STATIONARY SCATTERING THEORY FOR 1-BODY STARK OPERATORS

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Abstract. We study and develop the stationary scattering theory for a class of one-body Stark Hamiltonians with short-range potentials, including the Coulomb potential, continuing our study in [AIIS1]. The classical scattering orbits are parabolas parametrized by asymptotic orthogonal momenta, and the kernel of the (quantum) scattering matrix at a fixed energy is defined in these momenta. We study mapping properties of the scattering matrix, show that the singularities of its kernel are located at the diagonal and compute the leading order singularities. Our approach can be viewed as an adaption of the method of Isozaki-Kitada [IK] used for stydying the scattering matrix for one-body Schrödinger operators without an external potential. It is more flexible and more informative than the more standard method used previously by Kvitsinsky-Kostrykin [KK1] for this study in the case of a constant external potential (the Stark case). It relies on Sommerfeld's uniqueness result in Besov spaces proven in [AIIS1], microlocal analysis as well as on classical phase space constructions.

Contents

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1. Introduction

In this paper we study and develop the stationary scattering theory for a class of one-body Stark Hamiltonians. While the time-dependent scattering theory is well-understood [AH, He, Ya1, Ya2, Wh] the stationary scattering theory is a our opinion in a less complete form, even for short-range potentials. There are other papers in the literature on one-body Stark stationary scattering theory, see for example [KK1, KK2], however we find it useful and appealing for its intrinsic beauty to give a more systematic account done entirely within the framework of stationary theory. The time-dependent framework will only be discussed for the sake of motivation and interpretation.

Having the stationary apparatus well settled we then pass to a detailed study of the scattering matrix. This is also the subject of [KK1] with which we have overlapping results. Our approach is very different from the one of [KK1]. It can be considered as an adaption of the method of Isozaki-Kitada [IK] used for stydying the scattering matrix for one-body Schrödinger operators without an external potential. It is more flexible and more informative than 'the standard method'. While the paper by Kvitsinsky-Kostrykin can be seen as an application of the standard method in the case of a constant external potential, our scheme is closer to the one invented by Isozaki-Kitada. In particular it relies on microlocal analysis and on classical phase space constructions. By using such notions the accomplishment of [IK] is a 'trivialization' of the detailed study of the scattering matrix. More precisely Isozaki-Kitada extracted the singularities of the scattering matrix in the form of an explicit PsDO (or a FIO in the case of long-range potentials).

In this paper we more or less show how to do the same in the Stark case with short-range potentials. (Note that the Coulomb potential is a 'short-range' potential in the Stark case). In particular, and more precisely, we show how to isolate the local singularities to be present only in a term expressed as an explicit oscillatory integral, with properties conforming with characteristica of a pseudodifferential operator. For example this allows us to compute the leading order local singularities for the Coulomb potential, reproducing a result in [KK1].

Let us outline the relationship of our purely stationary setup to time-dependent scattering theory. We consider a d-dimensional particle (with $d \geq 2$) subject to a constant nonzero field pointing in the x_1-direction. For simplicity we assume that its strength as well as the particle mass and charge are all taken to 1. We split the coordinates in $\mathbb{R}^d$ into x_1 and the coordinates for orthogonal directions, decomposing the configuration space variable as

$$(x, y) \in \mathbb{R} \times \mathbb{R}^{d-1}; \quad x = x_1,\ y = (x_2, \dots, x_d).$$

Then the classical free Stark Hamiltonian is given by

$$h_0(x, y, \eta, \zeta) = \tfrac{1}{2}(\eta^2 + \zeta^2) - x, \quad (x, y, \eta, \zeta) \in T^*\mathbb{R}^d \cong \mathbb{R}^{2d},$$

and hence the associated Hamilton equations are

$$\dot{x} = \eta, \quad \dot{y} = \zeta, \quad \dot{\eta} = 1, \quad \dot{\zeta} = 0.$$

The solution with the initial data $(x_0, y_0, \eta_0, \zeta_0) \in T^*\mathbb{R}^d$, defining the free classical flow (say denoted by $\Theta(t)$), is given by

$$x = \tfrac{1}{2}t^2 + t\eta_0 + x_0, \quad y = t\zeta_0 + y_0, \quad \eta = t + \eta_0, \quad \zeta = \zeta_0. \tag{1.1}$$

In particular the classical orbits are parabolas of the form $x = \frac{1}{2\zeta^2}y^2 + O(t)$. The same property holds for $h = h_0 + q$, where q is short-range, for example given as $q = q_1$ in the following condition which will be imposed throughout this paper.

Condition 1.1. The potential q splits into real-valued functions as $q = q_1 + q_2$, where q_2 has compact support, $q_2(-\Delta + 1)^{-1}$ is compact, q_1 is smooth and for some $\delta \in (0, 1/2]$

$$\partial^\beta q_1 = O\big(r^{-(1+2\delta+|\beta|)/2}\big); \quad r = (x^2 + y^2)^{1/2}. \tag{1.2}$$

We introduce for any scattering orbit (with potential $q = q_1$) the *asymptotic orthogonal momenta* $\zeta^\pm = \lim_{t\to\pm\infty} \zeta(t)$. The orbit is incoming and outgoing along parabolas given as sections of the paraboloids $x = \frac{1}{2(\zeta^\mp)^2}y^2$, respectively. It is part of the classical scattering problem to determine the transition from an incoming asymptotic parabola to an outgoing asymptotic parabola, or stated differently the transition from an incoming value ζ^- to an outgoing value ζ^+. As we will outline below (with further details given in the bulk of the paper) this information is in quantum mechanics encoded in the subject of study in this paper, the scattering matrix.

Under Condition 1.1 the free and the perturbed Stark operators on $L^2(\mathbb{R}^d)$ are given by $H_0 = p^2/2 - x$ and $H = p^2/2 - x + q$ (with $p = -\mathrm{i}\nabla$), respectively. It is a well-established fact that asymptotic completeness holds, i.e. that the wave operators

$$W^\pm = \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}$$

exist and map onto $L^2(\mathbb{R}^d)$. The asymptotic orthogonal momenta read in this case

$$p_y^\pm = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} p_y \mathrm{e}^{-\mathrm{i}tH} = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} y/t\, \mathrm{e}^{-\mathrm{i}tH},$$

where the limits are taken in the strong resolvent sense (see [Ad1]).

In terms of the *stationary wave operators* $\mathcal{F}^-$ and $\mathcal{F}^+$ we can simultaneously diagonalize either H and p_y^- or H and p_y^+, respectively. These wave operators have several representations, for example given in terms of asymptotic properties of the boundary values $\lim_{\epsilon\to 0}(H - \lambda \mp \mathrm{i}\epsilon)^{-1}$ (taken in an appropriate space). However they are also connected to the time-depending wave operators by the formulas $\mathcal{F}_0(W^\pm)^* = \mathcal{F}^\pm$, where $\mathcal{F}_0$ is given in terms of asymptotic properties of the boundary values $\lim_{\epsilon\to 0}(H_0 - \lambda \mp \mathrm{i}\epsilon)^{-1}$, or alternatively and more useful, given by a Fourier-Airy transformation which in turn is defined by an explicit oscillatory integral. By joint diagonalization we mean more precisely the assertions

$$H = \big(\mathcal{F}^\pm\big)^* M_\lambda \mathcal{F}^\pm \quad \text{and} \quad p_y^\pm = \big(\mathcal{F}^\pm\big)^* \Big(\int_{\mathbb{R}} \oplus M_\zeta \,\mathrm{d}\lambda\Big)\mathcal{F}^\pm,$$

where $M_{(\cdot)}$ refers to multiplication in $L^2(\mathbb{R}, \mathrm{d}\lambda; \Sigma)$ or in $\Sigma := L^2\big(\mathbb{R}_\zeta^{d-1}, \mathrm{d}\zeta\big)$, respectively.

The *scattering operator* $S = (W^+)^*W^-$ is represented as

$$\mathcal{F}_0 S \mathcal{F}_0^{-1} = \int_{\mathbb{R}} \oplus S(\lambda)\,\mathrm{d}\lambda,$$

where $S(\lambda)$ is a unitary operator on Σ called the *scattering matrix* at energy λ. Its Schwartz kernel $S(\lambda)(\zeta, \zeta')$ is defined in terms of the variables ζ and ζ' which may be interpreted as incoming and outgoing asymptotic orthogonal momenta, respectively. This explains the physical relevance of detailed information on $S(\lambda)$ and its kernel.

In this paper we study several representations of $S(\lambda)$ based on Sommerfeld's uniqueness result in Besov spaces proven in [AIIS1]. We show mapping properties and we show that the principal symbol of $T(\lambda) := S(\lambda) - I$ viewed of as a PsDO (although not justified to be a classical PsDO) is given by

$$t_{\rm psym}(\zeta, y) = -2\mathrm{i}\int_0^\infty \tfrac{q_1(x,-y)}{\sqrt{2x}}\,\mathrm{d}x.$$

Applied to $q = \kappa r^{-1}$ for $d \geq 3$ the singularity structure of the kernel of the scattering matrix at the diagonal is

$$S(\lambda)(\zeta, \zeta') - \delta(\zeta, \zeta') = \kappa C|\zeta - \zeta'|^{3/2-d} + O\big(|\zeta - \zeta'|^{2-d}\big),$$

locally uniformly in ζ, ζ' and λ.

The latter result conforms with [KK1] for $d = 3$ in which case $C = -\mathrm{i}(2\pi)^{-1/2}$.

In the bulk of the paper we use Condition 1.1 with the extra condition $q_2 = 0$ imposed. It is a minor technical issue (and hardly interesting for the reader) to do the general case by modifying the arguments of the paper.

We use the standard notation $\langle z\rangle = (1+|z|^2)^{1/2}$ for z in a normed space, while we for any $m \in \mathbb{N}$ let $\langle z\rangle_m = (m^2 + |z|^2)^{1/2}$ and $\hat{z}_m = z/\langle z\rangle_m$. We use the (standard) notation $F(x \in M) = 1_M$ for the characteristic function of a set M. For any $\kappa \in \mathbb{R}$ the notation $\chi(\cdot < \kappa)$ stands for any smooth real function χ on $\mathbb{R}$ with $\chi' \in C^\infty_{\rm c}(\mathbb{R})$ and $\chi(t) = 0$ for $t \geq \kappa$. If $\kappa > 0$ we require in addition $\chi(t) = 1$ for $t \leq \kappa/2$, and if $\kappa < 0$ we also require $\chi(t) = 1$ for $t \leq 2\kappa$. Similarly we introduce $\chi(\cdot > \kappa)$ which by definition have $\chi(t > \kappa) = 0$ for $t \leq \kappa$. Let $\chi^\perp(\cdot < \kappa) = 1 - \chi(\cdot < \kappa)$ and $\chi^\perp(\cdot > \kappa) = 1 - \chi(\cdot > \kappa)$.

2. Airy function asymptotics

One can write up explicitly a diagonalizing transform $\int_{\mathbb{R}} \oplus \mathcal{F}_0(\lambda)\,\mathrm{d}\lambda$ so that $\delta(H_0 - \lambda) = \mathcal{F}_0(\lambda)^*\mathcal{F}_0(\lambda)$ and also $\mathcal{F}_0^*(\lambda)$ becomes explicit, cf. [He, Ya1]. Writing the Airy function by its Fourier transform the expression for $\mathcal{F}_0(\lambda)^*$ (it is not unique) is an oscillatory integral. One can look at stationary points and find by stationary phase method considerations, see [Hö] (or for example [II, St]), what the asymptotics should be. Below we state the results without giving details of proof. The reader can find relevant details in Section 13, and for simplicity we take below $\lambda = 0$ (in general we just need to replace x by $x + \lambda$).

$$\begin{aligned}\big(\mathcal{F}_0(0)^*\xi\big)(x, y) &= c\int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\eta;\\ c = (2\pi)^{-\frac{d+1}{2}}, &\quad \theta = y\cdot\zeta - \eta^3/6 + (x - \zeta^2/2)\eta.\end{aligned}\tag{2.1}$$

We look for critical points

$$\begin{aligned}0 &= \partial_\eta\theta = -\eta^2/2 - \zeta^2/2 + x \quad \text{(energy relation)},\\ 0 &= \partial_\zeta\theta = y - \eta\zeta \quad \text{(velocity relation)}.\end{aligned}$$

Note that considering the momentum η as an effective time indeed the last equation written as $\zeta = y/\eta$ is a 'velocity relation'. If we substitute $\zeta = y/\eta$ in the argument of ξ, interchange limits of integration and do the ζ-integration we end up with

$$c\int \mathrm{e}^{\mathrm{i}\theta_0}\xi(y/\eta)\big(\mathrm{i}\eta/(2\pi)\big)^{\frac{1-d}{2}}\,\mathrm{d}\eta;$$
$$\theta_0(\eta)=y^2/(2\eta)-\eta^3/6+x\eta.$$

