') the *radial and spherical components* of the spherical eikonal coordinates, respectively.

The Euclidean metric splits into the radial and spherical components in the spherical eikonal coordinates. Let us present it as a corollary, although we will not use it in the present paper. The entries of θ' are distinguished by Greek indices always running over $2, \ldots, d$, while the entries of y canonically are distinguished by Roman ones always running over $1, \ldots, d$.

Corollary 4.7. *Let (t, θ') be spherical eikonal coordinates at any $\lambda \in I$. Then,*

$$(\partial_t y_i(\lambda, t, \theta'))(\partial_t y_i(\lambda, t, \theta')) = |(\nabla S_{\mathrm{L}})(\lambda, y(\lambda, t, \theta'))|^{-2},$$
$$(\partial_t y_i(\lambda, t, \theta'))(\partial_\alpha y_i(\lambda, t, \theta')) = 0 \quad \textit{for } \alpha = 2, \ldots, d.$$

In addition, the Euclidean metric takes the form

$$\mathrm{d}x^2 = |\nabla S_{\mathrm{L}}|^{-2}\, \mathrm{d}t^2 + g_{\alpha\beta}\, \mathrm{d}\theta'_\alpha \mathrm{d}\theta'_\beta.$$

Proof. The former formulas follow from (4.3a) and (4.5), and the last formula is an immediate consequence of the former ones. ■

4.2.2. Volume and surface measures. Let $J\colon I \times \mathbb{R}_+ \times \mathbb{S}^{d-1} \to [0, \infty)$ be a function such that the Euclidean volume measure can be expressed in (λ, t, θ) as

$$\mathrm{d}x(\lambda, t, \theta) = \mathrm{d}x_1 \cdots \mathrm{d}x_d(\lambda, t, \theta) = J(\lambda, t, \theta)\, \mathrm{d}t \mathrm{d}A(\theta), \tag{4.8}$$

where $\mathrm{d}A$ denotes the standard surface measure on $\mathbb{S}^{d-1}$. In fact, if we take any local coordinates $\theta' = (\theta'_2, \ldots, \theta'_d)$ of $\mathbb{S}^{d-1}$, and let J' be the Jacobian from the proof of Lemma 4.4, then J can be computed through the relation

$$\mathrm{d}A_{\lambda,t}(\theta(\theta')) := J(\lambda, t, \theta(\theta'))\, \mathrm{d}A(\theta(\theta')) = J'(\lambda, t, \theta')\, \mathrm{d}\theta'_2 \cdots \mathrm{d}\theta'_d. \tag{4.9}$$

Note that, for any $\phi \in L^1(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} \phi(x)\, \mathrm{d}x = \int_0^\infty \mathrm{d}t \int_{\mathbb{S}^{d-1}} \phi(y(\lambda, t, \theta))\, \mathrm{d}A_{\lambda,t}(\theta). \tag{4.10}$$

By the co-area formula [7, Theorem C.5], the element $|\nabla S_{\mathrm{L}}|(\lambda, y(\lambda,t,\theta))\,\mathrm{d}A_{\lambda,t}(\theta)$ is the Euclidean surface element on the distorted sphere $\{S_L = t\}$.

Lemma 4.8. *The following statements hold.*

(1) *One has an explicit formula*

$$J(\lambda,t,\theta) = \sqrt{2\lambda}R^{d-1}|(\nabla S_{\mathrm{L}})(\lambda, y(\lambda,t,\theta))|^{-2} \cdot \exp\Big(\int_{(2\lambda)^{1/2}R}^{t} (|\nabla S_{\mathrm{L}}|^{-2}\Delta S_{\mathrm{L}})(\lambda, y(\lambda,\tau,\theta))\,\mathrm{d}\tau\Big).$$

(2) *There exist the following limits uniformly in $(\lambda,\theta) \in I \times \mathbb{S}^{d-1}$:*

$$\lim_{t\to 0_+} t^{-(d-1)}J(\lambda,t,\theta) = (2\lambda)^{-d/2},$$
$$\lim_{t\to\infty} t^{-(d-1)}J(\lambda,t,\theta) =: J_+(\lambda,\theta) > 0.$$

Remark 4.9. For similar assertions in a wider geometric setting, see [18].

Proof. (1) Note that, for any $(\lambda,t,\theta) \in I \times \mathbb{R}_+ \times \mathbb{S}^{d-1}$,

$$\partial_t J(\lambda,t,\theta) = (\nabla \cdot |\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}})(\lambda, y(\lambda,t,\theta))J(\lambda,t,\theta). \tag{4.11}$$

In fact, (4.11) follows from (4.7) since in any local coordinates of $\mathbb{S}^{d-1}$, J'/J is a function independent of t, cf. (4.9). Then, since

$$\nabla \cdot (|\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}}) = |\nabla S_{\mathrm{L}}|^{-2}\Delta S_{\mathrm{L}} - \partial_t \ln(|\nabla S_{\mathrm{L}}|^2),$$

it follows from (4.11) that, for some $C(\lambda,\theta) \geq 0$,

$$J(\lambda,t,\theta) = C(\lambda,\theta)|(\nabla S_{\mathrm{L}})(\lambda, y(\lambda,t,\theta))|^{-2} \cdot \exp\Big(\int_{(2\lambda)^{1/2}R}^{t} (|\nabla S_{\mathrm{L}}|^{-2}\Delta S_{\mathrm{L}})(\lambda, y(\lambda,\tau,\theta))\,\mathrm{d}\tau\Big).$$

We can determine $C(\lambda,\theta) = \sqrt{2\lambda}R^{d-1}$ by (1.6) and (4.6), which shows the assertion.

(2) The assertion is clear for $t \to 0_+$ thanks to the explicit expression (4.6). Let $t \geq (2\lambda)^{1/2}R$. Then, by (1.6), Theorem 1.3, and (4.5), it follows that

$$||(\nabla S_{\mathrm{L}})(\lambda, y(\lambda,t,\theta))|^{-2} - (2\lambda)^{-1}| \leq C_1 t^{-\sigma},$$
$$|(|\nabla S_{\mathrm{L}}|^{-2}\Delta S_{\mathrm{L}})(\lambda, y(\lambda,\tau,\theta)) - (d-1)\tau^{-1}| \leq C_1\tau^{-1-\sigma}.$$

This verifies the asymptotics for $t \to \infty$. ∎

4.2.3. Change of coordinates at infinity. Here we investigate relation between the spherical eikonal coordinates and the ordinary spherical coordinates. For each $\lambda \in I$, we can change from $(t,\theta) \in \mathbb{R}_+ \times \mathbb{S}^{d-1}$ to $(r,\omega) \in \mathbb{R}_+ \times \mathbb{S}^{d-1}$ through

$$r(\lambda,t,\theta) = |y(\lambda,t,\theta)|, \quad \omega(\lambda,t,\theta) = \hat{y}(\lambda,t,\theta) = |y(\lambda,t,\theta)|^{-1} y(\lambda,t,\theta). \tag{4.12}$$

We claim that (4.12) induces a C^1-diffeomorphism of $\mathbb{S}^{d-1}$ at infinity provided "s_{L} is small" (which thanks to Corollary 2.14 can be assumed by taking R sufficiently big). More precisely, we claim the following assertion.

Lemma 4.10. *Uniformly in $\lambda \in I$, there exists the limit*

$$\omega_+(\lambda,\cdot) := \lim_{t\to\infty} \omega(\lambda,t,\cdot)\colon \mathbb{S}^{d-1} \to \mathbb{S}^{d-1} \tag{4.13}$$

in the C^1-topology. Moreover, possibly for enlarged $R > 0$ only, the map $\omega_+(\lambda,\cdot)$ is a C^1-diffeomorphism on $\mathbb{S}^{d-1}$ depending continuously on $\lambda \in I$, and, for any $(\lambda,\theta) \in I \times \mathbb{S}^{d-1}$,

$$\mathrm{d}A(\omega_+(\lambda,\theta)) = (2\lambda)^{d/2} J_+(\lambda,\theta)\, \mathrm{d}A(\theta), \tag{4.14}$$

where J_+ is from Lemma 4.8.

Remark 4.11. For fixed $\lambda \in I$, the map $\omega_+(\lambda,\cdot)$ on $\mathbb{S}^{d-1}$ is called the *asymptotic direction map* and its inverse $\theta_+(\lambda,\cdot) = \omega_+^{-1}(\lambda,\cdot) = (\omega_+(\lambda,\cdot))^{-1}$ the *inverse asymptotic direction map*.

Proof. Take $R_0 > 0$ as in Corollary 2.14, and let $\sigma' \in (0,\sigma)$. For the moment, all the estimates below are uniform in $R \geq R_0$. We will possibly need R to be larger in Step IV.

Step I. For any fixed $(\lambda,\theta) \in I \times \mathbb{S}^{d-1}$, we prove the existence of the limit (4.13) in the pointwise sense. For each $i = 1,\dots,d$, we compute and bound, omitting the arguments, as

$$\begin{aligned}
\frac{\partial}{\partial t}\omega_i &= |y|^{-1}|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_i - |y|^{-3} y_i y_j |\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_j \\
&= |y|^{-1}|\nabla S_{\mathrm{L}}|^{-2}(\delta_{ij} - |y|^{-2} y_i y_j)((\nabla S_{\mathrm{L}})_j - (2\lambda)^{1/2}|y|^{-1} y_j) \\
&= \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'}),
\end{aligned} \tag{4.15}$$

where we have used Theorem 1.3 and Lemma 4.4. The integrability of (4.15) in $t \in (1,\infty)$ implies that there exists the limit (4.13) in the pointwise sense. In addition, $\omega_+\colon I \times \mathbb{S}^{d-1} \to \mathbb{S}^{d-1}$ is continuous since (4.15) is uniform in $(\lambda,\theta) \in I \times \mathbb{S}^{d-1}$.

Step II. Take any local coordinates $\theta' = (\theta'_2, \dots, \theta'_d)$ of $\mathbb{S}^{d-1}$, and set, for any $\alpha = 2, \dots, d$,

$$\Omega(\lambda, t, \theta') = (\partial_\alpha \omega_1(\lambda, t, \theta'))^2 + \cdots + (\partial_\alpha \omega_d(\lambda, t, \theta'))^2.$$

We claim that, for any compact subset K of the associated (open) coordinate region, there exist $c_1, C_1 > 0$ such that, for any $(\lambda, t, \theta') \in I \times \mathbb{R}_+ \times K$,

$$c_1 \le \Omega(\lambda, t, \theta') \le C_1. \tag{4.16}$$

For that, we compute and bound the t-derivative of Ω as in Step I. Since we have

$$(\partial_\alpha \omega_i) = |y|^{-1}(\partial_\alpha y_i) - |y|^{-3} y_i y_j (\partial_\alpha y_j), \tag{4.17}$$

we can write, by using (4.3a),

$$\begin{aligned}
\frac{\partial}{\partial t}(\partial_\alpha \omega_i) = & -|y|^{-3} y_j |\nabla S_{\mathrm{L}}|^{-2} (\nabla S_{\mathrm{L}})_j (\partial_\alpha y_i) + |y|^{-1} (\nabla |\nabla S_{\mathrm{L}}|^{-2})_j (\nabla S_{\mathrm{L}})_i (\partial_\alpha y_j) \\
& + |y|^{-1} |\nabla S_{\mathrm{L}}|^{-2} (\nabla^2 S_{\mathrm{L}})_{ij} (\partial_\alpha y_j) \\
& + 3|y|^{-5} |\nabla S_{\mathrm{L}}|^{-2} (\nabla S_{\mathrm{L}})_k y_i y_j y_k (\partial_\alpha y_j) \\
& - |y|^{-3} |\nabla S_{\mathrm{L}}|^{-2} (\nabla S_{\mathrm{L}})_i y_j (\partial_\alpha y_j) - |y|^{-3} y_i |\nabla S_{\mathrm{L}}|^{-2} (\nabla S_{\mathrm{L}})_j (\partial_\alpha y_j) \\
& - |y|^{-3} y_i y_j (\nabla |\nabla S_{\mathrm{L}}|^{-2})_k (\nabla S_{\mathrm{L}})_j (\partial_\alpha y_k) \\
& - |y|^{-3} y_i y_j |\nabla S_{\mathrm{L}}|^{-2} (\nabla^2 S_{\mathrm{L}})_{jk} (\partial_\alpha y_k) \\
=: & \, B_1 + \cdots + B_8.
\end{aligned} \tag{4.18}$$

To bound the terms on the right-hand side of (4.18), we will first prove that

$$|y|^{-1}(\partial_\alpha y_i) = (\partial_\alpha \omega_i) + \mathcal{O}(R^{-\sigma+\sigma'} \langle t \rangle^{-\sigma'}) \Omega^{1/2}. \tag{4.19}$$

To keep the notation simple, we prefer henceforth to state errors like $\mathcal{O}(R^{-\sigma+\sigma'} \langle t \rangle^{-\sigma'})$ as $\mathcal{O}(R^{-\sigma+\sigma'} t^{-\sigma'})$. Now, with this convention, it follows by (4.5) and Theorem 1.3 that

$$|y| = (2\lambda)^{-1/2} t + \mathcal{O}(R^{-\sigma+\sigma'} t^{1-\sigma'}), \quad (\partial_\alpha y_i)(\nabla S_{\mathrm{L}})_i = 0, \tag{4.20}$$

so that (again thanks to Theorem 1.3) we can rewrite (4.17) as

$$\begin{aligned}
|y|^{-1}(\partial_\alpha y_i) &= (\partial_\alpha \omega_i) - |y|^{-2} y_i ((2\lambda)^{-1/2} (\nabla S_{\mathrm{L}})_j - |y|^{-1} y_j)(\partial_\alpha y_j) \\
&= (\partial_\alpha \omega_i) + \mathcal{O}(R^{-\sigma+\sigma'} t^{-\sigma'}) \sum_{j=1}^{d} |y|^{-1} |\partial_\alpha y_j|,
\end{aligned}$$

Hence, by a summation and subtraction,

$$\sum_{j=1}^{d} |y|^{-1} |\partial_\alpha y_j| \le C \sum_{i=1}^{d} |\partial_\alpha \omega_i| \le C \sqrt{d}\, \Omega^{1/2},$$

which verifies (4.19).

Now, we bound term by term

$$B_1 + \cdots + B_8 = (B_2 + B_7) + (B_4 + B_5 + B_6) + B_8 + (B_1 + B_3).$$

By (1.6) and (4.19),

$$B_2 + B_7 = \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega^{1/2}$$

By (4.20), (4.19), and Theorem 1.3,

$$\begin{aligned} B_4 + B_5 + B_6 &= 3|y|^{-4}|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_k y_i y_k ((2\lambda)^{-1/2}(\nabla S_{\mathrm{L}})_j - |y|^{-1} y_j)(\partial_\alpha y_j) \\ &\quad + |y|^{-2}|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_i ((2\lambda)^{-1/2}(\nabla S_{\mathrm{L}})_j - |y|^{-1} y_j)(\partial_\alpha y_j) \\ &= \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega^{1/2}. \end{aligned}$$

By (3.12), (4.20), (4.19), and Theorem 1.3,

$$\begin{aligned} B_8 &= |y|^{-2} y_i ((2\lambda)^{-1/2}(\nabla S_{\mathrm{L}})_j - |y|^{-1} y_j)|\nabla S_{\mathrm{L}}|^{-2}(\nabla^2 S_{\mathrm{L}})_{jk}(\partial_\alpha y_k) \\ &\quad - \frac{1}{2}(2\lambda)^{-1/2}|y|^{-2} y_i |\nabla S_{\mathrm{L}}|^{-2}(\nabla|\nabla S_{\mathrm{L}}|^2)_k(\partial_\alpha y_k) \\ &= \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega^{1/2}. \end{aligned}$$

Finally, by (4.20), (4.19), Theorem 1.3, and (3.2c) (see also Remark 3.2),

$$\begin{aligned} B_1 + B_3 &= -(2\lambda)^{-1/2}|y|^{-2}(\partial_\alpha y_i) \\ &\quad + |y|^{-2}((2\lambda)^{-1/2}(\nabla S_{\mathrm{L}})_j - |y|^{-1} y_j)|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})_j(\partial_\alpha y_i) \\ &\quad + (2\lambda)^{1/2} f^{-1}|y|^{-1}|\nabla S_{\mathrm{L}}|^{-2}((\partial_i f)(\partial_j f) + f(\nabla^2 f)_{ij})(\partial_\alpha y_j) \\ &= \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega^{1/2}. \end{aligned}$$

Therefore, combining the above estimates, we obtain

$$\frac{\partial}{\partial t}(\partial_\alpha \omega_i) = \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega^{1/2}, \quad \text{or} \quad \frac{\partial}{\partial t}\Omega = \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'})\Omega. \tag{4.21}$$

This implies $\ln \Omega$ is bounded, and thus the claim (4.16) is verified.

