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CLASSICAL SCATTERING AT LOW ENERGIES

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ABSTRACT. For a class of negative slowly decaying potentials, including the attractive Coulombic one, we study the classical scattering theory in the low-energy regime. We construct a (continuous) family of classical orbits parameterized by initial position $x \in \mathbb{R}^d$, final direction $\omega \in S^{d-1}$ of escape (to infinity), and the energy $\lambda \geqslant 0$, yielding a complete classification of the set of outgoing scattering orbits. The construction is given in the outgoing part of phase-space (a similar construction may be done in the incoming part of phase-space). For fixed $\omega \in S^{d-1}$ and $\lambda \geqslant 0$ the collection of constructed orbits constitutes a smooth manifold that we show is Lagrangian. The family of those Lagrangians can be used to study the quantum mechanical scattering theory in the low-energy regime for the class of potentials considered here. We devote this study to a subsequent paper [7].

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1. INTRODUCTION

In this paper we shall address a classical low-energy scattering problem for a two-body system. In a subsequent paper [7] we shall combine the results of this paper and some of [8] in a study of the quantum mechanical low-energy scattering theory within the same class of potentials; this will include construction of wave operators, corresponding generalized eigenfunctions and S-matrices and the establishment of regularity/asymptotics of these quantities at the threshold energy $\lambda = 0$ (for a review see [6]). A related programme has been carried out for positive energies for a wide class of potentials, see [14, 15, 22, 18]; for this case the study is based on a relatively simple

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structure of a class of outgoing (or incoming) classical orbits used in the construction of certain Fourier integral operators.

However there are severe difficulties if one tries to incorporate the low energy regime $\lambda \approx 0$ in this approach. Some of the difficulties already show up at the classical level, and therefore one needs additional conditions on the potential from the very outset of the analysis. In our opinion these "additional conditions" naturally count the virial condition and spherical symmetry of the leading term of the potential (both conditions to be imposed at infinity only).

To simplify the presentation, let us in this introduction assume that the potential takes the form (with $x \in \mathbb{R}^d$ for $d \geqslant 2$)

$$V(x) = -\gamma |x|^{-\mu} + O(|x|^{-\mu-\epsilon}), \tag{1.1}$$

where $\mu \in (0,2)$ and $\gamma, \epsilon > 0$. For derivatives, assume $\partial^\beta \{V(x) + \gamma |x|^{-\mu}\} = O(|x|^{-\mu-\epsilon-|\beta|})$. We look at the classical Hamiltonian $h(x,\xi) = \frac{1}{2}\xi^2 + V(x)$.

With (1.1) one can prove the existence of the *asymptotic normalized velocities* for any *classical scattering orbit*, i.e. a solution to Newton's equation with $|x(t)| \to \infty$,

$$\omega^\pm = \pm \lim_{t\to\pm\infty} \frac{x(t)}{|x(t)|}; \tag{1.2}$$

notice that this includes orbits with arbitrary energy $\lambda \geqslant 0$. In particular we see that there is a well defined classical scattering theory for $\lambda = 0$ (the quantities $\omega^\pm$ are outgoing and incoming directions).

We look at the following mixed problem (restricted to outgoing and incoming regions): Consider the momentum $\xi = \sqrt{2\lambda}\omega$ as depending on the two independent variables $\lambda \geqslant 0$ and $\omega \in S^{d-1}$ and solve

$$\begin{cases} \ddot{y}(t) = -\nabla V(y(t)), \\ \lambda = \frac{1}{2}\dot{y}(t)^2 + V(y(t)), \\ y(\pm 1) = x, \\ \omega = \pm \lim_{t\to\pm\infty} \frac{y(t)}{|y(t)|}. \end{cases} \tag{1.3}$$

The bulk of the paper is devoted to solving (1.3) and deriving various regularity properties. Given solutions to (1.3), we then construct phases $\phi^\pm(x,\omega,\lambda)$ in terms of the velocity fields

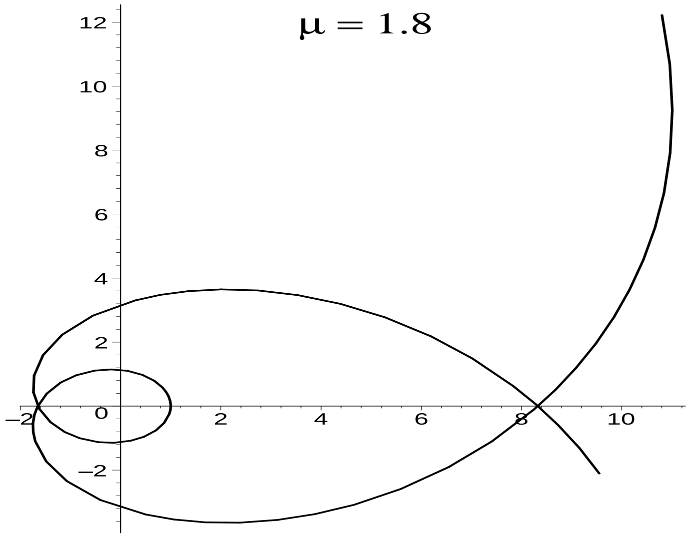
$$\nabla_x \phi^\pm(x,\omega,\lambda) = \dot{y}(\pm 1) = \dot{y}(t = \pm 1; x, \omega, \lambda).$$

It turns out that the constructed phases $\phi^\pm(x,\omega,\lambda)$ are jointly continuous but lack smoothness in the λ-variable at $\lambda = 0$.

We give a complete classification of the set of scattering orbits: For any scattering orbit $x(t)$ with asymptotic velocities $\omega^\pm$ given by (1.2) and energy $\lambda \geqslant 0$, there exists a (large) $T_0 > 0$ such that for all $\pm t \geqslant T \geqslant T_0$

$$x(t) = y(t \mp T \pm 1; x(\pm T), \omega^\pm, \lambda),$$
$$\dot{x}(t) = \nabla_x \phi^\pm(x(t), \omega^\pm, \lambda).$$

A typical orbit $x(t)$ for $\lambda = 0$ is depicted below, see Example 4.3 for an elaboration.



The paper is organized as follows: In Section 2 we impose conditions on the potential. In the case we allow the potential to have a non-spherically symmetric term we shall need certain regularity properties of the leading spherically symmetric term. These properties are stated in Condition 2.2; they are fulfilled for the example (1.1) discussed above.

In Section 3 we show the existence of the asymptotic normalized velocity in the classical theory (only the $+\infty$ case is treated).

In Sections 4 and 6 we solve the mixed problem (1.3) (the $+\infty$ case only), first in the case of spherical symmetry, then in the more general non-spherically symmetric case, and we derive smoothness properties of the solution. The first case is treated by the implicit function theorem, while our study of the second case is based on a perturbation and Taylor expansion argument (similar to [20, 21]), allowing us to set up a fixed point problem. The material is technically somewhat complicated, and to improve the presentation we devote Section 5 to some (abstract) preliminaries for Section 6 related to the uncertainty principle lemma (Hardy inequality). The basic issue of Section 5 is a limiting absorption principle at zero energy for a one-dimensional vector-valued problem, in which the time variable plays the role of a configuration space variable!

In Section 7 we prove that the outgoing velocity field $(x, F(x))$ from Definition 6.3 is Lagrangian, so that $F = \nabla\phi$ for some phase function ϕ. Then we fix $\phi^+ = \phi$ by specifying its value at a (local) point. We also explain how to define ϕ^-. These constructions will be the outset for studying quantum mechanics in [7]. Finally we show that the family of orbits (1.3) yields a complete classification of the set of scattering orbits.

2. CONDITIONS

We shall consider a classical Hamiltonian $h = \frac{1}{2}\xi^2 + V$ on $\mathbb{R}^d \times \mathbb{R}^d$, where $d \geqslant 2$ and V satisfies Condition 2.1 and possibly Conditions 2.2 and 2.3 (all stated below). We shall use the standard notation $\langle x\rangle = (1 + x^2)^{1/2}$ for $x \in \mathbb{R}^d$.

Condition 2.1. The function V can be written as a sum of two real-valued smooth functions, $V = V_1 + V_2$, such that: For some $\mu \in (0,2)$ we have:

(1) V_1 is a negative function that only depends on the radial variable $r = |x|$ in the region $r \geqslant 1$ (that is $V_1(x) = V_1(r)$ for $r \geqslant 1$). There exists $\epsilon_1 > 0$ such that
$$V_1(r) \leqslant -\epsilon_1 r^{-\mu}, \quad r \geqslant 1.$$
(2) For all $\gamma \in (\mathbb{N} \cup \{0\})^d$ there exists $C_\gamma > 0$ such that
$$\langle x\rangle^{\mu+|\gamma|}\left|\partial^\gamma V_1(x)\right| \leqslant C_\gamma.$$
(3) There exists $\tilde{\epsilon}_1 > 0$ such that
$$rV_1'(r) \leqslant -(2-\tilde{\epsilon}_1)V_1(r), \quad r \geqslant 1. \tag{2.1}$$
(4) There exists $\epsilon_2 > 0$ such that, for all $\gamma \in (\mathbb{N} \cup \{0\})^d$,
$$\langle x\rangle^{\mu+\epsilon_2+|\gamma|}\left|\partial^\gamma V_2(x)\right| \leqslant C_\gamma.$$

We introduce the quantity
$$\tilde{t}(r) = \int_1^r (-2V_1(\rho))^{-1/2}\mathrm{d}\rho, \quad r \geqslant 1, \tag{2.2}$$
which is the time of arrival at distance r from the origin for a purely outgoing zero-energy orbit starting at $r = 1$ at time $t = 0$ (assuming $V_2 = 0$).

The following condition will be needed only in the case $V_2 \neq 0$. We notice that (2.1) and (2.3) tend to be somewhat strong conditions for $\mu \approx 2$. On the other hand Conditions 2.1 and 2.2 hold for all $\epsilon_2 > 0$ for the particular example $V_1(r) = -\gamma r^{-\mu}$ (with $\epsilon_1 = \gamma$, $\tilde{\epsilon}_1 = 2-\mu$ and some $\bar{\epsilon}_1 < 1-\alpha\mu$), cf. Section 1.

Condition 2.2. Let V_1 be given as in Condition 2.1, and define $\alpha = \frac{2}{2+\mu}$. There exists $\bar{\epsilon}_1 > \max\{0, 1-\alpha(\mu+2\epsilon_2)\}$ such that
$$\limsup_{r\to\infty} r^{-1}V_1'(r)\tilde{t}(r)^2 < \tfrac{1}{4}(1-\bar{\epsilon}_1^2), \tag{2.3}$$
$$\limsup_{r\to\infty} V_1''(r)\tilde{t}(r)^2 < \tfrac{1}{4}(1-\bar{\epsilon}_1^2). \tag{2.4}$$

Let us for convenience assume under Condition 2.1 that
$$\epsilon_2 \leqslant \tfrac{1}{4}(2-\mu). \tag{2.5}$$
Notice that under Condition 2.2, inequality (2.5) is not in conflict with the condition $\bar{\epsilon}_1 > \max\{0, 1-\alpha(\mu+2\epsilon_2)\}$.

The following condition will be needed only in Subsection 7.2.

Condition 2.3. Let V_1, V_2 and $\bar{\epsilon}_1$ be given as in Conditions 2.1 and 2.2. Then
$$\limsup_{r\to\infty} \frac{-V_1'(r)}{\sqrt{-2V_1(r)}}\tilde{t}(r) < \tfrac{1}{2}(1+\bar{\epsilon}_1). \tag{2.6}$$

In the (typical) situation where $V_1(r)$ is concave at infinity obviously the bounds (2.4) and (2.6) are fulfilled.

We remark that the condition $\mu < 2$ is essential for the problems of this paper, due to the fact that only with this restriction the potential will be dominating the "centrifugal potential" $\frac{L^2}{2r^2}$ at infinity. Thus the regime $\mu \geqslant 2$ is qualitatively very different. On the other hand the Conditions 2.2 and 2.3 tend to be more technical, and we shall not here argue that these conditions are "natural". However from a practical point of view they are definitely needed for the fixed point approach we shall follow.

We shall often use the notation $x = r\hat{x}$ with $r = |x|$ and $\hat{x} = \frac{x}{r}$ for vectors $x \in \mathbb{R}^d \setminus \{0\}$. The notation $F(s > \epsilon)$ denotes a smooth increasing function $= 1$ for $s > \frac{3}{4}\epsilon$ and $= 0$ for $s < \frac{1}{2}\epsilon$; $F(\cdot < \epsilon) := 1 - F(\cdot > \epsilon)$. Throughout the paper the notation μ refers to the number μ appearing in Condition 2.1 and $\alpha := \frac{2}{2+\mu}$, cf. Condition 2.2. The function $g(r) := \sqrt{2\lambda - 2V_1(r)}$ (for V_1 obeying Condition 2.1) will also be used extensively. This quantity represents the speed of any orbit with energy λ and located at distance r from the origin (assuming $V_2 = 0$).

3. Asymptotic normalized velocity

We define a *classical outgoing scattering orbit* to be a solution to Newton's equation $\ddot{x}(t) = -\nabla V(x(t))$ obeying $|x(t)| \to \infty$ for $t \to +\infty$ (we consider for convenience here only the case of $t \to +\infty$). In this section we investigate various general properties of scattering orbits. Note that all the conditions on the potentials used in this section are implied by Condition 2.1.

The energy of the orbit is given by

$$\lambda = \tfrac{1}{2}\dot{x}(t)^2 + V(x(t)).$$

We start with a well known consequence of the positivity of the virial.

Proposition 3.1. *Suppose that for* $|x| \geqslant R$

$$-2V(x) - x \cdot \nabla V(x) \geqslant 0.$$

Then, for any outgoing scattering orbit, there exists T *such that for* $t \geqslant T$

$$x(t) \cdot \dot{x}(t) \geqslant 2(t-T)\lambda, \quad x^2(t) \geqslant 2\lambda(t-T)^2 + R^2.$$

Proof. For $|x(t)| \geqslant R$ we have

$$\begin{aligned} \frac{1}{2} \cdot \frac{\mathrm{d}^2}{\mathrm{d}t^2} x^2(t) = \frac{\mathrm{d}}{\mathrm{d}t}\big(x(t)\cdot\dot{x}(t)\big) &= 2\lambda - 2V(x(t)) - x(t)\cdot\nabla V(x(t)) \\ &\geqslant 2\lambda. \end{aligned} \tag{3.1}$$

If $x(t)$ is a scattering orbit, we can find T such that $\frac{\mathrm{d}}{\mathrm{d}t}x^2(T) \geqslant 0$ and $|x^2(T)| > R^2$. So (3.1) is satisfied for all $t \geqslant T$, and the result follows from integration. □

The following proposition can be traced back to [9], see also [8, Theorem 4.7].