The critical points of θ_0 fulfill

$$0=\partial_\eta\theta_0=-\tfrac12 y^2/\eta^2-\tfrac12\eta^2+x,$$

which in turn fulfill

$$\eta^2=x\pm\big(x^2-y^2\big)^{1/2}.$$

We choose '+' (the case of '−' does not contribute to the asymptotics) leading to the two critical points

$$\eta=\pm\sqrt{x+\big(x^2-y^2\big)^{1/2}}\approx\pm(2x)^{1/2}.$$

The second order derivative is $-\eta(1+O(y^2/x^2))$. Whence the asymptotics of the integral is given as the sum of the following two terms,

$$\begin{aligned}&c\mathrm{e}^{\pm\mathrm{i}\theta_1}\xi(y/\eta)\big(\mathrm{i}\eta/(2\pi)\big)^{-d/2}\\&\quad=\tfrac{\mathrm{e}^{\mp\mathrm{i}\pi d/4}}{\sqrt{2\pi}}(2x)^{-d/4}\mathrm{e}^{\pm\mathrm{i}\theta_1}\xi(\pm\omega);\\&\quad\theta_1=\sqrt{x+\big(x^2-y^2\big)^{1/2}}\Big(\tfrac12 y^2/\eta^2-\eta^2/6+x\Big),\\&\quad\eta^2=x+\big(x^2-y^2\big)^{1/2},\quad\omega=(2x)^{-1/2}y.\end{aligned}$$

3. Computations for a phase function

The phase θ_1 is more explicitly given as

$$\theta_1=\tfrac43\sqrt{x+\big(x^2-y^2\big)^{1/2}}\Big(x-\tfrac12\big(x^2-y^2\big)^{1/2}\Big).$$

Note that indeed

$$\begin{aligned}\theta_1&=\eta\left(y^2/(2\eta^2)-\eta^2/6+x\right)\\&=\sqrt{x+\big(x^2-y^2\big)^{1/2}}\left\{y^2\left(x+\big(x^2-y^2\big)^{1/2}\right)^{-1}/2-\left(x+\big(x^2-y^2\big)^{1/2}\right)/6+x\right\}\\&=\sqrt{x+\big(x^2-y^2\big)^{1/2}}\left\{\left(x-\big(x^2-y^2\big)^{1/2}\right)/2-x/6-\big(x^2-y^2\big)^{1/2}/6+x\right\}\\&=\tfrac43\sqrt{x+\big(x^2-y^2\big)^{1/2}}\left(x-\tfrac12\big(x^2-y^2\big)^{1/2}\right).\end{aligned}$$

We compute $\nabla\theta_1$ and $|\nabla\theta_1|^2$ as follows.

$$\begin{aligned}\nabla\theta_1&=\tfrac43\frac{x-\tfrac12\big(x^2-y^2\big)^{1/2}}{2\sqrt{x+\big(x^2-y^2\big)^{1/2}}}\left(1+x\big(x^2-y^2\big)^{-1/2},-y\big(x^2-y^2\big)^{-1/2}\right)\\&\quad+\tfrac43\sqrt{x+\big(x^2-y^2\big)^{1/2}}\left(1-\tfrac{x}{2}\big(x^2-y^2\big)^{-1/2},\tfrac{y}{2}\big(x^2-y^2\big)^{-1/2}\right)\\&=\sqrt{x+\big(x^2-y^2\big)^{1/2}}\left(1,y\left(x+\big(x^2-y^2\big)^{1/2}\right)^{-1}\right),\end{aligned}$$

$$\begin{aligned}|\nabla\theta_1|^2 &= \Big(x + \big(x^2 - y^2\big)^{1/2}\Big)\bigg(1 + y^2\Big(x + \big(x^2 - y^2\big)^{1/2}\Big)^{-2}\bigg)\\ &= x + \big(x^2 - y^2\big)^{1/2} + y^2\Big(x + \big(x^2 - y^2\big)^{1/2}\Big)^{-1}\\ &= 2x.\end{aligned}$$

Therefore θ_1 is a solution to the eikonal equation

$$\tfrac{1}{2}|\nabla\theta_1|^2 - x = 0. \tag{3.1}$$

The second order derivatives of θ_1 are given as follows.

$$\begin{aligned}(\nabla^2\theta_1)^{11} &= \tfrac{1}{2}\big(x^2 - y^2\big)^{-1/2}\sqrt{x + \big(x^2 - y^2\big)^{1/2}},\\ (\nabla^2\theta_1)^{1\alpha} &= -\tfrac{1}{2}\frac{y^\alpha}{|y|}\big(x^2 - y^2\big)^{-1/2}\sqrt{x - \big(x^2 - y^2\big)^{1/2}},\\ (\nabla^2\theta_1)^{\alpha\beta} &= \tfrac{1}{2}\frac{y^\alpha y^\beta}{|y|^2}\big(x^2 - y^2\big)^{-1/2}\sqrt{x + \big(x^2 - y^2\big)^{1/2}}\\ &\quad + \frac{1}{|y|}\sqrt{x - \big(x^2 - y^2\big)^{1/2}}\bigg(\delta^{\alpha\beta} - \frac{y^\alpha y^\beta}{|y|^2}\bigg);\end{aligned} \tag{3.2}$$

here the Greek indices run over $2, \dots, d$ and $\delta^{\alpha\beta}$ denotes Kronecker's δ.

4. Parabolic coordinates

It is known since a long time ago that parabolic coordinates are useful for stydying problems for Stark Hamiltonians, see [Ti]. Here we introduce a slight modification similar to the one used in [AIIS1].

Let $\breve{f} \in C^\infty(\mathbb{R})$ be a convex function such that $\breve{f}(t) = 1$ for $t \le 1/2$ and $\breve{f}(t) = t$ for $t \ge 2$. Let then $f \in C^\infty(\mathbb{R}^d)$ be given by

$$f(x, y) = \sqrt{\breve{f}(r + x)}; \quad r = (x^2 + y^2)^{1/2}. \tag{4.1a}$$

Note that

$$\nabla^2 f^2 \ge 0. \tag{4.1b}$$

Of course a classical scattering orbit will have $x > 1$ eventually so that for large time $f = (r + x)^{1/2}$. Since we will use the parabolic variable $(r + x)^{1/2}$ in quantum mechanics as well it is convenient to introduce the regularization f already at this stage. We choose other 'parabolic variables',

$$g = y/f, \quad g_i = y_i/f; \quad i = 2, \dots, d. \tag{4.1c}$$

We note the property

$$\nabla f \cdot \nabla g_i = 0 \ \text{ for } \ r + x > 2; \quad i = 2, \dots, d. \tag{4.2}$$

In Section 7 we will need a few calculus formulas in parabolic coordinates. Below we assume tacitly that $r + x > 2$. It may be convenient to note that

$$f^2 + g^2 = 2r \text{ and } 2r|\nabla f|^2 = 1.$$

Clearly we also have

$$f^2 - g^2 = 2x \text{ and } f|g| = |y|.$$

Introducing $\theta = f^3/3$ we compute

$$\begin{aligned}
\nabla\theta &= \tfrac{1}{2r}(f^3, fy),\\
(\nabla^2\theta)^{11} &= -\tfrac{1}{2}\tfrac{xf^3}{r^3} + \tfrac{3}{4}\tfrac{f^3}{r^2},\\
(\nabla^2\theta)^{1\alpha} &= -\tfrac{1}{2}\tfrac{y^\alpha f^3}{r^3} + \tfrac{3}{4}\tfrac{y^\alpha f}{r^2},\\
(\nabla^2\theta)^{\alpha\beta} &= -\tfrac{1}{2}\tfrac{y^\alpha y^\beta f}{r^3} + \tfrac{1}{4}\tfrac{y^\alpha y^\beta}{r^2 f} + \tfrac{1}{2}\tfrac{f}{r}\delta^{\alpha\beta},\\
\Delta\theta &= \tfrac{d}{2}\tfrac{f}{r}.
\end{aligned} \tag{4.3}$$

Moreover

$$\nabla\big(\tfrac{2r}{f^2}\big) = \tfrac{2}{rf^4}(-y^2, xy). \tag{4.4}$$

Letting T denote the change to parabolic coordinates, $T(x,y) = (f,g)$, then a computation using (4.2) shows that

$$J := |\det T'| = \tfrac{f^{2-d}}{f^2+g^2}. \tag{4.5}$$

Using again (4.2) we easily compute the partial derivative with respect to f

$$\partial_f = |\nabla f|^{-2}\nabla f\cdot\nabla = F\cdot\nabla;\quad F := \tfrac{2r}{f^2}\nabla\theta. \tag{4.6}$$

Using (4.3)–(4.5) we compute

$$\partial_f \ln\big(J^{-1/2}\big) = \tfrac{1}{2}\mathrm{div}F. \tag{4.7}$$

5. Phase space localization, classical mechanics

We note the following very rough bounds for free classical orbits. For any $\epsilon > 0$ eventually (i.e. for $t >> 1$)

$$\begin{aligned}
&|(x,y)/t^2 - (1/2,0)| \le \epsilon,\\
&|(\eta,\zeta)/t - (1,0)| \le \epsilon.
\end{aligned} \tag{5.1}$$

The same properties hold for scattering orbits of $h = h_0 + q$, where q fulfills Condition 1.1. In particular we can think of both of the quantities $\pm\sqrt{2x}$ and η as an 'effective time' allowing us to consider time-dependent observables as effective time-independent observables. In particular we obtain the following assertion for scattering orbits for $t \to +\infty$.

For any $\epsilon > 0$ eventually

$$x > 1,\quad |\tfrac{\eta}{\sqrt{2x}} - 1| \le \epsilon,\quad |\tfrac{y}{x}| \le \epsilon\quad |\tfrac{\zeta}{\eta}| \le \epsilon. \tag{5.2}$$

In [Ad2] quantum analogues of the bounds (5.1) is proven (including a Stark short-range potential), and thanks to those bounds a similar effective substitution will be possible in quantum mechanics as well. More precisely this should mean that the bounds (5.2) hold in the quantum case also, stated for evolved states (initially being well-localized) as strong bounds on the complement of the indicated phase-space localization.

We show here sharper results than (5.2) for classical orbits. This will be by a method that can be generalized to quantum mechanics, see Section 6.

In a region of the form $x > C$ and $|y|/x < C^{-1}$, with $C >> 1$ fixed, we define uniquely $f_1 > 0$ solving $3\theta_1 = f_1^3$. We are interested in showing decay estimates of the quantity $|y/x|$ along classical scattering orbits. Note that (5.2) does not assert more than $|y/x| \to 0$ for $t \to +\infty$.

We compute

$$\begin{aligned}\theta &= \tfrac{(2x)^{3/2}}{3}\bigl(1+\tfrac{3}{8}|y/x|^2+O\bigl(|y/x|^4\bigr)\bigr),\\ \theta_1-\theta &= f^3O\bigl(|y/x|^4\bigr),\\ \nabla\theta_1-\nabla\theta &= fO\bigl(|y/x|^3\bigr),\\ f-f_1 &= fO\bigl(|y/x|^4\bigr).\end{aligned}\tag{5.3}$$

Let

$$\begin{aligned}&\gamma=(\eta,\zeta)-\nabla\theta_1,\ \gamma=(\gamma_1,\dots,\gamma_d),\\ &\tilde\gamma=g/f=y/f^2=(\tilde\gamma_2,\dots,\tilde\gamma_d),\\ &\Gamma=(\gamma,\tilde\gamma).\end{aligned}\tag{5.4}$$

Note that Γ is a $(2d-1)$-dimensional variable. We are interested in a fixed energy-shelf, say $\lambda=0$, in which case we might think of Γ as a complete set of variables (here being unjustified). More importantly we are going to show sharper estimates on Γ than a priori can be read off (5.2).

Using the formula obtained by differentiating (3.1) we compute the time-derivative

$$D\Gamma^2/2=\frac{\mathrm{d}}{\mathrm{d}t}\Gamma^2/2=-\gamma\cdot\nabla^2\theta_1\gamma+\tilde\gamma\cdot D\tilde\gamma-\nabla q\cdot\gamma.\tag{5.5a}$$

We estimate

$$-\nabla q\cdot\gamma\le\epsilon\tfrac{f}{2r}\gamma^2+C(\epsilon)f|\nabla q|^2;\quad \epsilon>0.\tag{5.5b}$$

Due to Condition 1.1 we can bound

$$f|\nabla q|^2\le Cf^{-3}.\tag{5.5c}$$

From (3.2) we obtain

$$\nabla^2\theta_1=\tfrac{f}{2r}\bigl(I+O\bigl(|y/x|\bigr)\bigr).\tag{5.5d}$$

As for the second term we compute as

$$D\tilde\gamma=-\bigl(f^{-1}Df\bigr)\tilde\gamma+f^{-1}\nabla g\cdot\gamma+f^{-1}\nabla g\cdot\nabla\theta_1.$$

Note that due to (5.2) effectively

$$f^{-1}Df\approx\tfrac{f}{2r}\approx t^{-1}.$$

Clearly

$$f^{-1}\nabla g\cdot\gamma=O(f^{-2})\gamma=\tfrac{f}{2r}O(f^{-1})\gamma.$$

Due to (4.2) and (5.3) we can write

$$\begin{aligned}f^{-1}\nabla g\cdot\nabla\theta_1&=f^{-1}\nabla g\cdot(\nabla\theta_1-\nabla\theta)\\ &=f^{-1}O\bigl(|y/x|^3\bigr)=\tfrac{f}{2r}O(|\tilde\gamma|^3).\end{aligned}$$

We conclude that

$$D\tilde\gamma\approx-\tfrac{f}{2r}\bigl(\tilde\gamma+O(|\tilde\gamma|^3)+O(f^{-1})\gamma\bigr)+Cf^{-3}.\tag{5.5e}$$

Now the calculations (5.5a)–(5.5e) and elementary estimates yield that for any $\epsilon>0$

$$D\Gamma^2/2\le-\tfrac{f}{2r}(1-\epsilon)\Gamma^2,$$

from which we finally conclude that

$$\forall \epsilon > 0: \quad \Gamma = O\big(t^{\epsilon-1}\big) \text{ for } t \to +\infty. \tag{5.6}$$

Due to (5.3) and (5.6) it follows that

$$\forall \epsilon > 0: \quad (\eta, \zeta) - \nabla\theta = O\big(t^{\epsilon-1}\big) \text{ for } t \to +\infty.$$

Obviously it follows from (5.6) that $\Gamma^2 = O\big(t^{2\epsilon-2}\big)$, however it is more promising that a proof of this fact can be given by using again the above differential inequality. This proof generalizes to the quantum setting along the lines of [Sk] using the quantum analogues of (5.2) from [Ad2], see Section 6.