Step III. Next, we show $\omega_+(\lambda, \cdot)\colon \mathbb{S}^{d-1} \to \mathbb{S}^{d-1}$ is continuously differentiable. This is straightforward due to Step II. By (4.21) and (4.16), it follows that

$$\frac{\partial}{\partial t}(\partial_\alpha \omega_i) = \mathcal{O}(R^{-\sigma+\sigma'} t^{-1-\sigma'}) \tag{4.22}$$

uniformly in $\lambda \in I$ and locally uniformly in θ' in the coordinate region. It is integrable in $t \in (1, \infty)$, and this implies there exists the limit

$$\lim_{t\to\infty} \partial_\alpha \omega_i(\lambda, t, \theta')$$

uniformly in $\lambda \in I$ and locally uniformly in θ' in this region. Hence, the convergence (4.13) is in the C^1-topology, and $\omega_+(\lambda, \cdot)$ is continuously differentiable as wanted. Note that $\partial_\alpha \omega_+$ is continuous also in $\lambda \in I$ since these estimates are uniform in $\lambda \in I$.

Step IV. We prove that $\omega_+(\lambda, \cdot)$ is a C^1-diffeomorphism, provided $R \geq R_0$ is large. By (4.15), (4.22), and the fact that $\omega(\lambda, t, \theta) = \theta$ for any $t \in (0, (2\lambda)^{1/2} R]$, see (4.6), it follows that for, any sufficiently large $R \geq R_0$ and any $(\lambda, \theta) \in I \times \mathbb{S}^{d-1}$,

$$|\omega_+(\lambda, \theta) - \theta| \leq \frac{1}{2} \quad \text{and} \quad |\nabla_\theta(\omega_+(\lambda, \theta) - \theta)| \leq \frac{1}{2}. \tag{4.23}$$

Due to the second bound of (4.23), we can apply the inverse function theorem to $\omega_+(\lambda, \cdot)$, and hence the image $\omega_+(\lambda, \mathbb{S}^{d-1}) \subseteq \mathbb{S}^{d-1}$ is open. On the other hand, since $\mathbb{S}^{d-1}$ is compact and ω_+ is continuous, $\omega_+(\lambda, \mathbb{S}^{d-1})$ is also closed. Thus, $\omega_+(\lambda, \cdot)$ is surjective due to the connectedness of $\mathbb{S}^{d-1}$.

Now, it suffices to show the injectivity of $\omega_+(\lambda, \cdot)$. Suppose that, for some $\lambda \in I$ and $\theta_1, \theta_2 \in \mathbb{S}^{d-1}$,

$$\omega_+(\lambda, \theta_1) = \omega_+(\lambda, \theta_2).$$

Then, if we let γ be a grand circle segment, or a geodesic of minimal length, on $\mathbb{S}^{d-1}$ connecting θ_1 and θ_2, we can estimate, by using (4.23),

$$\begin{aligned} \mathrm{dist}_{\mathbb{R}^d}(\theta_1, \theta_2) &= \mathrm{dist}_{\mathbb{R}^d}(\theta_1 - \omega_+(\lambda, \theta_1), \theta_2 - \omega_+(\lambda, \theta_2)) \\ &\leq \int_0^1 |\nabla_\theta(\theta - \omega_+(\lambda, \theta))_{|\theta=\gamma(t)}|\, |\dot{\gamma}(t)|\, \mathrm{d}t \\ &\leq \frac{1}{2} \mathrm{dist}_{\mathbb{S}^{d-1}}(\theta_1, \theta_2) \leq \frac{\pi}{4} \mathrm{dist}_{\mathbb{R}^d}(\theta_1, \theta_2), \end{aligned}$$

where $\mathrm{dist}_{\mathbb{R}^d}$ and $\mathrm{dist}_{\mathbb{S}^{d-1}}$ are the standard metrics there. This implies $\theta_1 = \theta_2$, since $\pi < 4$. Thus, we conclude that $\omega_+(\lambda, \cdot) \colon \mathbb{S}^{d-1} \to \mathbb{S}^{d-1}$ is a C^1–diffeomorphism.

Step V. Finally, we show identity (4.14) by rewriting the Euclidean volume measure as follows. In the standard spherical coordinates (r, ω'), we can write

$$\mathrm{d}x(r, \omega') = r^{d-1}\, \mathrm{d}r \mathrm{d}A(\omega(\omega')) = r^{d-1} a(\omega')\, \mathrm{d}r \mathrm{d}\omega'_2 \cdots \mathrm{d}\omega'_d.$$

Let us further change the variables to (λ, t, θ') by using (4.12). We compute the Jacobian by the cofactor expansion. Some of the first order derivatives of (4.12) are bounded by (4.15) and (4.16), and we only have to note that by Theorem 1.3, (4.19), and (4.16),

$$\begin{aligned} \frac{\partial}{\partial t} r &= |y|^{-1} y \cdot (\nabla S_{\mathrm{L}}) / |\nabla S_L|^2 = (2\lambda)^{-1/2} + \mathcal{O}(t^{-\sigma'}), \\ \partial_\alpha r &= |y|^{-1} y \cdot \partial_\alpha y = (|y|^{-1} y - (2\lambda)^{-1/2} \nabla S_{\mathrm{L}}) \cdot \partial_\alpha y = \mathcal{O}(t^{1-\sigma'}). \end{aligned}$$

Then, the cofactor expansion yields

$$\begin{aligned}&\mathrm{d}x(r(\lambda,t,\theta'),\omega'(\lambda,t,\theta'))\\&\quad = t^{d-1}((2\lambda)^{-d/2}K'(\lambda,t,\theta') + \mathcal{O}(t^{-\sigma'}))a(\omega'(\lambda,t,\theta'))\,\mathrm{d}t\,\mathrm{d}\theta'_2\cdots\mathrm{d}\theta'_d,\end{aligned}$$

where $K'(\lambda,t,\cdot)$ is the Jacobian of $\omega(\lambda,t,\cdot)\colon \mathbb{S}^{d-1}\to\mathbb{S}^{d-1}$ in the local coordinates θ' and ω'. The above expression has to coincide with (4.8), so that

$$\begin{aligned}&t^{d-1}((2\lambda)^{-d/2}K'(\lambda,t,\theta') + \mathcal{O}(t^{-\sigma'}))a(\omega'(\lambda,t,\theta'))\,\mathrm{d}\theta'_2\cdots\mathrm{d}\theta'_d\\&\quad = J(\lambda,t,\theta(\theta'))\,\mathrm{d}A(\theta(\theta')),\end{aligned}$$

or

$$\begin{aligned}\mathrm{d}A(\omega(\omega'(\lambda,t,\theta'))) &= K'(\lambda,t,\theta')a(\omega'(\lambda,t,\theta'))\,\mathrm{d}\theta'_2\cdots\mathrm{d}\theta'_d\\&= ((2\lambda)^{d/2}t^{-(d-1)}J(\lambda,t,\theta(\theta')) + \mathcal{O}(t^{-\sigma}))\,\mathrm{d}A(\theta(\theta')).\end{aligned}$$

Hence, by letting $t\to\infty$, we obtain (4.14). We are done. ∎

4.2.4. Comparison of eikonal distances. Here we compare S_{L} (solving the eikonal equation for V_{L}) with the function S from Theorem 1.5 (solving the eikonal equation for V, with λ in the same interval I). We show that their difference has a radial limit at infinity (as a step of the proof we first establish the eikonal radial limit). We present a slightly generalized assertion localized to a conic subset of $\mathbb{R}^d$. For any $R'>0$ and any open subset $U\subseteq\mathbb{S}^{d-1}$ we set

$$\Gamma_{R',U} = \{x\in\mathbb{R}^d \mid |x|>R' \text{ and } \hat{x}\in U\},\quad \hat{x}=|x|^{-1}x.$$

Lemma 4.12. *Let $R>0$ be large enough as in Lemma 4.10. Let $R'>0$, and $U\subseteq\mathbb{S}^{d-1}$ be open, and assume $S=\sqrt{2\lambda}|x|(1+s)\in C(I;C^2(\Gamma_{R',U}))$ satisfies thte followivng conditions.*

(i) *For each $\lambda\in I$, $S(\lambda,\cdot)$ solves (1.3a) on $\Gamma_{R',U}$.*

(ii) *For any compact subset $I'\subseteq I$, there exist $\varepsilon, C>0$ such that, for any $|\alpha|\le 2$ and $(\lambda,x)\in I'\times\Gamma_{R',U}$,*

$$|\partial_x^\alpha s(\lambda,x)|\le C\langle x\rangle^{-\varepsilon-|\alpha|}.$$

Then the following assertions hold.

(1) *There exists the limit*

$$\Sigma_{\mathrm{L}}(\lambda,\theta) := \lim_{t\to\infty}(S(\lambda,y(\lambda,t,\theta)) - S_{\mathrm{L}}(\lambda,y(\lambda,t,\theta)))$$

taken locally uniformly in (λ, θ), *with* $\lambda \in I$ *and* $\theta \in \omega_+^{-1}(\lambda, U) = \theta_+(\lambda, U)$. *In particular, if* $S_1 \in C(I; C^2(\Gamma_{R',U}))$ *also satisfies the above conditions* (i) *and* (ii), *then there exists the limit*

$$\Sigma(\lambda, \theta) := \lim_{t \to \infty} (S_1(\lambda, y(\lambda, t, \theta)) - S(\lambda, y(\lambda, t, \theta)))$$

taken locally uniformly in (λ, θ) *with* $\lambda \in I$ *and* $\theta \in \theta_+(\lambda, U)$.

(2) *The quantities in* (1) *can also be computed as the limits*

$$\Theta_{\mathrm{L}}(\lambda, \omega) := \Sigma_{\mathrm{L}}(\lambda, \theta_+(\lambda, \omega)) = \lim_{r \to \infty} (S(\lambda, r\omega) - S_{\mathrm{L}}(\lambda, r\omega)),$$
$$\Theta(\lambda, \omega) := \Sigma(\lambda, \theta_+(\lambda, \omega)) = \lim_{r \to \infty} (S_1(\lambda, r\omega) - S(\lambda, r\omega)),$$

both taken locally uniformly in $(\lambda, \omega) \in I \times U$.

Proof. We proceed in two steps.

Step I. To prove the assertions of (1), we only show the first one. The second assertion is obvious from the first one. The following bounds are locally uniform in (λ, θ) with $\lambda \in I$ and $\theta \in \theta_+(\lambda, U)$, however we shall not elaborate on that feature. By (4.3a), (1.3a), and (1.6), we compute for large $t > 0$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(S - S_{\mathrm{L}}) &= |\nabla S_{\mathrm{L}}|^{-2}(\nabla S - \nabla S_{\mathrm{L}}) \cdot (\nabla S_{\mathrm{L}}) \\ &= -\frac{1}{2}|\nabla S_{\mathrm{L}}|^{-2}(\nabla S - \nabla S_{\mathrm{L}})^2 - |\nabla S_{\mathrm{L}}|^{-2} V_{\mathrm{S}}.\end{aligned} \tag{4.24}$$

We are going to show the integrability of (4.24) at infinity. The second term on the right-hand side of (4.24) is clearly integrable due to Theorem 1.3 and (4.5), and we discuss only the first term. It suffices to show that, for some small $\delta > 0$,

$$u := (\nabla S - \nabla S_{\mathrm{L}})^2 = \mathcal{O}(t^{-1-\delta}), \tag{4.25}$$

see also [9, Theorem 2.3 and its proof]. Similarly to (4.24), we can compute the derivative of u as

$$\begin{aligned}\frac{1}{2}|\nabla S_{\mathrm{L}}|^2 \frac{\mathrm{d}}{\mathrm{d}t} u &= (\nabla S - \nabla S_{\mathrm{L}}) \cdot (\nabla^2 S - \nabla^2 S_{\mathrm{L}})(\nabla S_{\mathrm{L}}) \\ &= -(\nabla S - \nabla S_{\mathrm{L}}) \cdot (\nabla^2 S)(\nabla S - \nabla S_{\mathrm{L}}) - (\nabla V_{\mathrm{S}}) \cdot (\nabla S - \nabla S_{\mathrm{L}}).\end{aligned} \tag{4.26}$$

From the assumptions on S, we deduce that

$$\nabla^2 S \geq 2\lambda S^{-1} I - C_2 S^{-1-\varepsilon} I - S^{-1}(\nabla S) \otimes (\nabla S).$$

We apply this bound to (4.26), use (1.3a) and (1.6) (as in (4.24)), and conclude that

$$\begin{aligned}\frac{1}{2}|\nabla S_{\mathrm{L}}|^2\frac{\mathrm{d}}{\mathrm{d}t}u \leq &-2\lambda S^{-1}u + C_2 S^{-1-\varepsilon}u\\ &+ S^{-1}((\nabla S-\nabla S_{\mathrm{L}})\cdot(\nabla S))^2 + |\nabla V_{\mathrm{S}}|u^{1/2}\\ = &-2\lambda S^{-1}u + C_2 S^{-1-\varepsilon}u + 4^{-1}S^{-1}(u-2V_{\mathrm{S}})^2 + |\nabla V_{\mathrm{S}}|u^{1/2}.\end{aligned} \tag{4.27}$$

By Theorem 1.3, (4.5), and the assumptions on S, we observe, letting $\delta\in(0,\varepsilon)$ be small enough, that

$$|\nabla S_{\mathrm{L}}|^2 = 2\lambda + \mathcal{O}(t^{-\delta}),\quad S = t+\mathcal{O}(t^{1-\delta}),\quad u=(\nabla S-\nabla S_{\mathrm{L}})^2=\mathcal{O}(t^{-\delta}).$$

Substituting these estimates into (4.27), we obtain, for large $t>0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}u \leq -2t^{-1}u + C_3 t^{-1-\delta}u + C_3 t^{-2-\delta} \leq -(2-\delta)t^{-1}u + C_3 t^{-2-\delta}.$$

This differential inequality implies (4.25). Hence, we are done with (1).