Proposition 3.2. *Suppose that*

$$2V(x) + x \cdot \nabla V(x) \leqslant -c|x|^{-\mu}, \quad c > 0, \quad |x| \geqslant R. \tag{3.2}$$

Then for any outgoing scattering orbit for large enough time and some $\epsilon > 0$,

$$|x(t)| \geqslant \epsilon t^{\alpha}. \tag{3.3}$$

Proof. For large enough T and $t \geqslant T$ we have $|x(t)| \geqslant R$. Then

$$\frac{1}{2} \cdot \frac{\mathrm{d}^2}{\mathrm{d}t^2} x^2(t) = 2\lambda - 2V(x(t)) - x(t) \cdot \nabla V(x(t)) \geqslant c|x(t)|^{-\mu}. \tag{3.4}$$

We multiply (3.4) from both sides by $\frac{\mathrm{d}}{\mathrm{d}t} x^2(t)$ and, using $\mu < 2$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{d}}{\mathrm{d}t} x^2(t)\right)^2 \geqslant c_1 \frac{\mathrm{d}}{\mathrm{d}t}(x^2(t))^{1-\mu/2}.$$

This yields

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} x^2(t)\right)^2 \geqslant c_1 (x^2(t))^{1-\mu/2} + c_2.$$

By Proposition 3.1 we know that for large times $\frac{\mathrm{d}}{\mathrm{d}t} x^2(t) \geqslant 0$ is positive, and hence

$$\frac{\mathrm{d}}{\mathrm{d}t} x^2(t) \geqslant \left(c_1 (x^2(t))^{1-\mu/2} + c_2\right)^{1/2}.$$

This implies for large enough time (3.3). □

The upper bound on the zero energy orbit (3.5) can be traced back to [3, 4].

Proposition 3.3. *Assume that* $V(x) = O(|x|^{-\mu})$. *Then the outgoing scattering orbits with* $\lambda = 0$ *satisfy the bound*

$$x(t) = O(t^{\alpha}). \tag{3.5}$$

If in addition, for $|x| \geqslant R$, $V(x) \leqslant -c_0|x|^{-\mu}$, $c_0 > 0$, *then all outgoing scattering orbits for large enough time satisfy the bound*

$$|\dot{x}(t)| \geqslant \epsilon t^{\alpha-1}. \tag{3.6}$$

If also for (3.2) *holds, then the orbits with* $\lambda = 0$ *satisfy*

$$\dot{x}(t) = O(t^{\alpha-1}). \tag{3.7}$$

Proof. For zero energy orbits we have

$$\frac{\mathrm{d}}{\mathrm{d}t}|x(t)| \leqslant |\dot{x}(t)| \leqslant \sqrt{|2V(x(t))|} \leqslant C_1 |x(t)|^{-\mu/2}.$$

This implies (3.5) for large time.

Again, for zero energy orbits

$$|\dot{x}(t)| = \sqrt{-2V(x(t))} \geqslant c_2 x(t)^{-\mu/2}, \quad c_2 > 0,$$

which together with (3.5) yields (3.6) for large time. For positive energy orbits we clearly have $|\dot{x}(t)| \to \sqrt{2\lambda}$, which also implies (3.6) for large time.

Finally, (3.3) and

$$|\dot{x}(t)| = \sqrt{-2V(x(t))} = O(|x(t)|^{-\mu/2})$$

yield (3.7). □

For a given outgoing scattering orbit $x(t)$ we define the *asymptotic normalized velocity* to be

$$\omega^+ = \lim_{t\to+\infty} \omega(t), \quad \omega(t) = \frac{x(t)}{|x(t)|}, \tag{3.8}$$

provided that this limit exists. We also define

$$\tilde{\omega}^+ := \lim_{t\to+\infty} \tilde{\omega}(t), \quad \tilde{\omega}(t) = \frac{\dot{x}(t)}{|\dot{x}(t)|},$$

provided that this limit exists.

Proposition 3.4. *Suppose that*

$$\begin{aligned} \nabla^n V(x) &= O(|x|^{-n-\mu}), \quad n = 1,2, \\ V(x) &\leqslant -c_0|x|^{-\mu}, \quad c_0 > 0, \quad |x| \geqslant R, \\ 2V(x) + x\cdot\nabla V(x) &\leqslant -c|x|^{-\mu}, \quad c > 0, \quad |x| \geqslant R, \\ \nabla V(x) - \hat{x}\hat{x}\cdot\nabla V(x) &= O(|x|^{-1-\mu-\epsilon_2}), \quad \epsilon_2 > 0. \end{aligned} \tag{3.9}$$

Then for any outgoing scattering orbit $x(t)$ there exists ω^+ and $\tilde{\omega}^+$ and they are equal. Moreover,

$$\omega(t) = \omega^+ + O(t^{-\alpha\epsilon_2}) = \tilde{\omega}(t) + O(t^{-\alpha\epsilon_2}). \tag{3.10}$$

Proof. Let $L_{ij} = x_i\dot{x}_j - x_j\dot{x}_i$ be the ij'th component of the angular momentum. Note that

$$L^2 := \sum_{i<j} L_{ij}^2 = x^2\dot{x}^2 - (x\cdot\dot{x})^2 = x^2\dot{x}^2\big(1-(\omega\cdot\tilde{\omega})^2\big).$$

By (3.9),

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}L_{ij}\right| = |x|\,|\nabla V(x) - \omega\omega\cdot\nabla V(x)| = O(|x|^{-\mu-\epsilon_2}) = O(t^{-\alpha(\mu+\epsilon_2)}),$$

and therefore,

$$L_{ij} = O(t^{1-\alpha(\mu+\epsilon_2)}). \tag{3.11}$$

We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}\omega(t) = \frac{\dot{x}(t) - \omega(t)\,\omega(t)\cdot\dot{x}(t)}{|x(t)|}.$$

Hence,

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\omega(t)\right| = \frac{\sqrt{\dot{x}^2(t) - (\omega(t)\dot{x}(t))^2}}{|x(t)|} = \frac{|L(t)|}{|x(t)|^2} = O(t^{-1-\alpha\epsilon_2}) \in L^1(\mathrm{d}t).$$

Hence ω^+ is well defined, and the first estimate in (3.10) holds.

Now

$$\begin{aligned} \frac{\mathrm{d}\tilde{\omega}(t)}{\mathrm{d}t} &= -\frac{\nabla V(x(t)) - \tilde{\omega}(t)\cdot\nabla V(x(t))\tilde{\omega}(t)}{|\dot{x}(t)|} \\ &= -\frac{\omega(t)\cdot\nabla V(x(t))(\omega(t) - \omega(t)\cdot\tilde{\omega}(t)\tilde{\omega}(t))}{|\dot{x}(t)|} + O(t^{-1-\alpha\epsilon_2}). \end{aligned}$$

The norm of the first term equals

$$\frac{|\omega(t)\cdot\nabla V(x(t))||L(t)|}{|\dot{x}(t)|^2|x(t)|} = O(t^{-1-\alpha\epsilon_2}).$$

Hence

$$\frac{\mathrm{d}\tilde{\omega}(t)}{\mathrm{d}t} = O(t^{-1-\alpha\epsilon_2}) \in L^1(\mathrm{d}t).$$

Hence $\tilde{\omega}^+$ is well defined, and the second estimate in (3.10) holds.

We have

$$1-(\omega(t)\cdot\tilde{\omega}(t))^2 = \frac{L(t)^2}{x^2(t)\dot{x}^2(t)} = O(t^{-2\alpha\epsilon_2}).$$

Hence, $|\omega^+\cdot\tilde{\omega}^+| = 1$.

By Proposition 3.1 (or [8, (4.38)]), we have $\omega(t)\cdot\tilde{\omega}(t) \geqslant 0$, for large t. Hence, $\omega^+\cdot\tilde{\omega}^+ \geqslant 0$. Therefore, $\omega^+ = \tilde{\omega}^+$. □

Example 3.5 (Extension of an example in a preliminary version of the book [5])**.** Consider the potential $V = r^{-\mu}\chi(\theta - c\ln r)$ specified in two dimensions using polar coordinates. Here $\chi \in C^\infty(S^1)$ is negative, $\chi'(0) < 0$ and $c > 0$ (and $\mu \in (0,2)$). A computation shows that there is a classical scattering orbit with $\theta = c\ln r$ if

$$\chi(0) = \mu^{-1}\left(c\Big(\frac{\alpha}{1-\alpha\mu} - 1\Big) + c^{-1}\frac{1-\alpha}{1-\alpha\mu}\right)\chi'(0). \tag{3.12}$$

So in this case the asymptotic normalized velocity ω^+ does not exist. This shows the importance of the smallness condition of Condition 2.1 (4), viz. $\epsilon_2 > 0$. We also see from (3.12) that a weaker notion of smallness would not suffice neither: If χ is taken to be almost constant, say $\chi \approx -1$, which may be viewed as an example of another type of perturbed radial potential, then there is still a solution to (3.12), in fact one with $c \approx 0$.

4. Mixed problem for radial potentials

In this section we assume that the potential is radial and for $r \geqslant 1$,

$$\begin{aligned} |\partial_r^n V(r)| &\leqslant C_n r^{-n-\mu}, \quad n = 0,1,\dots, \\ V(r) &\leqslant -cr^{-\mu}, \quad c > 0, \quad rV'(r) + 2V(r) < 0. \end{aligned} \tag{4.1}$$

Clearly, Condition 2.1 with $V_2(r) = 0$ implies (4.1).

For radial potentials all orbits are confined to a plane. Let us first investigate the two-dimensional problem. We will use polar coordinates $(y_1, y_2) = (r\cos\theta, r\sin\theta)$.

The angular momentum L is a preserved quantity, at our disposal. We need to solve the system

$$\begin{cases} \dot{\theta} = Lr^{-2}, \\ \dot{r} = \sqrt{2\lambda - 2V(r) - L^2 r^{-2}}. \end{cases} \tag{4.2}$$

We impose the conditions

$$r(1) = r_1, \quad \frac{\mathrm{d}}{\mathrm{d}t}r(1) > 0, \quad \lim_{t\to+\infty}\theta(t) = 0. \tag{4.3}$$

Our assumption implies that for any $\lambda \geqslant 0$ and $L \in \mathbb{R}$, there exists at most one $r_{\mathrm{tp}} = r_{\mathrm{tp}}(\lambda, L) \geqslant 1$ that solves

$$2\lambda - 2V(r_{\mathrm{tp}}) - L^2 r_{\mathrm{tp}}^{-2} = 0.$$

Note that the function

$$(1,\infty) \ni r \mapsto rg(r) = r\sqrt{2\lambda - 2V(r)} \quad \text{is increasing.} \tag{4.4}$$

Clearly, for any $\lambda \geqslant 0$, $L \in \mathbb{R}$ and $r_1 > r_{\rm tp} \geqslant 1$ the problem (4.2) subject to (4.3) has a unique solution. This solution is a scattering orbit and it has turning point at $r_{\rm tp}$. Writing $\theta_1 = \theta(1)$ we obtain

$$-\theta_1 = L\int_{r_1}^{\infty} r^{-2}(2\lambda - 2V(r) - L^2 r^{-2})^{-1/2}\mathrm{d}r. \tag{4.5}$$

The angle between the asymptotic direction and the turning point equals

$$-\theta_{\rm tp} = L\int_{r_{\rm tp}}^{\infty} r^{-2}(2\lambda - 2V(r) - L^2 r^{-2})^{-1/2}\mathrm{d}r. \tag{4.6}$$

Clearly, $\lim_{t\to-\infty}\theta(t) = 2\theta_{\rm tp}$.

Let $\theta_{\rm al} = \theta_{\rm al}(\lambda, r_1)$ denote the largest allowed angle such that for $|\theta_1| < \theta_{\rm al}$ there exists a solution to Newton's equation with energy λ obeying the conditions (4.3) as well as $\theta(1) = \theta_1$.

Proposition 4.1. *Introduce the constant*

$$C = \sup_{r' \geqslant r \geqslant 1} \frac{V(r')}{V(r)}. \tag{4.7}$$

Then $\theta_{\rm al} \geqslant \frac{\pi}{2} - \arctan\sqrt{C-1}$. *In particular, if* $V(r)$ *is increasing, so that* $C = 1$, *then* $\theta_{\rm al} \geqslant \frac{\pi}{2}$.

Proof. We write $L = r_1 g(r_1)\kappa$ with $\kappa \in [-1,1]$. It follows from (4.4) that for any such κ

$$2\lambda - 2V(r) - L^2 r^{-2} > 0 \quad \text{for} \quad r > r_1.$$

After a change of variable we may then write (4.5) as

$$-\theta_1 = \kappa\int_1^{\infty} s^{-1}\left(s^2\frac{\lambda - V(sr_1)}{\lambda - V(r_1)} - \kappa^2\right)^{-1/2}\mathrm{d}s. \tag{4.8}$$

Note that

$$cs^{-\mu} \leqslant \frac{\lambda - V(sr_1)}{\lambda - V(r_1)} = \frac{g(sr_1)^2}{g(r_1)^2} \leqslant C. \tag{4.9}$$

Clearly the right hand side of (4.8) is an increasing function of κ. Therefore, we get the lower bound

$$\int_1^{\infty} s^{-1}\left(s^2\frac{\lambda - V(sr_1)}{\lambda - V(r_1)} - 1\right)^{-1/2}\mathrm{d}s \geqslant \int_1^{\infty} s^{-1}(s^2 C - 1)^{-1/2}\mathrm{d}s = \frac{\pi}{2} - \arctan\sqrt{C-1}$$

for the largest allowed angle. □

Example 4.2. For the purely Coulombic case $V(r) = -\gamma r^{-1}$ one can compute the orbit

$$L^2\gamma^{-1} r(t)^{-1} = 1 - \frac{\cos(\theta_{\rm tp} - \theta(t))}{\cos(\theta_{\rm tp})},$$

where $\theta_{\rm tp}(\lambda, L) = \pi - \arctan\sqrt{2\lambda L^2\gamma^{-2}}$ (see [16, p. 126], for example). Therefore, the allowed angle equals

$$\theta_{\rm al}(\lambda, r_1) = \pi - \arctan\sqrt{2\lambda(2\lambda\gamma^{-2} r_1^2 + 2\gamma^{-1} r_1)}. \tag{4.10}$$

In particular, for $\lambda > 0$ the allowed angle is at least $\frac{\pi}{2}$ and for $\lambda = 0$ it is π.