Next we introduce

$$\gamma_{\|} = \tfrac{\nabla f}{|\nabla f|^2} \cdot \gamma \quad \text{ and } \quad \gamma_{\|}^{\rm exact} = \tfrac{\nabla f_1}{|\nabla f_1|^2} \cdot \gamma.$$

Using (3.1) we compute

$$\gamma_{\|}^{\rm exact} \approx \tfrac{2x}{f_1^2}\gamma_{\|}^{\rm exact} = \nabla\theta_1 \cdot \gamma = h - \gamma^2/2 - q. \tag{5.7a}$$

Using (5.3) we obtain

$$\gamma_{\|} - \gamma_{\|}^{\rm exact} = \Big(\tfrac{\nabla f}{|\nabla f|^2} - \tfrac{\nabla f_1}{|\nabla f_1|^2}\Big) \cdot \gamma = fO\big(|y/x|^3\big) \cdot \gamma = fO\big(|\Gamma|^4\big). \tag{5.7b}$$

For any zero-energy classical orbit we conclude from (1.2), (5.6), (5.7a) and (5.7b) that

$$\forall \epsilon > 0: \quad \gamma_{\|} = O\big(t^{2\epsilon-1-2\delta}\big) \text{ for } t \to +\infty. \tag{5.8}$$

6. Phase space localization, quantum mechanics

In quantum mechanics we introduce $H = p^2/2 - x + q$, $R(z) = (H - z)^{-1}$ and *simplified* quantum versions of the 'gamma observables' considered in classical mechanics above. Let

$$\gamma^{\rm si} = p - \nabla\theta \quad \text{ and } \quad \gamma_{\|}^{\rm si} = \operatorname{Re}\big(\nabla\theta \cdot \gamma^{\rm si}\big). \tag{6.1}$$

We call these operators *radiation operators* and note that a version of $\gamma_{\|}^{\rm si} = \operatorname{Re}\big(\nabla\theta \cdot \gamma^{\rm si}\big)$ appears already in [AIIS1]. The radiation operators are globally defined, while

$$p - \nabla\theta_1 \quad \text{ and } \quad \operatorname{Re}\big(\nabla\theta \cdot \big(p - \nabla\theta_1\big)\big) \tag{6.2}$$

are not. However the latter operators correspond more closely to the 'gamma observables' considered in Section 5 and regularized quantizations need to be considered to mimic the previous arguments in quantum mechanics. This means, more precisely, that regularizing symbols corresponding to (5.2) need to be introduced as cutoffs in the expression for the 'gamma observables' of Section 5. The quantization of those symbols would be the right regularization substituting (6.2) in similar differential inequality arguments as used previously in classical mechanics. Rather than stating resolvent bounds in terms of these regularized observables we prefer below to state bounds in terms of the observables in (6.1), which appear somewhat 'cleaner'. The latter bounds would follow by combining (5.3) and the more ugly looking bounds more or less as in (5.7b). In conclusion we can obtain analogues of (5.6) and (5.8) by using the scheme of [Sk] in combination with bounds of [Ad2]. We skip the details of proof stating the following useful bounds (of independent interest).

Let $\Gamma^{\mathrm{si}} = (\gamma^{\mathrm{si}}, y/f^2)$ and let Γ^{si}_k for $k = 1, \dots, 2d-1$ denote the corresponding components. Note that Γ^{si} is a simplified quantization of the classical Γ of (5.4). Let $L^2_s = \langle (x,y)\rangle^{-s} L^2(\mathbb{R}^d)$ for $s \in \mathbb{R}$ and $L^2_\infty = \cap_s L^2_s$.

Proposition 6.1. *Let $\epsilon > 0$ and $\psi \in L^2_\infty$ be given. Let $\phi = R(0 + \mathrm{i}0)\psi$. Then for all $k, l = 1, \dots, 2d-1$*

$$\|f^{1/2-\epsilon}\,\Gamma^{\mathrm{si}}_k \phi\| < \infty, \tag{6.3a}$$

$$\|f^{3/2-\epsilon}\,\Gamma^{\mathrm{si}}_k\,\Gamma^{\mathrm{si}}_l \phi\| < \infty, \tag{6.3b}$$

$$\|f^{1/2+2\delta-\epsilon}\gamma^{\mathrm{si}}_\| \phi\| < \infty. \tag{6.3c}$$

At this stage let us note that the commutator $[\Gamma^{\mathrm{si}}_k, \Gamma^{\mathrm{si}}_l]$ is a non-vanishing function if $k \le d$ and $l \ge d+1$ (or vice versa), but the order of decay of this function is f^{-2}, which conforms completely with (6.3a) and (6.3b).

The bound (6.3c) is an improvement of the radiation bound from [AIIS1] for which for a certain parameter β the value $\beta = 1/2$ is critical for fastly decaying potentials. This restriction is an artifact of the choice of 'radiation operator' in [AIIS1] and cannot possibly be removed. The bound (6.3c) for the 'radiation operator' $\gamma^{\mathrm{si}}_\|$ would in comparison mean that '$\beta = 4$ is critical' for $\delta = 1/2$.

To be demonstrated in Section 7 the construction of stationary wave operators is almost trivial with Proposition 6.1 at our disposal.

7. Wave operators

Recall the notation $\partial_f = F \cdot \nabla$ from (4.6) valid in the region $r + x > 2$. Under the conditions of Proposition 6.1 we introduce the function

$$\mathcal{R}(f,g) := \big(J^{-1/2}\mathrm{e}^{-\mathrm{i}\theta}\phi\big)(f,g), \quad J = |\det T'|,$$

and want to show that the limit

$$\lim_{f\to\infty} \mathcal{R}(f,\cdot) \text{ exists in } \Sigma := L^2\big(\mathbb{R}^{d-1}\big). \tag{7.1}$$

This leads us to computing the f-derivative of the Σ-valued function $\mathcal{R}$; we are done by showing that the derivative is integrable. Let us introduce $p_f = -\mathrm{i}\partial_f$. Then we compute using (4.4), (4.6) and (4.7)

$$\begin{aligned} p_f\mathcal{R} &= -\mathrm{i}\big(\partial_f \ln\big(J^{-1/2}\big)\big)\mathcal{R} + J^{-1/2}\mathrm{e}^{-\mathrm{i}\theta} F\cdot\gamma^{\mathrm{si}}\phi \\ &= J^{-1/2}\mathrm{e}^{-\mathrm{i}\theta}\mathrm{Re}\,\big(\tfrac{2r}{f^2}(\nabla\theta)\cdot\gamma^{\mathrm{si}}\big)\phi \\ &= \tfrac{2r}{f^2} J^{-1/2}\mathrm{e}^{-\mathrm{i}\theta}\gamma^{\mathrm{si}}_\|\phi - \tfrac{\mathrm{i}}{2}\Big(\tfrac{2}{rf^4}(-y^2, xy)\cdot\nabla\theta\Big)J^{-1/2}\mathrm{e}^{-\mathrm{i}\theta}\phi. \end{aligned}$$

By using the first identity in (4.3) and (4.4) we see that the right-hand side is of the form

$$J^{-1/2}\Big(O(1)\gamma^{\mathrm{si}}_\|\phi + O\big(\tfrac{y^2}{r^{5/2}}\big)\phi\Big) = J^{-1/2}\Big(O(1)\gamma^{\mathrm{si}}_\|\phi + O(f^{-1})\sum_{k=d+1}^{2d-1}\big(\Gamma^{\mathrm{si}}_k\big)^2\phi\Big). \tag{7.2}$$

Proposition 7.1. *Under the conditions of Proposition 6.1 the wave operator*

$$\mathcal{F}^+(0)\psi := \frac{\mathrm{e}^{\mathrm{i}\pi(d-2)/4}}{\sqrt{2\pi}} \lim_{f\to\infty}\mathcal{R}(f,\cdot) \text{ exists in } \Sigma.$$

Proof. Using Proposition 6.1 and (7.2) we estimate for any $\epsilon \in (0, 2\delta)$

$$\begin{aligned}\int_2^\infty \|p_f\mathcal{R}\|_\Sigma \,\mathrm{d}f &\le C_1 \int_2^\infty \|f^{1/2+\epsilon} p_f \mathcal{R}\|_\Sigma^2 \,\mathrm{d}f \\ &\le C_2\Big(\|f^{1/2+\epsilon}\gamma_\parallel^{\mathrm{si}}\phi\|_{L^2}^2 + \sum_{k=d+1}^{2d-1} \|f^{-1/2+\epsilon}\big(\Gamma_k^{\mathrm{si}}\big)^2\phi\|_{L^2}^2\Big) < \infty.\end{aligned}$$

□

Letting T_λ denote translation by λ in the direction of $(-1, 0, \dots, 0)$ on $L^2(\mathbb{R}^d)$, i.e. $(T_\lambda\psi)(x, y) = \psi(x + \lambda, y)$, we introduce $J_\lambda = T_\lambda J T_{-\lambda}$, $\theta_\lambda = T_\lambda \theta T_{-\lambda}$ and (in terms of parabolic coordinates)

$$\mathcal{R}^{\lambda\pm}_{\psi,f}(\zeta) := \big(J_\lambda^{-1/2} \mathrm{e}^{\mp \mathrm{i}\theta_\lambda} R(\lambda \pm \mathrm{i}0)\psi\big)(f, \pm\zeta).$$

By an easy extension of Proposition 6.1 to the case $\lambda \neq 0$ combined with the proof of Proposition 7.1 it follows that $\lim_{f\to\infty} \mathcal{R}^{\lambda+}_{\psi,f}$ exists, and by time-invariance it then follows that also $\lim_{f\to\infty} \mathcal{R}^{\lambda-}_{\psi,f}$ exists. In conclusion we have justified the existence of the wave operators

$$\mathcal{F}^\pm(\lambda)\psi := \tfrac{\mathrm{e}^{\pm \mathrm{i}\pi(d-2)/4}}{\sqrt{2\pi}} \,\Sigma\text{-}\!\lim_{f\to\infty} \mathcal{R}^{\lambda\pm}_{\psi,f}.$$

We note the formula

$$\|\mathcal{F}^\pm(\lambda)\psi\|^2 = \langle\psi, \delta(H-\lambda)\psi\rangle; \quad \delta(H-\lambda) = \pi^{-1}\operatorname{Im} R(\lambda + \mathrm{i}0). \tag{7.3}$$

In fact, giving the proof only for $\lambda = 0$, by integration by parts and by using Proposition 6.1 we can compute with $\chi = \chi(\cdot < 1)$

$$\begin{aligned}2\pi\langle\psi, \delta(H-\lambda)\psi\rangle &= 2\mathrm{Im}\langle (H-\lambda)\phi, \phi\rangle = -\lim_{\rho\to\infty} \mathrm{Re}\langle \nabla f \cdot p\phi, \rho^{-1}\chi'(f/\rho)\phi\rangle \\ &= -\lim_{\rho\to\infty} \mathrm{Re}\langle \nabla f \cdot \big(\gamma^{\mathrm{si}} + \nabla\theta\big)\phi, \rho^{-1}\chi'(f/\rho)\phi\rangle \\ &= -\lim_{\rho\to\infty} \mathrm{Re}\langle \tfrac{f^2}{2r}\phi, \rho^{-1}\chi'(f/\rho)\phi\rangle = 2\pi\|\mathcal{F}^\pm(\lambda)\psi\|^2.\end{aligned}$$

It follows from (7.3) that $\|\mathcal{F}^+(\lambda)\psi\| = \|\mathcal{F}^-(\lambda)\psi\|$ and that $\mathcal{F}^\pm(\lambda)\psi \in \Sigma$ are defined for any $\psi \in \mathcal{B}$. (For explicit formulas, see (7.6).) It follows from (8.2d) stated below that

$$C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1}) \subseteq \operatorname{Ran}\mathcal{F}^\pm(\lambda). \tag{7.4}$$

In particular $\mathcal{F}^\pm(\lambda)$ map onto a dense subspaces of Σ and we can define the *scattering matrix* as the unique unitary operator $S(\lambda)$ on Σ obeying

$$\mathcal{F}^+(\lambda)\psi = S(\lambda)\mathcal{F}^-(\lambda)\psi. \tag{7.5}$$

By construction the map $\mathbb{R} \ni \lambda \to S(\lambda) \in \mathcal{L}(\Sigma)$ is strongly continuous. Let us also note that for any $\psi \in \mathcal{B}$ the maps $\mathcal{F}^\pm(\cdot)\psi \in \Sigma$ are continuous.