Step II. We prove the first assertion of (2) (the other one in (2) follows from that). Fixing any compact subset $K\subset I\times U$, we are going to prove

$$\lim_{r\to\infty}\sup_{(\lambda,\omega)\in K}|\Sigma_{\mathrm{L}}(\lambda,\theta_+(\lambda,\omega)) - S(\lambda,r\omega) + S_{\mathrm{L}}(\lambda,r\omega)| = 0.$$

Using (4.12) and Lemma 4.10, let us first note that

$$\lim_{r\to\infty}\sup_{(\lambda,\omega)\in K}|\theta_+(\lambda,\omega)-\theta(\lambda,r\omega)| = 0. \tag{4.28}$$

In fact, changing variables from (r,ω) to (t,θ) and using $t=S_{\mathrm{L}}(\lambda,r\omega)$, it follows that, uniformly in $(\lambda,\omega)\in K$, one has $\mathrm{d}t/\mathrm{d}r = \nabla S_L\cdot\omega > \sqrt{\lambda}$ for large r, and hence taking $r\to\infty$ corresponds to taking $t\to\infty$. Thus, for some compact subset $K'\subset\{(\lambda,\theta);\ \lambda\in I,\ \theta\in\theta_+(\lambda,U)\}$, we can compute (thanks to Lemma 4.10)

$$\begin{aligned}&\lim_{r\to\infty}\sup_{(\lambda,\omega)\in K}|\theta_+(\lambda,\omega)-\theta(\lambda,r\omega)|\\ &\quad\leq \lim_{t\to\infty}\sup_{(\lambda,\theta)\in K'}|\theta_+(\lambda,\omega(\lambda,t,\theta)) - \theta(\lambda,y(\lambda,t,\theta))|\\ &\quad= \sup_{(\lambda,\theta)\in K'}|\theta_+(\lambda,\omega_+(\lambda,\theta))-\theta| = 0.\end{aligned}$$

Now, by (4.28), the above change of variables, and assertion (1), it follows that

$$\begin{aligned}&\lim_{r\to\infty}\sup_{(\lambda,\omega)\in K}|\Sigma_{\mathrm{L}}(\lambda,\theta_+(\lambda,\omega)) - S(\lambda,r\omega)+S_{\mathrm{L}}(\lambda,r\omega)|\\ &\quad= \lim_{r\to\infty}\sup_{(\lambda,\omega)\in K}|\Sigma_{\mathrm{L}}(\lambda,\theta(\lambda,r\omega)) - S(\lambda,r\omega)+S_{\mathrm{L}}(\lambda,r\omega)|\end{aligned}$$

$$= \lim_{t\to\infty} \sup_{(\lambda,\theta)\in K'} |\Sigma_{\mathrm{L}}(\lambda, \theta(\lambda, y(\lambda, t, \theta))) - S(\lambda, y(\lambda, t, \theta)) + S_{\mathrm{L}}(\lambda, y(\lambda, t, \theta))|$$
$$= \lim_{t\to\infty} \sup_{(\lambda,\theta)\in K'} |\Sigma_{\mathrm{L}}(\lambda, \theta) - S(\lambda, y(\lambda, t, \theta)) + S_{\mathrm{L}}(\lambda, y(\lambda, t, \theta))| = 0.$$

We are done. ∎

Remark 4.13. Such a localized version has an application in 3-body long-range stationary scattering theory [23], for which we should take $U \subseteq \mathbb{S}^{d-1}$ such that the closure $\overline{U}$ does not intersect the "collision planes." For such U, the function

$$\mathrm{e}^{\mathrm{i}\Theta(\lambda,\omega)} = \mathrm{e}^{\mathrm{i}\Sigma(\lambda,\theta_+(\lambda,\omega))}; \quad \theta_+(\lambda,\cdot) = \omega_+^{-1}(\lambda,\cdot), \tag{4.29}$$

induces a well-defined family of unitary multiplication operators on $L^2(U)(\subseteq \mathcal{G})$ being strongly continuous in λ. Upon varying U under the above constraint, the function (4.29) is defined almost everywhere on $\mathbb{S}^{d-1}$ and constitutes a strongly continuous $\mathcal{L}(\mathcal{G})$–valued function of λ. The transformation factor $\mathrm{e}^{\mathrm{i}\Theta(\lambda,\omega)}$ (exhibiting "covariance") and (1.10) are applicable to the 3-body problem [23], cf. Section 1.2.5. In particular, it is not possible to take $U = \mathbb{S}^{d-1}$ in that application. However, in the present paper we only use Lemma 4.12 with $U = \mathbb{S}^{d-1}$, see for example Remark 1.9 (3) and Theorem 1.12 (3).

4.3. Stationary wave operators

4.3.1. Construction for the regularized potential. Here, we discuss an analogue of Theorem 1.5 for H_{L} in the spherical eikonal coordinates. Once the strong radiation condition bounds from Theorem 1.24 are established and the spherical eikonal coordinates are fixed, the construction is rather straightforward, following the schemes of [9, 22]. Set, for any $\xi \in \mathcal{G}$,

$$\phi_\pm^{S_{\mathrm{L}}}[\xi](\lambda, x) = \frac{(2\pi)^{1/2}}{(2\lambda)^{1/4}} \chi(r) r^{-(d-1)/2} \mathrm{e}^{\pm \mathrm{i} S_{\mathrm{L}}(\lambda,x)} \xi(\hat{x}), \quad r = |x|, \ \hat{x} = |x|^{-1} x, \tag{4.30}$$

where χ is from (1.4) (see also (1.9)).

Proposition 4.14. *The following statements hold.*

(1) *For any $\lambda \in I$, there exist unique $E^\pm(\lambda) \in \mathcal{L}(\mathcal{B}, \mathcal{G})$ such that, for any $\psi \in \mathcal{B}$,*

$$R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)\psi - \phi_\pm^{S_{\mathrm{L}}}[E^\pm(\lambda)\psi](\lambda, \cdot) \in \mathcal{B}_0^*. \tag{4.31}$$

(2) *The mappings $E^\pm: I \times \mathcal{B} \to \mathcal{G}$ are continuous.*

(3) *For any $\lambda \in I$,*

$$E^\pm(\lambda)^* E^\pm(\lambda) = \delta(H_{\mathrm{L}} - \lambda),$$

Before proving Proposition 4.14, we present a trace-type theorem in a form appropriate for our application. Note that, by Fubini's theorem, we can identify

$$L^2_{\mathrm{loc}}(\mathbb{R}_+ \times \mathbb{S}^{d-1}) \simeq L^2_{\mathrm{loc}}(\mathbb{R}_+; \mathcal{G}).$$

To be precise, we denote the above identification operator for the moment by ι, i.e., for any $\psi \in L^2_{\mathrm{loc}}(\mathbb{R}_+ \times \mathbb{S}^{d-1})$, we let

$$\iota(\psi)(t) = \psi(t,\cdot) \in \mathcal{G} \quad \text{for a.e. } t \in \mathbb{R}_+.$$

Lemma 4.15. *Let $k \in \mathbb{N}_0$ and $\psi \in H^s_{\mathrm{loc}}(\mathbb{R}_+ \times \mathbb{S}^{d-1})$ with $s > k + 1/2$. Then,*

$$\iota(\psi) \in C^k(\mathbb{R}_+; \mathcal{G}), \quad \text{and} \quad \frac{\mathrm{d}^l}{\mathrm{d}t^l}\iota(\psi) = \iota\Big(\frac{\partial^l}{\partial t^l}\psi\Big) \quad \text{for } l = 0, \dots, k.$$

Proof of Lemma 4.15. By a partition-of-unity argument, we can reduce the claims to similar ones in a coordinate region. Then, we can mimic the proof of the familiar Sobolev embedding theorem. We omit the details. ■

Proof of Proposition 4.14. We proceed in four steps.

Step I. Let $\lambda \in I$ and $\psi \in C^\infty_c(\mathbb{R}^d)$ be given, and then let

$$\Psi(t) = J(\lambda,t,\cdot)^{1/2} \mathrm{e}^{\mp \mathrm{i} S_{\mathrm{L}}(\lambda, y(\lambda,t,\cdot))} (R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)\psi)(y(\lambda,t,\cdot)) \in \mathcal{G}; \quad t \in \mathbb{R}_+.$$

Since $R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)\psi \in H^2_{\mathrm{loc}}(\mathbb{R}^d)$, it follows from Lemma 4.15 that $\Psi \in C^1(\mathbb{R}_+; \mathcal{G})$. We first show the existence of the limits

$$D^{\pm}(\lambda)\psi = \mathcal{G}\text{–}\lim_{t\to\infty} \Psi(t). \tag{4.32}$$

By the fundamental theorem of calculus, we have

$$\Psi(t) = \Psi(1) + \int_1^t \frac{\mathrm{d}}{\mathrm{d}t}\Psi(\tau)\,\mathrm{d}\tau,$$

and it suffices to show that the last integrand is integrable as a $\mathcal{G}$-valued function. We can compute it, by Lemma 4.15, (4.11), (4.5), (4.3a), and (1.20), as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Psi &= J^{1/2}\mathrm{e}^{\mp \mathrm{i} S_{\mathrm{L}}}\big(\mathrm{i}|\nabla S_{\mathrm{L}}|^{-2}(\nabla S_{\mathrm{L}})\cdot\gamma + \tfrac{1}{2}(\nabla\cdot|\nabla S_{\mathrm{L}}|^{-2}\nabla S_{\mathrm{L}})\big)R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)\psi \\ &= J^{1/2}\mathrm{e}^{\mp \mathrm{i} S_{\mathrm{L}}}\big(\mathrm{i}|\nabla S_{\mathrm{L}}|^{-2}\gamma_{\|} + \tfrac{1}{2}(\nabla|\nabla S_{\mathrm{L}}|^{-2})\cdot(\nabla S_{\mathrm{L}})\big)R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)\psi.\end{aligned}$$

By (1.21a) and (3.12), we can find $\delta > 0$ and $\Phi \in L^2_{(1+\delta)/2}$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = J(\lambda,t,\cdot)^{1/2}\Phi(\lambda, y(\lambda,t,\cdot)).$$

Then, by the Cauchy–Schwarz inequality and (4.10),

$$\begin{aligned}
&\int_1^\infty \|\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t)\|_{\mathcal{G}}\,\mathrm{d}t \\
&\quad = \int_1^\infty \mathrm{d}t\Big(\int_{\mathbb{S}^{d-1}} |\Phi(\lambda, y(\lambda,t,\theta))|^2\,\mathrm{d}A_{\lambda,t}(\theta)\Big)^{1/2} \\
&\quad \le C_1\Big(\int_1^\infty t^{-1-\delta}\,\mathrm{d}t\Big)^{1/2}\Big(\int_1^\infty \mathrm{d}t\int_{\mathbb{S}^{d-1}} |(|\cdot|^{(1+\delta)/2}\Phi)(\lambda, y(\lambda,t,\theta))|^2\,\mathrm{d}A_{\lambda,t}(\theta)\Big)^{1/2} \\
&\quad \le C_2\|\Phi\|_{L^2_{(1+\delta)/2}}.
\end{aligned}$$

Hence, there exist the limits (4.32). We note that $D^{\pm}(\lambda)\psi$ are continuous in $\lambda \in I$, since $\Psi(t)$ is continuous in $\lambda \in I$, and the above estimates are locally uniform in this variable.

Step II. Next, we set, for any $\lambda \in I$ and $\psi \in C_c^\infty(\mathbb{R}^d)$,

$$\begin{aligned}
E^{\pm}(\lambda)\psi &= c(\lambda)(2\lambda)^{-d/4} J_+(\lambda, \theta_+(\lambda,\cdot))^{-1/2}(D^{\pm}(\lambda)\psi)(\theta_+(\lambda,\cdot)), \\
c(\lambda) &= (2\pi)^{-1/2}(2\lambda)^{1/2},
\end{aligned} \tag{4.33a}$$

and verify that they satisfy (4.31). For completeness of presentation, note that

$$\|E^{\pm}(\lambda)\psi\|_{\mathcal{G}} = c(\lambda)\|D^{\pm}(\lambda)\psi\|_{\mathcal{G}},$$

cf. Lemma 4.10. By (4.32), it follows that

$$\begin{aligned}
&\lim_{t\to\infty} t^{-1}\int_0^t \|D^{\pm}(\lambda)\psi - J(\lambda,\tau,\cdot)^{1/2}\mathrm{e}^{\mp\mathrm{i}S_{\mathrm{L}}(\lambda,y(\lambda,\tau,\cdot))}(R_{\mathrm{L}}(\lambda\pm\mathrm{i}0)\psi)(y(\lambda,\tau,\cdot))\|_{\mathcal{G}}^2\,\mathrm{d}\tau \\
&\quad = 0,
\end{aligned}$$

and, along with (4.10), Lemma 4.8, and the asymptotics $|y(\lambda,\tau,\cdot)|/\tau \to (2\lambda)^{-1/2}$, this implies

$$\begin{aligned}
\lim_{t\to\infty} t^{-1}\int_{\{S_L\le t\}} &|(2\lambda)^{-(d-1)/4}|x|^{-(d-1)/2}\mathrm{e}^{\pm\mathrm{i}S_{\mathrm{L}}(\lambda,x)} J_+(\lambda,\theta(\lambda,x))^{-1/2} \\
&\cdot (D^{\pm}(\lambda)\psi)(\theta(\lambda,x)) - (R_{\mathrm{L}}(\lambda\pm\mathrm{i}0)\psi)(x)|^2\,\mathrm{d}x = 0.
\end{aligned}$$

Hence, it suffices to prove

$$\begin{aligned}
\lim_{t\to\infty} t^{-1}\int_{\{S_L\le t\}} &|x|^{-(d-1)/2}|J_+(\lambda,\theta(\lambda,x))^{-1/2}(D^{\pm}(\lambda)\psi)(\theta(\lambda,x)) \\
&- J_+(\lambda,\theta_+(\lambda,\hat{x}))^{-1/2}(D^{\pm}(\lambda)\psi)(\theta_+(\lambda,\hat{x}))|^2\,\mathrm{d}x = 0.
\end{aligned}$$

In turn, if we let $u(\lambda,\theta) = J_+(\lambda,\theta)^{-1/2}(D^{\pm}(\lambda)\psi)(\theta)$ and again use eikonal spherical coordinates, it suffices to prove that

$$\lim_{t\to\infty} t^{-1}\int_0^t \|u(\lambda,\cdot) - u(\lambda,\theta_+(\lambda,\omega(\lambda,\tau,\cdot)))\|_{\mathscr{G}}^2\,\mathrm{d}\tau = 0. \tag{4.34}$$

To prove (4.34), first note that, for any $v, w \in \mathscr{G}$,

$$\|v(\theta_+(\lambda,\omega(\lambda,\tau,\cdot))) - w(\theta_+(\lambda,\omega(\lambda,\tau,\cdot)))\|_{\mathscr{G}} \le C_3\|v-w\|_{\mathscr{G}};\quad \tau\in[1,\infty). \tag{4.35}$$

Here, we used that the coordinate change $\theta \to \theta_+(\lambda,\omega(\lambda,\tau,\cdot))$ converges to the identity map in the C^1-topology as $\tau\to\infty$. Next, we estimate, for any $v \in C^\infty(\mathbb{S}^{d-1})$,

$$\begin{aligned}
&\|u(\lambda,\cdot) - u(\lambda,\theta_+(\lambda,\omega(\lambda,\tau,\cdot)))\|_{\mathscr{G}}\\
&\quad\le \|u(\lambda,\cdot) - v\|_{\mathscr{G}} + \|v - v(\theta_+(\lambda,\omega(\lambda,\tau,\cdot)))\|_{\mathscr{G}}\\
&\qquad + \|v(\theta_+(\lambda,\omega(\lambda,\tau,\cdot))) - u(\lambda,\theta_+(\lambda,\omega(\lambda,\tau,\cdot)))\|_{\mathscr{G}}.
\end{aligned} \tag{4.36}$$

The first term on the right-hand side of (4.36) can be arbitrarily small by choosing appropriate $v \in C^\infty(\mathbb{S}^{d-1})$. Due to (4.35), then also the third term is small (uniformly in τ). For any such v fixed, clearly the second term converges to 0 as $\tau\to\infty$. This verifies (4.34).