Example 4.3. We look at scattering for the example $V(r) = -\gamma r^{-\mu}$ at energy $\lambda = 0$. The angle between asymptotic direction and the turning point is independent of the orbit and is equal to $\theta_{\rm tp} = \frac{\pi}{2-\mu}$. The fact that this angle is independent of the orbit may be seen independently by invoking the scaling and rotational symmetry of Newton's equation; thus there is essentially only one scattering orbit at $\lambda = 0$ (see the illustration in Section 1 for the case $\mu = 1.8$). The implicit equation for this orbit is

$$\frac{2}{1+\cos\big((2-\mu)(\theta_{\rm tp}-\theta(t))\big)} = r(t)^{2-\mu}. \tag{4.11}$$

4.1. **Dependence of the angular momentum on data.**

Lemma 4.4. *We fix $\kappa_0 \in (0,1)$. Then for any $L \in \mathbb{R}$, $\lambda \geqslant 0$ and $r_1 \geqslant 1$, satisfying*

$$\frac{L^2}{r_1^2} \leqslant \kappa_0^2 g(r_1)^2, \tag{4.12}$$

we have a unique outgoing scattering orbit with the conditions (4.3)*, the energy λ and angular momentum L. The initial angle is given by* (4.5)*, and we have the following estimates:*

$$\partial_{r_1}^n \partial_{L^2}^m \frac{\theta_1}{L} = O(r_1^{-1-n-2m} g(r_1)^{-1-2m}), \quad n, m \geqslant 0. \tag{4.13}$$

Proof. Only (4.13) needs elaboration. For $n \geqslant 1$, we have

$$\begin{aligned}\partial_r^n(2\lambda - 2V(r) - L^2/r^2) &= O(r^{-\mu-n}) + O(L^2 r^{-2-n})\\ &= O(r^{-\mu-n}) + O(r^2 g(r)^2 r^{-2-n})\\ &= O(r^{-n} g(r)^2).\end{aligned}$$

The quantity $\partial_r^n(2\lambda - 2V(r) - L^2/r^2)^{-p}$ is a linear combination of terms of the following form (where $n_1 + \cdots + n_k = n$):

$$\begin{aligned}(2\lambda - 2V(r) - L^2/r^2)^{-p-k}\partial_r^{n_1}(2\lambda - 2V(r) - L^2/r^2)\cdots\partial_r^{n_k}(2\lambda - 2V(r) - L^2/r^2)\\ = O(g(r)^{-2p-2k} g(r)^2 r^{-n_1}\cdots g(r)^2 r^{-n_k})\\ = O(r^{-n} g(r)^{-2p}).\end{aligned}$$

Hence,

$$\partial_r^n(2\lambda - 2V(r) - L^2/r^2)^{-p} = O(r^{-n} g(r)^{-2p}).$$

Using (4.4) and (4.9) we obtain that

$$\begin{aligned}\partial_{L^2}^m \frac{\theta_1}{L} &= C_m \int_{r_1}^\infty r^{-2-2m}(2\lambda - 2V(r) - L^2/r^2)^{-1/2-m}\mathrm{d}r\\ &= O(r_1^{-1-2m} g(r_1)^{-1-2m}).\end{aligned}$$

For $n \geqslant 1$, $\partial_{r_1}^n \partial_{L^2}^m \frac{\theta_1}{L}$ is a linear combination of terms of the form

$$r_1^{-k-2m-1}\partial_{r_1}^{n-k}(2\lambda - 2V(r_1) - L^2/r_1^2)^{-1/2-m} = O(r_1^{-n-2m-1} g(r_1)^{-1-2m}). \qquad \square$$

Lemma 4.5. *Let* $\theta_0 \in (0, \frac{\pi}{2} - \arctan\sqrt{C-1})$ *where* C *is given by* (4.7)*. Then for all* $r_1 \geqslant 1$, $|\theta_1| \leqslant \theta_0$ *and* $\lambda \geqslant 0$ *we can find a unique outgoing scattering orbit satisfying* (4.3)*, with* $\theta(1) = \theta_1$ *and* $|\theta(t)| \leqslant |\theta_1|$ *for all* $t \geqslant 1$*. We have the following estimates:*

$$\partial_{r_1}^n \partial_{\theta_1^2}^m L^2 = O(r_1^{2-n} g(r_1)^2), \quad n, m \geqslant 0, \tag{4.14}$$

$$\partial_{r_1}^n \partial_{\theta_1^2}^m \frac{L}{\theta_1} = O(r_1^{1-n} g(r_1)), \quad n, m \geqslant 0. \tag{4.15}$$

Proof. We can solve the equation (4.5) for L such that (4.12) is fulfilled for some $\kappa_0 \in (0,1)$. Treating L^2 as an independent variable, obviously

$$\partial_{r_1}^n \partial_{L^2}^m L^2 = O(r_1^{2-2m-n} g(r_1)^{2-2m}). \tag{4.16}$$

We apply $\partial_{r_1}^n \partial_{L^2}^m$ to

$$\theta_1^2 = \left(\frac{\theta_1}{L}\right)^2 L^2,$$

use (4.13) and (4.16), and obtain

$$\partial_{r_1}^n \partial_{L^2}^m \theta_1^2 = O(r_1^{-n-2m} g(r_1)^{-2m}). \tag{4.17}$$

Next we note

$$\begin{aligned} \partial_{L^2} \theta_1^2 &= \int_{r_1}^{\infty} r^{-2}(2\lambda - 2V(r) - L^2 r^{-2})^{-1/2} \mathrm{d}r \\ &\quad \times \int_{r_1}^{\infty} r^{-2}(2\lambda - 2V(r))(2\lambda - 2V(r) - L^2 r^{-2})^{-3/2} \mathrm{d}r \\ &\geqslant c_0 r_1^{-2} g(r_1)^{-2}, \quad \text{for some } c_0 > 0. \end{aligned} \tag{4.18}$$

We claim that the quantity $\partial_{r_1}^n \partial_{\theta_1^2}^m L^2$ is a linear combination of terms of the form

$$\partial_{r_1}^{n_1} \partial_{L^2}^{m_1} \theta_1^2 \cdots \partial_{r_1}^{n_p} \partial_{L^2}^{m_p} \theta_1^2 (\partial_{L^2} \theta_1^2)^{-m-p} = O(r_1^{2-n} g(r_1)^2), \tag{4.19}$$

where $n = n_1 + \cdots + n_p$ and $m + p = m_1 + \cdots + m_p + 1$, which obviously proves (4.14). To see that indeed the terms are of the form given to the left of (4.19) we use induction with respect to $n + m$. The first step (justified by the implicit function theorem and the chain rule) is

$$\begin{aligned} \partial_{\theta_1^2} L^2 &= (\partial_{L^2} \theta_1^2)^{-1}, \\ \partial_{r_1} L^2 &= -\partial_{r_1} \theta_1^2 (\partial_{L^2} \theta_1^2)^{-1}. \end{aligned}$$

The inductive step uses the following identities:

$$\begin{aligned} \partial_{\theta_1^2}(\partial_{r_1}^{n_1} \partial_{L^2}^{m_1} \theta_1^2) &= \partial_{r_1}^{n_1} \partial_{L^2}^{m_1+1} \theta_1^2 (\partial_{L^2} \theta_1^2)^{-1}, \\ \partial_{r_1}(\partial_{r_1}^{n_1} \partial_{L^2}^{m_1} \theta_1^2) &= \partial_{r_1}^{n_1+1} \partial_{L^2}^{m_1} \theta_1^2 - \partial_{r_1}^{n_1} \partial_{L^2}^{m_1+1} \theta_1^2 \partial_{r_1} \theta_1^2 (\partial_{L^2} \theta_1^2)^{-1}. \end{aligned}$$

Finally we use (4.17) and (4.18) yielding the bound (4.19).

The quantity $\partial_{r_1}^n \partial_{\theta_1^2}^m \frac{\theta_1}{L}$ is a linear combination of terms of the form

$$\partial_{r_1}^{n_1} \partial_{\theta_1^2}^{m_1} L^2 \cdots \partial_{r_1}^{n_p} \partial_{\theta_1^2}^{m_p} L^2 \partial_{r_1}^k \partial_{L^2}^p \frac{\theta_1}{L} = O(r_1^{-1-n} g(r_1)^{-1}),$$

where $n = n_1+\cdots+n_p+k$ and $m = m_1+\cdots+m_p$; for the bound we use (4.13) and (4.14). Thus

$$\partial_{r_1}^n \partial_{\theta_1^2}^m \frac{\theta_1}{L} = O(r_1^{-1-n} g(r_1)^{-1}). \tag{4.20}$$

We note the inequality

$$-\frac{\theta_1}{L} \geqslant r_1^{-1} g(r_1)^{-1}. \tag{4.21}$$

Finally, the quantity $\partial_{r_1}^n \partial_{\theta_1^2}^m \frac{L}{\theta_1}$ is a linear combination of terms of the form

$$\partial_{r_1}^{n_1} \partial_{\theta_1^2}^{m_1} \frac{\theta_1}{L} \cdots \partial_{r_1}^{n_k} \partial_{\theta_1^2}^{m_k} \frac{\theta_1}{L} \left(\frac{L}{\theta_1}\right)^{k+1} = O(r_1^{1-n} g(r_1)),$$

where $n_1+\cdots+n_k = n$ and $m_1+\cdots+m_k = m$; for the bound we use (4.20) and (4.21). This proves (4.15). □

Finally, we consider orbits in arbitrary dimension. For $R \geqslant 1$ and $\sigma > 0$ we introduce

$$\Gamma_{R,\sigma}^+(\omega) = \{y \in \mathbb{R}^d : y\cdot\omega \geqslant (1-\sigma)|y|, |y| \geqslant R\}, \quad \omega \in S^{d-1},$$
$$\Gamma_{R,\sigma}^+ = \{(y,\omega) \in \mathbb{R}^d \times S^{d-1} : y \in \Gamma_{R,\sigma}^+(\omega)\}.$$

The mixed problem consists in finding a solution $y(t)$ to Newton's equation subject to mixed boundary conditions and an energy constraint given in terms of data $x \in \mathbb{R}^d$, $\omega \in S^{d-1}$ and $\lambda \geqslant 0$:

$$\begin{cases} \ddot{y}(t) = -\nabla V(y(t)), \\ \lambda = \frac{1}{2}\dot{y}(t)^2 + V(y(t)), \\ y(1) = x, \\ \omega = \lim_{t\to+\infty} \omega(t), \quad \omega(t) = \frac{y(t)}{|y(t)|}. \end{cases} \tag{4.22}$$

Proposition 4.6. *For all small enough $\sigma > 0$, the problem* (4.22) *has a solution $y(t)$, $t \geqslant 1$, for all data $(x,\omega) \in \Gamma_{1,\sigma}^+$ and $\lambda \geqslant 0$. Moreover this solution $y(t) \in \Gamma_{1,\sigma}^+(\omega)$ for all $t \geqslant 1$, and given the latter invariance property it is unique and*

$$\partial_x^\alpha \partial_\omega^\beta L^2 = O(|x|^{2-|\alpha|} g(|x|)^2). \tag{4.23}$$

Proof. Note that $(r_1, \sin^2\theta_1) = (|x|, 1-(\omega\cdot\hat{x})^2)$. Therefore, θ_1^2 and $r_1 = |x|$ are smooth function of x and ω with

$$\partial_\omega^\delta \partial_x^\gamma \theta_1^2 = O(|x|^{-|\gamma|}), \quad \partial_x^\gamma r_1 = O(|x|^{1-|\gamma|}). \tag{4.24}$$

In conjunction with (4.14) and the Faá di Bruno formula we obtain (4.23). (Recall that the Faá di Bruno formula is a basic combinatorial formula for computing derivatives of composite functions used frequently in the literature see for example [5, proof of Theorem 1.10.1]). □

Remarks 4.7. 1) The function L^2 is continuous in all variables at $\lambda = 0$, however as may readily be checked it is not smooth in λ at this point. This function is smooth for $\lambda > 0$.

2) The derivatives in ω and x of the function L^2 are also continuous in λ at $\lambda = 0$. This follows by an abstract argument (the proof is very simple, see for example [12, proof of Lemma 7.7.2]): Suppose $\mathscr{U}$ is an open subset of $\mathbb{R}^n$, and that $f : \mathscr{U} \times [0,1] \to \mathbb{R}$ is smooth in $z \in \mathscr{U}$ (for any fixed $\lambda \in [0,1]$) with $|\partial_z^\beta f| \leqslant C_\beta$ uniformly on $\mathscr{U} \times [0,1]$, and

suppose f is continuous in $(z,\lambda)\in\mathscr{U}\times[0,1]$. Then all z-derivatives are continuous in $(z,\lambda)\in\mathscr{U}\times[0,1]$.

3) For the uniqueness statement of Proposition 4.6 the stated invariance property is crucial due to the fact that orbits may wind around the center of attraction several times before escaping to infinity along an asymptotic direction, cf. the illustration in Section 1.

4.2. **Dependence of flow on data.** Let us examine the dependence of the flow on the boundary conditions. We start with the dependence on (r_1,θ_1) of the two-dimensional flow $(\theta,r)=(\theta(t),r(t))$.

Lemma 4.8. *The orbits described in Lemma 4.5 obey*

$$\partial^n_{r_1}\partial^m_{\theta_1^2} r = O(r_1^{1-n} g(r_1) g(r)^{-1}),\quad n+m\geqslant 1, \tag{4.25}$$

$$\partial^n_{r_1}\partial^m_{\theta_1^2}\theta^2 = O(r_1^{2-n} r^{-2} g(r_1)^2 g(r)^{-2}),\quad n+m\geqslant 0, \tag{4.26}$$

$$\partial^n_{r_1}\partial^m_{\theta_1^2}\frac{\theta}{\theta_1} = O(r_1^{1-n} r^{-1} g(r_1) g(r)^{-1}),\quad n+m\geqslant 0. \tag{4.27}$$

Proof. To prove (4.25) we note that the second equation of (4.2) is solved by

$$\int_{r_1}^{r}(2\lambda-2V(\rho)-L^2\rho^{-2})^{-1/2}\mathrm{d}\rho = t-1. \tag{4.28}$$

We use induction with respect to $n+m$. We apply to (4.28) the derivative $\partial^n_{r_1}\partial^m_{\theta_1^2}$, obtaining that zero is a linear combination of terms of the following form:

$$\begin{aligned}&\partial^{n_1}_{r_1}\partial^{m_1}_{\theta_1^2}L^2\cdots\partial^{n_k}_{r_1}\partial^{m_k}_{\theta_1^2}L^2\\ &\quad\times r_1^{-2k-u}\partial^v_{r_1}(2\lambda-2V(r_1)-L^2/r_1^2)^{-1/2-k},\end{aligned} \tag{4.29}$$

with $n_1+\cdots+n_k+u+v+1=n$, $m_1+\cdots+m_k=m$;

$$\begin{aligned}&\partial^{p_1}_{r_1}\partial^{q_1}_{\theta_1^2}r\cdots\partial^{p_l}_{r_1}\partial^{q_l}_{\theta_1^2}r\\ &\quad\times\partial^{n_1}_{r_1}\partial^{m_1}_{\theta_1^2}L^2\cdots\partial^{n_k}_{r_1}\partial^{m_k}_{\theta_1^2}L^2\\ &\quad\times r^{-2k-u}\partial^v_r(2\lambda-2V(r)-L^2/r^2)^{-1/2-k},\end{aligned} \tag{4.30}$$

with $n_1+\cdots+n_k+p_1+\cdots+p_l=n$, $u+v+1=l$, $m_1+\cdots+m_k+q_1+\cdots+q_l=m$; and

$$\begin{aligned}&\partial^{n_1}_{r_1}\partial^{m_1}_{\theta_1^2}L^2\cdots\partial^{n_k}_{r_1}\partial^{m_k}_{\theta_1^2}L^2\\ &\quad\times\int_{r_1}^{r}\rho^{-2k}(2\lambda-2V(\rho)-L^2/\rho^2)^{-1/2-k}\mathrm{d}\rho,\end{aligned} \tag{4.31}$$

with $n_1+\cdots+n_k=n$, $m_1+\cdots+m_k=m$.