Introduce the spaces

$$\mathcal{H} = L^2(\mathbb{R}^d), \quad \widetilde{\mathcal{H}} = L^2(\mathbb{R}, \mathrm{d}\lambda; \Sigma),$$

and let M_λ be the operator of multiplication by λ on $\widetilde{\mathcal{H}}$. We define

$$\mathcal{F}^\pm = \int_{\mathbb{R}} \oplus \mathcal{F}^\pm(\lambda)\,\mathrm{d}\lambda \colon \mathcal{B} \to C(\mathbb{R}; \Sigma).$$

These operators can be extended to proper spaces which is stated as the first part of the following result. For vector-valued functions ξ on $\mathbb{R}$ (or on $\mathbb{R}_+$) we use the notation $⨍_\rho \xi(r)\,\mathrm{d}r = \rho^{-1}\int_\rho^{2\rho}\xi(r)\,\mathrm{d}r$, $\rho > 0$.

Proposition 7.2. *The operators $\mathcal{F}^\pm$ considered as maps $\mathcal{B}\cap\mathcal{H} \to \widetilde{\mathcal{H}}$ extend uniquely to isometries $\mathcal{H} \to \widetilde{\mathcal{H}}$. These extensions obey $\mathcal{F}^\pm H \subseteq M_\lambda \mathcal{F}^\pm$. Moreover for any $\psi \in \mathcal{B}$ the vectors $\mathcal{F}^\pm(\lambda)\psi$ are given as averaged limits, i.e.*

$$\mathcal{F}^\pm(\lambda)\psi = \Sigma\text{–}\lim_{\rho\to\infty} ⨍_\rho \frac{\mathrm{e}^{\pm\mathrm{i}\pi(d-2)/4}}{\sqrt{2\pi}}\,\mathcal{R}^{\lambda\pm}_{\psi,f}\,\mathrm{d}f, \tag{7.6}$$

and the limits (7.6) *are attained locally uniformly in $\lambda \in \mathbb{R}$.*

It is an easy consequence of (8.2d) stated below combined with a density argument (as in [IS2] for example) that the above operators $\mathcal{F}^\pm$, called *stationary wave operators*, map onto $\widetilde{\mathcal{H}}$. Whence stationary completeness is fulfilled, and in fact $\mathcal{F}^\pm H = M_\lambda \mathcal{F}^\pm$.

The adjoint of the operators $\mathcal{F}^\pm(\lambda)$ in Proposition 7.2, i.e. $\mathcal{F}^\pm(\lambda)^* \in \mathcal{L}(\Sigma, \mathcal{B}^*)$, are called *stationary wave matrices.*

In Section 9 we show that the stationary and the time-dependent wave operators coincide.

8. Scattering matrix and generalized eigenfunctions

Let us discuss other results similar to the stationary theories of [Sk, IS2].

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

$$\phi^\pm_\lambda[\xi](f,g) = \frac{\mathrm{e}^{\mp\mathrm{i}\pi d/4}}{\sqrt{2\pi}} J_\lambda^{1/2}(f,g)\,\mathrm{e}^{\pm\mathrm{i}\theta_\lambda(f,g)}\,\xi(\pm g) \tag{8.1}$$

These are for $\xi \in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1})$ (zeroth order) WKB-approximations of exact generalized eigenfunctions. In fact we can compute $\psi^\pm_\lambda[\xi] := (H-\lambda)\phi^\pm_\lambda[\xi] \in \mathcal{B}$ and therefore we can consider the exact solutions

$$\phi^\pm_{\lambda,\mathrm{ex}}[\xi] := \phi^\pm_\lambda[\xi] - R(\lambda \mp \mathrm{i}0)\psi^\pm_\lambda[\xi]; \quad \xi \in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}). \tag{8.2a}$$

As in [Sk, IS2] we can compute (now using Proposition 6.1)

$$\phi^\pm_{\lambda,\mathrm{ex}}[\xi] = \mathcal{F}^\pm(\lambda)^*\xi. \tag{8.2b}$$

For comparison we obtain from the Sommerfeld uniqueness result of [AIIS1] that

$$0 = \phi^\pm_\lambda[\xi] - R(\lambda \pm \mathrm{i}0)\psi^\pm_\lambda[\xi], \tag{8.2c}$$

leading to

$$\xi = \pm\mathrm{i}2\pi\mathcal{F}^\pm(\lambda)\psi^\pm_\lambda[\xi]; \quad \xi \in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}). \tag{8.2d}$$

The elements of the space

$$\mathcal{E}_\lambda := \{\phi \in \mathcal{B}^* \,|\, (H-\lambda)\phi = 0\}$$

may be called *minimum generalized eigenfunctions.* They are all of the form (8.2b), as stated in the following theorem. We introduce

$$\gamma^{\mathrm{si}}_{\lambda\pm} = p \mp \nabla\theta_\lambda = T_\lambda \gamma^{\mathrm{si}}_\pm T_{-\lambda} \quad \text{and} \quad \gamma^{\mathrm{si}}_{\|\lambda\pm} = \mathrm{Re}\,\big(\nabla\theta_\lambda \cdot \gamma^{\mathrm{si}}_{\lambda\pm}\big). \tag{8.3}$$

The sharp cutoff functions F_m (with $m \in \mathbb{N}_0$), also used below, are given as $F_m = 1_{\{2^m \le f < 2^{m+1}\}}$.

Proposition 8.1. *(i) For any one of $\xi_\pm\in\Sigma$ or $\phi\in\mathcal{E}_\lambda$ the two other quantities in $\{\xi_-,\xi_+,\phi\}$ uniquely exist such that*

$$\phi-\phi_\lambda^+[\xi_+]-\phi_\lambda^-[\xi_-]\in\mathcal{B}_0^*. \tag{8.4a}$$

(ii) The correspondences in (8.4a) *are given by the formulas*

$$\phi=\mathcal{F}^\pm(\lambda)^*\xi_\pm,\quad \xi_+=S(\lambda)\xi_-, \tag{8.4b}$$

$$\xi_\mp=\mp\tfrac12\tfrac{\sqrt{2\pi}}{\mathrm{e}^{\pm\mathrm{i}\pi d/4}}\,\Sigma\text{–}\lim_{\rho\to\infty}⨍_\rho\big(T_\lambda J^{1/2}\,\mathrm{e}^{\pm\mathrm{i}\theta}\tfrac{2r}{f^4}T_{-\lambda}\gamma^{\mathrm{si}}_{\|\lambda\pm}\phi\big)(f,\mp\cdot)\,\mathrm{d}f. \tag{8.4c}$$

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

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

$$\|\xi_\pm\|_\Sigma^2=\pi\lim_{m\to\infty}2^{-m}\|F_m\phi\|^2. \tag{8.4d}$$

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

Note for example that the combination of (8.2a), (8.2b) and (8.2d) leads to (8.4a) for any $\xi_-\in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ with $\xi_+=S(\lambda)\xi_-$ and $\phi=\mathcal{F}^-(\lambda)^*\xi_-$. By continuity the same assertion then holds for any $\xi_-\in\Sigma$. The other assertions follow by mimicking similarly [Sk, IS2].

It follows by (8.2a), (8.2b), (8.4a) and (8.4b) that $S(\lambda)\xi$, $\xi\in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$, is characterized by the formula

$$-R(\lambda+\mathrm{i}0)\psi_\lambda^-[\xi]-\phi_\lambda^+[S(\lambda)\xi]=\mathcal{F}^-(\lambda)^*\xi-\phi_\lambda^+[S(\lambda)\xi]-\phi_\lambda^-[\xi]\in\mathcal{B}_0^*, \tag{8.5}$$

leading in turn to the following formula for the scattering matrix.

Corollary 8.2. *For any any $\xi\in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$*

$$S(\lambda)\xi=-\tfrac{\sqrt{2\pi}}{\mathrm{e}^{-\mathrm{i}\pi d/4}}\,\Sigma\text{–}\lim_{\rho\to\infty}⨍_\rho\mathcal{R}^{\lambda+}_{\psi_\lambda^-,f}\,\mathrm{d}f. \tag{8.6}$$

Note that (8.6) is an alternative to the more general formula (8.4c) (with $\xi_+=S(\lambda)\xi$ and subscripts to the right chosen to be minus and with $\phi=\mathcal{F}^-(\lambda)^*\xi$).

Yet another formula for the scattering matrix is the following expression (shown by integration by parts and by using (8.6)). We assume $\xi,\xi'\in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ and note that then

$$\tfrac{1}{2\pi\mathrm{i}}\langle\xi',S(\lambda)\xi\rangle=\langle\psi_\lambda^+[\xi'],R(\lambda+\mathrm{i}0)\psi_\lambda^-[\xi]\rangle-\langle\phi_\lambda^+[\xi'],\psi_\lambda^-[\xi]\rangle. \tag{8.7}$$

There are other representations like (8.7) of the scattering matrix, which we will examine. The derivation uses in any case the Sommerfeld uniqueness result.

We also note that our choice of notation is consistent in the case $q=0$ in the following sense.

Corollary 8.3. *For $q=0$*

$$\mathcal{F}_0(\lambda)=\mathcal{F}^+(\lambda)=\mathcal{F}^-(\lambda).$$

In particular $S(\lambda)=I$ in this case.

Proof. We use the considerations of Section 2 (the stationary phase method) in combination with Proposition 8.1 (i) and (ii). □

9. Identificaton of wave operators

It follows from the Avron-Herbst formula [AH] that for any $\varphi \in L^2(\mathbb{R}^d)$

$$\big(\mathrm{e}^{-\mathrm{i}tH_0}\varphi\big)(x,y) \approx \mathrm{e}^{-\mathrm{i}\pi d/4} t^{-d/2} \mathrm{e}^{\mathrm{i}\{-t^3/6+tx+[(x-t^2/2)^2+y^2]/(2t)\}} \hat{\varphi}((x-t^2/2)/t, y/t)$$

as $|t| \to \infty$.

To identify wave operators it would be tempting, cf. [IS3], to try to compute directly the L^2-asymptotics of integrals of the form

$$\int \mathrm{e}^{-\mathrm{i}t\lambda} J_\lambda^{1/2} \mathrm{e}^{\mathrm{i}\theta_\lambda} \xi(y/f_\lambda) h(\lambda)\,\mathrm{d}\lambda,$$

where $\xi \in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ and $h \in C_{\mathrm{c}}^\infty(\mathbb{R})$ and compare with the right-hand side of the above formula, however this does not seem doable. We proceed differently introducing, cf. (2.1),

$$\begin{gathered}\big(\check{F}_0^\pm(\lambda)^*\xi\big)(x,y) = c\int \mathrm{d}\zeta\, \xi(\zeta) \int \mathrm{e}^{\mathrm{i}\theta_\lambda} \chi_\pm(\eta)\,\mathrm{d}\eta;\\ c = (2\pi)^{-\frac{d+1}{2}},\quad \theta_\lambda = y\cdot\zeta - \eta^3/6 + (x+\lambda-\zeta^2/2)\eta,\end{gathered} \tag{9.1}$$

in terms of the partition $\chi_+ + \chi_- = 1$, $\chi_+ = \chi(\cdot > 0)$ and $\chi_- = \chi^\perp(\cdot > 0)$. Using the formula

$$(H_0-\lambda)\mathrm{e}^{\mathrm{i}\theta_\lambda} = -(\partial_\eta\theta_\lambda)\mathrm{e}^{\mathrm{i}\theta_\lambda} = \mathrm{i}\partial_\eta \mathrm{e}^{\mathrm{i}\theta_\lambda}, \tag{9.2}$$

we can integrate by parts and get

$$(H_0-\lambda)\check{F}_0^\pm(\lambda)^*\xi = -\mathrm{i}c\int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta_\lambda}\chi_\pm'(\eta)\,\mathrm{d}\eta.$$

By the method of non-stationary phase this integral decays rapidly (here smoothness of ξ is needed, see Section 13).

Next by Sommerfeld's theorem the generalized eigenfunctions in the formula (8.2a) are given by

$$\phi^\pm_{\lambda,\mathrm{ex}}[\xi] = \check{F}_0^\pm(\lambda)^*\xi - R(\lambda\mp\mathrm{i}0)(H-\lambda)\check{F}_0^\pm(\lambda)^*\xi. \tag{9.3}$$

Now it should be easy to analyse the integral

$$I^+(t;x,y) := \int \mathrm{e}^{-\mathrm{i}t\lambda}\big(\check{F}_0^+(\lambda)^*\xi\big)h(\lambda)\,\mathrm{d}\lambda;\quad t>0.$$

In fact by the method of non-stationary phase

$$I^+(t;x,y) \approx \int \mathrm{e}^{-\mathrm{i}t\lambda}\big(\mathcal{F}_0(\lambda)^*\xi\big)h(\lambda)\,\mathrm{d}\lambda = \big(\mathrm{e}^{-\mathrm{i}tH_0}\varphi\big)(x,y) \text{ as } t\to+\infty, \tag{9.4}$$

with $\varphi\in\mathcal{H}$ fixed by $\mathcal{F}_0\varphi = h\otimes\xi\in\tilde{\mathcal{H}}$. This is what we want!