Step III. We next show that, for any $\lambda \in I$ and $\psi \in C_c^\infty(\mathbb{R}^d)$,

$$\|E^{\pm}(\lambda)\psi\|_{\mathscr{G}}^2 = \langle\psi, \delta(H_L - \lambda)\psi\rangle. \tag{4.37}$$

Using for $T > 0$ the function χ_T from (1.5), we set

$$\eta_T = 1 - \chi_T,\quad \eta_T' = -T^{-1}\chi'(|\cdot|/T). \tag{4.38}$$

Introducing also the notation $\phi = R_L(\lambda \pm \mathrm{i}0)\psi$, we then write

$$2\pi\langle\psi,\delta(H_L-\lambda)\psi\rangle = \pm 2\,\mathrm{Im}\langle(H_L-\lambda)\phi,\phi\rangle = \pm 2\lim_{T\to\infty}\mathrm{Im}\langle(H_L-\lambda)\phi,\eta_T\phi\rangle.$$

By an integration by parts, this leads to

$$\begin{aligned}
2\pi\langle\psi,\delta(H_L-\lambda)\psi\rangle &= \mp\lim_{T\to\infty}\mathrm{Re}\langle\hat{x}\cdot p\phi,\eta_T'\phi\rangle\\
&= \mp\lim_{T\to\infty}\mathrm{Re}\langle\hat{x}\cdot\gamma\phi,\eta_T'\phi\rangle - \lim_{T\to\infty}\langle|\nabla\chi_1 S_L|\phi,\eta_T'\phi\rangle.
\end{aligned} \tag{4.39}$$

The contribution from the first term on the right-hand side of (4.39) vanishes due to (1.21c). As for the second term we rewrite the integral in the standard spherical coordinates, substitute (4.31) and conclude that

$$-\lim_{T\to\infty}\langle|\nabla\chi_1 S_L|\phi,\eta_T'\phi\rangle = 2\pi\|E^{\pm}(\lambda)\psi\|_{\mathscr{G}}^2,$$

hence the claim (4.37) for $\psi \in C_c^\infty(\mathbb{R}^d)$.

Step IV. Now, we prove assertions (1)–(3). Identity (4.37) immediately implies that $E^{\pm}(\lambda)$ extend continuously as $\mathcal{B} \to \mathcal{G}$, and the extensions obviously satisfy (4.31) and (4.37). This verifies assertions (1) and (3). To see the joint continuity of the morphism $E^{\pm}: I \times \mathcal{B} \to \mathcal{G}$, we let $\lambda, \mu \in I$ and $\psi, \varphi \in \mathcal{B}$. We take another $\zeta \in C_c^\infty(\mathbb{R}^d)$, and split

$$\begin{aligned}
&\|E^{\pm}(\lambda)\psi - E^{\pm}(\mu)\varphi\|_{\mathcal{G}} \\
&\quad \le \|E^{\pm}(\lambda)\psi - E^{\pm}(\lambda)\zeta\|_{\mathcal{G}} + \|E^{\pm}(\lambda)\zeta - E^{\pm}(\mu)\zeta\|_{\mathcal{G}} \\
&\qquad + \|E^{\pm}(\mu)\zeta - E^{\pm}(\mu)\varphi\|_{\mathcal{G}} \\
&\quad \le \langle \psi - \zeta, \delta(H_{\mathrm{L}} - \lambda)(\psi - \zeta)\rangle^{1/2} + \|E^{\pm}(\lambda)\zeta - E^{\pm}(\mu)\zeta\|_{\mathcal{G}} \\
&\qquad + \langle \zeta - \varphi, \delta(H_{\mathrm{L}} - \mu)(\zeta - \varphi)\rangle^{1/2}.
\end{aligned}$$

By the locally uniform boundedness of $R_{\mathrm{L}}(\lambda \pm \mathrm{i}0) \in \mathcal{L}(\mathcal{B}, \mathcal{B}^*)$, the first and third terms on the right-hand side above can be arbitrarily small (uniformly in the spectral parameter) if we choose ψ, φ, and ζ close to each other. For such a fixed ζ, the second term can be arbitrarily small if λ and μ are close. This is easily seen using formula (4.33a) and the continuity of $D^{\pm}(\cdot)\zeta$ recorded in Step I. Hence, (2) is verified. ∎

4.3.2. Construction in general. Now, we prove Theorem 1.5 and Corollary 1.8. We implement the effects from $V_{\mathrm{S}} + q$ by the second resolvent identities

$$R(\lambda \pm \mathrm{i}0) = R_{\mathrm{L}}(\lambda \pm \mathrm{i}0)(1 - (V_{\mathrm{S}} + q)R(\lambda \pm \mathrm{i}0)) \in \mathcal{L}(\mathcal{B}, \mathcal{B}^*). \tag{4.40}$$

Proof of Theorem 1.5 (1) *and* (2). Take the function Σ_{L} from Lemma 4.12 with $U = \mathbb{S}^{d-1}$, and we define $F^{\pm}(\lambda)\psi \in \mathcal{G}$ for any $(\lambda, \psi) \in I \times \mathcal{B}$ as

$$F^{\pm}(\lambda)\psi = \mathrm{e}^{\mp \mathrm{i}\Theta_{\mathrm{L}}(\lambda, \cdot)} E^{\pm}(\lambda)(1 - (V_{\mathrm{S}} + q)R(\lambda \pm \mathrm{i}0))\psi, \tag{4.41}$$

where

$$\Theta_{\mathrm{L}}(\lambda, \omega) = \Sigma_{\mathrm{L}}(\lambda, \theta_+(\lambda, \omega)); \quad \theta_+(\lambda, \cdot) = \omega_+(\lambda, \cdot)^{-1}.$$

Then, we can deduce (1.10) by (4.40), (4.41), and (4.31), verifying assertion (1). As for (2), note that the mappings

$$I \times \mathcal{B} \to \mathcal{B},\ (\lambda, \psi) \mapsto (1 - (V_{\mathrm{S}} + q)R(\lambda \pm \mathrm{i}0))\psi$$

are continuous thanks to Theorem 3.17. Then, assertion (2) is clear from Lemmas 4.10 and 4.12 and Proposition 4.14. ∎

To prove assertions (3) and (4) in Theorem 1.5 we will use the *Sommerfeld uniqueness* for H, or a characterization of the limiting resolvents $R(\lambda \pm \mathrm{i}0)$. The following version of the property is almost a direct consequence from Theorem 1.24 and (4.40), cf. [1, 14]; however, let us present it for completeness of the paper.

Proposition 4.16. *Let $\lambda \in I$, $\psi \in \mathcal{B}$, and $\phi \in \mathcal{B}^*$. Then, $\phi = R(\lambda \pm \mathrm{i}0)\psi$ holds if and only if both of the following assertions hold:*

(1) *ϕ solves the Helmholtz equation $(H - \lambda)\phi = \psi$ in the distributional sense;*

(2) *ϕ satisfies the outgoing/incoming radiation condition $\gamma_\| \phi \in \mathcal{B}_0^*$.*

Remarks 4.17. (1) Here, $\gamma_\|$ is defined by (1.20) with respect to $S = S_\mathrm{L}$. In the proposition we can equally well use the more natural $\gamma_\|$ defined by (1.20) with respect to the general S, or in fact $\gamma_\|$ given in terms of the expression $S = S_0 = \sqrt{2\lambda}|x|$.

(2) For $\psi = 0$, the above result implies the (sharp) version of a *Rellich theorem*: if $\phi \in \mathcal{B}_0^*$ solves $(H - \lambda)\phi = 0$, then $\phi = 0$.

Proof. The necessity is clear from (4.40), (4.1a), and (1.21a). Thus, it remains to prove the sufficiency. Assume 4.16 (1) and (2), and set

$$\phi' = \phi - R(\lambda \pm \mathrm{i}0)\psi \in \mathcal{B}^*.$$

Then by (4.40), (4.1a), and (1.21a), ϕ' satisfies

$$(H - \lambda)\phi' = 0, \quad \gamma_\| \phi' \in \mathcal{B}_0^*.$$

We can further verify $\phi' \in \mathcal{B}_0^*$. Using a notation similar to (4.38),

$$\eta_T = 1 - \chi(\chi_1 S_L/T), \quad \eta_T' = -T^{-1}\chi'(\chi_1 S_L/T),$$

we have

$$2\,\mathrm{Im}(\eta_T(H - \lambda)) = \pm|\nabla \chi_1 S_\mathrm{L}|^2 \eta_T' + \mathrm{Re}(\eta_T' \gamma_\|).$$

Hence,

$$0 \le -\langle \phi', |\nabla \chi_1 S|^2 \eta_T' \phi' \rangle \le \pm\,\mathrm{Re}\langle \phi', \eta_T' \gamma_\| \phi' \rangle.$$

By letting $T \to \infty$, it follows that indeed $\phi' \in \mathcal{B}_0^*$.

Since H does not have positive eigenvalues, it neither has generalized eigenfunctions with positive eigenvalues in $\mathcal{B}_0^*$, see [1, Theorem 1.4], and we certainly obtain that $\phi' = 0$. Hence, $\phi = R(\lambda \pm \mathrm{i}0)\psi$. ∎

The Sommerfeld uniqueness provides the following useful representations. We recall (4.30), and we define, for any $\xi \in C^\infty(\mathbb{S}^{d-1})$,

$$\psi_\pm^{S_\mathrm{L}}[\xi](x) = \psi_\pm^{S_\mathrm{L}}[\xi](\lambda, x) = (H - \lambda)\phi_\pm^{S_\mathrm{L}}[\xi](\lambda, x) = (H - \lambda)\phi_\pm^{S_\mathrm{L}}[\xi](x).$$

Proposition 4.18. *Let $(\lambda, \xi) \in I \times C^\infty(\mathbb{S}^{d-1})$. Then*

$$\phi_\pm^{S_\mathrm{L}}[\xi] \in \mathcal{B}^*, \quad \gamma_\| \phi_\pm^{S_\mathrm{L}}[\xi] \in \mathcal{B}_0^*, \quad \psi_\pm^{S_\mathrm{L}}[\xi] \in \mathcal{B}. \tag{4.42a}$$

Moreover,

$$\phi_{\pm}^{S_{\mathrm{L}}}[\xi] = R(\lambda \pm \mathrm{i}0)\psi_{\pm}^{S_{\mathrm{L}}}[\xi] \tag{4.42b}$$

and

$$F^{\pm}(\lambda)^*(\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi) = \pm\frac{1}{2\pi\mathrm{i}}(\phi_{\pm}^{S_{\mathrm{L}}}[\xi] - R(\lambda \mp \mathrm{i}0)\psi_{\pm}^{S_{\mathrm{L}}}[\xi]). \tag{4.42c}$$

Proof. The first inclusion from (4.42a) is obvious. To prove the last one, we use (1.6) to rewrite it for $|x| \geq 2R$ as

$$\begin{aligned}\psi_{\pm}^{S_{\mathrm{L}}}[\xi] = \frac{(2\pi)^{1/2}}{2(2\lambda)^{1/4}} r^{-(d-1)/2}\mathrm{e}^{\pm\mathrm{i}S_{\mathrm{L}}}\Big(&p^2 \pm 2(\nabla S_{\mathrm{L}})\cdot p\\ &+\mathrm{i}(d-1)r^{-1}(\nabla r)\cdot p \mp \mathrm{i}(\Delta S_{\mathrm{L}})\\ &\pm \mathrm{i}(d-1)r^{-1}(\nabla r)\cdot(\nabla S_{\mathrm{L}})\\ &+\frac{(d-1)(d-3)}{4}r^{-2} + 2(V_{\mathrm{S}}+q)\Big)\xi.\end{aligned}$$

Noting that

$$\begin{aligned}&(\nabla S_{\mathrm{L}})\cdot p = ((\nabla S_{\mathrm{L}})\cdot(\nabla r))(\nabla r)\cdot p + (\nabla(S_{\mathrm{L}} - \sqrt{2\lambda}r))\cdot(1-(\nabla r)\otimes(\nabla r))p,\\ &(\nabla r)\cdot p\xi = 0, \quad p\xi = \mathcal{O}(r^{-1})\end{aligned}$$

and using Theorem 1.3, we obtain the last inclusion of (4.42a). The second one can be verified similarly.

Now, (4.42b) follows from (4.42a) and Proposition 4.16, and it remains to verify (4.42c). We can write, for any $\psi \in C_{\mathrm{c}}^{\infty}(\mathbb{R}^d)$,

$$\begin{aligned}\langle\psi, F^{\pm}(\lambda)^*(\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi)\rangle &= \langle F^{\pm}(\lambda)\psi, \mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi\rangle_{\mathcal{G}}\\ &= \frac{(2\lambda)^{1/2}}{2\pi}\lim_{T\to\infty}\langle R(\lambda\pm\mathrm{i}0)\psi, \chi_T'\phi_{\pm}^{S_{\mathrm{L}}}[\xi]\rangle,\end{aligned}$$

where

$$\chi_T' = T^{-1}\chi'\Big(\frac{|x|}{T}\Big),$$

cf. (4.38). We use Theorem 1.3 to proceed as

$$\begin{aligned}\langle\psi, F^{\pm}(\lambda)^*(\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi)\rangle &= \pm\frac{1}{2\pi}\lim_{T\to\infty}\langle R(\lambda\pm\mathrm{i}0)\psi, \mathrm{Re}((\nabla\chi_T)\cdot p)\phi_{\pm}^{S_{\mathrm{L}}}[\xi]\rangle\\ &= \pm\frac{1}{2\pi\mathrm{i}}\lim_{T\to\infty}\langle R(\lambda\pm\mathrm{i}0)\psi, [H-\lambda, 1-\chi_T]\phi_{\pm}^{S_{\mathrm{L}}}[\xi]\rangle\\ &= \pm\frac{1}{2\pi\mathrm{i}}\langle\psi, \phi_{\pm}^{S_{\mathrm{L}}}[\xi] - R(\lambda\mp\mathrm{i}0)\psi_{\pm}^{S_{\mathrm{L}}}[\xi]\rangle.\end{aligned}$$

This implies (4.42c). ∎

Proof of Theorem 1.5 (3) *and* (4). To prove the first identity of (3), it suffices to show that, for any $\lambda \in I$, $\xi \in \mathcal{G}$ and $\psi \in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$,

$$\langle (H-\lambda)F^\pm(\lambda)^*\xi, \psi\rangle = 0. \tag{4.43}$$

However, by Proposition 4.16, we have

$$R(\lambda \pm \mathrm{i}0)(H-\lambda)\psi = \psi \in C_{\mathrm{c}}^\infty(\mathbb{R}^d),$$

so that

$$F^\pm(\lambda)(H-\lambda)\psi = 0.$$

Thus, (4.43) follows. On the other hand, by (4.41), Proposition 4.14, and (4.40), we have, for any $\psi \in \mathcal{B}$,

$$\begin{aligned}\|F^\pm(\lambda)\psi\|_{\mathcal{G}}^2 &= \langle (1-(V_{\mathrm{S}}+q)R(\lambda\pm\mathrm{i}0))\psi, \\ &\qquad \delta(H_{\mathrm{L}}-\lambda)(1-(V_{\mathrm{S}}+q)R(\lambda\pm\mathrm{i}0))\psi\rangle \\ &= \langle \psi, \delta(H-\lambda)\psi\rangle.\end{aligned}$$

This implies the second identity of (3).

To prove (4), we use (4.42b). In fact, along with (1.10) and Lemma 4.12, it says, for any $(\lambda,\xi) \in I \times C^\infty(\mathbb{S}^{d-1})$,

$$F^\pm(\lambda)\psi_\pm^{S_{\mathrm{L}}}[\xi] = \mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi \tag{4.44}$$

or $\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}C^\infty(\mathbb{S}^{d-1}) \subseteq F^\pm(\lambda)\mathcal{B} \subseteq \mathcal{G}$. Hence, we obtain assertion (4). ∎

Proof of Corollary 1.8. The existence of the wave operators $F^\pm(\lambda)$ is already shown in Theorem 1.5. Next, by Theorem 1.5 (3) and (4), the scattering matrix $\mathsf{S}(\lambda)$ is defined at least on a dense subspace of $\mathcal{G}$, and in fact it preserves the norm and maps onto a dense set. Therefore, $\mathsf{S}(\lambda)$ extends uniquely to a unitary operator on $\mathcal{G}$.