Using (4.14) the terms (4.29) are estimated by

$$O(r_1^{-n+1}g(r_1)^{-1}). \tag{4.32}$$

The terms (4.30) are divided into the single term

$$\partial^n_{r_1}\partial^m_{\theta_1^2}\, r(2\lambda-2V(r)-L^2/r^2)^{-1/2} \tag{4.33}$$

and the remaining ones, which by (4.4) and (4.14) can be estimated by

$$C\big|\partial_{r_1}^{p_1}\partial_{\theta_1^2}^{q_1} r\big|\cdots\big|\partial_{r_1}^{p_l}\partial_{\theta_1^2}^{q_l} r\big| r_1^{p_1+\cdots+p_l-n} r^{1-l} g(r)^{-1}. \tag{4.34}$$

By the induction assumption, and using $l \geqslant 1$ and (4.9), (4.34) is bounded by

$$C r_1^{1-n} g(r_1) g(r)^{-2}. \tag{4.35}$$

Using $k \geqslant 1$ and (4.9), the terms (4.31) are estimated by

$$\begin{aligned} C_1 g(r_1)^{2k} r_1^{2k-n} \int_{r_1}^{r} \rho^{-2k} g(\rho)^{-1-2k} \mathrm{d}\rho &\leqslant C_2 g(r_1)^2 g(r)^{-2} r_1^{2-n} \int_{r_1}^{r} \rho^{-2} g(\rho)^{-1} \mathrm{d}\rho \\ &\leqslant C_3 g(r_1) g(r)^{-2} r_1^{1-n}. \end{aligned}$$

Thus we obtain the estimate

$$\big|\partial_{r_1}^{n}\partial_{\theta_1^2}^{m} r\big| g(r)^{-1} = O(g(r_1) g(r)^{-2} r_1^{1-n}),$$

from which (4.25) follows.

Next we would like to prove (4.26). We start from the identity

$$\frac{\theta}{L} = -\int_r^{\infty} \rho^{-2}(2\lambda - V(\rho) - L^2/\rho^2)^{-1/2} \mathrm{d}\rho. \tag{4.36}$$

This shows $\frac{\theta}{L} = O(r^{-1} g(r)^{-1})$. Next we obtain that $\partial_{r_1}^{n}\partial_{\theta_1^2}^{m}\frac{\theta}{L}$ is a linear combination of terms of the following form:

$$\begin{aligned} &\partial_{r_1}^{p_1}\partial_{\theta_1^2}^{q_1} r \cdots \partial_{r_1}^{p_l}\partial_{\theta_1^2}^{q_l} r \\ &\times \partial_{r_1}^{n_1}\partial_{\theta_1^2}^{m_1} L^2 \cdots \partial_{r_1}^{n_k}\partial_{\theta_1^2}^{m_k} L^2 \\ &\times r^{-2-2k-u} \partial_r^{v} (2\lambda - 2V(r) - L^2/r^2)^{-1/2-k}, \end{aligned} \tag{4.37}$$

with $n_1 + \cdots + n_k + p_1 + \cdots + p_l = n$, $u + v + 1 = l$, $m_1 + \cdots + m_k + q_1 + \cdots + q_l = m$; and

$$\begin{aligned} &\partial_{r_1}^{n_1}\partial_{\theta_1^2}^{m_1} L^2 \cdots \partial_{r_1}^{n_k}\partial_{\theta_1^2}^{m_k} L^2 \\ &\times \int_r^{\infty} \rho^{-2-2k} (2\lambda - 2V(\rho) - L^2/\rho^2)^{-1/2-k} \mathrm{d}\rho, \end{aligned} \tag{4.38}$$

with $n_1 + \cdots + n_k = n$, $m_1 + \cdots + m_k = m$.

The term (4.37) is estimated by

$$C_1 r_1^{-n+l+2k} r^{-1-l-2k} g(r_1)^{l+2k} g(r)^{-1-l-2k} \leqslant C_2 r_1^{-n} r^{-1} g(r)^{-1}.$$

The term (4.38) is estimated by

$$C_1 r_1^{-n+2k} r^{-1-2k} g(r_1)^{2k} g(r)^{-1-2k} \leqslant C_2 r_1^{-n} r^{-1} g(r)^{-1}.$$

Thus

$$\partial_{r_1}^{n}\partial_{\theta_1^2}^{m}\frac{\theta}{L} = O(r_1^{-n} r^{-1} g(r)^{-1}). \tag{4.39}$$

Now by

$$\theta^2 = \left(\frac{\theta}{L}\right)^2 L^2,$$

(4.14) and (4.39) we obtain (4.26).

By

$$\frac{\theta}{\theta_1} = \frac{\theta}{L} \cdot \frac{L}{\theta_1},$$

(4.15) and (4.39), we obtain (4.27). □

We go back to the case of arbitrary dimension.

Proposition 4.9. *The orbits considered in Proposition 4.6 satisfy*

$$\partial_\omega^\delta \partial_x^\gamma y = \begin{cases} O(|y|) & \textit{for } \gamma = 0, \\ O\big(|x|^{1-|\gamma|} g(|x|) g(|y|)^{-1}\big) & \textit{for } |\gamma| \geqslant 1. \end{cases} \tag{4.40}$$

In particular,

$$\partial_\omega^\delta \partial_x^\gamma y = O(|x|^{-|\gamma|}|y|). \tag{4.41}$$

Proof. We use the formula

$$y = r\cos\theta\,\omega + r\frac{\sin\theta}{\sin\theta_1}(\hat{x} - \hat{x}\cdot\omega\,\omega). \tag{4.42}$$

Now, $\partial_\omega^\delta \partial_x^\gamma r\cos\theta\omega$ is a linear combination of terms of the form

$$\begin{aligned} &\partial_\omega^{\pi_1}\partial_x^{\rho_1} r_1 \cdots \partial_\omega^{\pi_n}\partial_x^{\rho_n} r_1 \\ &\quad\times \partial_\omega^{\sigma_1}\partial_x^{\tau_1}\theta_1^2 \cdots \partial_\omega^{\sigma_m}\partial_x^{\tau_m}\theta_1^2 \\ &\quad\times \partial_{r_1}^{n_1}\partial_{\theta_1^2}^{m_1} r \partial_{r_1}^{n_2}\partial_{\theta_1^2}^{m_2}\cos\theta \\ &\quad\times \partial_\omega^{\delta_0}\omega. \end{aligned} \tag{4.43}$$

Likewise, $\partial_\omega^\delta \partial_x^\gamma \frac{r\sin\theta}{r_1\sin\theta_1}(x - x\cdot\omega\,\omega)$ is a linear combination of terms of the form

$$\begin{aligned} &\partial_\omega^{\pi_1}\partial_x^{\rho_1} r_1 \cdots \partial_\omega^{\pi_n}\partial_x^{\rho_n} r_1 \\ &\quad\times \partial_\omega^{\sigma_1}\partial_x^{\tau_1}\theta_1^2 \cdots \partial_\omega^{\sigma_m}\partial_x^{\tau_m}\theta_1^2 \\ &\quad\times \partial_{r_1}^{n_1}\partial_{\theta_1^2}^{m_1} r \partial_{r_1}^{n_2}\partial_{\theta_1^2}^{m_2}\frac{\sin\theta}{\sin\theta_1} \\ &\quad\times \partial_\omega^{\delta_0}\partial_x^{\gamma_0}(\hat{x} - \hat{x}\cdot\omega\,\omega). \end{aligned} \tag{4.44}$$

Note that

$$\partial_\omega^{\delta_0}\omega = O(1), \tag{4.45}$$

$$\partial_\omega^{\delta_0}\partial_x^{\gamma_0}(\hat{x} - \hat{x}\cdot\omega\,\omega) = O(|x|^{-|\gamma_0|}). \tag{4.46}$$

Moreover by Lemma 4.8,

$$\partial_{r_1}^{n_1}\partial_{\theta_1^2}^{m_1} r = \begin{cases} O(r) & \text{if } n_1 + m_1 = 0, \\ r_1^{1-n_1} g(r_1) g(r)^{-1} & \text{if } n_1 + m_1 \geqslant 1, \end{cases} \tag{4.47}$$

$$\partial_{r_1}^{n_2}\partial_{\theta_1^2}^{m_2}\cos\theta = \begin{cases} O(1) & \text{if } n_2 + m_2 = 0, \\ r_1^{2-n_2} r^{-2} g(r_1)^2 g(r)^{-2} & \text{if } n_2 + m_2 \geqslant 1, \end{cases} \tag{4.48}$$

$$\partial_{r_1}^{n_2}\partial_{\theta_1^2}^{m_2}\frac{\sin\theta}{\sin\theta_1} = r_1^{1-n_2} r^{-1} g(r_1) g(r)^{-1}. \tag{4.49}$$

(For (4.49) we use the decomposition $\frac{\sin\theta}{\sin\theta_1} = \frac{\theta}{\theta_1} \cdot \frac{\sin(\theta)/\theta}{\sin(\theta_1)/\theta_1}$.)

Now, applying (4.24) and (4.45)–(4.49) to (4.43) and (4.44) yields (4.40). □

One may also estimate derivatives of $\dot{y}$:

Proposition 4.10.

$$\partial_\omega^\delta \partial_x^\gamma (\dot{y} - \sqrt{2\lambda}\omega) = O\big(|x|^{-|\gamma|}|y|^{-\mu} g(|y|)^{-1}\big). \tag{4.50}$$

In particular

$$\partial_\omega^\delta \partial_x^\gamma \dot{y} = O\big(|x|^{-|\gamma|} g(|y|)\big). \tag{4.51}$$

Proof. First we represent

$$\dot{y}(t) - \sqrt{2\lambda}\omega = \int_t^\infty \nabla V(y) \mathrm{d}t', \tag{4.52}$$

Now $\partial_\omega^\delta \partial_x^\gamma (\dot{y}(t) - \sqrt{2\lambda}\omega)$ is a linear combination of terms of the form

$$\begin{aligned} &\int_t^\infty \partial_\omega^{\delta_1} \partial_x^{\gamma_1} y(t') \cdots \partial_\omega^{\delta_n} \partial_x^{\gamma_n} y(t') \nabla^{n+1} V(y(t')) \mathrm{d}t' \\ &\quad = O\left(|x|^{-|\gamma|} \int_{|y|}^\infty \rho^{-1-\mu} g(\rho)^{-1} \mathrm{d}\rho\right), \end{aligned} \tag{4.53}$$

which are $O(|x|^{-|\gamma|}|y|^{-\mu} g(|y|)^{-1})$. □

We also notice the uniform bounds

$$|y|^{-1} g(|y|) \leqslant \frac{C}{t-1}, \quad |y|^{-1} \leqslant C t^{-\alpha}, \tag{4.54}$$

Since $|y|^{-1} \leqslant |x|^{-1}$ the second estimate of (4.54) may be generalized as

$$|y|^{-1} \leqslant C|x|^{-\delta} t^{-\alpha(1-\delta)}, \quad \delta \in [0,1]. \tag{4.55}$$

5. TIME–DEPENDENT LINEAR FORCE PROBLEM

We consider the following one-dimensional matrix-valued ODE

$$\ddot{z}(t) - q(t) z(t) = \tilde{z}(t), \quad t \geqslant 1, \tag{5.1}$$

where $q(t) \in M_d(\mathbb{C})$ is self-adjoint for all $t \geqslant 1$, and as a function of t, q is continuous and bounded. Moreover we assume the following bound for some $\epsilon > 0$

$$(t-1)^2 q(t) \geqslant -\tfrac{1}{4}(1-\epsilon^2) \quad \text{for } t \geqslant 1. \tag{5.2}$$

The goal of this section is to study the initial value problem given by (5.1) and the initial value condition $z(1) = 0$. As the reader will see the relevant tools come from functional analysis.

Throughout the section we fix any

$$r \in \big(-\tfrac{\epsilon}{2}, \tfrac{\epsilon}{2}\big). \tag{5.3}$$

We introduce for any such r the following form on the domain $\mathscr{D}(Q_r) = W_0^{1,2}(1,\infty) \subseteq L^2(1,\infty)$ ($W_0^{1,2} \subseteq W^{1,2}$ refers to standard Sobolev spaces, see for example [2], although we are here dealing with $\mathbb{C}^d$-valued functions): Let $p_t = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$ and

$$Q_r(\psi, \phi) = \langle p_t \psi, p_t \phi \rangle + \langle \psi, \{q(t) - r^2 t^{-2} + \mathrm{i} r (p_t t^{-1} + t^{-1} p_t)\} \phi \rangle. \tag{5.4}$$

Formally this is the form of the operator $H_r = t^r H t^{-r}$, where H is the Schrödinger operator $H = p_t^2 + q(t)$ with Dirichlet boundary condition at $t = 1$. To justify this we invoke [17, Theorem VIII.16] and the Hardy inequality [2, Lemma 5.3.1]. Due to this inequality and to (5.2), there exists $\delta = \delta(\epsilon, r) > 0$ such that

$$\mathrm{Re}\, Q_r(\phi) = \mathrm{Re}\, Q_r(\phi,\phi) \geqslant \delta \left\langle \phi, \{p_t^2 + (t-1)^{-2}\}\phi \right\rangle. \tag{5.5}$$

Whence, in the terminology of [17], the form Q_r is strictly m-accretive. There is an associated operator H_r for which the open left half-plane $\mathbb{C}_- = \{\zeta \in \mathbb{C} : \mathrm{Re}\zeta < 0\}$ is a subset of the resolvent set, cf. [17, Lemma after Theorem VIII.16].

Lemma 5.1. *The $\mathscr{B}(L^2(1,\infty))$-valued functions*

$$B_r(\zeta) := (t-1)^{-1}(H_r - \zeta)^{-1}(t-1)^{-1}$$

and

$$p_t(H_r - \zeta)^{-1}(t-1)^{-1} \tag{5.6}$$

are uniformly bounded on $\mathbb{C}_-$.

Proof. Applying (5.5) to $\phi = (H_r - \zeta)^{-1}(t-\sigma)^{-1} f$ where $\sigma < 1$ and $f \in L^2(1,\infty)$ yields (by the Cauchy Schwarz inequality)

$$\left\| (t-\sigma)^{-1}(H_r - \zeta)^{-1}(t-\sigma)^{-1} f \right\| \leqslant \delta^{-1} \|f\|. \tag{5.7}$$

Letting $\sigma \to 1$ and using the Lebesgue convergence theorems we conclude that $(H_r - \zeta)^{-1}(t-1)^{-1} f \in \mathscr{D}((t-1)^{-1})$ for all $f \in \mathscr{D}((t-1)^{-1})$, and that (5.7) with $\sigma = 1$ holds for such f's.