In the paper [II] completeness for Schrödinger operators is considered/proven from the stationary point of view. In our setting one would look at exact solutions to the Schrödinger equation of the form

$$\int \mathrm{e}^{-\mathrm{i}t\lambda}\phi^+_{\lambda,\mathrm{ex}}[\xi]h(\lambda)\,\mathrm{d}\lambda. \tag{9.5}$$

Using (9.3) and [II, Lemma 5.1] we obtain that this wave packet behaves like $\mathrm{e}^{-\mathrm{i}tH_0}\varphi$ as $t\to+\infty$ with the above L^2-function φ.

Given the above identification of wave packets we can show that the scattering matrix for the wave operators

$$W^\pm := \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}$$

agrees with the construction $S(\lambda)$ of (7.5). To see this we write the integral (9.5) as $\mathrm{e}^{-\mathrm{i}tH}\varphi'$ with $\varphi' = W^+\varphi$. On the other hand we can compute

$$\varphi' = \lim_{\epsilon\to 0_+} \epsilon \int_0^\infty \mathrm{e}^{-\epsilon t}\mathrm{e}^{\mathrm{i}tH} I^+(t)\,\mathrm{d}t = \lim_{\epsilon\to 0_+} \epsilon \int_0^\infty \int \cdots \,\mathrm{d}\lambda \mathrm{d}t$$

by first integrating with respect to t and then using the stationary phase method (cf. Section 2) and Proposition 6.1, see for example [IS3]. The resulting formula is

$$\mathcal{F}_0(W^+)^* = \mathcal{F}^+. \tag{9.6a}$$

Similarly we derive

$$\mathcal{F}_0(W^-)^* = \mathcal{F}^-. \tag{9.6b}$$

In particular the *scattering operator* $S = (W^+)^*W^-$ is represented as

$$\mathcal{F}_0 S \mathcal{F}_0^{-1} = \mathcal{F}^+\big(\mathcal{F}^-\big)^{-1} = \int_{\mathbb{R}} \oplus S(\lambda)\,\mathrm{d}\lambda.$$

We also learn from (9.6a) and (9.6b) that there exist the *asymptotic orthogonal momenta*

$$p_y^\pm = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} p_y \mathrm{e}^{-\mathrm{i}tH} = \big(\mathcal{F}^\pm\big)^*\Big(\int_{\mathbb{R}} \oplus M_\zeta\,\mathrm{d}\lambda\Big)\mathcal{F}^\pm;$$

here the limit is taken in the strong resolvent sense and M_ζ denotes multiplication by (the components of) ζ in $\Sigma = L^2\big(\mathbb{R}^{d-1}_\zeta\big)$. Whence formally the (Schwartz) kernel $S(\lambda)(\zeta,\zeta')$ of the scattering matrix is defined in terms of incoming and outgoing asymptotic orthogonal momenta.

10. Resolvent bounds

For $\varphi \in \mathcal{H}$ and an operator T on $\mathcal{H}$ the notation $\langle T\rangle_\varphi$ means $\langle\varphi, T\varphi\rangle$. The notation $\mathcal{L}(\mathcal{H})$ refers to the set of bounded operators on $\mathcal{H}$.

Lemma 10.1. *For any $m \in \mathbb{N}$ and $h \in C_c^\infty(\mathbb{R})$*

$$|x|^{m/2}\chi(x<0)h(H) \in \mathcal{L}(\mathcal{H}). \tag{10.1}$$

Proof. We insert $-x = H - p^2/2 - q$ in

$$\langle -x\rangle_\varphi; \quad \varphi = \chi(x<0)h(H)\psi,$$

use the formula

$$\langle H\rangle_\varphi = \operatorname{Re}\langle \chi(x<0)^2 H\rangle_{h(H)\psi} + \tfrac{1}{2}\|\chi(x<0)' h(H)\psi\|^2,$$

showing (10.1) for $m = 1$.

For general m we can proceed by induction in a similar fashion.

□

Let $A_m = \mathrm{Re}\,\big(\nabla f_m \cdot p\big)$ where $f_m(x,y) = \sqrt{\breve f(2x + 2\langle y\rangle_m)}$ for $m \in \mathbb{N}$; recall the notation $\langle y\rangle_m = (m^2 + |y|^2)^{1/2}$. Let $A_{m,M} = \tfrac12 \mathrm{Re}\,\big(\nabla f_m^2 \cdot p\big) = f_m^{1/2} A_m f_m^{1/2}$.

We compute

$$\mathrm{i}[H, 2A_{m,M}] = p \cdot \big(\nabla^2 f_m^2\big)p + \partial_x f_m^2 - \big(\nabla f_m^2\big) \cdot \nabla q - \tfrac14 \Delta^2 f_m^2,$$

which leads to

$$\begin{aligned} \mathrm{i}[H, 2A_{m,M}] &\geq 2 - \big(\nabla f_m^2\big) \cdot \nabla q - \tfrac14 \big(\Delta^2 f_m^2\big) - C_1 F(2x + 2\langle y\rangle_m \leq 2) \\ &\geq 2 - C_2 \tfrac{1}{\langle r\rangle} - C_3 m^{-3} - C_4 \tfrac{x-1}{m} F(x - 1 + m \leq 0). \end{aligned}$$

In combination with Lemma 10.1 we conclude that for any given energy the Mourre estimate holds for $A_{m,M}$ with a constant as close to 1 as wished provided we take m large enough.

For convenience we abbreviate $A_m = A$ and $f_m = f$ and note the following estimates locally uniformly in $\lambda \in \mathbb{R}$, cf. [GIS, AIIS1, AIIS2]. The parameter m may depends on λ (locally uniformly though) as well as on the parameters t, t' appearing in the estimates below (in our application we consider fixed parameters only).

$$f^{-s} R(\lambda \pm \mathrm{i}0) f^{-s} \in \mathcal{L}(\mathcal{H}); \quad s > 1/2. \tag{10.2a}$$

$$\begin{aligned} f^s \chi(\pm A < t) R(\lambda \pm \mathrm{i}0) f^{-1-s} &\in \mathcal{L}(\mathcal{H}); \\ &s > -1/2,\ t < 1. \end{aligned} \tag{10.2b}$$

$$\begin{aligned} f^s \chi(\pm A < t) R(\lambda \pm \mathrm{i}0) \chi(\pm A > t') f^s &\in \mathcal{L}(\mathcal{H}); \\ &s \in \mathbb{R},\ -1 < t < t' < 1. \end{aligned} \tag{10.2c}$$

$$\forall k \in \mathbb{N}: \quad f^{-s} R(\lambda \pm \mathrm{i}0)^k f^{-s} \in \mathcal{L}(\mathcal{H}); \quad s > 1/2 + k. \tag{10.3}$$

The latter estimate is a consequence of (10.2a)–(10.2c) and an algebraic argument, in fact there are 'microlocal bounds' in the spirit of (10.2a)–(10.2c) for powers also (obtained by the same argument). These estimates are useful for obtaining regularity of the S-matrix in the spectral parameter.

11. Classical mechanics bounds

We would like to associate to the operator $A = A_m$ of the previous section the symbol $a = \frac{\eta + \hat y_m \cdot \zeta}{\sqrt{2x + 2\langle y\rangle_m}}$; $\hat y_m = y/\langle y\rangle_m$ and m is a fixed large positive integer. Of course this requires as a minimum a localization to the region where $x + \langle y\rangle_m > 0$.

We consider for any such m and for any $\varepsilon \in (0,1)$

$$\mathcal{X}_\varepsilon^\pm = \mathcal{X}_{m,\varepsilon}^\pm := \Big\{ x + \langle y\rangle_m > 0, \quad \pm(\eta + \hat y_m \cdot \zeta) > -\varepsilon \sqrt{2x + 2\langle y\rangle_m} \Big\}; \quad \hat y_m = \tfrac{y}{\langle y\rangle_m}.$$

We claim that $\mathcal{X}_\varepsilon^+$ and $\mathcal{X}_\varepsilon^-$ are preserved by the free classical flow Θ (1.1), forward and backward, respectively. To see this we estimate on $\mathcal{X}_\varepsilon^\pm$,

$$\begin{aligned}2x(t)+2\langle y(t)\rangle_m &= t^2+2t(\eta+\hat{y}_m\cdot\zeta)+(2x+2\langle y\rangle_m)\\ &\quad+2\Big(\sqrt{2ty\cdot\zeta+\langle y\rangle_m^2+(t\zeta)^2}-t\hat{y}_m\cdot\zeta-\langle y\rangle_m\Big)\\ &\geq t^2-2|t|\varepsilon\sqrt{2x+2\langle y\rangle_m}+(2x+2\langle y\rangle_m)\\ &\geq(1-\varepsilon)\big(t^2+2x+2\langle y\rangle_m\big)\\ &>0;\quad \pm t\geq 0.\end{aligned}\tag{11.1}$$

Let on $\mathcal{X}_\varepsilon^+\cup\mathcal{X}_\varepsilon^+$

$$a:=\tfrac{\eta+\hat{y}_m\cdot\zeta}{\sqrt{2x+2\langle y\rangle_m}}.$$

By the free classical Mourre estimate

$$\tfrac{\mathrm{d}}{\mathrm{d}t}a(t)\geq\big(1-a(t)^2\big)/\sqrt{2x(t)+2\langle y(t)\rangle_m}\quad\text{on } \mathcal{X}_\varepsilon^\pm \text{ and for } \pm t\geq 0.$$

In particular, indeed if $\pm a(0)>-\varepsilon$, then $\pm a(t)>-\varepsilon$ for all $\pm t\geq 0$.

12. Transport equations

Let $n\in\mathbb{N}$ be a fixed big number. We construct $a_n^\pm=\sum_0^n b_k^\pm$ as follows (omitting superscripts). Let $b_0=1$ and $q_0=q$. Suppose that b_k and q_k, $0\leq k\leq n-1$, are constructed, then these quantities with k replaced by $k+1$ are given by

$$\begin{aligned}b_{k+1}&=\mathrm{i}\int_0^{\pm\infty}q_k(\Theta(t))\,\mathrm{d}t,\\ q_{k+1}&=qb_{k+1}-\tfrac12(\Delta_{(x,y)}b_{k+1}).\end{aligned}$$

The motivation for introducing this system comes from the fact that

$$\mathrm{i}\big(\partial_\eta+(\eta,\zeta)\cdot\nabla_{(x,y)}\big)b_{k+1}=q_k,\tag{12.1}$$

see Sections 13 and 14. Using the notation of Subsection 11 we are going to localize these constructions to $\mathcal{X}_\varepsilon^\pm=\mathcal{X}_{m,\varepsilon}^\pm$. Recall that $\mathcal{X}_\varepsilon^+$ and $\mathcal{X}_\varepsilon^-$ are preserved by the flow Θ, forward and backward, respectively.

Note the elementary bounds

$$\begin{aligned}\forall b>0:\quad \int_0^\infty(t^2+b^2)^{-s_1}t^{s_2}\,\mathrm{d}t&=C_{s_1,s_2}\,b^{s_2+1-2s_1};\\ s_2+1-2s_1&<0,\quad -1<s_2.\end{aligned}\tag{12.2}$$

It follows from (11.1), (12.2) and induction that for any $0\leq k\leq n$ and any $\varepsilon\in(0,1)$

$$\begin{aligned}\partial_{\eta,\zeta}^\alpha\,\partial_{x,y}^\beta b_k&=O\Big(\langle x+\langle y\rangle_m\rangle^{-(k\delta+|\beta|/2)}\Big),\\ \partial_{\eta,\zeta}^\alpha\,\partial_{x,y}^\beta q_k&=O\Big(\langle x+\langle y\rangle_m\rangle^{-(1/2+(k+1)\delta+|\beta|/2)}\Big);\quad (x,y,\eta,\zeta)\in\mathcal{X}_\varepsilon^\pm.\end{aligned}\tag{12.3}$$

In particular it follows that for $k=n$

$$\partial_{\eta,\zeta}^\alpha\,\partial_{x,y}^\beta q_n^\pm=O\Big(\langle x+\langle y\rangle_m\rangle^{-(1/2+(n+1)\delta+|\beta|/2)}\Big);\quad (x,y,\eta,\zeta)\in\mathcal{X}_\varepsilon^\pm.\tag{12.4}$$

Remark 12.1. The appearance of the expression $|\beta|/2$ to the right in (12.3) and (12.4) rather than just $|\beta|$ is a consequence of Condition 1.1. If we replace $|\beta|$ in (1.2) by $2|\beta|$ (which is doable for homogeneous potentials for example) then indeed the stronger versions of (12.3) and (12.4) are fulfilled.