Finally, we are left with the strong continuity. By (1.11) and (4.44), it follows that, for any $\eta \in C^\infty(\mathbb{S}^{d-1})$,

$$F^+(\lambda)\psi_-^{S_{\mathrm{L}}}[\eta] = \mathsf{S}(\lambda)F^-(\lambda)\psi_-^{S_{\mathrm{L}}}[\eta] = \mathsf{S}(\lambda)\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\eta. \tag{4.45}$$

Note that the above left-hand side is continuous in $\lambda \in I$, and so is the right-hand side. Now, we fix any $\xi \in \mathcal{G}$ and $\lambda \in I$, and, for any $\varepsilon > 0$, choose $\eta \in C^\infty(\mathbb{S}^{d-1})$ and $\delta > 0$ such that, for any $\mu \in (\lambda-\delta, \lambda+\delta)$,

$$\|\xi - \mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\mu,\cdot)}\eta\|_{\mathcal{G}} < \varepsilon.$$

Then, by the unitarity of the scattering matrix, for any $\mu \in (\lambda-\delta,\lambda+\delta)$,

$$\begin{aligned}\|\mathsf{S}(\lambda)\xi - \mathsf{S}(\mu)\xi\|_{\mathcal{G}} &\le \|\mathsf{S}(\lambda)(\xi - \mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\eta)\|_{\mathcal{G}} + \|\mathsf{S}(\lambda)\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\eta - \mathsf{S}(\mu)\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\mu,\cdot)}\eta\|_{\mathcal{G}} \\ &\quad + \|\mathsf{S}(\mu)(\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\mu,\cdot)}\eta - \xi)\|_{\mathcal{G}} \\ &< 2\varepsilon + \|\mathsf{S}(\lambda)\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\eta - \mathsf{S}(\mu)\mathrm{e}^{\mathrm{i}\Theta_{\mathrm{L}}(\mu,\cdot)}\eta\|_{\mathcal{G}}.\end{aligned}$$

By letting $\delta > 0$ be smaller if necessary, the above right-hand side is bounded by 3ε. Thus, we obtain the desired strong continuity. ■

4.4. Generalized eigenfunctions

We next prove Theorem 1.10.

Proof of Theorem 1.10. We proceed in five steps.

Step I. We first show that, if $\phi \in \mathcal{E}_\lambda$ and $\xi_\pm \in \mathcal{G}$ satisfy (1.12a), then (1.12c) holds. For that, we first compute

$$\begin{aligned}
&\lim_{m\to\infty} 2^{-m}\|1_m\phi\|^2\\
&\quad= \lim_{m\to\infty} 2^{-m}\|1_m(\phi^S_+[\xi_+] - \phi^S_-[\xi_-])\|^2\\
&\quad= \frac{\pi}{(2\lambda)^{1/2}}\Bigg(\|\xi_+\|^2_{\mathcal{G}} + \|\xi_-\|^2_{\mathcal{G}}\\
&\qquad\qquad - \lim_{m\to\infty} 2^{2-m}\,\mathrm{Re}\int_{[2^{m-1},2^m)\times\mathbb{S}^{d-1}} \mathrm{e}^{2\mathrm{i}S(\lambda,r\omega)}\overline{\xi_-(\omega)}\xi_+(\omega)\,\mathrm{d}r\,\mathrm{d}A(\omega)\Bigg).
\end{aligned}$$

Here, the last limit vanishes. In fact, we can integrate by parts as

$$\begin{aligned}
\int_{2^{m-1}}^{2^m} \mathrm{e}^{2\mathrm{i}S(\lambda,r\omega)}\,\mathrm{d}r &= \frac{1}{2\mathrm{i}}(\partial_r S(\lambda,r\omega))^{-1}\mathrm{e}^{2\mathrm{i}S(\lambda,r\omega)}\Big|_{2^{m-1}}^{2^m}\\
&\quad + \frac{1}{2\mathrm{i}}\int_{2^{m-1}}^{2^m}(\partial_r S(\lambda,r\omega))^{-2}(\partial_r^2 S(\lambda,r\omega))\mathrm{e}^{2\mathrm{i}S(\lambda,r\omega)}\,\mathrm{d}r,
\end{aligned}$$

and it does not contribute to the limit by the conditions of Theorem 1.5. Thus, we obtain

$$\|\xi_+\|^2_{\mathcal{G}} + \|\xi_-\|^2_{\mathcal{G}} = \frac{(2\lambda)^{1/2}}{\pi}\lim_{m\to\infty} 2^{-m}\|1_m\phi\|^2. \tag{4.46}$$

On the other hand, proceeding as in the proof of Proposition 4.18 and using in the last step the integration by parts from above, we compute

$$\begin{aligned}
0 &= \lim_{T\to\infty}\langle\phi, \mathrm{i}[H-\lambda, 1-\chi_T]\phi\rangle\\
&= -\lim_{T\to\infty}\langle\phi, \mathrm{Re}((\nabla r)\cdot p)\chi_T'\phi\rangle\\
&= -\lim_{T\to\infty}\langle\phi^S_+[\xi_+] - \phi^S_-[\xi_-], \mathrm{Re}((\nabla r)\cdot p)\chi_T'\phi\rangle\\
&= -(2\lambda)^{1/2}\lim_{T\to\infty}\langle\phi^S_+[\xi_+] + \phi^S_-[\xi_-], \chi_T'\phi\rangle\\
&= 2\pi(\|\xi_-\|^2_{\mathcal{G}} - \|\xi_+\|^2_{\mathcal{G}}).
\end{aligned}$$

In combination with (4.46), this verifies (1.12c).

Step II. Here we prove the uniqueness asserted in (1). Suppose $\phi' \in \mathcal{E}_\lambda$ and $\xi'_\pm \in \mathcal{G}$ also satisfy (1.12a). Then we have

$$(\phi - \phi') - \phi^S_+[\xi_+ - \xi'_+] + \phi^S_-[\xi_- - \xi'_-] \in \mathcal{B}^*_0. \tag{4.47}$$

If $\phi = \phi'$, it follows that $\xi_\pm = \xi'_\pm$ by the result of Step I. On the other hand, if either of $\xi_\pm = \xi'_\pm$ hold, then we have $\xi_\mp = \xi'_\mp$, respectively, again by the result of Step I. This and (4.47) imply $\phi - \phi' \in \mathcal{B}_0$, but then it follows that $\phi - \phi' = 0$ thanks to Remark 4.17 (2). Thus, we obtain the uniqueness.

Step III. Here we complete assertions (1) and (2). Note that, for any $\xi \in \mathcal{G}$,

$$F^\pm(\lambda)^*\xi \mp \frac{1}{2\pi \mathrm{i}}(\phi^S_\pm[\xi] - \phi^S_\mp[\mathsf{S}(\lambda)^{\mp 1}\xi]) \in \mathcal{B}^*_0. \tag{4.48}$$

In fact, by (4.42c), (1.10), (1.11), and (4.44) (the latter applied as in (4.45)), we have, for any $\xi \in C^\infty(\mathbb{S}^{d-1})$,

$$F^\pm(\lambda)^*(\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi) \mp \frac{1}{2\pi\mathrm{i}}(\phi^S_\pm[\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi] - \phi^S_\mp[\mathsf{S}(\lambda)^{\mp 1}\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}\xi]) \in \mathcal{B}^*_0,$$

and then – by density of $\mathrm{e}^{\mp\mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)}C^\infty_{\mathrm{c}}(\mathbb{R}^d) \subseteq \mathcal{G}$ and the continuity of $F^\pm(\lambda)^*$, $\phi^S_\pm$, and $\mathsf{S}(\lambda)^{\pm 1}$ – we obtain (4.48). Now, if either of $\xi_\pm \in \mathcal{G}$ is given, then the vectors $\phi \in \mathcal{E}_\lambda$ and $\xi_\mp \in \mathcal{G}$ are given by (1.12b), respectively, and obviously satisfy (1.12a), thanks to (4.48). By the uniqueness, from Step II we are done with the case where either of $\xi_\pm \in \mathcal{G}$ is given first.

Next, let $\phi \in \mathcal{E}_\lambda$ be given first. By the above arguments and Step II, it suffices to show there exist $\xi_\pm \in \mathcal{G}$ satisfying $\phi = 2\pi\mathrm{i}F^\pm(\lambda)^*\xi_\pm$. For each $T \geq 1$, we can find $\xi_{\pm,T} \in \mathcal{G}$ such that, for any $\eta \in \mathcal{G}$,

$$\langle \eta, \xi_{\pm,T}\rangle_{\mathcal{G}} = \pm\frac{(2\lambda)^{1/2}}{2\pi}\langle \phi^S_\pm[\eta], \chi'_T\phi\rangle.$$

Obviously, such $\xi_{\pm,T} \in \mathcal{G}$ are uniformly bounded for $T \geq 1$, and we can choose weakly convergent subsequences $(\xi_{\pm,T_n})_{n\in\mathbb{N}}$, cf. [25, Theorem 1, p. 126]. Denote the weak limits by $\xi_\pm \in \mathcal{G}$. Then, for any $\psi \in C^\infty_{\mathrm{c}}(\mathbb{R}^d)$, we compute

$$\begin{aligned}\langle \psi, F^\pm(\lambda)^*\xi_\pm\rangle &= \langle F^\pm(\lambda)\psi, \xi_\pm\rangle_{\mathcal{G}} \\ &= \pm\frac{(2\lambda)^{1/2}}{2\pi}\lim_{n\to\infty}\langle \phi^S_\pm[F^\pm(\lambda)\psi], \chi'_{T_n}\phi\rangle \\ &= \pm\frac{(2\lambda)^{1/2}}{2\pi}\lim_{n\to\infty}\langle R(\lambda \pm \mathrm{i}0)\psi, \chi'_{T_n}\phi\rangle.\end{aligned}$$

Then, as in the proof of Proposition 4.18, we use Proposition 4.16, Theorem 1.3, and the assumption $\phi \in \mathcal{E}_\lambda$ to proceed as

$$\begin{aligned}\langle \psi, F^{\pm}(\lambda)^* \xi_\pm \rangle &= \frac{1}{2\pi} \lim_{n\to\infty} \langle \mathrm{Re}((\nabla r)\cdot p) R(\lambda \pm \mathrm{i}0)\psi, \chi'_{T_n}\phi \rangle \\ &= \frac{1}{2\pi\mathrm{i}} \lim_{n\to\infty} \langle R(\lambda \pm \mathrm{i}0)\psi, [H-\lambda, 1-\chi_{T_n}]\phi \rangle \\ &= \frac{1}{2\pi\mathrm{i}} \langle \psi, \phi \rangle.\end{aligned}$$

Thus, we obtain that $\phi = 2\pi\mathrm{i}F^{\pm}(\lambda)^*\xi_\pm$. The assertions (1) and (2) are done.

Step IV. Here we prove (3). Note that the identities (1.12c) are already established in Step I. Then, in combination with (1) and (2), we see that $F^{\pm}(\lambda)^*\colon \mathcal{G} \to \mathcal{E}_\lambda \subseteq \mathcal{B}^*$ are indeed bi-continuous. Hence, we obtain (3).

Step V. Finally, we prove (4). Since $F^{\pm}(\lambda)^*$ are injective with closed ranges in $\mathcal{B}^*$ by (3), Theorem 1.5 (4) and Banach's closed range theorem [25, Theorem p. 205] imply that the ranges of $F^{\pm}(\lambda)$ coincide with $\mathcal{G}$. This, along with (3) and Theorem 1.5 (3), in turn implies that the range of $\delta(H-\lambda)$ coincides with $\mathcal{E}_\lambda$. Hence, we are done. ∎

4.5. Generalized Fourier transforms

We close this section with the proof of Theorem 1.12, which is rather routine thanks to Theorem 1.5, see also [18, 22].

Proof of Theorem 1.12. We proceed in five steps.

Step I. We may let I be compact. In fact, if I is unbounded, decompose

$$I = \bigcup_{n\in\mathbb{N}} [\lambda_n, \lambda_{n+1}]; \quad \lambda_1 < \lambda_2 < \cdots < \lambda_n \to \infty \quad \text{as } n \to \infty,$$

and, supposing that the assertion holds true for compact intervals, we define

$$\mathcal{F}_I = \bigoplus_{n\in\mathbb{N}} \mathcal{F}_{[\lambda_n,\lambda_{n+1}]}\colon \mathcal{H}_I \to \widetilde{\mathcal{H}}_I.$$

Then the assertion for I follows due to absence of positive eigenvalues for H_I and M_λ and closedness of H_I and M_λ. Thus, we let I be compact in the following.

Step II. Let us construct the isometries $\mathcal{F}^{\pm}\colon \mathcal{H}_I \to \widetilde{\mathcal{H}}_I$. By Theorem 1.5 and Stone's formula [20, Theorem VII.13], it follows that, for any $\psi \in \mathcal{B}$,

$$\|\mathcal{F}_0^{\pm}\psi\|^2_{\widetilde{\mathcal{H}}_I} = \int_I \|F^{\pm}(\lambda)\psi\|^2_{\mathcal{G}}\,\mathrm{d}\lambda = \int_I \langle \psi, \delta(H-\lambda)\psi\rangle\,\mathrm{d}\lambda = \|P_H(I)\psi\|^2_{\mathcal{H}_I}. \tag{4.49}$$

Since $\mathcal{B} \subseteq \mathcal{H}$ is dense, also $P_H(I)\mathcal{B} \subseteq \mathcal{H}_I$ is dense. Thus, for any $\psi \in \mathcal{H}_I$ we can choose a sequence $(\psi_n)_{n\in\mathbb{N}}$ on $\mathcal{B}$ such that $P_H(I)\psi_n \to \psi$ in $\mathcal{H}_I$, and then we can define

$$\mathcal{F}^{\pm}\psi = \lim_{n\to\infty} \mathcal{F}_0^{\pm}\psi_n.$$

By (4.49), these limits are well defined and certainly define isometries as wanted.

To be used below, we note that, by construction, for any $\psi \in \mathcal{B}$,

$$\mathcal{F}^{\pm}P_H(I)\psi = \mathcal{F}_0^{\pm}\psi \in C(I;\mathcal{G}).$$

Step III. Next, we show $\mathcal{F}^{\pm}H_I = M_\lambda\mathcal{F}^{\pm}$. Note all the involved operators are bounded. Take any $\psi \in C_c^\infty(\mathbb{R}^d)$ and $\lambda \in I$. If we then set $\psi' = (H-\lambda)\psi$, it follows from Proposition 4.16 that $\psi = R(\lambda \pm \mathrm{i}0)\psi'$. Consequently,

$$R(\lambda \pm \mathrm{i}0)H\psi = \lambda R(\lambda \pm \mathrm{i}0)\psi + \psi.$$

This implies that, for any $\psi \in C_c^\infty(\mathbb{R}^d)$,

$$\mathcal{F}_0^{\pm}H\psi = M_\lambda\mathcal{F}_0^{\pm}\psi.$$

Similarly to Step I, for any $\psi \in \mathcal{H}_I$, we can choose a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R}^d)$ such that $P_H(I)\psi_n \to \psi$, hence $P_H(I)H\psi_n \to H_I\psi$, in $\mathcal{H}_I$. Then, it follows that

$$\mathcal{F}^{\pm}H_I\psi = \lim_{n\to\infty}\mathcal{F}_0^{\pm}H\psi_n = \lim_{n\to\infty}M_\lambda\mathcal{F}_0^{\pm}\psi_n = M_\lambda\mathcal{F}^{\pm}\psi.$$

The claim is verified.