As for bounding (5.6) we combine (5.5) and (5.7) to obtain uniform boundedness of $p_t(H_r - \zeta)^{-1}(t-\sigma)^{-1}$. Again we let $\sigma \to 1$. □

Lemma 5.2. *There exists the weak limit*

$$B_r(0) = \mathrm{w-}\lim_{\zeta \to 0, \mathrm{Re}\zeta < 0} B_r(\zeta).$$

Proof. Let $f \in L^2(1,\infty)$. For any sequence $\zeta_n \to 0$ with $\mathrm{Re}\zeta_n < 0$, $B_r(\zeta_{n_k}) f \rightharpoonup g$ for some g and some subsequence ζ_{n_k} (cf. Lemma 5.1 and [23, Theorem V.2.1]). Writing $g = B_r(0) f$ it remains to show that for any $f \in \mathscr{D}((t-1)^{-1})$, g is independent of choice of sequences. So suppose that for such f, $B_r(\zeta_{1,n}) f \rightharpoonup g_1$ and $B_r(\zeta_{2,n}) f \rightharpoonup g_2$. We need to show that $\psi := g_1 - g_2 = 0$. We readily obtain that for all $\phi \in C_c^\infty(1,\infty)$

$$\left\langle (t-1) H_{-r}\phi, \psi \right\rangle = 0. \tag{5.8}$$

Using this we can show that, indeed, $\psi = 0$ by the following approximation argument. Pick a real-valued $\chi \in C^\infty[1,\infty)$ such that $\chi(t) = 1$ for $t < 2$ and $\chi(t) = 0$ for $t > 3$, and let $\chi_n(t) = \chi(\frac{t}{n})$, $n \in \mathbb{N}$. We introduce $\Psi(t) = (t-1)\psi(t)$ and $\psi_n = \chi_n \Psi$. By elliptic regularity we obtain from (5.8) that $\Psi(t)$ is smooth up to (and including) $t = 1$. Since $\psi \in L^2(1,\infty)$ we must have $\Psi(1) = 0$, in particular $\psi_n \in \mathscr{D}(Q_r)$. Using (5.8) with this input we compute

$$Q_r(\psi_n) = \|\chi_n' \Psi\|^2. \tag{5.9}$$

Since $(t-1)\chi_n'(t) = (t-1)\chi'(\frac{t}{n})$ is uniformly bounded, the Lebesgue dominated convergence theorem yields that the right hand side of (5.9) vanishes as $n \to \infty$. Whence by (5.5)

$$\|\psi\| = \lim_{n\to\infty} \|\chi_n \psi\| = 0. \qquad \square$$

Lemma 5.3. *For all $\zeta \in \mathbb{C}_-$*

$$(H_r - \zeta)^{-1} = t^r (H-\zeta)^{-1} t^{-r}.$$

Proof. We shall only consider the case $r \geqslant 0$ (the case $r \leqslant 0$ may be treated similarly). It suffices to show that

$$t^{-r}(H_r - \zeta)^{-1} = (H-\zeta)^{-1} t^{-r}. \tag{5.10}$$

Clearly $t^{-r}(H_r-\zeta)^{-1} f \in \mathcal{D}(Q_0)$ for any $f \in L^2(1,\infty)$. For all $\phi \in C_c^\infty(1,\infty)$ we compute

$$Q_0(\phi, t^{-r}(H_r-\zeta)^{-1} f) = \langle \phi, t^{-r} H_r (H_r-\zeta)^{-1} f\rangle. \tag{5.11}$$

Since $C_c^\infty(1,\infty)$ is a core for Q_0 we deduce that (5.11) is valid for all $\phi \in \mathcal{D}(Q_0)$. Whence

$$H t^{-r}(H_r-\zeta)^{-1} f = t^{-r} H_r (H_r-\zeta)^{-1} f,$$

from which we readily obtain (5.10). $\square$

Using Lemma 5.3 we can show strong convergence of $T_r(\zeta) := t^{-1}(H_r-\zeta)^{-1}t^{-1}$. Notice that by Lemma 5.2 there exists

$$T_r(0) = \mathrm{w}-\lim_{\zeta\to 0, \mathrm{Re}\,\zeta<0} T_r(\zeta),$$

and that by Lemma 5.3, $T_r(0) = t^r T_0(0) t^{-r}$.

Lemma 5.4.

$$T_r(0) = \mathrm{s}-\lim_{\zeta\to 0, \mathrm{Re}\,\zeta<0} T_r(\zeta). \tag{5.12}$$

Proof. Pick $\delta \in (0, \frac{\epsilon}{2} - |r|)$. We claim that for all $f \in \mathcal{D}(t^\delta)$

$$T_r(\zeta) f = t^{-\delta} T_{r+\delta}(\zeta) t^\delta f \to t^{-\delta} T_{r+\delta}(0) t^\delta f. \tag{5.13}$$

Since $t^{-\delta} t^{-1}(H_r+1)^{-1} t$ is compact the (norm-) convergence, (5.13) follows from the first resolvent equation and weak convergence. Since $t^{-\delta} T_{r+\delta}(0) t^\delta = T_r(0)$ this proves (5.12). $\square$

Remark 5.5. Using the uniform boundedness of the family (5.6) and Lemma 5.2, one may show the existence of the weak limit

$$\mathrm{w}-\lim_{\zeta\to 0, \mathrm{Re}\,\zeta<0} R_r(\zeta), \quad R_r(\zeta) = p_t (H_r-\zeta)^{-1} t^{-1}.$$

Assuming in addition to the given conditions on q that $tq(t)$ is bounded, one may show using the proof of Lemma 5.4 the existence of the strong limit, $\mathrm{s}-\lim_{\zeta\to 0, \mathrm{Re}\,\zeta<0} R_r(\zeta)$.

We introduce for $s \in \mathbb{R}$ the weighted spaces

$$Z_{-s} = L^2_{-s}(1,\infty) = t^s L^2(1,\infty). \tag{5.14}$$

Here L^2 refers to the space of $\mathbb{C}^d$-valued square integrable functions.

Lemma 5.6. *Suppose $s < 1 + \frac{\epsilon}{2}$, where $\epsilon > 0$ is given as in* (5.2)*. Suppose $z \in L^2_{-s}(1,\infty)$ satisfies the homogeneous analogue of* (5.1) *in $\mathscr{D}'(1,\infty)$ (i.e. we assume that the right hand side vanishes and that the equation holds in distributional sense), and $z(1) = 0$. Then $z = 0$.*

Proof. We consider for any $\tilde{z} \in \mathscr{D}(1,\infty)$

$$0 = \lim_{\zeta\to 0,\,\mathrm{Re}\,\zeta<0} \left\langle (H-\zeta)^{-1}\tilde{z}, Hz \right\rangle.$$

By Lemmas 5.3 and 5.4 we may compute the limit as to obtain

$$0 = \langle H^{-1}\tilde{z}, Hz\rangle$$

with $H^{-1}\tilde{z} := t^{1-r}T_r(0)\,t^{1+r}\tilde{z}$, provided $|r| < \frac{\epsilon}{2}$. For a later application we need $r \geqslant s-1$ which by assumption is feasible.

The idea is to integrate by parts in the expression on the right. First we notice that $p_t H^{-1}\tilde{z} \in L^2_r$, cf. Remark 5.5. Next we claim that

$$p_t z \in L^2_{1-s}. \tag{5.15}$$

For that we introduce for $n \in \mathbb{N}$ the multiplication operator $F_n(t) = F(\frac{t}{n} < 1)$, and consider the expression

$$\left\langle p_t z, F_n(t)\,t^{2-2s} p_t z\right\rangle + \left\langle z, q(t)F_n(t)\,t^{2-2s} z\right\rangle. \tag{5.16}$$

Up to a term that can be bounded uniformly in n (using the assumption that $z \in L^2_{-s}$) this expression is equal to $\mathrm{Re}\langle Hz, F_n(t)\,t^{2-2s}z\rangle$. Whence (5.15) follows from (5.16) and the monotone convergence theorem.

Now integration by parts yields (this is a version of Green's identity)

$$0 = \left[-\overline{H^{-1}\tilde{z}}\cdot \frac{\mathrm{d}}{\mathrm{d}t} z + \left\{ \frac{\mathrm{d}}{\mathrm{d}t}\overline{H^{-1}\tilde{z}} \right\}\cdot z \right]_1^\infty + \langle HH^{-1}\tilde{z}, z\rangle.$$

Obviously the last term to the right is equal to $\langle \tilde{z}, z\rangle$. We claim that the first term vanishes. The lower boundary term (at $t = 1$) vanishes. The upper limit should be interpreted as a limit along a suitable sequence $t_m \to \infty$. Specifically, since the form is $[tf(t)]_1^\infty$ with f integrable (here we use (5.15)) it follows indeed that $t_m f(t_m) \to 0$ along such sequence.

We conclude that

$$0 = \langle \tilde{z}, z\rangle,$$

and since this holds for all $\tilde{z} \in \mathscr{D}(1,\infty)$ the proof is complete. □

Corollary 5.7. *Suppose $\tilde{z} \in L^2_{1+r}(1,\infty)$ where $r > -\frac{\epsilon}{2}$ with $\epsilon > 0$ given as in* (5.2)*. Then there exists a uniquely determined $z \in \cup_{s<1+\epsilon/2} L^2_{-s}(1,\infty)$ satisfying the equation* (5.1) *in $\mathscr{D}'(1,\infty)$ and $z(1) = 0$.*

Proof. For the existence part we may assume that $r < \frac{\epsilon}{2}$. Take $z = -t^{1-r}T_r(0)\,t^{1+r}\tilde{z}$. The uniqueness part follows immediately from Lemma 5.6. □

6. Mixed problem in the case $V_2 \neq 0$

In the section we impose Conditions 2.1 and 2.2. We shall find an analogue of Proposition 4.6.

6.1. **Solving a fixed point problem.** We are interested in solving (4.22) for $(x,\omega) \in \Gamma^+_{R,\sigma}$ where $R \geqslant 1$ is large and $\sigma > 0$ is small. For that we write the solution as $y = z + y_1$, where $y_1(t)$ is the solution constructed in Section 4 (with $V_2 = V_3 = 0$). We shall derive a fixed point problem for the "perturbation" z. By Newton's equation

$$\begin{aligned}\ddot{z} &= -\nabla V(z+y_1) + \nabla V_1(y_1) = -\nabla^2 V_1(y_1) z + \mathscr{R}(z),\\ \mathscr{R}(z) &= -\int_0^1 (1-l)\nabla^3 V_1(lz+y_1)\{z,z\}\mathrm{d}l - \nabla V_2(z+y_1).\end{aligned} \tag{6.1}$$

The Hessian in the first term on the right hand side of (6.1) is given by

$$\nabla^2 V_1(y_1) = V_1''(|y_1|)P_\parallel(y_1) + |y_1|^{-1} V_1'(|y_1|)P_\perp(y_1), \tag{6.2}$$

where $P_\parallel(y_1) = |y_1|^{-2}|y_1\rangle\langle y_1|$ projects onto the span of y_1, and $P_\perp(y_1) = I - P_\parallel(y_1)$.

Using Condition 2.2, (4.28) and representation (6.2) we see that $q(t) := -\nabla^2 V_1(y_1)$ satisfies condition (5.2) with $\epsilon = \bar{\epsilon}_1$. The equation (6.1) has the form of (5.1)

$$\ddot{z} - qz = \tilde{z} := \mathscr{R}(z). \tag{6.3}$$

We shall solve (6.3) using Banach's fixed point theorem. In this section the notation $Z_{-s} = L^2_{-s}(1,\infty)$ refers to weighted L^2-spaces of $\mathbb{R}^d$-valued square integrable functions, cf. (5.14).

We will choose s of the form

$$s = \alpha + \tfrac{1}{2} - \epsilon, \tag{6.4}$$

where $\epsilon > 0$ satisfies

$$\left|\alpha - \tfrac{1}{2} - \epsilon\right| < \tfrac{\bar{\epsilon}_1}{2}, \tag{6.5}$$

$$\epsilon < \alpha\epsilon_2. \tag{6.6}$$

By taking $\epsilon < \alpha\epsilon_2$ sufficiently close to $\alpha\epsilon_2$, indeed (6.5) and (6.6) are fulfilled (here we use (2.5)).

We shall prove the following result.

Proposition 6.1. *Suppose Conditions 2.1 and 2.2. Fix $\epsilon > 0$ sufficiently close to $\alpha\epsilon_2$ (but smaller). Then there exist $R_0 \geqslant 1$ and $\sigma_0 > 0$ such that for all $R \geqslant R_0$ and for all positive $\sigma \leqslant \sigma_0$ the problem (4.22) is solved by some function $y(t) = z(t) + y_1(t)$, $t \geqslant 1$, for all data $(x,\omega) \in \Gamma^+_{R,\sigma}$ and $\lambda \geqslant 0$. The function $z(t)$ is constructed as a fixed point of (6.7) stated below. Moreover this solution $y(t) \in \Gamma^+_{R,\sigma}(\omega)$ for all large enough $t \geqslant 1$.*

Proof. We shall use the operator $T_r(0)$ from Lemma 5.4 with $r = 1 - s$ and s given by (6.4). Notice that then (5.3) is fulfilled upon replacing $\epsilon \to \bar{\epsilon}_1$ due to (6.5).

Consider the following fixed point problem for $z \in Z_{-s}$:

$$z = \mathscr{P}(z), \tag{6.7}$$

where

$$\mathscr{P}(z) = -t^s T_r(0) t^{2-s}\tilde{\mathscr{R}}(z), \quad \tilde{\mathscr{R}}(z) = \chi_1\chi_2\mathscr{R}(z). \tag{6.8}$$

Here χ_j are auxiliary operators introduced in a first step; once the fixed point is constructed they can be removed. They are given in terms of $z \in Z_{-s}$ by $\chi_1 = F(\frac{|z|}{|y_1|} < \frac{2}{3})$ and $\chi_2 = F(\frac{|z|}{t^{\alpha-\epsilon}} < 2)$, respectively.

We claim that the map $\mathscr{P}$ is a contraction on Z_{-s} for all $(x,\omega) \in \Gamma^+_{R,\sigma}$ with $\sigma > 0$ small and R large, yielding by Banach's fixed point theorem a solution to (6.7).

We start by verifying that indeed $\mathscr{P} : Z_{-s} \to Z_{-s}$.

We may bound the vector $\tilde{\mathscr{R}}(z)$ in (6.8) as

$$\tilde{\mathscr{R}}(z)(t) = O(t^{-\alpha(1+\mu)-2\epsilon}) + O(t^{-\alpha(1+\mu+\epsilon_2)}), \tag{6.9}$$

using the second estimate of (4.54) and the support properties of the χ_j's. Since $T_r(0)$ is bounded on $L^2(1,\infty)$ we obtain from (6.9) and (6.6) that $t^s T_r(0) t^{2-s} \tilde{\mathscr{R}}(z) \in Z_{-s}$.