13. Analysis of the scattering matrix

We shall use (9.1) and (12.4) and the quantity

$$\begin{aligned} F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi &:= c\int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta_\lambda} a^{\pm}_n\,\chi_1\,\chi_2\,\mathrm{d}\eta;\\ \chi_1 &= \chi(x+\langle y\rangle_m > 1),\quad \chi_2=\chi_2^{\pm}=\chi\big(\pm a > -\varepsilon\big),\\ c &= (2\pi)^{-\frac{d+1}{2}},\quad a=\tfrac{\eta+\hat{y}_m\cdot\zeta}{\sqrt{2x+2\langle y\rangle_m}}. \end{aligned} \tag{13.1}$$

We calculate

$$\begin{aligned} c^{-1}(H-\lambda)F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi &= \int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta_\lambda}\big(q^{\pm}_n\,\chi_1\,\chi_2 + r^{\pm}_n\big)\,\mathrm{d}\eta;\\ r^{\pm}_n &= -\mathrm{i}a^{\pm}_n\,(\chi_1\partial_\eta\chi_2 + (\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi_2))\\ &\quad -(\nabla_{(x,y)}a^{\pm}_n)\cdot\nabla_{(x,y)}(\chi_1\chi_2) - \tfrac{a^{\pm}_n}{2}\,\Delta_{(x,y)}(\chi_1\chi_2). \end{aligned} \tag{13.2}$$

We fix the parameters m,n 'large' (they are considered as 'free parameters') and fix as well $\varepsilon\in(0,1/2)$. Introduce then

$$\begin{aligned} \phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] &= F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi,\\ \psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] &= (H-\lambda)\phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi]. \end{aligned}$$

It is not important precisely which cutoffs χ_1 and χ_1 are used in (13.1).

We claim the following formula for the generalized eigenfunction of (8.2a)

$$\phi^{\pm}_{\lambda,\mathrm{ex}}[\xi] = \phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] - R(\lambda\mp \mathrm{i}0)\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi];\quad \xi\in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}), \tag{13.3a}$$

and also that

$$0 = \phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] - R(\lambda\pm \mathrm{i}0)\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi], \tag{13.3b}$$

leading to

$$\xi = \pm\mathrm{i}2\pi\mathcal{F}^{\pm}(\lambda)\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi];\quad \xi\in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}). \tag{13.3c}$$

Given (13.3c), the analogue of (8.7) reads

$$\tfrac{1}{2\pi\mathrm{i}}\langle\xi, S(\lambda)\xi'\rangle = \langle\psi^{+}_{\lambda,m,n,\varepsilon}[\xi], R(\lambda+\mathrm{i}0)\psi^{-}_{\lambda,m,n,\varepsilon}[\xi']\rangle - \langle\phi^{+}_{\lambda,m,n,\varepsilon}[\xi], \psi^{-}_{\lambda,m,n,\varepsilon}[\xi']\rangle. \tag{13.4}$$

Lemma 13.1. *For all $\xi\in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1})$ the functions $\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi]\in L^2_s$ for a big $s=s(n)>1$, and the formulas* (13.3a) *and* (13.3b) *are valid.*

Proof. Write

$$\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] = \psi^{\pm}_{\lambda,m,n,\varepsilon,1}[\xi] + \psi^{\pm}_{\lambda,m,n,\varepsilon,2}[\xi].$$

corresponding to the splitting

$$\int \mathrm{e}^{\mathrm{i}\theta_\lambda}\big(q^{\pm}_n\,\chi_1\,\chi_2 + r^{\pm}_n\big)\,\mathrm{d}\eta = \int \mathrm{e}^{\mathrm{i}\theta_\lambda}\,q^{\pm}_n\,\chi_1\,\chi_2\,\mathrm{d}\eta + \int \mathrm{e}^{\mathrm{i}\theta_\lambda}\,r^{\pm}_n\,\mathrm{d}\eta$$

in (13.2).

There are two way of integrating by parts. These are based on the formulas

$$\begin{aligned} e^{i\theta_\lambda} = \Big(1+\big(x+\lambda-\eta^2/2-\zeta^2/2\big)^2\Big)^{-1} \\ \big(1-i\big(x+\lambda-\eta^2/2-\zeta^2/2\big)\partial_\eta\big)e^{i\theta_\lambda}, \end{aligned} \tag{13.5a}$$

$$e^{i\theta_\lambda} = \Big(1+\big(y-\eta\zeta\big)^2\Big)^{-1}\big(1-i\big(y-\eta\zeta\big)\partial_\zeta\big)e^{i\theta_\lambda}. \tag{13.5b}$$

I: The contribution from $q_n^\pm$ takes the desired form since (12.4) effectively provides a factor $\langle x+\langle y\rangle_m\rangle^{-t_1}$ with $t_1>1$ large. We can use a part of this factor to obtain a high power of $\langle(\eta,\zeta)\rangle^{-1}$ as well as a high power of $\langle x\rangle^{-1}$ by integrating by parts using (13.5a) repeatedly. We can then use the decay in x (for $x<0$ only) and another part of the factor $\langle x+\langle y\rangle_m\rangle^{-t_1}$ to obtain a high power of $\langle y\rangle^{-1}$ as well. Altogether we obtain the desired factor $\langle x\rangle^{-s}\langle y\rangle^{-s}$ with $s=s(n)>1$ big for the contribution from $q_n^\pm$.
II: As for the contribution from $r_n^\pm$ we observe that terms for which the factor χ_1 is differentiated can be treated exactly as above.
III: It remains to consider the contributions from terms where at least one derivative falls on the factor χ_2. By definition any such term is supported in $\{x+\langle y\rangle_m>1,\ -\varepsilon/2\geq\pm a\geq-\varepsilon\}$. Since ξ is compactly supported the variable ζ is localized and we may for any such term consider

$$\tfrac{|\eta|}{\sqrt{x+\langle y\rangle_m}}\approx|a|\in[\varepsilon/2,\varepsilon]\quad\text{effectively}. \tag{13.6}$$

By the integration by parts in η we can obtain high inverse powers of of $\langle(\eta,\zeta)\rangle^{-1}$ and $\langle x\rangle^{-1}$ in any region of the form $\{x>1,\ |\eta^2/(2x)-1|>\epsilon\}$, $\epsilon>0$. Using then repeatedly integrating by parts in ζ (using (13.5b)) we obtain in this case a high power of $\langle y\rangle^{-1}$ as well. We can treat the region $\{x<2R\}$ for any $R>2$ in the same way.

In a region of the form $\{x>R,\ |\eta^2/(2x)-1|<2\epsilon\}$ for a small $\epsilon>0$ we consider separately the regions $M_1=\{\langle y\rangle_m/\langle\eta\rangle>C\}$ and $M_2=\{\langle y\rangle_m/\langle\eta\rangle<2C\}$, where $C>1$ is taken such that $\operatorname{supp}\xi\subset\{|\zeta|<C/2\}$. In the region M_1 we may obtain a high power of $\langle y\rangle^{-1}$ by repeated use of (13.5b) and therefore in turn a high power of $\langle\eta\rangle^{-1}$ as well. From integration by parts in η we then obtain a high power of $\langle x\rangle^{-1}$ also. It remains to treat the region M_2 and for that purpose we implement (13.6) by estimating

$$\varepsilon\geq|a|\geq\tfrac{|\eta|-C/2}{\sqrt{2x+4C\langle\eta\rangle}}\quad\text{on }\{x>R,\ -\varepsilon/2\geq\pm a\geq-\varepsilon\}\cap M_2.$$

But for $x>1$ large the estimate $\varepsilon^2(2x+4C\langle\eta\rangle)\geq(|\eta|-C/2)^2$ for $2C\leq|\eta|$ yields $\eta^2/(2x)\leq\epsilon'$ for any given $\epsilon'>\varepsilon^2$. Whence if we first fix $\epsilon<(1-\varepsilon^2)/2$, then for $R>2$ sufficiently large

$$\{x>R,\ |\eta^2/(2x)-1|<2\epsilon,\ -\varepsilon/2\geq\pm a\geq-\varepsilon\}\cap M_2=\emptyset.$$

This proofs the first assertion of the lemma.
IV: As for the second assertion, the difference of the left- and right-hand sides in (13.3a) is a purely outgoing or incoming generalizes eigenfunction in $\mathcal{B}^*$, respectively. Hence it must vanish. The argument for (13.3b) is similar.

□

Lety $\mathcal{E}'_{d-1}$ denote the space of compactly supported distributions on $\mathbb{R}^{d-1}$. Any $\xi \in \mathcal{E}'_{d-1}$ can be written as $\xi = \langle p_y \rangle^{2m'} \xi'$, where $m' \in \mathbb{N}$ and $\xi' \in C_c(\mathbb{R}^{d-1})$. Let

$$\chi_\varepsilon(t) = \chi(t < -\varepsilon/4)\chi(t > -2\varepsilon);\ t \in \mathbb{R}.$$

Lemma 13.2. *Let $m' \in \mathbb{N}$ and consider a fixed $\xi \in \mathcal{E}'_{d-1}$ on the above form $\xi = \langle p_y \rangle^{2m'} \xi'$. The functions $\psi^\pm_{\lambda,m,n,\varepsilon}[\xi]$ can for n sufficiently big, say $n \geq n'$ for some $n' = n'(m')$, be written as*

$$\psi^\pm_{\lambda,m,n,\varepsilon}[\xi] = f^{s'} \chi_\varepsilon(\pm A)\varphi_1^\pm + f^{-s}\varphi_2^\pm \text{ with } \varphi_1^\pm,\ \varphi_2^\pm \in \mathcal{H}, \tag{13.7}$$

and with $s' = s'(m')$ being independent of n and for a big $s = s(n) > 1$ (more precisely $s(n) \to \infty$ for $n \to \infty$).

Proof. **I**: The powers of p_y in the definition of the ξ can be moved to other factors of the ζ-integral thereby essentially producing an addition factor $\langle y \rangle^{2m'}$. By the proof of Lemma 13.1 the contribution from the term $q_n^\pm$ did not use integration by parts in the other direction, i.e. (13.5b) was not used. In fact a large negative power $\langle x \rangle^{-s} \langle y \rangle^{-s}$ with $s = s(n) > 1$ was produced. This can bound a factor $\langle y \rangle^{2m'}$, and we conclude that the contribution from the term $q_n^\pm$ takes the form of the second term on the right-hand side of (13.7).
II: As for the contribution from $r_n^\pm$ we observe that terms for which the factor χ_1 is differentiated offer a factor f^{-s} right away (in fact for any s) and we can also bound an additional factor $\langle y \rangle^{2m'}$, so again there is agreement with the form of the second term on the right-hand side of (13.7).
III: As for the contribution from the terms of $r_n^\pm$ for which the factor χ_2 is differentiated is more complicated. We can use part of Step III of the proof of Lemma 13.1, but obviously now (13.5b) is not useful. In a region of the form

$$\{x > 1,\ |\eta^2/(2x) - 1| > \epsilon\} \cup \{x < 4\}; \quad \epsilon > 0, \tag{13.8}$$

we obtain a high power of $\langle (x, \eta) \rangle^{-1}$ by the η-integration by parts. This power in combination with the growing factor $\langle y \rangle^{s'}$, $s' = 2m' + d$, can be bounded by $f^{s'}$ on $\operatorname{supp} \chi_1$. This leads us to writing the contribution from any term given by first localizing to (13.8) as $f^{s'}\varphi^\pm$, and therefore in turn as

$$f^{s'}\varphi^\pm = f^{2m'}\chi_\varepsilon(\pm A)\varphi^\pm + f^{2m'}\big(1 - \chi_\varepsilon(\pm A)\big)\varphi^\pm. \tag{13.9}$$

The first term agrees with the first term on the right-hand side of (13.7), so it remains for show that the second term agrees with the second term on the right-hand side of (13.7). For the latter task we observe that if we replace A by its Weyl symbol $a_{\mathrm{w}} = \frac{\eta + \hat{y}_m \cdot \zeta}{f}$ then since $a_{\mathrm{w}} = a$ for $x + \langle y \rangle \geq 1$ obviously

$$\big(1 - \chi_\varepsilon(\pm a_{\mathrm{w}})\big)\chi'\big(\pm a > -\varepsilon\big) = O(f^{-s-2m'}). \tag{13.10}$$

Note that the prime for the second factor denotes the derivative of the function (we are discussing the case where χ_2 is differentiated). To leading order we may move the factor $1 - \chi_\varepsilon(\pm A)$ inside the integrals pass the exponential $\mathrm{e}^{\mathrm{i}\theta_\lambda}$ thereby indeed replacing the operator by it symbol and (13.10) would apply. However there are 'errors' since there is some (x, y)-dependence in our constructed symbols. We will proceed slightly differently.

Pick $\chi \in C_{\mathrm{c}}^\infty(\mathbb{R})$ with $\chi(t) = 1$ on $\operatorname{supp} \chi'\big(\cdot > -\varepsilon\big)$ but $\chi(t) = 0$ on $\operatorname{supp}(1 - \chi_\varepsilon)$. Take an almost analytic extension $\tilde\chi \in C^\infty(\mathbb{C})$ of χ, and set

$$\mathrm{d}\mu_\chi(z) = \pi^{-1}(\bar\partial\tilde\chi)(z)\,\mathrm{d}u\mathrm{d}v; \quad z = u + \mathrm{i}v.$$

Then

$$\chi(t) = \int_{\mathbb{C}} (t-z)^{-1}\,\mathrm{d}\mu_\chi(z); \quad t \in \mathbb{R}.$$

In particular

$$\begin{aligned}&\big(1 - \chi_\varepsilon(\pm A)\big)\chi_1\chi'\big(\pm a > -\varepsilon\big)\\ &= \big(1 - \chi_\varepsilon(\pm A)\big)\big(\chi(\pm a) - \chi(\pm A)\big)\chi_1\chi'\big(\pm a > -\varepsilon\big)\\ &= \pm\int_{\mathbb{C}} \big(1 - \chi_\varepsilon(\pm A)\big)(\pm A - z)^{-1}\big(A - a\big)\chi_1(\cdot)(\pm a - z)^{-1}\chi'\big(\pm a > -\varepsilon\big)\,\mathrm{d}\mu_\chi(z).\end{aligned}$$

We insert this formula in the expression for $\varphi^\pm$ for those terms with a single derivative of χ_2 (the one with a double derivative can be treated similarly). Then we move the middle factor $(A-a)\chi_1$ to the far right including passing the exponential $\mathrm{e}^{\mathrm{i}\theta_\lambda}$. This produces altogether an extra factor f^{-1} since all derivatives are bounded except when passing through the exponential where cancellation occur. Repeating this procedure we gain a large power of f^{-1}, say $f^{-s-2m'}$, which is exactly what is needed for showing that the second term of (13.9) agrees with the second term on the right-hand side of (13.7).