Step IV. In order to complete (1) and (2), it remains to show that the morphisms $\mathcal{F}^{\pm}\colon \mathcal{H}_I \to \widetilde{\mathcal{H}}_I$ are surjective. It suffices to show that the ranges $\mathcal{F}^{\pm}\mathcal{H}_I \subseteq \widetilde{\mathcal{H}}_I$ are dense. Take any $\Xi \in C(I;\mathcal{G}) \subseteq \widetilde{\mathcal{H}}_I$, and fix any $\varepsilon > 0$. By the compactness, the result from Step II and Theorem 1.10 (4) we can find a finite open covering $I \subseteq U_1 \cup \cdots \cup U_n$ and $\psi_1,\dots,\psi_n \in P_H(I)\mathcal{B} \subseteq \mathcal{H}_I$ such that for any $i = 1,\dots,n$ and $\lambda \in I \cap U_i$

$$\|\Xi(\lambda) - (\mathcal{F}^{\pm}\psi_i)(\lambda)\|_{\mathcal{G}} < \varepsilon.$$

If we let $\{\chi_i\}_i$ be a partition of unity subordinate to $\{U_i\}_i$, then, for any $\lambda \in I$,

$$\Big\|\Xi(\lambda) - \sum_{i=1}^n \chi_i(\lambda)(\mathcal{F}^{\pm}\psi_i)(\lambda)\Big\|_{\mathcal{G}} < \varepsilon.$$

Since $\mathcal{F}^{\pm}\psi_i \in C(I;\mathcal{G})$, we can replace the above χ_i by some polynomials $\tilde{\chi}_i$ due the Weierstrass approximation theorem with an additional ε error. Then set

$$\psi = \sum_{i=1}^n \tilde{\chi}_i(H)\psi_i \in \mathcal{H}_I,$$

and we obtain, by the result from Step III, that, for any $\lambda \in I$,

$$\|\Xi(\lambda) - (\mathcal{F}^{\pm}\psi)(\lambda)\|_{\mathcal{G}} < 2\varepsilon.$$

Hence, (1) and (2) are done.

Step V. Assertion (3) is clear from the definition of the generalized Fourier transforms, see e.g. (4.41), and Lemma 4.12 with $U = \mathbb{S}^{d-1}$. We are done. ■

5. Time-dependent scattering theory

We discuss the time-dependent scattering theory, proving Theorems 1.14, 1.17, and 1.20. Our arguments are heavily dependent on the stationary theory from the previous sections in parallel to [17], however for 2-admissible potentials the low degree of smoothness entails some complication. In Section 5.1, we prove Theorem 1.14 by rigorously justifying the Legendre transform, and then we compare the asymptotics of solutions to the time-dependent eikonal equation. With these results in place, we show Theorem 1.17 in Section 5.2, hence obtaining the existence and covariance of the time-dependent wave operators. Finally, Theorem 1.20, in particular including asymptotic completeness, is shown by comparing the time-dependent wave operators with the generalized Fourier transforms.

5.1. Time-dependent eikonal equation

Here, we prove Theorem 1.14. We justify the Legendre transform, investigating its properties.

Proof of Theorem 1.14. Fix μ, μ', I, R, and $S = (2\lambda)^{1/2}|x|(1+s)$ as in the assertion. We first claim, letting $R > 0$ be larger if necessary, that for each $(t,x) \in \Omega_\mu$ we can find a unique critical point of the function (1.14) in the variable $\lambda \in I$. In fact, we can compute

$$\begin{aligned} \partial_\lambda \widetilde{K} &= (2\lambda)^{-1/2}|x|(1 + s + 2\lambda(\partial_\lambda s)) - t, \\ \partial_\lambda^2 \widetilde{K} &= -(2\lambda)^{-3/2}|x|(1 + s - 4\lambda(\partial_\lambda s) - 4\lambda^2(\partial_\lambda^2 s)), \end{aligned} \tag{5.1}$$

and thus, by Corollary 2.14, for sufficiently large $R > 0$,

$$(\partial_\lambda \widetilde{K})(\mu'^2/2, t, x) \geq \Big(\frac{\mu + \mu'}{2}\Big)^{-1}|x| - t > 0, \quad \lim_{\lambda\to\infty}(\partial_\lambda \widetilde{K})(\lambda, t, x) = -t < 0,$$

and, for any $\lambda \in I$,

$$(\partial_\lambda^2 \widetilde{K})(\lambda, t, x) \leq -\frac{1}{2}(2\lambda)^{-3/2}|x| < 0.$$

This implies that there uniquely exists $\lambda_c = \lambda_c(t, x) \in I$ such that

$$(\partial_\lambda \widetilde{K})(\lambda_c, t, x) = (2\lambda_c)^{-1/2}|x|(1 + s(\lambda_c, x) + 2\lambda_c(\partial_\lambda s)(\lambda_c, x)) - t = 0. \quad (5.2)$$

By the implicit function theorem, $\lambda_c \in C^{l-1}(\Omega_\mu)$. Now, we set

$$K = \widetilde{K}(\lambda_c, \cdot, \cdot), \quad (5.3)$$

and then we can easily see by (5.2) that

$$\partial_t K = -\lambda_c, \quad \nabla_x K = (\nabla_x S)(\lambda_c, \cdot), \quad (5.4)$$

which verifies $K \in C^l(\Omega_\mu)$ and (1.15). We have proven Theorem 1.14 (1).

Next, we prove assertion (2). For that, we claim for any $k + |\alpha| \le 1$

$$\Big|\partial_t^k \partial_x^\alpha \Big(\lambda_c - \frac{x^2}{2t^2}\Big)\Big| \le C_1 t^{-k} \langle x\rangle^{-\sigma-|\alpha|}. \quad (5.5)$$

In fact, note that (5.2) and Corollary 2.14 imply (uniformly in large $R > 0$)

$$c_2 t^{-2} x^2 \le \lambda_c \le C_2 t^{-2} x^2. \quad (5.6)$$

Note also that $\lambda_c = x^2/2t^2$ for $|x| \le R$; so, to show the bounds (5.5) and (1.16), we can indeed assume that $|x| > R$. Then, by combining (5.2), Theorem 1.3, Corollary 2.14, and (5.6), we obtain

$$\Big|\lambda_c - \frac{x^2}{2t^2}\Big| = \frac{x^2}{2t^2}|s + 2\lambda_c(\partial_\lambda s)||2 + s + 2\lambda_c(\partial_\lambda s)| \le C_3\langle x\rangle^{-\sigma}. \quad (5.7)$$

This shows the claim for $k + |\alpha| = 0$. For $k + |\alpha| = 1$, we compute the derivatives of λ_c by the Leibniz rule applied to (5.2), equivalently written as

$$1 = \frac{x^2}{2t^2}\lambda_c^{-1}(1 + s + 2\lambda_c\partial_\lambda s)^2.$$

In fact, we have, for $k = 1$ and $|\alpha| = 0$,

$$\begin{aligned} 0 = &-\frac{x^2}{t^3}\lambda_c^{-1}(1 + s + 2\lambda_c\partial_\lambda s)^2 \\ &- \frac{x^2}{2t^2}(\partial_t\lambda_c)\lambda_c^{-2}(1 + s - 4\lambda_c\partial_\lambda s - 4\lambda_c^2\partial_\lambda^2 s)(1 + s + 2\lambda_c\partial_\lambda s), \end{aligned}$$

and, for $k = 0$ and $|\alpha| = 1$,

$$\begin{aligned} 0 = &\Big(\partial_x^\alpha \frac{x^2}{2t^2}\Big)\lambda_c^{-1}(1 + s + 2\lambda_c\partial_\lambda s)^2 \\ &- \frac{x^2}{2t^2}(\partial_x^\alpha\lambda_c)\lambda_c^{-2}(1 + s - 4\lambda_c\partial_\lambda s - 4\lambda_c^2\partial_\lambda^2 s)(1 + s + 2\lambda_c\partial_\lambda s) \\ &+ \frac{x^2}{t^2}\lambda_c^{-1}(\partial_x^\alpha s + 2\lambda_c\partial_\lambda\partial_x^\alpha s)(1 + s + 2\lambda_c\partial_\lambda s). \end{aligned}$$

Possibly by taking $R > 0$ larger from the beginning (if necessary) and by using Corollary 2.14, we can write, for $k = 1$ and $|\alpha| = 0$,

$$\partial_t \lambda_c = -\frac{2}{t}\lambda_c(1 + s + 2\lambda_c\partial_\lambda s)(1 + s - 4\lambda_c\partial_\lambda s - 4\lambda_c^2\partial_\lambda^2 s)^{-1},$$

and, for $k = 0$ and $|\alpha| = 1$,

$$\begin{aligned}\partial_x^\alpha \lambda_c = {}& \frac{2t^2}{x^2}\Big(\partial_x^\alpha \frac{x^2}{2t^2}\Big)\lambda_c(1 + s + 2\lambda_c\partial_\lambda s)(1 + s - 4\lambda_c\partial_\lambda s - 4\lambda_c^2\partial_\lambda^2 s)^{-1} \\ & + 2\lambda_c(\partial_x^\alpha s + 2\lambda_c\partial_\lambda\partial_x^\alpha s)(1 + s - 4\lambda_c\partial_\lambda s - 4\lambda_c^2\partial_\lambda^2 s)^{-1}.\end{aligned}$$

The claim (5.5) follows from the above expressions, (5.7), and Theorem 1.3.

One can verify assertion (2) by (1.14), (5.3), (5.5), (5.4), and Theorem 1.3. While the bounds (1.16) follow immediately unless $k = 0$ and $|\alpha| = 2$, the latter case requires some other computations. We omit the details of proof for that case. ∎

We next investigate the asymptotics of general solutions to (1.3b).

Lemma 5.1. *Let $\mu, T, \Omega_{\mu,T}$, and K satisfy the assumption of Theorem 1.17, and let K_{L} be the Legendre transform of the function S_{L} taken from Section 4.1 with $I = I_{\mu'} = [\mu'^2/2, \infty)$, $\mu' \in (0, \mu)$, and $l' > 1 + 2/\rho$. In addition, let y be the flow associated with S_{L} as in Section 4.2, and set*

$$\tau(\lambda, t, \theta) = \int_0^t |\nabla S_{\mathrm{L}}(\lambda, y(\lambda, s, \theta))|^{-2}\, \mathrm{d}s.$$

Then, the following assertions hold.

(1) *There exists the limit*

$$\Xi_{\mathrm{L}}(\lambda, \theta) := \lim_{t\to\infty}(K(\tau(\lambda, t, \theta), y(\lambda, t, \theta)) - K_{\mathrm{L}}(\tau(\lambda, t, \theta), y(\lambda, t, \theta)))$$

taken locally uniformly in $(\lambda, \theta) \in J \times \mathbb{S}^{d-1}$, where $J = [\mu^2/2, \infty)$. In particular, if K_1 also satisfies the assumption of Theorem 1.17, there exists the limit

$$\Xi(\lambda, \theta) := \lim_{t\to\infty}(K_1(\tau(\lambda, t, \theta), y(\lambda, t, \theta)) - K(\tau(\lambda, t, \theta), y(\lambda, t, \theta)))$$

taken locally uniformly in $(\lambda, \theta) \in J \times \mathbb{S}^{d-1}$.

(2) *The quantities in (1) can also be computed as the limits*

$$\begin{aligned}\Phi_L(\lambda, \omega) &:= \Xi_L(\lambda, \theta_+(\lambda, \omega)) \\ &= \lim_{\tau\to\infty}(K(\tau, (2\lambda)^{1/2}\tau\omega) - K_L(\tau, (2\lambda)^{1/2}\tau\omega)),\end{aligned}$$

$$\Phi(\lambda,\omega) := \Xi(\lambda,\theta_+(\lambda,\omega))$$
$$= \lim_{\tau\to\infty}(K_1(\tau,(2\lambda)^{1/2}\tau\omega) - K(\tau,(2\lambda)^{1/2}\tau\omega)),$$

both taken locally uniformly in $(\lambda,\omega)\in J\times\mathbb{S}^{d-1}$.

Remark 5.2. The requirement $l' > 1 + 2/\rho$ (not used in the proof) will be needed in the proof of Lemma 5.3, cf. Remark 4.3. The above function τ should be considered as the "physical time," cf. Remark 4.5 (2).

Proof. We proceed in three steps.

Step I. The second assertion of (1) is clear from the first one, hence we only prove the first assertion of (1). It suffices to show existence of the limits

$$\Psi(\lambda,\theta) := \lim_{t\to\infty}(K(\tau(\lambda,t,\theta),y(\lambda,t,\theta)) - S_{\rm L}(\lambda,y(\lambda,t,\theta)) + \lambda\tau(\lambda,t,\theta)) \quad (5.8a)$$

and

$$\Psi_{\rm L}(\lambda,\theta) := \lim_{t\to\infty}(K_{\rm L}(\tau(\lambda,t,\theta),y(\lambda,t,\theta)) - S_{\rm L}(\lambda,y(\lambda,t,\theta)) + \lambda\tau(\lambda,t,\theta)) \quad (5.8b)$$

taken locally uniformly in $(\lambda,\omega)\in J\times\mathbb{S}^{d-1}$. We can prove them in the same manner, but it follows easily from the proof of (5.8a) that in fact

$$K_{\rm L}(\tau(\lambda,t,\theta),y(\lambda,t,\theta)) - S_{\rm L}(\lambda,y(\lambda,t,\theta)) + \lambda\tau(\lambda,t,\theta) = 0, \quad (5.8c)$$

hence we discuss only (5.8a).

Note that all the arguments below are locally uniform in $(\lambda,\theta)\in J\times\mathbb{S}^{d-1}$. Omitting the arguments, and using (1.15), (4.3a), and (1.6), we can compute the t-derivative for large $t>0$ as

$$\frac{\mathrm{d}}{\mathrm{d}t}(K - S_{\rm L} + \lambda\tau) = -\frac{1}{2}|\nabla S_{\rm L}|^{-2}(\nabla K - \nabla S_{\rm L})^2 - |\nabla S_{\rm L}|^{-2}V_{\rm S}. \quad (5.9)$$

The second term on the right-hand side of (5.9) is obviously integrable at infinity, and thus it suffices to show that, for some $\delta>0$,

$$u := (\nabla K - \nabla S_{\rm L})^2 = \mathcal{O}(t^{-1-\delta}). \quad (5.10)$$

For that, similarly to (5.9), we further differentiate it for large $t>0$ as

$$\frac{1}{2}|\nabla S_{\rm L}|^2\frac{\mathrm{d}}{\mathrm{d}t}u = -(\nabla K - \nabla S_{\rm L})(\nabla^2 K)(\nabla K - \nabla S_{\rm L}) - (\nabla V_{\rm S})\cdot(\nabla K - \nabla S_{\rm L}). \quad (5.11)$$

By (1.7), (1.16), and (4.1a), it follows that, for some (small) $\delta>0$ and (big) $C_1>0$ and any large $t>0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}u \le -(2-\delta)t^{-1}u + C_1 t^{-2-\delta}.$$

This certainly implies (5.10). Thus, we are done with (1).

Step II. To prove assertion (2), we discuss the following change of variables. We claim that, for all large $\tau > 0$ and any $(\lambda, \omega) \in J \times \mathbb{S}^{d-1}$, there exist $\bar\lambda$ and $\bar\theta$ such that

$$(\tau, (2\lambda)^{1/2}\tau\omega) = (\tau(\bar\lambda, t, \bar\theta), y(\bar\lambda, t, \bar\theta)) \quad \text{with } t = S_L(\bar\lambda, (2\lambda)^{1/2}\tau\omega), \tag{5.12a}$$

and that

$$\lim_{\tau\to\infty} \bar\lambda(\tau) = \lambda \quad \text{and} \quad \lim_{\tau\to\infty} \bar\theta(\tau) = \theta_+(\lambda, \omega). \tag{5.12b}$$

First, we solve, for fixed $\bar\lambda$ and $\bar\theta$, the equation

$$\tau = \int_0^t |\nabla S_{\mathrm{L}}(\bar\lambda, y(\bar\lambda, s, \bar\theta))|^{-2}\, \mathrm{d}s,$$

for $t = t(\tau, \bar\lambda, \bar\theta)$ (with a C^1-dependence by the implicit function theorem). For fixed large τ, we then need to solve the equation

$$(2\lambda)^{1/2}\omega = \frac{y(\bar\lambda, t, \bar\theta)}{\tau} =: F_\tau(\bar\lambda, \bar\theta) \tag{5.13}$$

for $\bar\lambda$ and $\bar\theta$. This can be done by using the inverse function theorem in a version applicable to parameter-dependent problems (note that τ is the relevant parameter), for example the version stated as [15, Theorem D.1]. We need to verify that the derivative of F_τ at $z_0 := (\lambda, \theta_+(\lambda, \omega))$ is non-degenerate near infinity.