As for the contraction property let $z_1, z_2 \in Z_{-s}$ be given. Straightforward estimations using (4.55) and (6.6) show

$$\|\mathscr{P}(z_1) - \mathscr{P}(z_2)\|_{-s} \leq C|x|^{-\delta} \|z_1 - z_2\|_{-s} \leq \tfrac{1}{2} \|z_1 - z_2\|_{-s}. \tag{6.10}$$

Here we have taken $\delta > 0$ small; see (6.11) and (6.13) stated below for a similar application of (4.55). Clearly $C|x|^{-\delta} \leq CR^{-\delta} \leq \frac{1}{2}$ if R is large enough.

Finally we show that the factors χ_j's in (6.7) and (6.8) can be removed for the constructed fixed point, say $z = z_{-s} \in Z_{-s}$. First we notice the bound

$$\begin{aligned} \|z\|_{-s} &\leq 2\|\mathscr{P}(z=0)\|_{-s} = 2\left\| t^s T_r(0) t^{2-s} \nabla V_2(y_1(\cdot)) \right\|_{-s} \\ &\leq C_\delta |x|^{-\delta} \leq C_\delta R^{-\delta}, \end{aligned} \tag{6.11}$$

obtained using the contraction property (6.10), (6.6) and (4.55). We shall need a pointwise Sobolev type of bound. Let $w(t) = \frac{\mathrm{d}}{\mathrm{d}t}(t^{1-2s}|z(t)|^2)$. By elementary estimations and by using (6.11) and Remark 5.5 (notice that in conjunction with the fixed point equation the uniform bound of Remark 5.5 yields a weighted bound of the time-derivative of z) we may show that

$$\int_1^\infty |w(t)| \mathrm{d}t \leq \tfrac{1}{4} \quad \text{for } R \text{ large enough.}$$

From this estimate we get (by integrating to infinity)

$$|z(t)| \leq \tfrac{1}{2} t^{\alpha-\epsilon}, \quad t \geq 1. \tag{6.12}$$

Combining (6.12) with the bound

$$t^{\epsilon-\alpha}|y_1| \geq c|x|^{\epsilon/\alpha} \geq cR^{\epsilon/\alpha} \geq 2, \tag{6.13}$$

we conclude that indeed $\chi_1 = F(\frac{|z|}{|y_1|} < \frac{2}{3}) = 1$ and $\chi_2 = F(\frac{|z|}{t^{\alpha-\epsilon}} < 2) = 1$ for all sufficiently large R's. Consequently those factors χ_j's can be removed.

Obviously $z(1) = 0$ and the problem (4.22) is solved by $y(t) = z(t) + y_1(t)$. □

Remarks 6.2. 1) The above analysis yields the following uniform bound of the fixed point (with ϵ as above)

$$|z(t)| \leq C_\delta |x|^{-\delta} t^{\alpha-\epsilon},$$

valid for some $\delta = \delta(\epsilon) > 0$.

2) For positive energies there is a simpler procedure, cf. [5, proof of Theorem 1.5.1]. This leads to the improved decay in time

$$y(t)-(t-1)\sqrt{2\lambda}\omega-x=O(t^{\delta}),\quad \delta>\max\{1-\mu,0\},\tag{6.14}$$

with the bounding constant being locally uniform in $(\omega,\lambda)\in S^{d-1}\times(0,\infty)$. Obviously (6.14) is not uniform in λ. Compared to the procedure for positive energies the present one is based on an additional Taylor expansion. In this way we circumvent a problem related to the fact that the quantity $\int t|\nabla^2V(y)|\mathrm{d}t$ is finite only for $\lambda>0$ (causing a difficulty for the contraction property at $\lambda=0$).

3) Although it is not stated in Proposition 6.1 that $\Gamma^+_{R,\sigma}(\omega)$ is invariant under the forward flow, this is indeed true; see Lemma 6.4 stated below. Notice that it follows from Proposition 4.6 that $\Gamma^+_{R,\sigma}(\omega)$ is invariant in the case $V_2=0$.

4) We have not proved that the solution to the problem (4.22) is unique in the sense used in Proposition 4.6 in the case $V_2=0$.

Definition 6.3. Under the conditions of Proposition 6.1 we define a vector field F on $\Gamma^+_{R_0,\sigma_0}(\omega)$ by

$$F(x)=\dot y(t=1;x,\omega,\lambda);\tag{6.15}$$

here y refers to the solution of (4.22) given in Proposition 6.1.

Lemma 6.4. *Let $y=y(t)=y(t;x,\omega,\lambda)$ be the solution from Proposition 6.1. Then $y\in\Gamma^+_{R,\sigma}(\omega)$ for all $t\geq 1$.*

Let F_1 be given as in Definition 6.3 in the case $V_2=0$, and let ϵ be given as in Proposition 6.1. Then for all positive $\epsilon'<\epsilon$ and $\epsilon_2'<\epsilon_2$

$$F(x)-F_1(x)=O(|x|^{-\mu/2-\breve\epsilon}),\quad \breve\epsilon:=\min\left\{\tfrac{\epsilon'}{\alpha},\epsilon_2'\right\}.\tag{6.16}$$

In particular for constants $C,c>0$ independent of x, ω and λ,

$$\left|\frac{F(x)}{|F(x)|}-\frac{F_1(x)}{|F_1(x)|}\right|\leq C|x|^{-\breve\epsilon},\tag{6.17}$$

and

$$\frac{F(x)}{|F(x)|}\cdot\hat x\geq 1-C(1-\hat x\cdot\omega)-C|x|^{-\breve\epsilon},\tag{6.18}$$

$$\frac{F(x)}{|F(x)|}\cdot\hat x\leq 1-c(1-\hat x\cdot\omega)+C|x|^{-\breve\epsilon},\tag{6.19}$$

$$\frac{F(x)}{|F(x)|}\cdot\omega\geq 1-C(1-\hat x\cdot\omega)-C|x|^{-\breve\epsilon}.\tag{6.20}$$

Proof. Let $y_1=y_1(t)$ signify the solution in the case $V_2=0$. From (4.52) and Taylor's formula we obtain

$$\dot y(t)-\dot y_1(t)=\int_t^\infty\left\{\int_0^1\nabla^2V_1(lz+y_1)z\mathrm{d}l+\nabla V_2(y)\right\}\mathrm{d}s.\tag{6.21}$$

To bound the contribution from the first term on the right hand side we use (4.54) and (6.12), and estimate with $\delta = \frac{1-\alpha+\epsilon'}{2}$ for $\epsilon' < \epsilon$

$$\begin{aligned}\int_t^\infty \int_0^1 \nabla^2 V_1(lz+y_1) z \mathrm{d}l \mathrm{d}s &= \int_t^\infty O(|y_1|^{-\delta(2+\mu)}) s^{-(1-\delta)\alpha(2+\mu)} s^{\alpha-\epsilon} \mathrm{d}s \\ &= O(|y_1(t)|^{-\mu/2-\epsilon'/\alpha}).\end{aligned} \tag{6.22}$$

The contribution from the second term on the right hand side is estimated similarly

$$\begin{aligned}\int_t^\infty \nabla V_2(y) \mathrm{d}s &= |y_1(t)|^{-\mu/2-\epsilon_2'} \int_t^\infty O(|y_1|^{-1-\mu/2+\epsilon_2'-\epsilon_2}) \mathrm{d}s \\ &= O(|y_1(t)|^{-\mu/2-\epsilon_2'}).\end{aligned} \tag{6.23}$$

We conclude that

$$\dot y(t) - \dot y_1(t) = O(|y_1(t)|^{-\mu/2-\check\epsilon}) = |\dot y_1(t)| O(|x|^{-\check\epsilon}). \tag{6.24}$$

We obtain (6.16) by taking $t = 1$ in (6.24). Clearly (6.17) follows from (6.16). Moreover (6.18) and (6.19) in turn follow from (6.17) and from Section 4 (possibly after diminishing σ_0), while (6.20) readily follows from (6.18) (for a new constant). Notice for (6.18) and (6.19) in the case $V_2 = 0$ that $1 - \frac{F(x)}{|F(x)|} \cdot \hat x = 1 - \cos\psi_1$ and $1 - \hat x \cdot \omega = 1 - \cos\theta_1$. Whence the statements are equivalent to the bounds $c\theta_1 \leqslant \psi_1 \leqslant C\theta_1$, which may be derived from the following formula (representing $\kappa = -\sin\psi_1$):

$$\frac{\partial \kappa^2}{\partial \theta_1^2}(\theta_1 = 0) = \left(\int_1^\infty s^{-2} \frac{g(r_1}{g(sr_1)} \mathrm{d}s \right)^{-2}. \tag{6.25}$$

Finally we obtain from (6.17), (6.24), and the above considerations (for the case $V_2 = 0$), that $y(t) \in \Gamma^+_{R,\sigma}(\omega)$ for all $t \geqslant 1$ given that $x = y(1) \in \Gamma^+_{R,\sigma}(\omega)$. □

We shall show in Section 7 that F is a smooth gradient field. The following result, the proof of which is somewhat complicated since we have not proved uniqueness, cf. Remarks 6.2 4), will be useful.

Lemma 6.5. *Let $y = y(t) = y(t; x, \omega, \lambda)$ be the solution from Proposition 6.1. Then $\dot y(t) = F(y(t))$ for all $t \geqslant 1$.*

Proof. Let us omit ω, λ in the notation, and consider the following equivalent statement, say $p(T)$,

$$y(t + \bar t - 1; x) = y(t; y(\bar t; x)) \quad \text{for all } t \geqslant 1 \text{ and all } \bar t \in [1, T]. \tag{6.26}$$

Here $T \geqslant 1$ is arbitrary.

Obviously $p(1)$ is true. Let us prove that $p(T)$ is true for a $T > 1$ that may be chosen to be independent of x: We consider

$$\tilde z(\,\cdot\,) := y(\,\cdot\, + \bar t - 1; x) - y_1(\,\cdot\,; y(\bar t; x))$$

for $\bar t \in (1, T]$. We claim that (with s given by (6.4))

$$\tilde z \in Z_{-s}, \tag{6.27}$$

$$|\tilde z| < \tfrac{1}{3} \left| y_1(\,\cdot\,; y(\bar t; x)) \right|, \tag{6.28}$$

$$|\tilde z| < t^{\alpha-\epsilon}. \tag{6.29}$$

Notice that by using (6.27)–(6.29), the fact that $\tilde z(1) = 0$, Lemma 5.6 and the uniqueness property for contractions we obtain that $\tilde z(t) = z(t; y(\bar t; x))$ and therefore indeed (6.26) (for suitably small $T - 1 > 0$). Here Lemma 5.6 is applied to the vector $\tilde z - \mathscr{P}(\tilde z)$.

We estimate

$$|\tilde z(t)| \leqslant |y(t+\bar t-1;x) - y(t;x)| + |z(t;x)| + |y_1(t;x) - y_1(t;y(\bar t;x))|, \tag{6.30}$$

$$|y(t+\bar t-1;x) - y(t;x)| \leqslant \int_0^{\bar t-1} |\dot y(s+t;x)|\mathrm{d}s = O(t^0), \tag{6.31}$$

and

$$\begin{aligned} y_1(t;x) - y_1(t;y(\bar t;x)) &= \int_0^1 (\nabla_x y_1)\big(t; l(x - y(\bar t;x)) + y(\bar t;x)\big)\cdot(x - y(\bar t;x))\mathrm{d}l \\ &= O(g(|y_1|)^{-1}) = O(t^{\alpha\mu/2}), \end{aligned} \tag{6.32}$$

cf. (4.40).

From (6.30)–(6.32) we obtain (6.27).

As for (6.28) we may use the estimates

$$\big|y_1(t;y(\bar t;x))\big| \geqslant |y_1(t;x)| - \big|y_1(t;y(\bar t;x)) - y_1(t;x)\big|, \tag{6.33}$$

$$|z(t;x)| \leqslant \tfrac14 |y_1(t;x)|, \tag{6.34}$$

and the previous estimates. (Here the smallness of $T - 1 > 0$ comes in.) The proof of (6.29) is similar.

Now to show (6.26) in the general case, suppose $p(T)$ for some $T > 1$. Then for $\triangle \bar t > 0$ small (in agreement with the previous step) we have, with $\bar t = T + \triangle \bar t$,

$$\begin{aligned} y(t+\bar t-1;x) &= y((t+\triangle\bar t)+T-1;x) = y(t+\triangle\bar t; y(T;x)) \\ &= y\big(t; y(\triangle\bar t+1; y(T;x))\big) = y\big(t; y(\bar t;x)\big). \end{aligned}$$

Here we used $p(T)$ as well as the previous step with x replaced by $y(T;x)$. Whence we have shown $p(T')$ for a $T' > T$, and therefore (6.26) for all $T \geqslant 1$. □

6.2. **Smoothness properties of solution y.** We shall compute and estimate derivatives with respect to initial position x and final direction ω of the constructed solution $y = z + y_1$ and of the vector field F given in Definition 6.3. We studied the derivatives of $y = y_1$ in Subsection 4.2. It is well-known that under general conditions a solution to a fixed point equation depending on parameters will be smooth in these variables, see for instance [13, Appendix C].

From the fixed point equation (6.7) one may derive (for example) the representation

$$\partial_x z = (I - \nabla_z \mathscr{P})^{-1}\partial_x \mathscr{P}. \tag{6.35}$$

Notice here the bound

$$\|\nabla_z \mathscr{P}\|_{\mathscr{B}(Z_{-s})} \leqslant \tfrac12, \tag{6.36}$$

cf. (6.10) (with s given by (6.4)). To deal with higher order derivatives we need a more elaborate analysis.

Motivated by (6.12) we introduce the following modification of the spaces $Z_{-\sigma}$ of (5.14). Let $Z_{-\sigma}^{\text{unif}}$ be the space of $\mathbb{R}^d$-valued continuous functions $\tilde z$ on $[1,\infty)$ obeying

$$\|\tilde z\|_{-\sigma}^{\text{unif}} := \sup_{t\geqslant 1} t^{-\sigma}|\tilde z(t)| < \infty.$$

We shall first estimate various derivatives of the contraction $\mathscr{P}$ on Z_{-s}.