IV: For a localized term in the region of the form $\{x > 2,\ |\eta^2/(2x) - 1| < 2\epsilon\}$ for a small $\epsilon > 0$ (actually any $\epsilon \in (0, 1/2)$ suffices), which remains to be treated, we can use the same argument as above. The only difference is that the η-integration by parts does not suffice. So to get a weight like $\langle(x,\eta)\rangle^{-2}$ to insure the Hilbert space bound we first bound an inverse power of $\langle x\rangle^{-1}$ by the same power of f. Then the η-integration by parts yields an inverse power of $\langle\eta\rangle^{-1}$ also. In this way we get a weight like $\langle(x,\eta)\rangle^{-2}$ at the price of an extra power of f, and we can indeed mimic Step III.

□

Corollary 13.3. *For all $\xi \in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ the vector $S(\lambda)\xi \in C^\infty(\mathbb{R}^{d-1})$.*

Proof. Let $\xi_+, \xi_- \in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ be given and pick n large.

I: We look at the first term $\langle\psi^+_{\lambda,m,n,\varepsilon}[\xi_+], R(\lambda + \mathrm{i}0)\psi^-_{\lambda,m,n,\varepsilon}[\xi_-]\rangle$ of (13.4). We use representations of $\psi^\pm_{\lambda,m,n,\varepsilon}[\xi_\pm]$ that do not use the regularity of $\xi_\pm$, more precisely we write $\xi_\pm = \langle p_y\rangle^{2m'}\xi'_\pm$ depending on an arbitrary m' as considered in Lemma 13.2 and use then Lemma 13.2 in combination with (10.2a)–(10.2c).

We conclude that the contribution from $S(\lambda)\xi_-$ from the first term of (13.4) is smooth up some high order (depending on n).

II: Obviously the good decay of $\psi^-_{\lambda,m,n,\varepsilon}[\xi_-]$ in (x,y) from Lemma 13.1 and repeated application of (13.5a) yield that also the second term of (13.4) contributes by a arbitrarily smooth term to $S(\lambda)\xi_-$. The degree of smoothness depends on n.

III: Since $S(\lambda)\xi_-$ is independent of n, indeed $S(\lambda)\xi_-$ is smooth. □

We note that the smoothness of $\xi_-(\in C_{\mathrm{c}}^\infty(\mathbb{R}^{d-1})$ was not used in Step I in the above proof, in fact for this part we could have assumed $\xi_- \in \mathcal{E}'_{d-1}$ only and concluded that the corresponding contribution to $S(\lambda)\xi_- \in C^{m'}(\mathbb{R}^{d-1})$ for an arbitrarily given $m' \in \mathbb{N}$, although this requires first taking n large enough. This means that the first term of (13.4) is a *smoothing operator*, and the local singularities of the kernel $S(\lambda)(\zeta,\zeta')$ up to any given order must be sitting in the second term of (13.4). This term is an explicit oscillatory integral. We have

$$\begin{aligned}&-2\pi\mathrm{i}\langle\phi^+_{\lambda,m,n,\varepsilon}[\xi],\psi^-_{\lambda,m,n,\varepsilon}[\xi']\rangle\\&=\tfrac{-\mathrm{i}}{(2\pi)^d}\iint\mathrm{d}x\mathrm{d}y\int\mathrm{d}\zeta\overline{\xi(\zeta)}\int\mathrm{e}^{-\mathrm{i}\theta_\lambda}\overline{a^+_n}\chi_1\chi_2^+\mathrm{d}\eta\int\mathrm{d}\zeta'\xi'(\zeta')\int\mathrm{e}^{\mathrm{i}\theta'_\lambda}\big(q^-_n\chi_1\chi_2^-+r^-_n\big)\mathrm{d}\eta',\end{aligned}$$

where the first exponential $\mathrm{e}^{-\mathrm{i}\theta_\lambda}$ is considered as a funtion of (η,ζ) (and of (x,y) as well) while the second exponential $\mathrm{e}^{\mathrm{i}\theta'_\lambda}=\mathrm{e}^{\mathrm{i}\theta_\lambda}$ is considered as a function of (η',ζ') (the prime superscipt for θ'_λ does not mean differentiation!). Of course the symbols q^-_n, χ^-_2 and r^-_n also depend of the variables (η',ζ'), while a^+ and χ^+_2 rather depend on (η,ζ). We write the right-hand side as

$$\iint\overline{\xi(\zeta)}\breve S(\zeta,\zeta')\xi'(\zeta')\,\mathrm{d}\zeta\mathrm{d}\zeta'$$

and then in turn $\breve S$ as a pseudodifferential operator

$$\begin{aligned}\breve S(\zeta,\zeta')&=(2\pi)^{1-d}\int\mathrm{e}^{\mathrm{i}(\zeta-\zeta')\cdot y}\,\breve s(\zeta,\zeta',-y)\,\mathrm{d}y;\\ \breve s(\zeta,\zeta',y)&=(2\pi\mathrm{i})^{-1}\int\mathrm{d}x\int\mathrm{e}^{\mathrm{i}\left(\eta^3/6-(x+\lambda-\zeta^2/2)\eta\right)}\overline{a^+_n}\chi_1\chi_2^+\,\mathrm{d}\eta\\&\qquad\int\mathrm{e}^{\mathrm{i}\left(-\eta'^3/6+(x+\lambda-\zeta'^2/2)\eta'\right)}\left(q^-_n\chi_1\chi_2^-+r^-_n\right)\mathrm{d}\eta'.\end{aligned}$$

The contribution from q^-_n is a smoothing operator, since we can use the bound $\langle x+\langle y\rangle_m\rangle^{-s}$, s large, and η- and η'-integration by parts to obtain a bound of the form

$$\forall|\alpha|\le m':\quad\partial^\alpha_{(\zeta,\zeta',y)}\breve s(\zeta,\zeta',y)=O(\langle(\zeta,\zeta',y)\rangle^{-m'})\text{ for a large }m'.$$

Using again the non-stationary phase argument we obtain similarly, computing up a smoothing operator, that only $\{x>R,\,\eta\approx\eta'\}$ with $R>1$ big matters. Whence we are left with

$$(2\pi\mathrm{i})^{-1}\int_R^\infty\mathrm{d}x\int\mathrm{e}^{\mathrm{i}\left(\eta^3/6-(x+\lambda-\zeta^2/2)\eta\right)}\overline{a^+_n}\,\mathrm{d}\eta\int\mathrm{e}^{\mathrm{i}\left(-\eta'^3/6+(x+\lambda-\zeta'^2/2)\eta'\right)}r^-_n\,\mathrm{d}\eta'.\quad(13.11)$$

We can use (13.11), the formula

$$\mathrm{e}^{\mathrm{i}(\zeta-\zeta')\cdot y}=-\mathrm{i}\tfrac{\zeta-\zeta'}{(\zeta-\zeta')^2}\cdot\partial_y\mathrm{e}^{\mathrm{i}(\zeta-\zeta')\cdot y};\quad\zeta\neq\zeta',\quad(13.12)$$

and integrate by parts repeatedly obtaining an arbitrary degree of smoothness away from the diagonal. Note that each integration by parts produces effectively at least a factor $\langle y\rangle^{-1/2}$. Whence we have the following result.

Theorem 13.4. *The kernel $S(\lambda)(\zeta,\zeta')$ is smooth away from the diagonal $\{\zeta=\zeta'\}$.*

14. Analysis of the kernel of the scattering matrix at the diagonal

We will derive yet another representation of the scattering matrix. This will be more suitable for possibly computing singularities at the diagonal of its kernel. We do a partial analysis of the latter problem in Subsection 14.

14.1. **Subtracting the δ-singularity at the diagonal.** We shall use notation of (9.1), (12.4) and the quantity

$$\begin{aligned} F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi &:= c\int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta_\lambda}\,\chi_1(a^{\pm}_n\chi_2+\chi_2^{\perp})\,\mathrm{d}\eta;\\ &\chi_1=\chi(x+\langle y\rangle>1),\\ &\chi_2=\chi_2^{\pm}=\chi\big(\pm a>-\varepsilon\big),\\ &\chi_2^{\perp}=\chi_2^{\perp\pm}=\chi^{\perp}\big(\pm a>-\varepsilon\big);\quad a=\tfrac{\eta+\hat y_m\cdot\zeta}{\sqrt{2x+2\langle y\rangle_m}}. \end{aligned}\tag{14.1}$$

Note in comparison with Section 13 the appearence of the factor $\chi_2^{\perp}$. As in Section 13 we fix the parameters m,n in (12.4) 'large', and we fix as well (any) $\varepsilon\in(0,1/2)$. Likewise it is not important precisely which cutoffs χ_1 and χ_2 are used in (14.1).

We calculate

$$\begin{aligned} c^{-1}(H-\lambda)F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi &= \int \mathrm{d}\zeta\,\xi(\zeta)\int \mathrm{e}^{\mathrm{i}\theta_\lambda}\big(q^{\pm}_n\,\chi_1\,\chi_2+r^{\pm}_n+r^{\perp\pm}_n\big)\,\mathrm{d}\eta;\\ r^{\pm}_n &= -\mathrm{i}a^{\pm}_n\,\big(\chi_1\partial_\eta\chi_2+(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi_2)\big)\\ &\quad-(\nabla_{(x,y)}a^{\pm}_n)\cdot\nabla_{(x,y)}(\chi_1\chi_2)-\tfrac{a^{\pm}_n}{2}\,\Delta_{(x,y)}(\chi_1\chi_2),\\ r^{\perp\pm}_n &= -\mathrm{i}\,\big(\chi_1\partial_\eta\chi_2^{\perp}+(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi_2^{\perp})\big)-\tfrac12\,\Delta_{(x,y)}(\chi_1\chi_2^{\perp})+q\chi_1\chi_2^{\perp}. \end{aligned}\tag{14.2}$$

These formulas simplify in terms of the notation $\breve a^{\pm}_n=\sum_1^n b^{\pm}_k$. Indeed $a^{\pm}_n\chi_2+\chi_2^{\perp}=1+\breve a^{\pm}_n$, and $\breve r^{\pm}_n:=r^{\pm}_n+r^{\perp\pm}_n$ takes the form

$$\begin{aligned} \breve r^{\pm}_n &= -\mathrm{i}\breve a^{\pm}_n\,\big(\chi_1\partial_\eta\chi_2+(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi_2)\big)\\ &\quad-(\nabla_{(x,y)}\breve a^{\pm}_n)\cdot\nabla_{(x,y)}(\chi_1\chi_2)-\tfrac{\breve a^{\pm}_n}{2}\,\Delta_{(x,y)}(\chi_1\chi_2)\\ &\quad-\mathrm{i}\,(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1)-\tfrac12\,\Delta_{(x,y)}(\chi_1)+q\chi_1\chi_2^{\perp}. \end{aligned}$$

Now we introduce

$$\begin{aligned} \phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] &= F^{\pm}_{m,n,\varepsilon}(\lambda)^*\xi,\\ \psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi] &= (H-\lambda)\phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi], \end{aligned}$$

and note the following formula for the generalized eigenfunction of (8.2a),

$$\phi^{\pm}_{\lambda,\mathrm{ex}}[\xi]=\phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi]-R(\lambda\mp\mathrm{i}0)\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi];\quad \xi\in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}).\tag{14.3a}$$

Also we note, cf. Theorem 8.1, that

$$\mathcal{F}^{\mp}(\lambda)^*\xi=\phi^{\mp}_{\lambda,\mathrm{ex}}[\xi]=\phi^{\pm}_{\lambda,m,n,\varepsilon}[\xi]-R(\lambda\pm\mathrm{i}0)\psi^{\pm}_{\lambda,m,n,\varepsilon}[\xi],\tag{14.3b}$$

leading to

$$\xi-S(\lambda)^{-1}\xi=-\mathrm{i}2\pi\mathcal{F}^{-}(\lambda)\psi^{-}_{\lambda,m,n,\varepsilon}[\xi];\quad \xi\in C^\infty_{\mathrm{c}}(\mathbb{R}^{d-1}).\tag{14.3c}$$

Now, the analogue of (8.7) reads

$$\begin{aligned} &\tfrac{1}{2\pi\mathrm{i}}\langle\xi,T(\lambda)\xi'\rangle\\ &\quad=\langle\psi^{+}_{\lambda,m,n,\varepsilon}[\xi],R(\lambda+\mathrm{i}0)\psi^{-}_{\lambda,m,n,\varepsilon}[\xi']\rangle-\langle\phi^{+}_{\lambda,m,n,\varepsilon}[\xi],\psi^{-}_{\lambda,m,n,\varepsilon}[\xi']\rangle;\\ &T(\lambda):=S(\lambda)-I. \end{aligned}\tag{14.4}$$

14.2. **Analysis of the kernel of $T(\lambda)$ at the diagonal.** Most likely the operator $T(\lambda)$ is a pseudodifferential operator of *order* $-\delta$, meaning that its kernel can be written as

$$T(\zeta,\zeta') = (2\pi)^{1-d}\int \mathrm{e}^{\mathrm{i}(\zeta-\zeta')\cdot y}\, t(\zeta,y)\,\mathrm{d}y,$$

where locally uniformly in ζ (possibly including λ as well)

$$\partial_\zeta^\alpha\,\partial_y^\beta t = O\big(\langle y\rangle^{-(\delta+|\beta|/2)}\big). \tag{14.5}$$

We shall not here prove this assertion but at least give some evidence. (The appearance of the expression $|\beta|/2$ to the right in (14.5) is an artifact of (1.2) of Condition 1.1 and can under a more restrictive condition be relaxed, see Remark 12.1.) First we use (14.4). The first term (with m,n chosen freely) is a smoothing term (to any order depending on n), cf. Step I of the proof of Corollary 13.3.