First, note that

$$F_\infty(\bar\lambda, \bar\theta) := \lim_{\tau\to\infty} F_\tau(\bar\lambda, \bar\theta) = (2\bar\lambda)^{1/2}\omega_+(\bar\lambda, \bar\theta) \text{ in a neighborhood of } z_0,$$

in particular that

$$F_\infty(z_0) = (2\lambda)^{1/2}\omega.$$

Next, note that

$$\omega_+(\bar\lambda, \bar\theta) = \int_0^\infty \frac{\partial}{\partial s}\omega(\bar\lambda, s, \bar\theta)\, \mathrm{d}s + \bar\theta \quad \text{and} \quad \partial_{\bar\lambda}\omega_+(\bar\lambda, \bar\theta) = \int_0^\infty \partial_{\bar\lambda}\partial_s\omega(\bar\lambda, s, \bar\theta)\, \mathrm{d}s.$$

By the latter formula, the representation (4.15), and Corollary 2.14, it follows that $\partial_{\bar\lambda}\omega_+(\bar\lambda, \bar\theta)$ is small when the parameter R is sufficiently big. When combined with (4.23), this leads to the conclusion that the map $(\bar\lambda, \bar\theta) \to F_\infty(\bar\lambda, \bar\theta) = (2\bar\lambda)^{1/2}\omega_+(\bar\lambda, \bar\theta)$ is non-degenerate C^1 near z_0 (uniformly in large R).

Now, to solve (5.13), by applying [15, Theorem D.1], all that remains to be seen is that the limits

$$\lim_{\tau\to\infty} \partial_{\bar\lambda, \bar\theta} F_\tau(\bar\lambda, \bar\theta)$$

exist, uniformly in a neighborhood of z_0. We skip the details of the verification of this uniform convergence, and conclude the solvability of (5.13). This justifies (5.12a) and (5.12b).

Step III. Now, we prove the first assertion of (2) (this implies the second one). We proceed partly in parallel to the proof of Lemma 4.12 (2). It suffices to show that, with notation from Step I,

$$\Psi(\lambda,\theta_+(\lambda,\omega)) - \Psi_{\mathrm{L}}(\lambda,\theta_+(\lambda,\omega)) = \lim_{\tau\to\infty}\big(K(\tau,(2\lambda)^{1/2}\tau\omega) - K_{\mathrm{L}}(\tau,(2\lambda)^{1/2}\tau\omega)\big),$$

locally uniformly in $(\lambda,\omega)\in J\times\mathbb{S}^{d-1}$. Take any compact subset $L\subset J\times\mathbb{S}^{d-1}$. Let $(\bar\lambda,\bar\theta)=(\bar\lambda(\tau),\bar\theta(\tau))$ be the change of variables from Step II. Using the locally uniform limit (4.28) along with (5.12a) and (5.12b), and noting that $\tau\to\infty$ corresponds to $t\to\infty$, it follows that, for some compact subset $L'\subset J\times\mathbb{S}^{d-1}$,

$$\begin{aligned}
&\lim_{\tau\to\infty}\sup_{(\lambda,\omega)\in L}\big|\Psi(\lambda,\theta_+(\lambda,\omega)) - \Psi_{\mathrm{L}}(\lambda,\theta_+(\lambda,\omega))\\
&\qquad\qquad - K(\tau,(2\lambda)^{1/2}\tau\omega) + K_{\mathrm{L}}(\tau,(2\lambda)^{1/2}\tau\omega)\big|\\
&\quad=\lim_{\tau\to\infty}\sup_{(\lambda,\omega)\in L}\big|\Psi(\bar\lambda,\theta(\bar\lambda,(2\lambda)^{1/2}\tau\omega)) - \Psi_{\mathrm{L}}(\bar\lambda,\theta(\bar\lambda,(2\lambda)^{1/2}\tau\omega))\\
&\qquad\qquad\qquad - K(\tau,(2\lambda)^{1/2}\tau\omega) + K_{\mathrm{L}}(\tau,(2\lambda)^{1/2}\tau\omega)\big|\\
&=\lim_{t\to\infty}\sup_{(\bar\lambda,\bar\theta)\in L'}\big|\Psi(\bar\lambda,\theta(\bar\lambda,y(\bar\lambda,t,\bar\theta))) - \Psi_{\mathrm{L}}(\bar\lambda,\theta(\bar\lambda,y(\bar\lambda,t,\bar\theta)))\\
&\qquad\qquad - K(\tau(\bar\lambda,t,\bar\theta),y(\bar\lambda,t,\bar\theta)) + K_{\mathrm{L}}(\tau(\bar\lambda,t,\bar\theta),y(\bar\lambda,t,\bar\theta))\big|\\
&=\lim_{t\to\infty}\sup_{(\bar\lambda,\bar\theta)\in L'}\big|\Psi(\bar\lambda,\bar\theta) - \Psi_{\mathrm{L}}(\bar\lambda,\bar\theta)\\
&\qquad\qquad - K(\tau(\bar\lambda,t,\bar\theta),y(\bar\lambda,t,\bar\theta)) + K_{\mathrm{L}}(\tau(\bar\lambda,t,\bar\theta),y(\bar\lambda,t,\bar\theta))\big|\\
&=0.
\end{aligned}$$

Thus, we are done. ∎

5.2. Time-dependent wave operators

Here we prove Theorems 1.17 and 1.20.

5.2.1. Existence

Proof of Theorem 1.17. We first prove the existence of the strong limits (1.17) by the familiar Cook–Kuroda method. Thanks to a density argument based on uniform boundedness of $U^\pm(t)$ and $\mathrm{e}^{\pm\mathrm{i}tH}$ in $t>T$, it suffices to show that, for any $h\in C_{\mathrm{c}}^\infty(\mathbb{R}_+\times\mathbb{S}^{d-1})$ with $\operatorname{supp}h\subseteq J\times\mathbb{S}^{d-1}$, there exist the limits

$$\lim_{t\to\infty}\mathrm{e}^{\pm\mathrm{i}tH}U^\pm(t)h. \tag{5.14}$$

For that, we show integrability of

$$\left\| \frac{\partial}{\partial t} \mathrm{e}^{\pm \mathrm{i}tH} U^{\pm}(t)h \right\|_{\mathcal{H}} = \left\| \Big(\frac{\partial}{\partial t} \pm \mathrm{i}H\Big) U^{\pm}(t)h \right\|_{\mathcal{H}}$$

at infinity. Using the Hamilton–Jacobi equation (1.3b) and letting $\omega' = (\omega'_2, \dots, \omega'_d)$ be any local coordinates of $\mathbb{S}^{d-1}$, we compute

$$\begin{aligned}\Big(\frac{\partial}{\partial t} \pm \mathrm{i}H\Big) U^{\pm}(t)h = {} & \mathrm{e}^{\mp 3\pi\mathrm{i}/4} t^{-1} |x|^{1-d/2} \mathrm{e}^{\pm \mathrm{i}K} \\ & \cdot \Big[\mp \frac{\mathrm{i}}{2} x^2 t^{-4} (\partial_\lambda^2 h) \mp \frac{\mathrm{i}}{2} |x|^{-2} (\Delta_{\mathbb{S}^{d-1}} h) + (\partial_i \omega'_\alpha)(\partial_i K)(\partial_\alpha h) \\ & + (-t^{-3} x^2 \mp \mathrm{i} t^{-2} + t^{-2} x \cdot (\nabla_x K))(\partial_\lambda h) \\ & + \Big(-t^{-1} \pm \mathrm{i}\frac{d}{4}\Big(1 - \frac{d}{2}\Big)|x|^{-2} \pm \mathrm{i}q \\ & + \Big(1 - \frac{d}{2}\Big)|x|^{-2} x \cdot (\nabla_x K) + \frac{1}{2}(\Delta_x K)\Big)h\Big].\end{aligned}$$

By the assumption on K and the support property of h, the last expression is of order $t^{-1-\min\{\varepsilon,\tau\}}$ with values in $\mathcal{H}$. Hence, the limits (5.14) exist. Since $U^{\pm}(t)$ and $\mathrm{e}^{\pm \mathrm{i}tH}$ are isometries, it is clear that so are $W^{\pm}$. By the above computation, we easily see that $W^{\pm} M_\lambda \subseteq H W^{\pm}$. In particular, the mapping property stated in the last part of Theorem 1.17 (1) follows.

Assertion (2) follows readily from (1) and Lemma 5.1 (2). ∎

We present alternative representations of $W^{\pm}$, which will be useful in the proof of their completeness. See also [17, Lemma 3.3].

Lemma 5.3. *In the setting of Lemma 5.1, define, for any $h \in C_{\mathrm{c}}^\infty(\mathbb{R}_+ \times \mathbb{S}^{d-1})$, with* $\operatorname{supp} h \subseteq J \times \mathbb{S}^{d-1}$ *the evolutions*

$$(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x) = (\pm 2\pi\mathrm{i})^{-1} \int_0^\infty \mathrm{e}^{\mp \mathrm{i}\lambda t} \phi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)](\lambda, x)\,\mathrm{d}\lambda, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d,$$

where $\phi_{\pm}^{S_{\mathrm{L}}}[\cdot]$ is from (4.30). Then, for each $t > 0$, it follows that $\widetilde{U}_{\mathrm{L}}^{\pm}(t)h \in \mathcal{H}$. Moreover,

$$W^{\pm} \mathrm{e}^{\mp \mathrm{i}\Phi_{\mathrm{L}}} h = \lim_{t \to \infty} \mathrm{e}^{\pm \mathrm{i}tH} \widetilde{U}_{\mathrm{L}}^{\pm}(t)h.$$

Remark 5.4. The above evolution map $\widetilde{U}_{\mathrm{L}}^{\pm}(t)$ motivates our free comparison dynamics $U^{\pm}(t)$. In fact, due to the stationary phase theorem, the leading term is very similar to that of $U^{\pm}(t)$, see the proof below. Note, however, that we need higher order derivatives of the phase function. This is why we substitute S_{L} for S in $\widetilde{U}_{\mathrm{L}}^{\pm}(t)$. The error is compensated by the factor $\mathrm{e}^{\mp \mathrm{i}\Phi_{\mathrm{L}}}$.

Proof. We proceed in six steps.

Step I. To show that $\widetilde{U}_{\mathrm{L}}^{\pm}(t)h \in \mathcal{H}$, we introduce

$$\widetilde{K}_{\mathrm{L}}(\lambda, t, x) = S_{\mathrm{L}}(\lambda, x) - \lambda t,$$

cf. (1.14). First, fix any $t > 0$, and let $R' > 0$ be sufficiently large. Then, by the expressions (5.1) corresponding to $\widetilde{K}_{\mathrm{L}}$, we have, for any $(\lambda, \hat{x}) \in \operatorname{supp} h$ with $|x| > R'$,

$$\partial_\lambda \widetilde{K}_{\mathrm{L}}(\lambda, t, x) \geq c_1 \langle x \rangle, \quad |\partial_\lambda^2 \widetilde{K}_{\mathrm{L}}(\lambda, t, x)| \leq C_1 \langle x \rangle. \tag{5.15}$$

Thus, we can integrate by parts as

$$\widetilde{U}_{\mathrm{L}}^{\pm}(t)h = (2\pi)^{-1/2} \chi |x|^{-(d-1)/2} \int_0^\infty \mathrm{e}^{\pm \mathrm{i} \widetilde{K}_{\mathrm{L}}} \partial_\lambda [(\partial_\lambda \widetilde{K}_{\mathrm{L}})^{-1} (2\lambda)^{-1/4} h] \, \mathrm{d}\lambda, \tag{5.16}$$

which implies, due to (5.15) again, that, for any $|x| > R'$,

$$|(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x)| \leq C_2 \langle x \rangle^{-(d+1)/2}.$$

Since $\widetilde{U}_{\mathrm{L}}^{\pm}(t)h$ is uniformly bounded for $|x| \leq R'$, we conclude that $\widetilde{U}_{\mathrm{L}}^{\pm}(t)h \in \mathcal{H}$.

We prove the second assertion in the remaining steps.

Step II. By the uniform boundedness of $\mathrm{e}^{\pm \mathrm{i} t H}$ and Lemma 5.1, it suffices to show that as $t \to \infty$

$$(U_{\mathrm{L}}^{\pm}(t)h)(x) = \mathrm{e}^{\mp 3\pi \mathrm{i}/4} t^{-1} |x|^{1-d/2} \mathrm{e}^{\pm \mathrm{i} K_{\mathrm{L}}(t,x)} h(x^2/(2t^2), \hat{x}) + o(t^0) \quad \text{in } \mathcal{H}.$$

Recall that S_{L} is defined for $I = [\mu'^2/2, \infty)$ as in Lemma 5.1. Let $\mu'' = (\mu' + \mu)/2$, and decompose $\mathbb{R}_+ \times \mathbb{R}^d = \Omega_{\mu''} \cup \Omega_{\mu''}^c$ and, correspondingly,

$$(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x) = 1_{\Omega_{\mu''}}(t, x)(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x) + 1_{\Omega_{\mu''}^c}(t, x)(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x). \tag{5.17}$$

Here, let us prove that the second term of (5.17) is negligible. In fact, using (5.1) for $\widetilde{K}_{\mathrm{L}}$, we can estimate, for any $\lambda \geq \mu^2/2$ and $(t, x) \notin \Omega_{\mu''}$ with sufficiently large t,

$$\partial_\lambda \widetilde{K}_{\mathrm{L}}(\lambda, t, x) \leq -c_2 t, \quad |\partial_\lambda^2 \widetilde{K}_{\mathrm{L}}(\lambda, t, x)| \leq C_3 \langle x \rangle.$$

This allows us to integrate by parts in the same way as for (5.16) and deduce the pointwise bound

$$|1_{\Omega_{\mu''}^c}(t, x)(\widetilde{U}_{\mathrm{L}}^{\pm}(t)h)(x)| \leq C_4 t^{-1} \langle x \rangle^{-(d-1)/2}.$$

By integration, we then conclude the norm-bound

$$1_{\Omega_{\mu''}^c} \widetilde{U}_{\mathrm{L}}^{\pm}(t)h = \mathcal{O}(t^{-1/2}) \quad \text{in } \mathcal{H}.$$

Step III. As for the first term of (5.17), we decompose it as follows. Using that $\mu'' > \mu'$, we can for any $(t, x) \in \Omega_{\mu''}$ find a unique critical point $\lambda_{L,c} = \lambda_{L,c}(t, x)$ of $\widetilde{K}_L$. Then, take any $\eta_0 \in C_c^\infty(\mathbb{R})$ such that $\eta_0(s) = 1$ for $|s| \leq 1/2$ while $\eta_0(s) = 0$ for $|s| \geq 1$, and set

$$\eta(\lambda, t, x) = \eta_0(\langle x\rangle^\delta(\lambda - \lambda_{L,c})), \quad \frac{1}{2} - \frac{\rho}{6} < \delta < \frac{1}{2} - \frac{1}{4(l'-1)}.$$

We recall that l' is the fixed integer obeying the condition $l' > 1 + 2/\rho$. Obviously, we can find δ fulfilling these constraints, henceforth taken fixed. We now decompose

$$\begin{aligned} 1_{\Omega_{\mu''}} \widetilde{U}_L^\pm(t)h &= \mp\mathrm{i}(2\pi)^{-1/2} 1_{\Omega_{\mu''}} \chi |x|^{-(d-1)/2} \int_0^\infty (\eta + (1-\eta)) \mathrm{e}^{\pm\mathrm{i}\widetilde{K}_L} (2\lambda)^{-1/4} h \, \mathrm{d}\lambda \\ &=: \psi_1(t, x) + \psi_2(t, x). \end{aligned}$$