Lemma 6.6. *For all multi-indices δ and γ, $k \in \mathbb{N} \cup \{0\}$, and $z_1, \dots, z_k \in Z^{\mathrm{unif}}_{\epsilon-\alpha} \cap Z_{-s}$,*

$$\left\| \partial^\delta_\omega \partial^\gamma_x \partial^k_z \mathscr{P}\{z_1, \dots, z_k\} \right\|_{-s} \leqslant C_{\delta,\gamma,k} |x|^{-|\gamma|} \|z_1\|^{\mathrm{unif}}_{\epsilon-\alpha} \cdots \|z_k\|^{\mathrm{unif}}_{\epsilon-\alpha}, \tag{6.37}$$

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} \partial^\delta_\omega \partial^\gamma_x \partial^k_z \mathscr{P}\{z_1, \dots, z_k\} \right\|_{1-s} \leqslant C_{\delta,\gamma,k} |x|^{-|\gamma|} \|z_1\|^{\mathrm{unif}}_{\epsilon-\alpha} \cdots \|z_k\|^{\mathrm{unif}}_{\epsilon-\alpha}. \tag{6.38}$$

Proof. We start by verifying (6.37) for $k = 0$, $\delta = 0$ and $|\gamma| = 1$. So we need to trace the x-dependence of $\mathscr{P}$ as defined by (6.8). There is a contribution from differentiating the factor $T_r(0)$ and another from differentiating the factor $\tilde{\mathscr{R}}(z)$. Using Lemma 5.4 we may use the formal computation

$$\partial_x T_r(0) = -T_r(0)\, t(\partial_x q)\, t\, T_r(0); \tag{6.39}$$

here

$$\partial_x q = -\nabla^3 V_1(y_1) \partial_x y_1. \tag{6.40}$$

Using (4.54), (4.41) and (6.40) we derive $t(\partial_x q)t = O(|x|^{-1})$, so $\partial_x T_r(0) = O(|x|^{-1})$. As for the x-dependence from the factor $\tilde{\mathscr{R}}(z)$ we may combine (4.41) and the arguments for (6.9) to pick up an extra factor $|x|^{-1}$ in the estimation of $\partial_x \tilde{\mathscr{R}}(z)$.

Higher derivatives are treated similarly.

As for (6.38) we use Remark 5.5 and the same estimates as before. □

Lemma 6.7. *For all multi-indices δ and γ*

$$\|\partial^\delta_\omega \partial^\gamma_x z\|_{-s} = O(|x|^{-|\gamma|}), \tag{6.41}$$

$$\|\partial_t \partial^\delta_\omega \partial^\gamma_x z\|_{1-s} = O(|x|^{-|\gamma|}), \tag{6.42}$$

$$\|\partial^\delta_\omega \partial^\gamma_x z\|^{\mathrm{unif}}_{\epsilon-\alpha} = O(|x|^{-|\gamma|}). \tag{6.43}$$

Proof. We notice that (6.41)–(6.43) in the case $|\delta| + |\gamma| = 0$ follow from (6.11), (6.12) and the arguments for (6.12).

By the same reasoning (the Sobolev bound) if (6.41) and (6.42) are known for $|\delta| + |\gamma| \leqslant n$ for some $n \in \mathbb{N}$, then also (6.43) for $|\delta| + |\gamma| \leqslant n$ is valid.

So suppose we know (6.41)–(6.43) for all multi-indices δ and γ with $|\delta| + |\gamma| \leqslant n - 1$ for some $n \in \mathbb{N}$, then we only need to verify the bounds (6.41) and (6.42) for $|\delta| + |\gamma| \leqslant n$. For this we fix multi-indices δ and γ with $|\delta| + |\gamma| = n - 1$ and look at the representation of $\check{z} = \partial^\delta_\omega \partial^\gamma_x z$ obtained from differentiating (6.7) (a Faá di Bruno formula)

$$\begin{aligned} \check{z} =& (\partial_z \mathscr{P})\{\check{z}\} + \partial^\delta_\omega \partial^\gamma_x \mathscr{P} \\ &+ \sum c_{\delta',\delta_1,\dots,\delta_k,\gamma',\gamma_1,\dots,\gamma_k} (\partial^{\delta'}_\omega \partial^{\gamma'}_x \partial^k_z \mathscr{P})\{\partial^{\delta_1}_\omega \partial^{\gamma_1}_x z, \dots, \partial^{\delta_k}_\omega \partial^{\gamma_k}_x z\}, \end{aligned} \tag{6.44}$$

where summation is over $k \geqslant 1$, $\delta' + \delta_1 + \cdots + \delta_k = \delta, \gamma' + \gamma_1 + \cdots + \gamma_k = \gamma$ and $n - 1 \geqslant k + |\delta'| + |\gamma'| \geqslant 2$. The meaning of (6.44) if $n = 1$ is (6.7), while for $n = 2$ the third term to the right should be omitted. Now we may compute $\partial \check{z}$ (meaning either $\partial^{e_i}_\omega \check{z}$ or $\partial^{e_j}_x \check{z}$) by differentiating (6.44). The result is, cf. (6.35),

$$\partial \check{z} = (\partial_z \mathscr{P})\{\partial \check{z}\} + \tilde{z},$$

where $\tilde{z}$ may be treated using (6.37) and the induction hypothesis. So (again) we may invoke (6.36). This yields (6.41) (as well as the representation (6.44)) for $|\delta| + |\gamma| = n$.

It remains to prove (6.42) in the inductive argument. For that we use the proven formula (6.44) for $|\delta|+|\gamma|=n$. We proceed somewhat similarly applying now $t\partial_t$ to both sides of this formula with $\check z$ now given in terms of indices with $|\delta|+|\gamma|=n$. This leads to

$$t\partial_t \check z = t\frac{\mathrm{d}}{\mathrm{d}t}\partial_z \mathscr{P}\{\check z\} + t\partial_t \bar z.$$

The first term to the right may be treated using Remark 5.5; it is estimated as

$$\left\| t\frac{\mathrm{d}}{\mathrm{d}t}\partial_z \mathscr{P}\{\check z\}\right\|_{-s} \leqslant C\|\check z\|_{-s},$$

cf. (6.10). The second term may be treated using (6.38) and the induction hypothesis (specifically only (6.43)). The estimate (6.42) follows. □

Proposition 6.8. *With F the vector field in Definition 6.3, there are uniform bounds valid for all multi-indices δ and γ:*

$$\partial_\omega^\delta \partial_x^\gamma F(x) = \langle x\rangle^{-|\gamma|} O(g(|x|)), \tag{6.45}$$

$$\partial_\omega^\delta \partial_x^\gamma (F(x)-F_1(x)) = \langle x\rangle^{-\breve\epsilon-|\gamma|} O(g(|x|)). \tag{6.46}$$

Here F_1 is given as F for the case $V_2=0$, and $\breve\epsilon>0$ is given as in Lemma 6.4.

Proof. As for (6.45) we shall use the same scheme as for proving (4.50). First we notice the following consequence of (6.43):

$$|\partial_\omega^\delta \partial_x^\gamma z(t)| \leqslant C_{\delta,\gamma}|y_1(t)|\,|x|^{-|\gamma|}. \tag{6.47}$$

By (4.41)

$$|\partial_\omega^\delta \partial_x^\gamma y_1(t)| \leqslant C_{\delta,\gamma}|y_1(t)|\,|x|^{-|\gamma|}. \tag{6.48}$$

The combination of (6.47) and (6.48) is

$$|\partial_\omega^\delta \partial_x^\gamma y(t)| \leqslant C_{\delta,\gamma}|y_1(t)|\,|x|^{-|\gamma|}. \tag{6.49}$$

As in the proof of (4.50), we represent

$$\partial_* F = \partial_* \dot y(t=1) = \partial_* \sqrt{2\lambda}\,\omega + \int_1^\infty \partial\nabla V(y)\partial_* y\,\mathrm{d}t, \tag{6.50}$$

from which we may derive a Faá di Bruno formula (by repeated differentiation) to which (6.49) applies. The argument for the case $\delta=0$ and $|\gamma|=1$ is similar to (4.53): By combining (6.49) and (6.50) we obtain

$$\begin{aligned}\partial_x \dot y(t=1;x,\omega,\lambda) &= \int_1^\infty \nabla^2 V(y) O\left(\frac{|y|}{|x|}\right)\mathrm{d}t\\ &= O(|x|^{-1-\mu/2}) = \langle x\rangle^{-1}O(g(|x|)),\end{aligned} \tag{6.51}$$

which obviously is a particular case of (6.45). The general case is similar.

As for (6.46) we need a more refined argument than (6.51); this is now based on (6.21). We need to differentiate and estimate the expressions to the left in (6.22) and (6.23). The estimation of the differentiated expressions is done using (6.43) and (6.48) in a similar manner as done in the proof of Lemma 6.4. Details are omitted. □

Lemma 6.9. *The vector field $F=F(x,\omega,\lambda)$ as well as all derivatives $\partial_\omega^\delta\partial_x^\gamma F$ are jointly continuous in the variables $(x,\omega)\in\Gamma^+_{R_0,\sigma_0}$ and $\lambda\geqslant 0$.*

Proof. Since in fact $F(x,\omega,\lambda)$ is smooth in $(x,\omega) \in \Gamma^+_{R_0,\sigma_0}$ and $\lambda > 0$, cf. Remarks 4.7 1), only continuity at $\lambda = 0$ is non-trivial. Due to Remarks 4.7 2) and Proposition 6.8 it suffices to show that

$$F(x,\omega,\lambda) \to F(x,\omega,0) \quad \text{as } \lambda \to 0. \tag{6.52}$$

For that we first notice that

$$y_1(t;x,\omega,\lambda) \to y_1(t;x,\omega,0) \quad \text{as } \lambda \to 0. \tag{6.53}$$

This may be seen by combining Remarks 4.7 1) and a standard continuity statement of a flow in terms of variation of the initial values and the vector field, see for example [1, Theorem 3, p.177].

Since $\mathscr{P} = \mathscr{P}(\zeta,\lambda) \in Z_{-s}$ is jointly continuous in $\lambda \geqslant 0$ and $\zeta \in Z_{-s}$ (as may readily be checked) and there is a uniform contraction constant, a general principle for contractions, cf. [13, Appendix C], yields continuity for the fixed points; viz.

$$z_\lambda \to z_0 = z_{\lambda=0} \quad \text{in} \quad Z_{-s}. \tag{6.54}$$

Next we represent, cf. (6.21),

$$F(x,\omega,\lambda) - F(x,\omega,0) = \int_1^\infty (\nabla V(y_\lambda) - \nabla V(y_0))\mathrm{d}t.$$

The norm of the integrand on the right is estimated uniformly by $Ct^{-\alpha(1+\mu)}$. Combining this fact, (6.53), (6.54) and [19, Theorems 1.34, 3.12] we conclude (6.52). □

We end this section by stating a somewhat similar approximation result needed in the next section; clearly there are results for higher derivatives as in Lemma 6.9 but they will not be needed. Let $V_{2,n}(x) = F(\frac{|x|}{n} < 1)V_2(x)$ for $n \in \mathbb{N}$, and let $z_n, y_n, \mathscr{P}_n$ and F_n be the quantities defined upon replacing V_2 by $V_{2,n}$ in previous constructions.

Lemma 6.10. *The vector field $F_n = F_n(x,\omega,\lambda)$ is defined on the same domain as F (possibly after a slight shrinking), and pointwisely*

$$\partial_x F_n \to \partial_x F \quad \text{as } n \to \infty.$$

Proof. Clearly for all multi-indices γ, the function $\langle x\rangle^{\mu+\epsilon_2+|\gamma|}\partial^\gamma V_{2,n}(x)$ is bounded uniformly in n. Employing this property one may check the first statement as well as the existence of uniform bounds on $\sup_x \langle x\rangle^{|\gamma|}\|\partial_x^\gamma z_n\|_{-s}$ and $\sup_x g(x)^{-1}\langle x\rangle^{|\gamma|}|\partial^\gamma F_n(x)|$. Whence it suffices to show that

$$F_n(x) \to F(x) \quad \text{as } n \to \infty, \tag{6.55}$$

cf. Remarks 4.7 2).

Since $\mathscr{P}_n(\zeta) \in Z_{-s}$ is jointly continuous in $n \in \mathbb{N}$ and $\zeta \in Z_{-s}$ (more precisely we have $\|\mathscr{P}_n(\zeta_n) - \mathscr{P}(\zeta)\|_{-s} \to 0$ for any sequence $\zeta_n \to \zeta$ in Z_{-s}) we have continuity for the fixed points; viz. $z_n \to z$ in Z_{-s}.

We represent

$$F_n - F = \int_1^\infty (\nabla V_n(y_n) - \nabla V(y))\mathrm{d}t.$$

As in the proof of Lemma 6.9 we have a uniform bound as well as pointwise convergence (along subsequences) for the integrand; we can argue as before and conclude (6.55). □

7. SOLUTION TO EIKONAL EQUATION

In this section we shall see that the vector field F of Definition 6.3 can be written as $F(x) = \nabla\phi(x)$ for some smooth function ϕ. We impose Conditions 2.1 and 2.2, however if $V_2 = 0$ Condition 2.1 suffices; in that case F is given by the same definition.

Definition 7.1. Under the conditions of Proposition 6.1 (or Proposition 4.6) we introduce for $(x,\omega) \in \Gamma^+_{R_0,\sigma_0}$ and $\lambda \geqslant 0$,

$$\phi(x) = \phi(x,\omega,\lambda) = (x - R_0\omega) \cdot \int_0^1 F(l(x - R_0\omega) + R_0\omega)\mathrm{d}l + \sqrt{2\lambda}R_0.$$

It follows from Lemma 6.9 that $\phi = \phi(x,\omega,\lambda)$, as well as all derivatives $\partial^\delta_\omega \partial^\gamma_x \phi$, are jointly continuous in the variables $(x,\omega) \in \Gamma^+_{R_0,\sigma_0}$ and $\lambda \geqslant 0$. We shall show that the image of the map $\Gamma^+_{R_0,\sigma_0}(\omega) \ni x \mapsto (x, F(x)$ is Lagrangian, so that indeed this function ϕ is an antiderivative of F.

Proposition 7.2. *Under the conditions of Definition 7.1*

$$F(x) = \nabla_x\phi(x),$$

and ϕ solves the eikonal equation

$$\tfrac{1}{2}(\nabla_x\phi)^2 + V(x) = \lambda, \quad x \in \Gamma^+_{R_0,\sigma_0}(\omega). \tag{7.1}$$

Proof. Let us denote by $\theta_t = (y, F(y))$ the Hamiltonian orbit located at time $t = 1$ at the point $(x, F(x))$, cf. Lemma 6.5. Viewing $\theta_t = \theta_t(x)$ as a function of x we shall show that

$$\theta_1^*\sigma = 0, \tag{7.2}$$

where here $\sigma = \sum \mathrm{d}\xi_i \wedge \mathrm{d}x_i$ is the canonical two-form. For that we invoke the continuity property in the dependence through the term V_2 as specified in Lemma 6.10. We obtain that $\theta_1^*\sigma = \lim_{n\to\infty}\theta^*_{1,n}\sigma$ (using obvious notation), and henceforth we may assume that V_2 is compactly supported.