As for the second term we write

$$\begin{aligned}&-2\pi\mathrm{i}\langle\phi^+_{\lambda,m,n,\varepsilon}[\xi],\psi^-_{\lambda,m,n,\varepsilon}[\xi']\rangle = \tfrac{-\mathrm{i}}{(2\pi)^d}\iint \mathrm{d}x\mathrm{d}y\int \mathrm{d}\zeta\,\overline{\xi(\zeta)}\\ &\int \mathrm{e}^{-\mathrm{i}\theta_\lambda}\chi_1\big(1+\overline{\check a^+_n}\big)\mathrm{d}\eta\int \mathrm{d}\zeta'\xi'(\zeta')\int \mathrm{e}^{\mathrm{i}\theta'_\lambda}\big(q^-_n\,\chi_1\,\chi^-_2+\check r^-_n\big)\mathrm{d}\eta',\end{aligned}$$

The contribution from the term $q^-_n\chi_1\,\chi^-_2$ is a smoothing operator, since we can use the bound $\langle x+\langle y\rangle_m\rangle^{-s}$, s large, and η- and η'-integration by parts to obtain a bound of the form

$$\forall|\alpha|\le m':\quad \partial^\alpha_{(\zeta,\zeta',y)}\check t(\zeta,\zeta',y) = O(\langle(\zeta,\zeta',y)\rangle^{-m'}) \text{ for a large } m'$$

for the corresponding symbol $\check t$.

Let us look at the leading order term of the remaining part. It is given by

$$\begin{aligned}&-2\pi\mathrm{i}\langle\phi^+_{\lambda,n,\varepsilon}[\xi],\psi^-_{\lambda,n,\varepsilon}[\xi']\rangle \approx \tfrac{-\mathrm{i}}{(2\pi)^d}\iint \mathrm{d}x\mathrm{d}y\int \mathrm{d}\zeta\,\overline{\xi(\zeta)}\int \mathrm{e}^{-\mathrm{i}\theta_\lambda}\chi_1\mathrm{d}\eta\int \mathrm{d}\zeta'\xi'(\zeta')\\ &\int \mathrm{e}^{\mathrm{i}\theta'_\lambda}\Big(-\mathrm{i}b^-_1\,\big(\chi_1\partial_\eta\chi^-_2+(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi^-_2)\big)+q\chi_1\chi^{\perp-}_2\Big)\mathrm{d}\eta'.\end{aligned}$$

Due to (12.1) in fact

$$\begin{aligned}&-\mathrm{i}b^-_1\,\big(\chi_1\partial_\eta\chi^-_2+(\eta,\zeta)\cdot\nabla_{(x,y)}(\chi_1\chi^-_2)\big)+q\chi_1\chi^{\perp-}_2\\ &\approx q\chi_1-\mathrm{i}\big(\partial_\eta+(\eta,\zeta)\cdot\nabla_{(x,y)}\big)\big(b^-_1\chi_1\chi^-_2\big)\big).\end{aligned}$$

Now the second term does not contribute to leading order and for the first term we get the expected 'Born term', which simplifies by using the stationary phase method. We end up with an explicit leading order term (given in terms of any big $R>1$ making $\eta=\sqrt{2x+2\lambda-\zeta^2}$ well-defined),

$$-2\mathrm{i}\int_R^\infty \tfrac{q(x,-y)}{\sqrt{2x+2\lambda-\zeta^2}}\,\mathrm{d}x \approx -2\mathrm{i}\int_R^\infty \tfrac{q(x,-y)}{\sqrt{2x}}\,\mathrm{d}x =: t_{\mathrm{psym}}(\zeta,y). \tag{14.6}$$

This suggests the following result (most likely within reach by a stationary phase method), which however will be left unproven in this paper.

Proposition 14.1. *The principal symbol of $T(\lambda)$ is given by*

$$t_{\mathrm{psym}}(\zeta,y) = -2\mathrm{i}\int_R^\infty \tfrac{q(x,-y)}{\sqrt{2x}}\,\mathrm{d}x$$

in the sense that the difference $t - t_{\mathrm{psym}}$ has order $-\delta - 1/2$ locally uniformly in ζ and λ.

We are interested in analyzing the singularity of the kernel of $T(\lambda)$ at the diagonal for slowly decaying potentials. The above unproven assertion would be a convenient tool for this issue, cf. [IK, Lemma 4.1]. However we can actually extract the leading singularity with less knowledge, i.e. by using a more standard stationary phase method. The leading order singularity is given in terms of t_{psym} as indicated above. We skip the details of proof. The corresponding operator T_{psym} has order $-\delta$ and in general no better, see the computation below.

For a homogeneous potential $q \approx \kappa r^{-\alpha}$, $1/2 < \alpha < d - 1/2$, we can compute in terms of (12.2)

$$\int_R^\infty \tfrac{q(x,-y)}{\sqrt{2x}}\,\mathrm{d}x \approx \int_0^\infty \tfrac{q(x,-y)}{\sqrt{2x}}\,\mathrm{d}x \approx \kappa c_1 |y|^{\frac{1}{2}-\alpha} \text{ for } |y| \to \infty,$$

with

$$c_1 = 2^{-3/2} \int_0^\infty (t+1)^{-\alpha/2} t^{-3/4}\,\mathrm{d}t = 2^{-3/2}\Gamma(1/4)\Gamma(\alpha/2 - 1/4)/\Gamma(\alpha/2),$$

cf. [AS, (13.2.5), (13.5.10)]. The Fourier transform of $|y|^{\frac{1}{2}-\alpha}$ is known. Whence in this case the leading order singularity of the kernel of $T(\lambda)$ is given by

$$\begin{aligned} T(\zeta,\zeta') &\approx \kappa c_2 |\zeta - \zeta|^{\frac{1}{2}+\alpha-d}; \\ c_2 =& c_1 (2\pi)^{1-d}(-2\mathrm{i})(2\pi)^{(d-1)/2} 2^{d/2-\alpha} \Gamma((d-1/2-\alpha)/2))/\Gamma((\alpha-1/2)/2)) \\ =& -\mathrm{i}(2\pi)^{(1-d)/2} 2^{(d-1)/2-\alpha}\Gamma(1/4)\Gamma(d/2-1/4-\alpha/2)/\Gamma(\alpha/2) \end{aligned}$$

For the Coulomb potential $q = \kappa r^{-1}$ with $d \geq 3$ the order of the symbol t_{psym} is $-1/2$, and the singularity (at the diagonal) is the form

$$T(\zeta,\zeta') \approx \kappa c_2 |\zeta - \zeta'|^{3/2-d}. \tag{14.7}$$

We more or less summarize this result as follows, skipping details of proof.

Corollary 14.2. *For $q = \kappa r^{-1}$ and $d \geq 3$ the kernel*

$$S(\lambda)(\zeta,\zeta') - \delta(\zeta,\zeta') = \kappa c_2 |\zeta - \zeta'|^{3/2-d} + O\big(|\zeta - \zeta'|^{2-d}\big)$$

at the diagonal, locally uniformly in ζ, ζ' and λ.

For $q = \kappa r^{-1}$ and $d = 3$, we can use that

$$\Gamma(1/4)\Gamma(d/2 - 1/4 - \alpha/2) = \sqrt{2}\pi \quad \text{and} \quad \Gamma(\alpha/2) = \sqrt{\pi},$$

yielding in that case $c_2 = -\mathrm{i}(2\pi)^{-1/2}$ and $T(\zeta,\zeta') \approx -\mathrm{i}\kappa(2\pi)^{-1/2}|\zeta - \zeta'|^{-3/2}$. This result agrees with [KK1]. In that paper the exact asymptotics at the diagonal is derived by a different method relying on explicit calculations of integrals involving powers of the potential and the free Stark resolvent kernel. This method seems restricted to homogeneous potentials. In our approach (which is valid for a wider class of potentials) the singularities are 'sitting' in an explicit oscillatory integral, which as indicated above in principle is 'computable'.

For a partial decomposition of the kernel of $S(\lambda)$ for the Coulomb potential, see [KK2], although this paper does not examine the singularity problem.

References

[Ad1] T. Adachi, *Asymptotic observables for N-body Stark Hamiltonians*, Ann. Inst. H. Poincaré **68** no. 3, (1998), 247–283.

[Ad2] T. Adachi, *Propagation estimates for N-body Stark Hamiltonians*, Ann. Inst. H. Poincaré **62** no. 4, (1995), 409–428.

[AH] J. E. Avron, I. W. Herbst, *Spectral and scattering theory of Schrödinger operators related to the Stark effect*. Comm. Math. Phys. **52** no. 3 (1977), 239–254.

[AIIS1] T. Adachi, K. Itakura, K. Ito, E. Skibsted, *Spectral theory for the Stark Hamiltonian*, preprint May 2019.

[AIIS2] T. Adachi, K. Itakura, K. Ito, E. Skibsted, *New methods in spectral theory of N-body Schrödinger operators*, arXiv:1804.07874, submitted.

[AS] M. Abramowitz, I.A. Stegun, *Handbook of mathematical functions*, Dover Publications, New York, 1972.

[GIS] C. Gérard, H. Isozaki and E. Skibsted, *N-body resolvent estimates*, J. Math. Soc. Japan **48** no. 1 (1996), 135–160.

[He] I. W. Herbst, *Unitary equivalence of stark Hamiltonians*. Math. Z. **155** (1977), no. 1, 55–70.

[Hö] L. Hörmander, *The Analysis of Linear Partial Differential Operators. I*, Springer, Berlin, 1990.

[II] T. Ikebe, H. Isozaki, *A stationary approach to the existence and completeness of long-range operators*, Integral equations and operator theory **5** (1982), 18–49.

[IK] H. Isozaki, H. Kitada *Scatttering matrices for two-body Schrödinger operators*, Scientific papers of the College of Arts and Sciences, Tokyo Univ. **35** (1985), 81–107.

[IS1] K. Ito, E. Skibsted, *Spectral theory on manifolds*, arXiv:1602.07488, submitted.

[IS2] K. Ito, E. Skibsted, *Stationary scattering theory on manifolds*, arXiv:1602.07487, submitted.

[IS3] K. Ito, E. Skibsted, *Time-dependent scattering theory on manifolds*, arXiv:1905.02942, submitted.

[KK1] A. Kvitsinsky, V. Kostrykin, *Potential scattering in homogeneous external electrostatic field*, Teoret. Mat. Fiz. **75** no. 3 (1988), 416–430; translation in Theoret. and Math. Phys.75 (1988), no. 3, 619–629.

[KK2] A. Kvitsinsky, V. Kostrykin, *S-matrix and Jost functions of Schrödinger Hamiltonian related to the Stark effect*, J. Math. Phys. **31** (1990), 2731–2736.

[Sk] E. Skibsted, *Renormalized two-body low-energy scattering*, J. d'Analyse Math. **122** (2014), 25–68.

[St] E.M. Stein, *Harmonic analysis: real-variable methods, orthogonality and oscillatory integrals*, Princeton University Press, Princeton New Jersey 1993.

[Ti] E.C. Titchmarsh, *Eigenfunction expansions associated with second-order differential equations. Vol. 2*. Oxford, at the Clarendon Press 1958.

[Ya1] K. Yajima, *Spectral and scattering theory for Schrödinger operators with Stark effect*. J. Fac. Sci. Univ. Tokyo Sect. IA Math. **26** no. 3 (1979), 377–390.

[Ya2] K. Yajima, *Spectral and scattering theory for Schrödinger operators with Stark effect, II*. J. Fac. Sci. Univ. Tokyo Sect. IA Math. **28** no. 1 (1981), 1–15.

[Wh] D. A. W. White, *The Stark effect and long range scattering in two Hilbert spaces*. Indiana Univ. Math. J. **39** (1990), no. 2, 517–546.

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