Step IV. The second term ψ_2 is negligible. In fact, for any $k = 2, \ldots, l'$, sufficiently large t, and $(\lambda, t, x) \in \operatorname{supp}(1-\eta)$ with $(\lambda, \hat{x}) \in \operatorname{supp} h$, $(t, x) \in \Omega_{\mu''}$, we can bound

$$|\partial_\lambda \widetilde{K}_L(\lambda, t, x)| \geq c_2 \langle x\rangle^{1-\delta}, \quad |\partial_\lambda^k \widetilde{K}_L(\lambda, t, x)| \leq C_3 \langle x\rangle^{1+\sigma-m(k)+k}.$$

This and the lower bound $\delta > 1/2 - \rho/6 > 1/2 - \rho/2$ imply that each time we integrate ψ_2 by parts as in (5.16) we at least gain a decay of order $\langle x\rangle^{-1+2\delta}$. Hence, by doing the integration by parts in total $(l'-1)$ times, we can conclude that

$$\psi_2 = o(t^0) \quad \text{in } \mathcal{H}.$$

Step V. It remains to investigate ψ_1. Let us expand the phase function as

$$\widetilde{K}_L(\lambda, t, x) = K_L(t, x) + \frac{1}{2} A(t, x)(\lambda - \lambda_{L,c})^2 + B(\lambda, t, x)(\lambda - \lambda_{L,c})^3$$

with

$$\begin{aligned} A(t, x) &= (\partial_\lambda^2 S_L)(\lambda_{L,c}, x), \\ B(\lambda, t, x) &= \frac{1}{2} \int_0^1 (1-\tau)^2 (\partial_\lambda^3 S_L)(\lambda_{L,c} + \tau(\lambda - \lambda_{L,c}), x) \, \mathrm{d}\tau. \end{aligned}$$

We substitute the expression into ψ_1, and split the integral as

$$\begin{aligned} \psi_1 &= \mp\mathrm{i}(2\pi)^{-1/2} 1_{\Omega_{\mu''}} \chi |x|^{-(d-1)/2} \mathrm{e}^{\pm\mathrm{i}K_L} \\ &\quad \cdot \Bigg((2\lambda_{L,c})^{-1/4} h(\lambda_{L,c}, \cdot) \int_0^\infty \mathrm{e}^{\pm\mathrm{i}A(\lambda-\lambda_{L,c})^2/2} \eta \, \mathrm{d}\lambda \\ &\qquad + \int_0^\infty \mathrm{e}^{\pm\mathrm{i}A(\lambda-\lambda_{L,c})^2/2} \eta [\mathrm{e}^{\pm\mathrm{i}B(\lambda-\lambda_{L,c})^3} (2\lambda)^{-1/4} h - (2\lambda_{L,c})^{-1/4} h(\lambda_{L,c}, \cdot)] \, \mathrm{d}\lambda \Bigg). \end{aligned}$$

Let us denote the last integral by T, and show that its contribution is negligible. By an integration by parts, we can rewrite it as

$$T = -\int_{|\lambda-\lambda_{\mathrm{L},c}|\le\langle x\rangle^{-\delta}} \Big(\int_{\lambda_{\mathrm{L},c}}^{\lambda} \mathrm{e}^{\pm\mathrm{i}A(\lambda'-\lambda_{\mathrm{L},c})^2/2}\,\mathrm{d}\lambda'\Big) \cdot \frac{\partial}{\partial\lambda}\eta[\mathrm{e}^{\pm\mathrm{i}B(\lambda-\lambda_{\mathrm{L},c})^3}(2\lambda)^{-1/4}h - (2\lambda_{\mathrm{L},c})^{-1/4}h(\lambda_{\mathrm{L},c},\cdot)]\,\mathrm{d}\lambda.$$

Then, by the van der Corput lemma, cf. [24, p. 332], and the assumed support property of h, it follows that on $\operatorname{supp}(1_{\Omega_{\mu''}}\chi)$

$$T = \mathcal{O}(\langle x\rangle^{-1/2-\delta'}), \quad \delta' = \delta - \frac{1}{2} + \frac{\rho}{6},$$

so that indeed

$$\psi_1 \pm \mathrm{i}(2\pi)^{-1/2}1_{\Omega_{\mu''}}|x|^{-(d-1)/2}\mathrm{e}^{\pm\mathrm{i}K_{\mathrm{L}}}(2\lambda_{\mathrm{L},c})^{-1/4}h(\lambda_{\mathrm{L},c},\cdot)\int_0^\infty \mathrm{e}^{\pm\mathrm{i}A(\lambda-\lambda_{\mathrm{L},c})^2/2}\eta\,\mathrm{d}\lambda$$
$$= o(t^0)$$

as a vector in $\mathcal{H}$.

Step VI. Finally, we remove η from the last integral with another admissible error, and then implement the Gaussian integral to obtain

$$\psi_1 = \mathrm{e}^{\mp\mathrm{i}3\pi/4}|x|^{-(d-1)/2}\mathrm{e}^{\pm\mathrm{i}K_{\mathrm{L}}}|A|^{-1/2}(2\lambda_{\mathrm{L},c})^{-1/4}h(\lambda_{\mathrm{L},c},\cdot) + o(t^0) \quad \text{in } \mathcal{H}.$$

Thus, using Lemma 5.1 and

$$A = -(2\lambda_{\mathrm{L},c})^{-3/2}|x| + \mathcal{O}(\langle x\rangle^{1-\sigma}), \quad \lambda_{\mathrm{L},c} = x^2/(2t^2) + \mathcal{O}(\langle x\rangle^{-\sigma}),$$

we obtain the second assertion of the lemma. ∎

5.2.2. Asymptotic completeness. Now, we are ready to prove the first part of Theorem 1.20.

Proof of Theorem 1.20 (1). It suffices to show the identity (1.19) since then the asymptotic completeness is obvious by the unitarity of $\mathcal{F}^{\pm}$. Let S_{L} be defined for an interval $I_{\mu'} = [\mu'^2/2, \infty)$, $0 < \mu' < \mu$, sufficiently big to include the given closed interval I. Then, for any $h \in C_{\mathrm{c}}^\infty(\mathbb{R}_+ \times \mathbb{S}^{d-1})$ with $\operatorname{supp} h \subseteq (I \cap J) \times \mathbb{S}^{d-1}$ and for any $\psi \in C_{\mathrm{c}}^\infty(\mathbb{R}^d)$, we can compute, by Lemma 5.3,

$$\langle\psi, W^{\pm}\mathrm{e}^{\mp\mathrm{i}\Phi_{\mathrm{L}}}h\rangle_{\mathcal{H}} = \lim_{\varepsilon\to 0_+}\int_0^\infty \varepsilon\mathrm{e}^{-\varepsilon t}\langle\psi, \mathrm{e}^{\pm\mathrm{i}tH}\tilde{U}_{\mathrm{L}}^{\pm}(t)h\rangle_{\mathcal{H}}\,\mathrm{d}t$$
$$= \lim_{\varepsilon\to 0_+}(\pm 2\pi\mathrm{i})^{-1}\int_0^\infty\Big(\int_0^\infty\langle\varepsilon\mathrm{e}^{\mp\mathrm{i}t(H-\lambda\mp\mathrm{i}\varepsilon)}\psi, \phi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)]\rangle_{\mathcal{H}}\,\mathrm{d}\lambda\Big)\,\mathrm{d}t.$$

By Fubini's theorem and (4.42c), we can further proceed as

$$\begin{aligned}
&\langle \psi, W^{\pm} \mathrm{e}^{\mp \mathrm{i}\Phi_{\mathrm{L}}} h\rangle_{\mathcal{H}} \\
&= \lim_{\varepsilon\to 0_+} (\pm 2\pi \mathrm{i})^{-1} \int_0^\infty \langle \mp \mathrm{i}\varepsilon R(\lambda \pm \mathrm{i}\varepsilon)\psi, \phi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)]\rangle_{\mathcal{H}}\,\mathrm{d}\lambda \\
&= \lim_{\varepsilon\to 0_+} (\pm 2\pi \mathrm{i})^{-1} \int_0^\infty \langle \psi - (H-\lambda)R(\lambda \pm \mathrm{i}\varepsilon)\psi, \phi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)]\rangle_{\mathcal{H}}\,\mathrm{d}\lambda \\
&= \lim_{\varepsilon\to 0_+} (\pm 2\pi \mathrm{i})^{-1} \int_0^\infty \langle \psi, \phi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)] - R(\lambda \mp \mathrm{i}\varepsilon)\psi_{\pm}^{S_{\mathrm{L}}}[h(\lambda,\cdot)]\rangle_{\mathcal{H}}\,\mathrm{d}\lambda \\
&= \int_0^\infty \langle \psi, F^{\pm}(\lambda)^*(\mathrm{e}^{\mp \mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)} h(\lambda,\cdot))\rangle_{\mathcal{H}}\,\mathrm{d}\lambda \\
&= \int_0^\infty \langle \mathrm{e}^{\mp \mathrm{i}\Theta_{\mathrm{L}}(\lambda,\cdot)} F^{\pm}(\lambda)\psi, h(\lambda,\cdot)\rangle_{\mathcal{G}}\,\mathrm{d}\lambda = \langle \mathrm{e}^{\pm \mathrm{i}\Theta_{\mathrm{L}}} \mathcal{F}^{\pm}\psi, h\rangle_{\widetilde{\mathcal{H}}}.
\end{aligned}$$

This implies, as operators $\mathcal{H}_{I\cap J} \to \widetilde{\mathcal{H}}_{I\cap J}$,

$$(W^{\pm})^* = \mathrm{e}^{\pm \mathrm{i}(\Theta_{\mathrm{L}} - \Phi_{\mathrm{L}})} \mathcal{F}^{\pm}.$$

We have proven (1.19) with $\Psi = \Phi_{\mathrm{L}} - \Theta_{\mathrm{L}}$, and we are done with (1). ■

To prove the remaining assertion (2), we use an approximation argument to be studied in the following. Fix any $\rho \in (0,\sigma)$ and $\delta \in (0, \sigma - \rho)$, and let $\varepsilon = 1/j$ for any $j \in \mathbb{N}$. For these parameters ρ, ε, and δ used as inputs in Lemma 4.1 (2) we decompose V, accordingly and the denote the decomposition as

$$V = V_{\mathrm{S},j} + V_{\mathrm{L},j}.$$

Lemma 5.5. *Let $\mu > \mu' > 0$, $I = [\mu'^2/2, \infty)$, and $J = [\mu^2/2, \infty)$, and fix a sufficiently large $R > 0$. Let $S, S_{\mathrm{L},j}$ be determined as in Theorem 1.3 for $V, V_{\mathrm{L},j}$, and let $K, K_{\mathrm{L},j}$ be their Legendre transforms as in Theorem 1.14, respectively. Then,*

$$\lim_{j\to\infty} \Theta_{\mathrm{L},j} = 0 \quad \textit{locally uniformly on } I \times \mathbb{S}^{d-1} \tag{5.18}$$

with $\Theta_{\mathrm{L},j}$ being the limit from Lemma 4.12 for S and $S_{\mathrm{L},j}$, and

$$\lim_{j\to\infty} \Phi_{\mathrm{L},j} = 0 \quad \textit{locally uniformly on } J \times \mathbb{S}^{d-1} \tag{5.19}$$

with $\Phi_{\mathrm{L},j}$ being the limit from Lemma 5.1 for K and $K_{\mathrm{L},j}$.

Remark 5.6. In the construction of S, $S_{\mathrm{L},j}$, K, $K_{\mathrm{L},j}$ we can use the same R, since it depends only on sizes of zeroth to second derivatives of V, $V_{\mathrm{L},j}$, which are uniformly estimated due to Lemma 4.1 (2). See the proofs of Theorems 1.3 and 1.14.

Proof. We proceed in two steps.

Step I. To prove (5.18), we can partially mimic the proof of Lemma 4.12. For details of the following computations, see the proof there, though one should note that S and $S_{\mathrm{L},j}$ now are more specific than before.

Let y_j be the flow from Section 4.2 associated with $S_{\mathrm{L},j}$; we discuss the limit

$$\Sigma_{\mathrm{L},j}(\lambda,\theta) := \lim_{t\to\infty}\big(S(\lambda, y_j(\lambda,t,\theta)) - S_{\mathrm{L},j}(\lambda, y_j(\lambda,t,\theta))\big).$$

Omitting the argument, we can compute its derivative in t as

$$\frac{\mathrm{d}}{\mathrm{d}t}(S - S_{\mathrm{L},j}) = -\frac{1}{2}|\nabla S_{\mathrm{L},j}|^{-2}(\nabla S - \nabla S_{\mathrm{L},j})^2 - |\nabla S_{\mathrm{L},j}|^{-2}\chi_R V_{\mathrm{S},j}. \tag{5.20}$$

Hence, we are led to consider

$$u = (\nabla S - \nabla S_{\mathrm{L},j})^2.$$

Its t-derivative is computed as

$$\begin{aligned}&\frac{1}{2}|\nabla S_{\mathrm{L},j}|^2\frac{\mathrm{d}}{\mathrm{d}t}u\\ &\quad= -(\nabla S - \nabla S_{\mathrm{L},j})\cdot(\nabla^2 S)(\nabla S - \nabla S_{\mathrm{L},j}) - (\nabla\chi_R V_{\mathrm{S},j})\cdot(\nabla S - \nabla S_{\mathrm{L},j}),\end{aligned}$$

and thus we can deduce that for any (small) $\delta > 0$ there exist $C_1, T > 0$, independent of $j \in \mathbb{N}$, such that

$$\frac{\mathrm{d}}{\mathrm{d}t}u \le -(2-\delta)t^{-1}u + C_1 j^{-1}t^{-2-\delta};\quad t \ge T.$$

By integration, we then deduce that

$$u(t) \le t^{\delta-2}T^{2-\delta}u(T) + C_1 j^{-1}t^{-1-\delta};\quad t \ge T. \tag{5.21}$$

By another integration, (5.20) and (5.21) imply a uniform bound

$$|S - S_{\mathrm{L},j}| \le |(S - S_{\mathrm{L},j})(T)| + C_2 T u(T) + C_3 j^{-1}.$$

On the other hand, by integrating a version of (4.26) from $t = 0$ (where u vanishes) to $t = T$ (for fixed T), we deduce that

$$|(S - S_{\mathrm{L},j})(T)| + C_2 T u(T) \le C_4 j^{-1/2}.$$

(In fact, the bound holds with $j^{-1/2}$ replaced by j^{-1}, if we invoke the variational principle of Lemma 2.5 to bound the first term.)

We conclude that, for large t,

$$|S - S_{\mathrm{L},j}| \leq C_5 j^{-1/2}.$$

In particular, $|\Sigma_{\mathrm{L},j}|$, $|\Theta_{\mathrm{L},j}| \leq C_3 j^{-1/2}$, and (5.18) follows.

Step II. The proof of (5.19) is similar. We consider versions of (5.8a) and (5.8b) using versions of (5.8c) and (5.11), omitting here the details. ∎

Proof of Theorem 1.20 (2). Let K be the Legendre transform of S from Theorem 1.3, as given in (2). Note that the phase corrections $\mathrm{e}^{\mp \mathrm{i}\Psi} = \mathrm{e}^{\pm \mathrm{i}(\Theta_{\mathrm{L}} - \Phi_{\mathrm{L}})}$ are independent of choice of V_{L} since so are $\mathcal{F}^{\pm}$ and $W^{\pm}$. Thus, it suffices to choose $V_{\mathrm{L},j}$ such that the associated difference $\Theta_{\mathrm{L},j} - \Phi_{\mathrm{L},j}$ converges to 0 as $j \to \infty$. However, this obviously follows from Lemma 5.5. ∎

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