Next, since $\theta_1^*\sigma = \theta_t^*\sigma$ for all $t \geqslant 1$, it suffices to show the strong limit equality

$$\lim_{t\to\infty}\theta_t^*\sigma = 0. \tag{7.3}$$

We pick $\bar t > 1$ so large that the first coordinate, say $\bar x$, of $\theta_{\bar t}(x)$ is outside the support of V_2 (and similarly for all later times). Considering $\bar x = \bar x(x)$ as a function of x we may write $\theta_t^*\sigma = \bar x^*\theta_{t-\bar t+1}(\bar x)^*\sigma$, cf. (6.26), and compute

$$\theta_{t-\bar t+1}(\bar x)^*\sigma = \sum_{k<l} \partial_{\bar x_l} y \cdot (F' - F'^{\mathrm{tr}})\partial_{\bar x_k} y \mathrm{d}\bar x_k \wedge \mathrm{d}\bar x_l.$$

Here F' signifies the derivative of F at y, and "tr" is used for the transposed operator. Now, using (4.40) and (6.45) we get

$$\partial_{\bar x_l} y \cdot (F' - F'^{\mathrm{tr}})\partial_{\bar x_k} y = O\big(g(|y|)|y|^{-1}\big)O\left(\frac{g(|\bar x|)^2}{g(|y|)^2}\right) = O\left(\frac{g(|\bar x|)^2}{|y|g(|y|)}\right).$$

The right hand side tends to 0, and therefore (7.3) follows. □

Remarks 7.3. 1) For $\lambda > 0$ the constructed phase function essentially coincides with the Isozaki-Kitada (outgoing) phase function, $\phi(x,\xi)$, $\xi = \sqrt{2\lambda}\omega$, cf. [14, Definition 2.3] or [5, Proposition 2.8.2]. In particular, according to the method of proof of Proposition 6.8, there are bounds

$$\partial_\lambda^k \partial_\omega^\kappa \partial_x^\gamma \{\phi(x,\omega,\lambda) - \sqrt{2\lambda} x\cdot\omega\} = O(|x|^{\delta-|\gamma|}) \quad \text{as } |x| \to \infty, \qquad \delta > \max\{1-\mu, 0\}. \tag{7.4}$$

However these bounds are not uniform in λ as opposed to (6.45). (In (6.45) we paid the price of weaker pointwise decay.)

2) We constructed the phase by integrating the vector field F. In [14] and [5] this is constructed by a different procedure. Since it is assumed there that λ keeps away from 0, one would need additional elaboration to include $\lambda = 0$ by that procedure. Our arguments are related to [10, p.16] and [11, proof of Theorem 2.1].

3) We may integrate from $R_0\hat{x}$ to x along the line segment joining the two points plus in addition on the (small) arc joining $R_0\omega$ and $R_0\hat{x}$ on a great circle of radius R_0. This gives the following representation in the case $V_2 = 0$

$$\phi(x,\omega,\lambda) = \tilde{\phi}(r, \hat{x}\cdot\omega, \lambda) + \phi_2(\hat{x},\omega,\lambda), \qquad \tilde{\phi} = r\int_{R_0/r}^1 g(lr)\sqrt{1-\kappa^2(lr,\theta^2)}\,\mathrm{d}l. \tag{7.5}$$

7.1. **Constructions in incoming region.** We introduce for $R \geqslant 1$ and $\sigma > 0$

$$\Gamma^-_{R,\sigma}(\omega) = \{y \in \mathbb{R}^d : y\cdot\omega \leqslant (\sigma-1)|y|,\ |y| \geqslant R\}, \quad \omega \in S^{d-1},$$
$$\Gamma^-_{R,\sigma} = \{(y,\omega) \in \mathbb{R}^d \times S^{d-1} : y \in \Gamma^-_{R,\sigma}(\omega)\}.$$

Mimicking the previous procedure, starting from the mixed problem

$$\begin{cases} \ddot{y}(t) = -\nabla V(y(t)), \\ \lambda = \frac{1}{2}\dot{y}(t)^2 + V_1(y(t)), \\ y(-1) = x, \\ \omega = -\lim\limits_{t\to-\infty} \omega(t), \quad \omega(t) = \frac{y(t)}{|y(t)|}, \end{cases} \tag{7.6}$$

cf. (4.22), we may similarly construct a solution $\phi^-(x,\omega,\lambda)$ to the eikonal equation in some $\Gamma^-_{R,\sigma}(\omega)$. In fact denoting by $\phi^+(x,\omega,\lambda)$ the solution from Definition 7.1 this amounts to taking

$$\phi^-(x,\omega,\lambda) = -\phi^+(x,-\omega,\lambda), \quad x \in \Gamma^-_{R_0,\sigma_0}(\omega) = \Gamma^+_{R_0,\sigma_0}(-\omega). \tag{7.7}$$

7.2. **Classification of scattering orbits.** The scattering orbits may be characterized in terms of the solutions to (4.22) and (7.6) as follows.

Proposition 7.4. *Suppose Conditions 2.1–2.3. For any scattering orbit $x(t)$ with asymptotic velocities $\omega^\pm$, given by* (1.2) *and energy $\lambda \geqslant 0$, there exists a* (*large*) $T_0 > 0$ *such that for all $\pm t \geqslant T \geqslant T_0$,*

$$x(t) = y(t \mp T \pm 1; x(\pm T), \omega^\pm, \lambda), \tag{7.8}$$

$$\dot{x}(t) = \nabla_x \phi^\pm(x(t), \omega^\pm, \lambda). \tag{7.9}$$

Proof. It suffices to look at the case $t \to +\infty$. The proof of (7.8) is somewhat similar to the proof of Lemma 6.5. We introduce

$$\tilde{z}(t) = x(t-1+T) - y_1(t; x(T), \omega^+, \lambda).$$

It needs to be shown that $\tilde{z}(t) = z(t; x(T), \omega^+, \lambda)$, $t \geqslant 1$.

Clearly $\tilde{z}(1) = 0$. We omit the notation ω^+ and λ. As in the proof of Lemma 6.5 it suffices to show (6.27)–(6.29) (with $y_1(\cdot) = y_1(\cdot\,; x(T))$ used to the right in (6.28)).

By Newton's equation

$$\ddot{\tilde{z}} = -\int_0^1 \nabla^2 V_1(l\tilde{z} + y_1)\{\tilde{z}\}\mathrm{d}l - \nabla V_2(\tilde{z} + y_1).$$

Writing $q = -\int_0^1 \nabla^2 V_1(l\tilde{z} + y_1)\mathrm{d}l$ and $\mathscr{R} = -\nabla V_2(\tilde{z} + y_1)$, the form is

$$\ddot{\tilde{z}} = q\tilde{z} + \mathscr{R},$$

or equivalently

$$(p_t^2 + q)\tilde{z} = -\mathscr{R}. \tag{7.10}$$

By (3.3) we may estimate $\mathscr{R}$ as follows in terms of any non-negative $\kappa < 1 + \mu + \epsilon_2$:

$$|\mathscr{R}(t)| \leqslant C t^{-\alpha(1+\mu+\epsilon_2-\kappa)} |x(T)|^{-\kappa}. \tag{7.11}$$

As for the matrix q we claim that indeed it satisfies the condition (5.2) with $\epsilon = \bar{\epsilon}_1$ provided $T > 0$ is large enough. (Notice that the particular case $l = 0$ was used in Section 6.) To see this it suffices to show that for any $\delta > 0$ there exists $T > 0$ large enough such that

$$t - 1 \leqslant (1+\delta)\tilde{t}\big(|l\tilde{z}(t) + y_1(t)|\big) \tag{7.12}$$

uniformly in $t \geqslant 1$ and $l \in [0,1]$, cf. Condition 2.2. Define $\theta = \theta(t) \in [0, \frac{\pi}{2}]$ by the relation $\cos\theta = \frac{x(t)\cdot y_1(t)}{|x(t)||y_1(t)|}$ (abusing here and henceforth notation $x(t-1+T) \to x(t)$). We may estimate

$$\big|lx(t) + (1-l)y_1(t)\big| \geqslant \cos\tfrac{\theta(t)}{2} \min\{|x(t)|, |y_1(t)|\},$$

and use this bound to the upper limit in the integral. Since $\theta(t) \to 0$ as $T \to \infty$ uniformly in $t \geqslant 1$, we are left with estimating

$$t - 1 \leqslant (1+\delta)\tilde{t}((1-\kappa)|x(t)|) \tag{7.13}$$

for a sufficiently small $\kappa > 0$. Notice that we need this also for the particular choice $x(t) = y_1(t)$.

Now since (7.13) is valid for $t = 1$ it suffices to show that the derivative

$$(1+\delta)(1-\kappa)\frac{x(t)}{|x(t)|}\cdot \dot{x}(t)\big(-2V_1((1-\kappa)|x(t)|)\big)^{-1/2} \geqslant 1. \tag{7.14}$$

Using Proposition 3.4 and elementary estimates we may see that uniformly in $t \geqslant 1$,

$$\lim_{T\to\infty} \frac{x(t)}{|x(t)|}\cdot\frac{\dot{x}(t)}{|\dot{x}(t)|} = 1,$$

$$\lim_{T\to\infty} |\dot{x}(t)|\big(-2V_1(|x(t)|)\big)^{-1/2} \geqslant 1,$$

$$\lim_{T\to\infty} \big(-2V_1(|x(t)|)\big)^{1/2}\big(-2V_1((1-\kappa)|x(t)|)\big)^{-1/2} = 1.$$

From this we obtain (7.14), and hence (7.13) and the above assertion for the matrix q.

If $\lambda > 0$ the condition (5.2) holds for the matrix q for any $\epsilon \in (0,1)$ (provided $T > 0$ is sufficiently large).

Next we claim that (7.10) is "solved" by

$$\tilde{z} = -(p_t^2 + q)^{-1}\mathscr{R}, \tag{7.15}$$

in agreement with the theory of Section 5. To see this we distinguish between the cases $\lambda = 0$ and $\lambda > 0$. Suppose first that $\lambda = 0$. The right hand side of (7.15) belongs to $L^2_{-\tilde{s}}(1,\infty)$ for some $\tilde{s} < 1 + \frac{\bar{\epsilon}_1}{2}$ due to (7.11) (this is similar to the argument following (6.9), in fact it holds with $\tilde{s} = s$). We also claim that

$$\tilde{z} \in L^2_{-\tilde{s}}(1,\infty) \quad \text{for some} \quad \tilde{s} < 1 + \tfrac{\bar{\epsilon}_1}{2}. \tag{7.16}$$

To show (7.16) we shall use (3.10) and the fact that

$$\bar{\epsilon}_1 > 1 - \alpha(\mu + 2\epsilon_2) \tag{7.17}$$

as follows: Abbreviate $\omega^+ = \omega$ and decompose

$$\tilde{z} = (x - x\cdot\omega\,\omega) - (y_1 - y_1\cdot\omega\,\omega) + \tilde{z}\cdot\omega\,\omega. \tag{7.18}$$

The first two terms on the right are of the form $O(t^{\alpha-\alpha\epsilon_2})$, cf. (3.10) and (3.5). By (7.17) the function $t^{\alpha-\alpha\epsilon_2} \in L^2_{-\tilde{s}}$ for some $\tilde{s} < 1 + \frac{\bar{\epsilon}_1}{2}$.

As for the third term to the right in (7.18) we write

$$\dot{\tilde{z}} = |\dot{x}|\frac{\dot{x}}{|\dot{x}|} - |\dot{y}_1|\frac{\dot{y}_1}{|\dot{y}_1|} = (|\dot{x}| - |\dot{y}_1|)\omega + O(t^{-\alpha\mu/2-\alpha\epsilon_2}),$$

cf. (3.7).

We estimate

$$|\dot{x}| = \sqrt{-2V_1(|x|)} + O(t^{-\alpha\mu/2-\alpha\epsilon_2}).$$

Combining this with the equation $|\dot{y}_1| = \sqrt{-2V_1(|y_1|)}$ and the estimate

$$\frac{lx + (1-l)y_1}{|lx + (1-l)y_1|} = \omega + O(t^{-\alpha\epsilon_2}),$$

we conclude that

$$|\dot{x}| - |\dot{y}_1| = \tilde{q}\tilde{z}\cdot\omega + O(t^{-\alpha\mu/2-\alpha\epsilon_2}),$$

where

$$\tilde{q} = \int_0^1 \frac{-V_1'(l\tilde{z} + y_1)}{\sqrt{-2V_1(l\tilde{z} + y_1)}}\mathrm{d}l.$$

It follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{z}\cdot\omega = \tilde{q}\tilde{z}\cdot\omega + O(t^{-\alpha\mu/2-\alpha\epsilon_2}),$$

which in turn yields

$$\tilde{z}\cdot\omega = \int_1^t \mathrm{e}^{\int_s^t \tilde{q}\mathrm{d}t'} O(s^{-\alpha\mu/2-\alpha\epsilon_2})\mathrm{d}s. \tag{7.19}$$

Using Condition 2.3 and (7.12) we get, uniformly in $t \geq 1$,

$$\tilde{q}(t) \leq \frac{\kappa}{t-1} \quad \text{for some} \quad \kappa < \frac{1}{2}(1 + \bar{\epsilon}_1). \tag{7.20}$$

We insert (7.20) into the right hand side of (7.19). Invoking (7.17) we get $\tilde{z}\cdot\omega = O(t^\kappa)$; in particular $\tilde{z}\cdot\omega \in L^2_{-\tilde{s}}(1,\infty)$ for some $\tilde{s} < 1 + \frac{\bar{\epsilon}_1}{2}$ and (7.16) is proven.

Finally by combining Lemma 5.6, the fact that $\tilde z(1)=0$, (7.10), (7.16) and the statement following (7.15) we conclude that indeed (7.15) holds in the case $\lambda=0$.

The case $\lambda>0$ may be treated similarly although the estimates are simpler in this case. Now it is enough to verify that both sides of (7.15) belong to $L^2_{-\tilde s}$ for some $\tilde s<\frac{3}{2}$. The right hand of (7.15) satisfies this by the same argument as for $\lambda=0$. As for the left hand of (7.15) the arguments above lead to

$$\tilde z-\tilde z\cdot\omega\omega=O(t^{1-\alpha\epsilon_2}), \tag{7.21}$$

and to the representation

$$\tilde z\cdot\omega=\int_1^t \mathrm{e}^{\int_s^t \tilde q\,\mathrm{d}t'}O(s^{-\alpha\epsilon_2})\mathrm{d}s. \tag{7.22}$$

In combination (7.21) and (7.22) lead to $\tilde z=O(t^{1-\alpha\epsilon_2})$. Consequently indeed $\tilde z\in L^2_{-\tilde s}$ for some $\tilde s<\frac{3}{2}$ in the case $\lambda>0$, and we may conclude (7.15) as before.

Using (7.11), (7.15) and the theory of Section 5 one may now verify (6.27)–(6.29) (with the same s) for $T>0$ sufficiently big, yielding (7.8) (by the arguments of the proof of Lemma 6.5). The arguments are similar to the proof of Proposition 6.1. (Notice for (6.28) that the estimate (3.3) with $x(t)\to y_1(t;x(T))$ holds uniformly in all large $T>0$.)

Clearly (7.9) follows from (7.8) and Lemma 6.5. □

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